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A Library Least Square approach in the Prompt-Gamma Neutron Activation Analysis (PGNAA) process in bulk coal samples

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Application possibility of Library Least Square (LLS) approach in Prompt-Gamma Neutron Activation (PGNA) technique in bulk coal samples elemental analysis is investigated this work. 14 MeV neutrons were produced by a neutron generator via the T(d,n)4He reaction. A polyethylene block as a neutron moderator. The prompt gamma ray spectra from five different powders of pure compounds (namely Ca(OH)2, Fe2O3, NaCl, SiO2 and TiO2) and, afterwards, several powder-mixtures of various composition were measured by a LaBr3(Ce) gamma detection system. The gamma detection system data was streamed directly to the computer, event-by-event. The experiment simulation was performed using GEANT4 instruments.

Simulation and experimental data were loaded into the algorithm based on LLS which sent out a volume coefficient for each component of a powder-mixture investigated. The results were compared in order to optimize GEANT4 model up to the most efficient version.

As an optimization process output, the simplest decision to increase results'accuracy was to remove a steel framework and a moderator from the experimental setup simulation. The reason was significant amount of iron, carbon and hydrogen located rather close to the sample and the scintillator what usually caused neutralization of needed characteristic radiation peaks in samples'spectra. Since a GEANT4 toolkit provides an opportunity to divide gamma rays spectra into neutron capture gamma-radiation (NCGR) spectrum and inelastic scattering gamma-radiation (ISGR) spectrum. The optimized model was used to obtain the reasonable results of an elemental analysis carried out for various model mixtures.

A set of remarkable functional dependences were derived using processed model data. Firstly, error dependence of an initial amount of a component was derived. The larger initial volumetric coefficient of a component is the lower measure of inaccuracy is.

Secondly, to show that a way of spectra calibration is rather important within PGNAA elemental analysis, a series of calculations were carried out using some particular results. The data contained different sets of components'volume coefficients which were obtained using various combinations of spectra displacements along the energy axis. The bigger is displacement of a component spectrum relative to other compounds' spectra, the larger is a value of ratio error. To make a conclusion, a list of recommendations was established in order to increase effectiveness of the PGNAA technique of elemental analysis:

• Providing an experimental detector responses library for pure compounds is advisable.

• There must be no massive objects made of high-density materials relatively close to the sample and a detector.

• A pulsed neutron generator is necessary to fix an impulse duration (in order to divide NCGR and ISGR spectra).

• A preferable energy range of detector's response is from 0.1 to 8.0 MeV.

• Spectra calibration should be carried out thoroughly (a pair of close characteristic radiation peaks must not be further than 15-30 keV from each other)

• The larger initial amount of a component in a mixture is, the more accurate the results of applying the LLS algorithm are.

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