

**The Henryk Niewodniczański
INSTITUTE OF NUCLEAR PHYSICS
Polish Academy of Sciences
152 Radzikowskiego Str., 31-342 Kraków, Poland**

www.ifj.edu.pl/reports/2005.html

Kraków, August 2005

Report No. 1965/AP

**Monte Carlo simulation of the upgraded,
neutron - gamma logging tool, SO-5-90-SN type.
Comparison of the simulations and measurements.**

Teresa Cywicka-Jakiel, Tomasz Zorski ¹

¹ AGH University of Science and Technology, Faculty of Geology, Geophysics and Environmental Protection, Dept. of Geophysics, Mickiewicza 30, PL-30-059 Kraków, Poland.

Abstract

For gas prospecting in the shaly-sand Miocene formations of the Carpathian Foredeep many complementary geophysical techniques are being used. The spectrometric Neutron-Gamma well Logging (sNGL) is one of the nuclear techniques being useful for the formation mineralogy identification.

The results of the real and simulated sNGL experiments are compared in this report. These benchmark experiments were performed for determination of the main rock constituents: Si, Ca, Fe and H in the rock models which belong to the Polish calibration station in Zielona Góra (BGW). The upgraded n-gamma spectrometer, SO-5-90-SN type, has been applied in the measurements and was simulated using the Monte Carlo code (MCNP). The results of the real and simulated sNGL experiments are in good conformity. The H, Ca and Fe concentrations obtained from the simulations ("MCNP") have been highly correlated with their reference ("chem") concentrations. Squares of the correlation coefficients (R^2) amount to 0.931, 0.969, 0.973, respectively. For the Si concentration (C_{Si}), dependence $C_{Si}^{MCNP}(C_{Si}^{chem})$ shows slightly lower R^2 (0.972) than for dependence $C_{Si}^{meas}(C_{Si}^{chem})$. This is mainly attributed to the unavailable B, Cl and Rare Earth Elements (REE) contents, of the BGW Zielona Góra rock models and to their geological inhomogeneities. Additional improvement of correlation between results of both experiments is also presented. It has been obtained when data from preliminary analyses for B, Cl and (REE) of two rock models were included in the simulations.

The Fe concentration can be used as one of the indicators of the formation clay content, therefore an accurate quantification of this element in the rocks is of high importance. The BGW calibration station in Zielona Góra has limited number of the rock models, and Fe content is poorly diversified in them. Therefore the artificial rocks of different Fe contents have been simulated and spectrometer sensitivity, to the changes of the Fe contents, has been estimated.

1. Introduction

Nowadays, the shaly-sand, thin - bedded formations are of special interest as they become an important field for the hydrocarbons exploration [Passey et al., 2004, Saxena et al., 2004, Zorski, 2004]. The precise determination of the clay type, can be crucial for the proper prediction of the reservoir properties. Nuclear methods are very useful not only for the porosity determination but also for formation lithology identification. Moreover their spatial ranges are suitable for the thin - bedded formations assuring higher vertical resolutions than in a deep range, electric resistivity logs.

The spectrometric Neutron-Gamma Logging (sNGL) offers possibility of identifying and quantifying of the rock elements by detecting the characteristic gamma-rays generated in neutron interactions [Hertzog et al., 1987, Schweitzer et al., 1988, Harvey et al., 1997]. The knowledge of the main rock elements: Si, Ca and Fe is of high importance for the lithology identification [Herron and Heron, 1996] and can be practically realized with the simple neutron-gamma spectrometer equipped with the highly efficient scintillation detector and an isotopic Am-Be neutron source. Other useful rock elements as K, U, Th can be obtained from the spectral, natural gamma ray logs (sGR) and additionally Al can be determined (under some conditions) from the neutron activation (NA) log. The obtained elements contents can be gathered and compared to the results of commonly used spectral litho-density logs and neutron (thermal or/and epithermal) logs. Such a complementary approach gives, as the final result, the precise "tool" for the determination of the formation mineralogical composition.

Nevertheless, full success in clay typing is possible under some conditions. First of all the proper, suitable for the local geological environment, mineralogical model have to be created, [Harvey et al., 1997, Środoń 2004]. Such a model enables obtaining mineral composition of the formations using elemental one. The second condition concerns the accuracy of the elements determination when the logs data are used. Higher accuracy of the elements predictions means higher reliability of the mineralogical model.

The proper transformation of the signals from the detector into the wide range of elemental contents needs the accurate calibration procedure to be available. The disturbing effects such as borehole diameter, salinities of the borehole fluids and formation fluids, rocks porosities etc. have to be included into calibration procedure, in the form of suitable correction factors. Usually, calibration standards, basing on the natural rock models, have the limited ranges of the elemental contents. Such a situation concerns the rock standards belonging to the Polish calibration station in Zielona Góra (Geofizyka Kraków Ltd.) [Massalski, 1988, Zorski, Massalski, 1997]. Distribution of the Si and Ca contents are limited to the ranges typical for the sandstone, limestone and dolomite lithologies. The only two models have the Fe contents slightly exceeding 1 wt %. This is evident that the more homogeneous distribution of the Si and Ca contents should be obtained for the calibration reliability and the extended range of Fe content, up to about 5 wt% (as in common rocks), should be reach.

As a remedy for this problem the numerical calculations (MCNP code) can be done allowing simulations of the rock models of required physical and geophysical parameters. A very important question concerning the reliability of the modelling calculation have to be answer before the industrial application. In this aim well controlled benchmark experiments are performed, in the real and numerically simulated conditions, which allow the full verification of the simulation results. Such a verification is presented in this paper.

The special n-gamma spectrometer SO-5-90 type [Pałka, Zorski, 1994] was recently upgraded to the new version: SO-5-90-SN [Zorski, Pałka, 2004] and is intended to the field measurements, in the boreholes not deeper than 2000 m. In the upgraded spectrometer double Am-Be source has been used with the optimised source housing and additional shielding for the BGO detector. The source-to-detector distance has been increased and a new photomultiplier has been used, improving the signal/noise ratio. The spectrometer belongs to the Faculty of Geology, Geophysics and Environmental Protection (University of Science and Technology in Kraków, Poland). This new tool, has been applied to the n-gamma measurements at the Polish calibration station in Zielona Góra and in the field logging of the Carpathian foredeep gas formations in Poland [Cywicka-Jakiel, Zorski, 2004b].

Comparisons between the Si, Ca, Fe and H contents, obtained from the real and simulated sNGL experiments, show a good agreement. Slightly higher discrepancies in a case of simulated Si contents are probably a consequence of the lack the chemical (reference) analyses for B, Cl and Rare Earth Elements (REE) for the Zielona Góra calibration standards. Data for B, Cl and REE were not included in the MCNP input files. At the moment the only two complete (preliminary) analyses exist for the Mucharz and Brenna sandstones, other are planned for the nearest future. As is shown in the paper, introducing preliminary B, Cl and REE contents into additional MCNP inputs, the better agreement is obtainable between measured and simulated elemental contents.

The positive verification of the sNGL simulations allows the artificial rock models to be simulated. The artificial rocks have been modelled to extend the range of the Fe contents. The simulated rocks were the homogeneous mixtures of silica and hematite. The Fe contents changed from 0 to 5 wt% and porosities (K_p) were 0 % and 10 % for every model. Probe sensitivity S_w to the changing Fe content has been evaluated.

2. Spectrometric n-gamma experiments at the BGW Zielona Góra calibration station.

The spectrometric n-gamma measurements, were performed at the BGW Zielona Góra calibration station in 2000 and 2001 [Zorski et al., 2000, 2001] to examine the potential possibility of quantifying the Si, Ca and Fe elements in the rocks. Firstly, the SO-5-90, secondly the SO-5-90-SN gamma spectrometers were used. The measurements and the Monte Carlo modeling for the SO-5-90 spectrometer has been described in [Cywicka-Jakiel., Zorski., 2004a]. The SO-5-90-SN spectrometer is equipped with 6 Ci double Am-Be source and an efficient ϕ 40 mm x 60 mm coaxial BGO detector shielded against the source neutrons and hard photons by the set of cylindrical shields made of Pb, Al and polyamide. The source-to-detector distance is 44 cm. Improved quality of the measured gamma-rays spectra has been obtained for the new spectrometer (Fig.1).

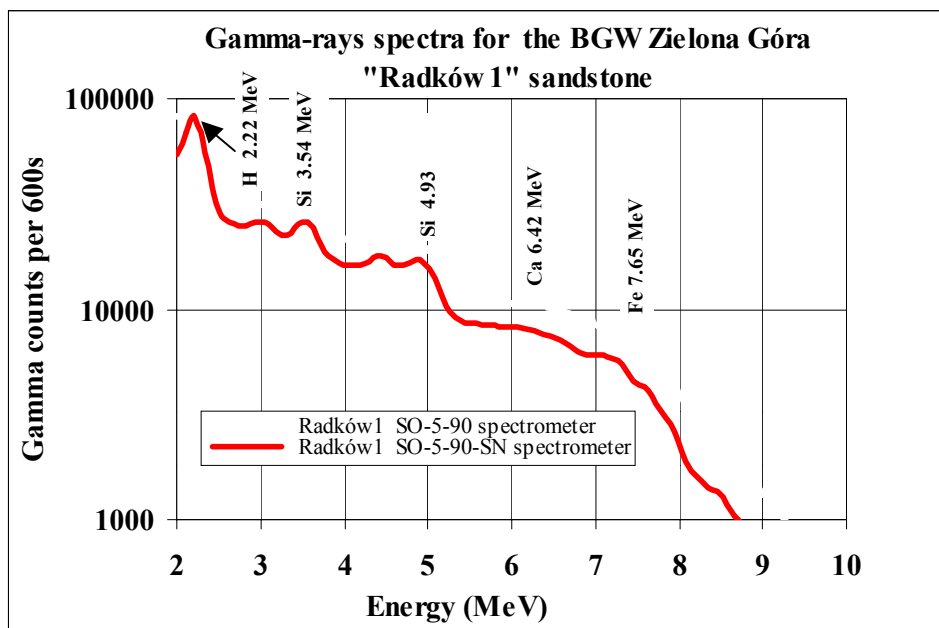


Fig.1. Gamma-rays spectra measured using the upgraded spectrometer SO-5-90-SN type and the previous one (SO-5-90 type).

The raw approximation of the peak/valley ratio for the hydrogen 2.22 MeV peak, gave about 3.32 and 2.69 for the spectrometers SO-5-90-SN and previous SO-5-90, respectively.

Three different gamma-rays spectra measured using the SO-5-90-SN spectrometer are presented in Fig.2 for different lithology models but for similar porosities and borehole diameters.

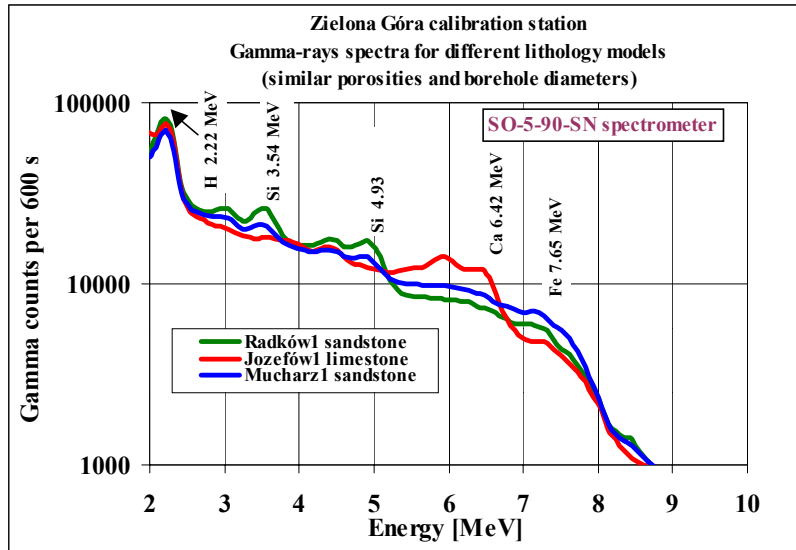


Fig.2. Gamma-rays spectra, measured using the SO-5-90-SN spectrometer, for different rock models of similar porosities and borehole diameters.

For the quantitative analyses of Si, Ca, Fe and H, the gross gamma counts from the appropriate spectral windows ΔE_γ around the characteristic gamma lines, were used. The energies of the major gamma lines from radiative capture and the selected energy windows ΔE_γ together with data for the previous spectrometer, are listed in Table 1.

Table 1. The major gamma lines from the (n, γ) interactions with H, Si, Ca, Fe and the selected energy windows ΔE_γ for the previous and upgraded spectrometers: SO-5-90 and SO-5-90-SN types respectively.

Element	E_γ [MeV]	ΔE_γ [MeV]	
		previous SO-5-90	SO-5-90-SN
H	2.22	1.71 ÷ 2.35	2.001÷2.521
Si	3.54; 4.93	2.67 ÷ 5.03	2.625÷5.228
Ca	6.42	5.25 ÷ 6.64	5.332÷6.789
Fe	7.631; 7.645	6.85 ÷ 10.0	6.893÷8.975

As mentioned in Introduction, the natural rock models of the BGW Zielona Góra calibration station are the natural lithology models - sandstones, limestones and dolomites. In consequence the Si, Ca and Fe contents in them are limited and poorly diversified showing, in some cases, the “bipolar” behavior. The porosities, matrix densities ρ_{matrix} and the average concentrations of the main rock constituents: Si, Ca, Fe together with H resulting from the water in the pores and from a bound water (sandstones) are included in Table 2.

Table 2. Parameters of the Zielona Góra rock models (standards) used for calibration of the SO-5-90-SN spectrometer – concentrations of H, Si, Ca, Fe (chemical analyses), porosity, matrix density, borehole diameter.

Rock model symbol – name - lithology	C_H (wt%)	C_{Si} (wt%)	C_{Ca} (wt%)	C_{Fe} (wt%)	porosity K_p (%)	ρ_{matrix} (g/cm ³)	Borehole diameter: Φ_2 (mm)
BM2 - Biała Marianna 2 -limestone	0.004	1.301	37.635	0.075	0.100	2.714	220
MO2 - Morawica 2 limestone	0.109	1.142	38.517	0.125	2.570	2.674	220
JO2 - Józefow 2 -limestone	0.704	0.685	36.161	0.079	15.240	2.659	216
Pi2 - Pińczow 2 - limestone	1.813	0.446	32.546	0.068	34.460	2.828	216
Li2 - Libiąż 2 –dolomite	0.664	0.252	20.694	0.115	15.240	2.697	220
Mu2 - Mucharz 2 - sandstone	0.326	28.073	6.127	1.202	2.600	2.710	220
Br2 - Brenna 2 – sandstone	0.484	34.700	1.923	1.667	7.670	2.648	215
Ra2 - Radków 2 - sandstone	0.784	39.831	0.223	0.238	14.700	2.620	216
Ze2 - Żerkowice 2 – sandstone	1.307	39.250	0.442	0.362	24.870	2.640	220

3. Description of the numerical modelling.

Numerical modelling of the sNGL experiments with the SO-5-90-SN spectrometer has been done using the MCNP4c – a general-purpose Monte Carlo N-Particle code [Briesmeister, 2000]. This code allows to simulate the neutron, photon, electron, or coupled neutron/photon/electron transport in a complex three-dimensional geometry.

The simplified scheme of the simulated sNGL arrangement is presented in Fig.3.

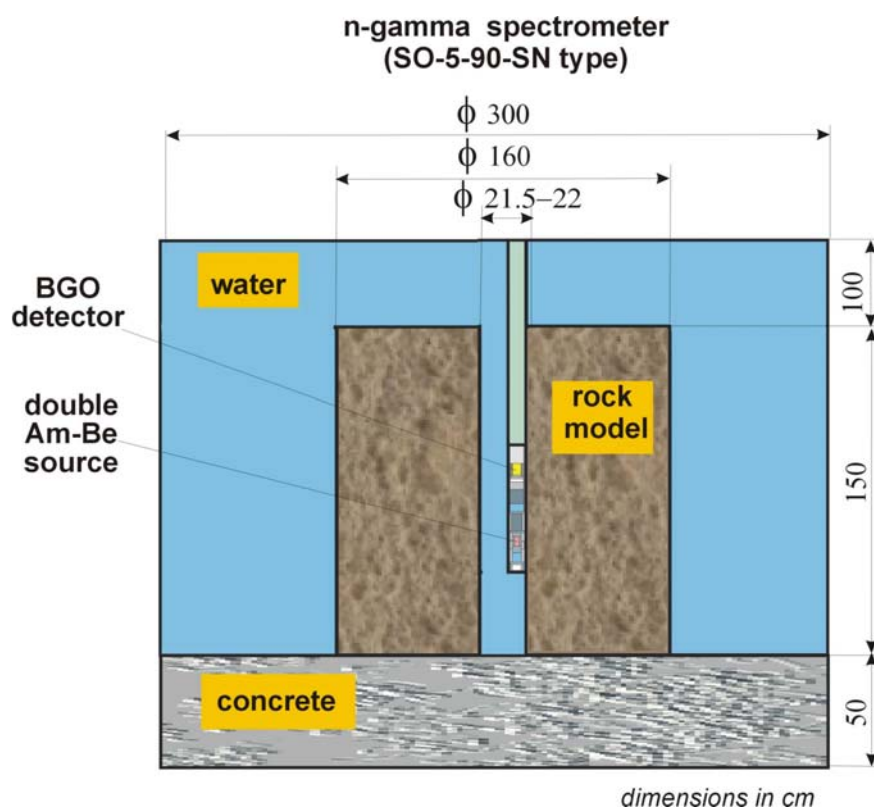


Fig.3. The simplified geometry of the sNGL experiment performed at the calibration station in Zielona Góra.

The cylindrical approximation of the rock models, boreholes and surrounding water has been established for numerical modelling. The rock models have been treated as the homogeneous ones.

Average porosities and matrix densities as well as an average elemental composition were established for the every rock model [Massalski et al., 1994]. Elements: H, C, O, Mg, Al, Si, K, Ca, Mn, Fe, Rb, Sr, Cd were taken into account. Actual diameters of the boreholes were used (220 mm, 215 and 216 mm). The bismuth germanate (BGO) crystal has been modelled as a regular cylinder, of diameter 4 cm and length of 6 cm, surrounded by the aluminium casing and the layer of teflon (3 mm). As in previous SO-5-90 spectrometer the photomultiplier and electronic setup have been simulated by a “diluted” aluminium having density of 1.35 g/cm³. The volume distributed, double ²⁴¹Am-Be source, has been simulated with neutrons picked with the same probability and emitted isotropically.

3.1 Cross sections data

For the MCNP code the comprehensive neutron/gamma cross sections libraries are obtainable with the continuous energy cross sections. Neutron data based mainly on the ENDF/B-V and ENDF/B-VI libraries (endf602, rmccs2, endf5p2, endf5u2, misc5xs2 files). The elements being introduced into MCNP4c input were: H, C, N, O, Na, Mg, Al, Si, K, Ca, Mn, Fe, Ge, Rb, Ni, Pb and Bi. S(α,β) treatment has been used for H cross sections in water (file tmccs2 for hydrogen in light water at 300 K). The cross sections data for Ge are not included into the MCNP4c package, they have been kindly obtained [Tickner, 2002]. Cross section data for gamma-rays interactions were taken from file mcplib22 and for electrons from el032 file.

3.2 Scoring

Several MCNP estimators determine scoring process at a point or region. In our case the track length estimator (tally type **F4**) has been mainly used which evaluates particle flux (or fluence) as a sum of particle track lengths crossing a detector region. Tally type F4 gives the neutron or γ-fluxes $\bar{\phi}_V$ averaged over a detector volume and normalized to be per starting particle:

$$\bar{\phi}_V = \frac{1}{V} \int_V \int_E \int_t \Phi(\mathbf{E}, \mathbf{r}, t) d\mathbf{E} dt dV \quad (5)$$

where $\Phi(\mathbf{E}, \mathbf{r}, t)$ is the neutron or γ-flux in a detector of volume V . The MCNP code estimates $\bar{\phi}_V$ by summing WT_i/V for all particle track lengths T_i :

$$\bar{\phi}_V = \sum \frac{WT_i}{V} \quad (6)$$

where W is the particle weight.

To obtain an average photon rates at the detector, which correspond to measurable γ-count rates in (cps), the **Fm4** card has been introduced which gives the number of photon collisions RR in a detector volume (in photons/cm³ per one source neutron and per energy bin). An energy binning is being assumed as for the real measurement (Table 1). RR is expressed as:

$$RR = C \int \phi(\mathbf{E}) R_m(\mathbf{E}) d\mathbf{E} \quad (7)$$

where C constant is used for normalization ($C = -1$ gives atomic density in atoms/(b·cm)), $\phi(\mathbf{E})$ is the energy-dependent γ flux (in photons/(MeV·cm²)), R_m is the microscopic reaction cross section (in barns) for the m type reaction taken from the MCNP libraries. To obtain the results in counts (cps) per energy bin, the factor $N = 995.25624 \cdot 10^6$ (cm³·n/s) was used which is a product of the source strength equal to $13.2 \cdot 10^6$ n/s and the volume of the BGO crystal amounted to 75.3982 cm³. The number of histories (nps) equal to 100 millions has been taken to obtain relative errors of photon rates in the range from 1 % to 4.2 % for tallies Fm4 type. MCNP simulations have run on the PC computer with the AMD Athlon 1.33 GHz processor.

The **F8** tally, an estimator of the pulse high spectra, has been used sporadically, as it is more time consuming and no variance reduction techniques can be applied for it. In F8 tally the energy (or charge) is deposited in a cell volume by source particles and their secondary particles (all the energy

tracks of the history). The F8 tally result for the Radków 2 sandstone together with the experimental spectrum is presented in Fig. 4. Special F8 tally option, GEB, has been used for Gaussian broadening of the gamma peaks. Good agreement between both spectra is visible.

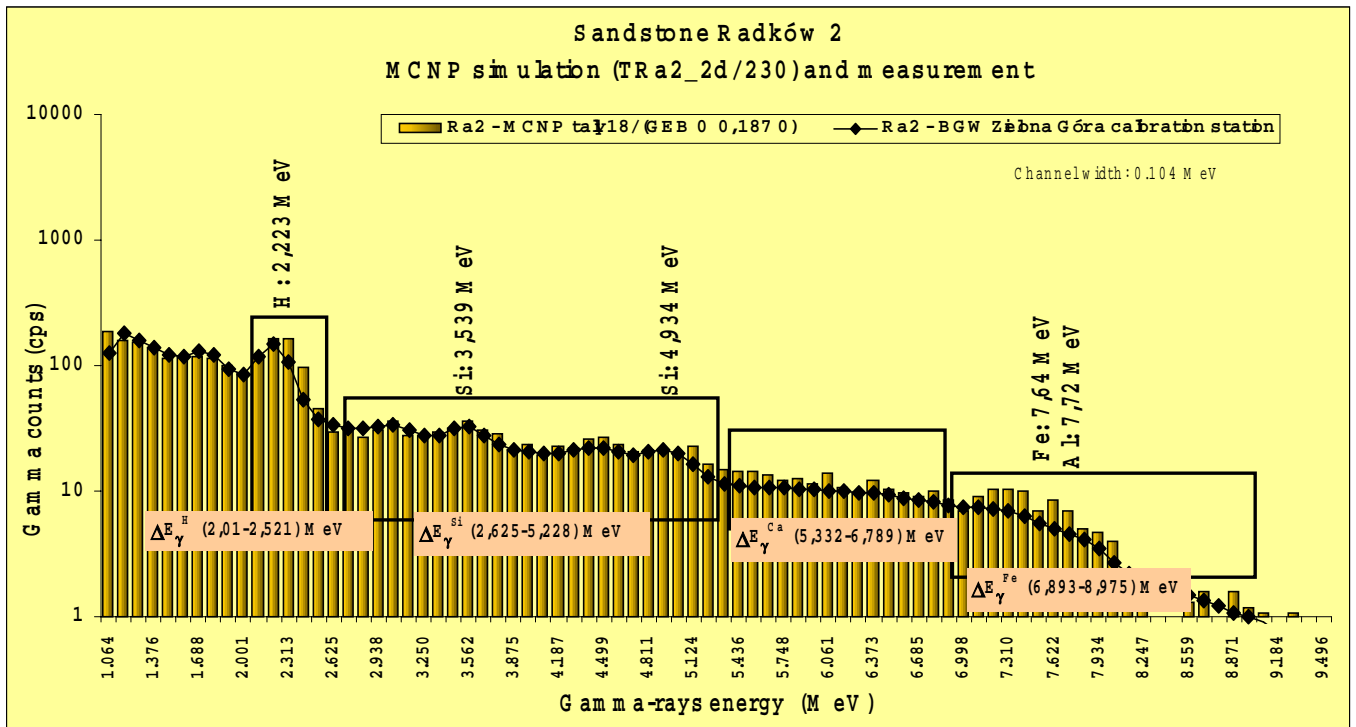


Fig. 4. The simulated (tally of F8 type) and the measured γ -rays spectra for the Radków 2 (Ra2) sandstone.

4. Results

The simulated gamma-rays spectra (F4 type), obtained from the MCNP code correspond to that from an idealized detector which registers all photons with 100 % efficiency at their primary energy. On the other side the real scintillation detector has efficiency less than 100 % because of the limited light collection and remarkable photomultiplier losses. Therefore one needs to renormalize (standardize) the raw MCNP spectra if they are evaluated together with experimental ones. Well controlled experiments (benchmark experiments) are needed for this aim.

4.1 Standardisation

The linear dependencies between simulated (“MCNP”) and measured (“meas”) gross gamma counts, attributed to the selected spectral windows (Table 1), for the BGW Zielona Góra rock models are visible in Figs. 5-8. These dependencies allow to obtain standardized (“stand”) counts using simulated (MCNP) ones (Tables A1-A2 of Appendix). Parameters of the regression lines: correlation coefficient squares R^2 , standard deviations S_Y are included in the Figs. 5-8.

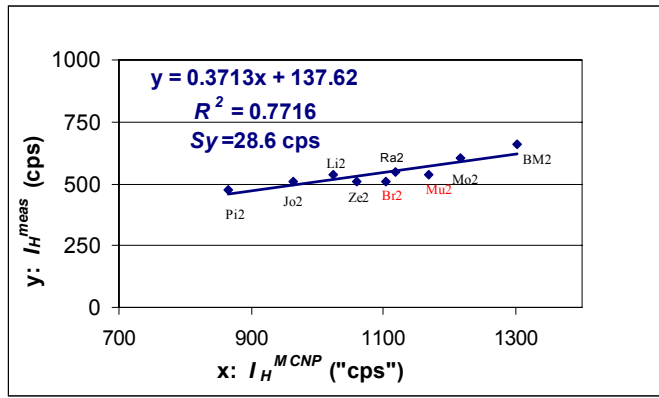


Fig. 5. The measured (*meas*) gross gamma counts vs simulated (*MCNP*) ones for H.

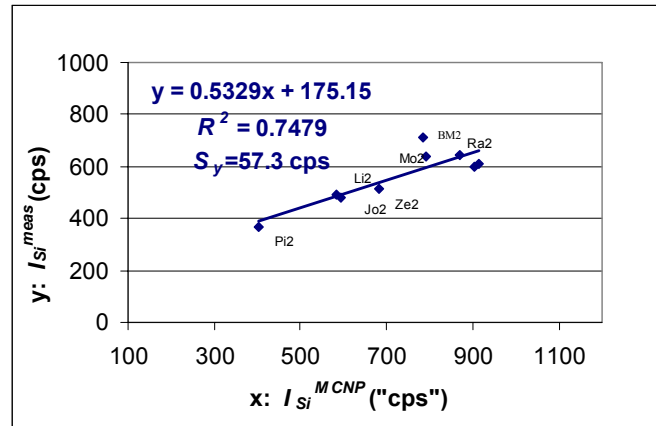


Fig. 6. The measured (*meas*) gross gamma counts vs simulated ("*MCNP*") ones for Si.

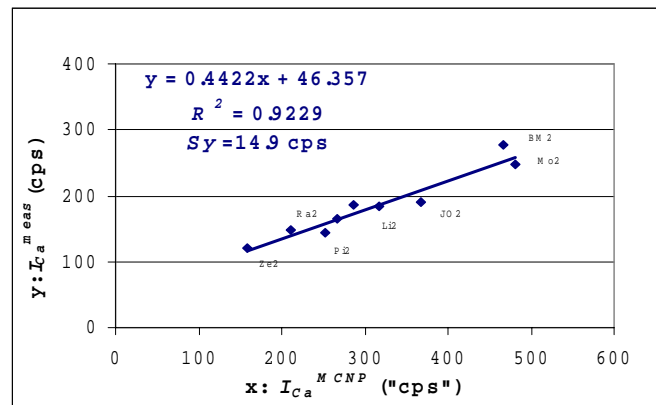


Fig. 7. The measured (*meas*) gross gamma counts vs simulated ("*MCNP*") ones for Ca.

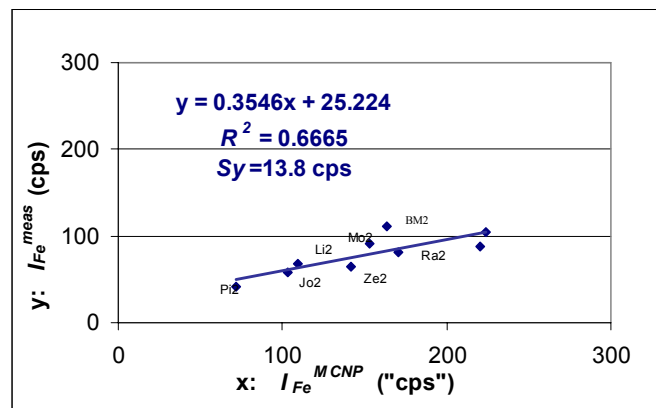


Fig.8. The measured (*meas*) gross gamma counts vs simulated ("*MCNP*") ones for Fe.

As can be seen from the Figs. 5-8 the highest correlation coefficient square R^2 exists for the linear dependence $I_{Ca}^{meas}(I_{Ca}^{MCNP})$. Lower correlation coefficients are visible for the linear dependencies $I_H^{meas}(I_H^{MCNP})$, $I_{Si}^{meas}(I_{Si}^{MCNP})$ and $I_{Fe}^{meas}(I_{Fe}^{MCNP})$. Main reasons are that no B, Cl and REE were included in the input files and that the BGW Zielona Góra rock models are not exactly homogeneous. For the MCNP calculations the homogeneous rock models have been assumed with the averaged elemental contents [Massalski et al., 1994]. However, distributions of the elemental contents obtained for every rock model from chemical analyses show, for several elements, rather high dispersions (standard deviations). For example for FeO in sandstones: Br2, Ra2, Ze2 and Mu2 relative dispersions (standard deviations to the averaged contents) amount to 30.4 %, 15.3%, 24.5%, 7.7% respectively. Also distributions of the CaO concentrations in the above sandstones show high relative dispersions: 46.9 %, 27.5 %, 42.8 % and 7.9 % respectively. Concentrations of SiO₂ in the limestones (BM2, JO2, Pi2) and in dolomite (Li2) have relative dispersions amounted to 61 %, 16.4 %, 28.6 % and 87.9 % respectively. Porosities show remarkable relative dispersions too, for limestones: Jozefow (Jo1), Morawica (Mo2), Pinczow (Pi 2) they amount to \approx 37 %, 22 % and 10 %, respectively.

4.2 Determination of the Si, Ca, Fe and H concentrations in the rocks.

The sNGL measurements performed in the unknown geological formations give the set of gamma-rays spectra which should be properly interpreted to determine the Si, Ca, Fe and H contents and thus to estimate mineralogical composition. To do this, the suitable calibration procedure has to be done using the rock models (calibration standards) of well known physical and chemical parameters.

Calibration equations for determination of the H, Si, Ca and Fe contents are of the form:

$$C_H^{opt} = b_{11}^{opt} + b_{12}^{opt} \cdot I_H^{opt} + b_{13}^{opt} \cdot I_{Si}^{opt} + b_{14}^{opt} \cdot I_{Ca}^{opt} + b_{15}^{opt} \cdot I_{Fe}^{opt} \quad (1)$$

$$C_{Si}^{opt} = b_{21}^{opt} + b_{22}^{opt} \cdot I_H^{opt} + b_{23}^{opt} \cdot I_{Si}^{opt} + b_{24}^{opt} \cdot I_{Ca}^{opt} + b_{25}^{opt} \cdot I_{Fe}^{opt} \quad (2)$$

$$C_{Ca}^{opt} = b_{31}^{opt} + b_{32}^{opt} \cdot I_H^{opt} + b_{33}^{opt} \cdot I_{Si}^{opt} + b_{34}^{opt} \cdot I_{Ca}^{opt} + b_{35}^{opt} \cdot I_{Fe}^{opt} \quad (3)$$

$$C_{Fe}^{opt} = b_{41}^{opt} + b_{42}^{opt} \cdot I_H^{opt} + b_{43}^{opt} \cdot I_{Si}^{opt} + b_{44}^{opt} \cdot I_{Ca}^{opt} + b_{45}^{opt} \cdot I_{Fe}^{opt} \quad (4)$$

The superscript *opt* was introduced to differentiate between the real (*meas*), simulated (*MCNP*) and standardized (*stand*) data. C_H^{opt} , C_{Si}^{opt} , C_{Ca}^{opt} , C_{Fe}^{opt} are concentrations (in wt.%) of the elements of interest, I_H^{opt} , I_{Si}^{opt} , I_{Ca}^{opt} , I_{Fe}^{opt} are the gross gamma counts (cps) from the appropriate spectral windows (Table 1). Coefficients b_{ij}^{opt} ($i: 1 \div 4$ and $j: 1 \div 5$) have been determined using multiple linear regression for N=9 rock models of the BGW Zielona Góra calibration station. The elemental concentrations of the models: C_H^{chem} , C_{Si}^{chem} , C_{Ca}^{chem} , C_{Fe}^{chem} , known from the chemical (*chem*) analyses, were regarded as the reference values.

The multiple linear regression (eqs 1 ÷ 4) has been used for determination of the Si, Ca, Fe and H concentrations in the rock models, independently for the real (“*meas*”) and simulated (“*MCNP*”) experiments. Coefficients b_{ij}^{opt} of equations 1 ÷ 4 and obtained elemental concentrations C_H^{opt} , C_{Si}^{opt} , C_{Ca}^{opt} , C_{Fe}^{opt} are listed in Appendix (Tables A3÷A7). Results for concentrations are also presented graphically (Appendix: Figs. A1÷A4). Parameters of multiple linear regression models (eqs. 1-4), correlation coefficient squares R^2 and standard deviations S_Y , are presented in Table 3.

Table 3. Parameters of the multiple linear regression (correlation coefficient squares R^2 and standard deviations S_y) for correlations between the reference (*chem*) and simulated (*MCNP*) concentrations of H, Si, Ca, Fe and between (*chem*) and (*meas*) concentrations.

Dependence (eqs. 1+4)	Without B, Cl, REE Simulations “MCNP”		Measurements “meas”		N
	R^2	S_y (wt %)	R^2	S_y (wt %)	
$Y = C_{Si}^{opt} (I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0,9721	4,395	0,9801	3,706	9
$Y = C_{Ca}^{opt} (I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0,9695	4,244	0,9691	4,269	9
$Y = C_{Fe}^{opt} (I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0,9733	0,135	0,8946	0,269	9
$Y = C_H^{opt} (I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0,9315	0,212	0,9292	0,216	9

As can be seen from Table 3 the correlation $C_{Si}^{MCNP}(C_{Si}^{chem})$ shows slightly lower correlation coefficients R^2 than $C_{Si}^{meas}(C_{Si}^{chem})$ mainly because of the mentioned lack of the B, Cl and REE in the simulated rock models. C_{Si}^{MCNP} concentrations show higher standard deviations (S_y) for the multiple linear regression model (eq. 2) than C_{Si}^{meas} . For dependence $C_{Fe}^{MCNP}(C_{Fe}^{chem})$ significantly stronger correlation exists ($R^2 = 0,9733$) than for $C_{Fe}^{meas}(C_{Fe}^{chem})$ with $R^2 = 0,8946$, probably because of the experimental instabilities and remarkable influence of the geological inhomogeneities on the measurements. It was mentioned that distribution of the FeO concentration, for example in Br2 sandstone, shows high relative dispersion (standard deviation to the averaged content) amounting to 30.4 %.

4.3. Preliminary simulations for BGW Zielona Góra sandstones with B, Cl and REE.

The remarkable amounts of B, Cl and REE were expected for Mucharz and Brenna sandstones as they show higher, measured thermal neutron absorption cross section than calculated using the existing chemical composition [Drabina et al., 2003]. Preliminary elemental analyses have been done, in Canada XRAL laboratories, for B, Cl and REE in these sandstones and are presented in Table 4 (as obtained from the XRAL laboratory).

Table 4. B, Cl and REE from the preliminary XRF analyses for Mucharz and Brenna sandstones.

Rock model	B (ppm)	Cl (ppm)	Gd (ppm)	Sm (ppm)	Eu (ppm)
Brenna Br 2	34	115	2.87	3.3	0.73
	39	117	2.93	3.3	0.76
Mucharz Mu 1	37	111	2.88	2.8	0.67
	39	124	2.79	2.9	0.67

Additional MCNP simulations have been done including these new elements. The new linear dependencies (new standardisation) between simulated (“MCNP”) and measured (“meas”) gross gamma counts have been obtained and compared to the previous ones (without B, Cl and REE). Correlation coefficient squares R^2 and standard deviations S_y for the fitted linear dependencies show remarkable improvement (Table 5) particularly for Si, Fe and H spectral windows.

Table 5. Parameters of the linear regression (correlation coefficient squares R^2 and standard deviations S_y) for measured and simulated gamma counts for Mucharz and Brenna with/without B, Cl and REE.

Linear dependence	With B, Cl, REE		Without B, Cl, REE	
	R^2	S_y (cps)	R^2	S_y (cps)
$Y = I_{Si}^{meas} (I_{Si}^{MCNP})$	0.8709	41.0	0.7479	57.3
$Y = I_{Ca}^{meas} (I_{Ca}^{MCNP})$	0.8569	20.3	0.9229	14.9
$Y = I_{Fe}^{meas} (I_{Fe}^{MCNP})$	0.7309	12.4	0.6665	13.8
$Y = I_H^{meas} (I_H^{MCNP})$	0.8977	19.0	0.7716	28.6

The quantitative analysis for determination of the Si, Ca, Fe and H contents has been done (equations 1 ÷ 4) for the set of MCNP simulations where Mu2 and Br2 sandstones have been included with B, Cl and REE in their compositions. Parameters of the multiple linear regression are included in Table 6.

Table 6. Parameters of the multiple linear regression (correlation coefficient squares R^2 and standard deviations S_y) for correlations between the reference (*chem*) and simulated (*MCNP*) concentrations of H, Si, Ca, Fe and between (*chem*) and (*meas*) concentrations. B, Cl and REE in Mu2 and Br2 – from preliminary analyses.

Dependence (eq. 1÷4)	with B, Cl and REE Simulations		Measurement		N
	R^2	S_y (wt %)	R^2	S_y (wt %)	
$Y = C_{Si}^{opt} (I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0.9773	3.965	0.9801	3.706	9
$Y = C_{Ca}^{opt} (I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0.9695	4.246	0.9691	4.269	9
$Y = C_{Fe}^{opt} (I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0.9949	0.059	0.8946	0.269	9
$Y = C_H^{opt} (I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0.9057	0.249	0.9292	0.216	9

Results from Tables 3 and 6 show that addition of B, Cl and REE to the simulated Mu2 and Br2 sandstones improved the accuracy of determining the Si and Fe concentrations as the better consistency was obtained between the “true” and simulated elemental composition of the rock models. The entire elemental analyses including B, Cl and REE are planned to be done for the all rock models of the BGW Zielona Góra calibration station.

4.4 Numerical modelling of the artificial rock models.

As mentioned, the BGW Zielona Góra calibration station has limited number of the rock models particularly those with Fe. Furthermore the only two rock models (Mu2, Br2) have the concentration of Fe exceeding 1 wt%. Moreover, as can be seen from Table 2, distribution of Fe content in the rock models shows “bipolar” behaviour. Construction of the new models is very expensive and time consuming. Therefore it is necessary to simulate artificial rock models particularly those with Fe concentration changing gradually from 0 wt % to 5 wt %. Such concentrations are attributed to the clay-sand of Miocene formations of the Carpathian Foredeep. Fe concentration is one of the indicators of the clay admixture [Herron et al., 1996].

The artificial rocks have been simulated as the homogeneous mixtures of silica SiO_2 (2.65 g/cm³) and hematite Fe_2O_3 (5.2 g/cm³). The Fe contents changed from 0 to 5 wt% and porosities K_p were 0 % and 10 % for every model. The porosities, main elements contents and volume densities for the new

rocks are presented in Table 7. Tables A8 of Appendix contains the simulated (*MCNP*) and standardized (*stand*) gross γ -counts from the selected spectral windows and the ratio of suitable γ -counts.

Table 7. The artificial rocks – concentrations of H, Si, Ca, Fe elements, porosities (water filled pores) and volume densities.

Nr, symbol of MCNP run wg. Kalibr2.xls	C_H (wt%)	C_{Si} (wt%)	C_{Ca} (wt%)	C_{Fe} (wt%)	Kp (%)	($SiO_2+Fe_2O_3$) ρ_{vol} (g/cm ³)
143/22.03.03.DFe0a	0.000	46.750	0.000	0.000	0	2.65
243/27.02.04.DFe1aa	0.000	46.082	0.000	1.000	0	2.686
145/24.03.03.DFe2a	0.000	45.413	0.000	2.000	0	2.723
146/25.03.03.DFe3a	0.000	44.745	0.000	3.000	0	2.759
147/26.03.03.DFe4a	0.000	44.076	0.000	4.000	0	2.796
148/27.03.03.DFe5a	0.000	43.408	0.000	5.000	0	2.832
149/27.03.03.DFe0_10a	0.447	44.792	0.000	0.000	10	2.485
244/28.02.04.DFe1_10b	0.441	44.175	0.000	0.960	10	2.517
151/29.03.03.DFe2_10a	0.436	43.558	0.000	1.922	10	2.551
152/01.04.03.DFe3_10a	0.430	42.939	0.000	2.884	10	2.583
153/02.04.03.DFe4_10a	0.425	42.319	0.000	3.847	10	2.616
154/02.04.03.DFe5_10a	0.419	41.698	0.000	4.811	10	2.649

To evaluate probe sensitivity to the varying Fe content, sensitivity parameter S_w has been introduced of the form:

$$S_w = \frac{(\Delta I/I)}{(\Delta w/w)} \cdot 100\% = \frac{(\Delta I/\Delta w)}{(I/w)} \cdot 100\% \quad (8)$$

where w is the wt. % of the Fe element (S_w is evaluated for the established $w = w_0$), I is the “signal” attributed to the element (e.q. the gross gamma counts from the selected spectral windows or the ratios of gamma counts). For the BGO detector of rather poor energy resolution and significant gamma background (Figs.1 and 2) it is more convenient to use, as “signals”, the ratios of the gross gamma counts which are less affected by the porosity and borehole diameters. Such “signals” are better correlated with the elemental concentration of Fe.

In Figs. 9 a and 9 b are shown dependencies (eq. 8) of “signal” I on Fe content when (a) “signal” I is the standardized gross γ -counts from the Fe spectral window or (b) “signal” I is the ratio of γ -counts from Fe and Si windows. Sensitivity parameters have been calculated for $w_0 = 2.5$ wt. % Fe. Significant improvement ($R^2 = 0.972$) of correlation between iron content and signal being γ -counts ratio is visible. Points are less scattered around regression line and sensitivity parameter of 22.3 % is more reliable than for dependence $I_{Fe}^{stand}(C_{Fe})$ deteriorated by significant porosity influence.

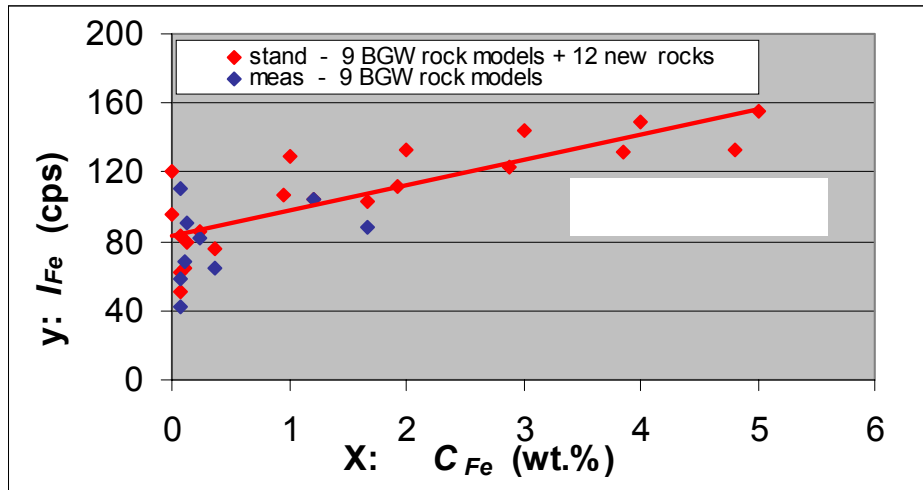


Fig. 9a. Linear dependence of the I_{Fe}^{opt} on the Fe content in the rock models.

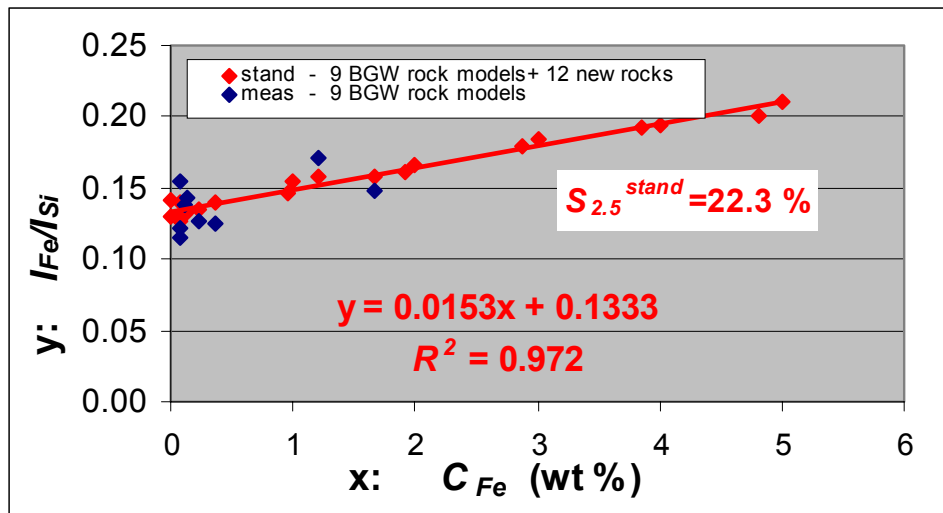


Fig. 9b. Linear dependence of the ratio $I_{Fe}^{opt}/I_{Si}^{opt}$ on the Fe content in the rock models.

The artificial rocks show the Fe concentration distributed uniformly in the range 0 ÷ 5 wt % and together with the rock models of BGW Zielona Góra give sufficient diversification of Fe element.

In Table 8 are presented the correlation coefficient squares R^2 and standard deviations S_Y for the Si, Ca, Fe and H contents, obtained from equations 1 ÷ 4, for the simulated set of $N = 21$ rock models (total number of the artificial and the BGW Zielona Góra models). Data for iron content seem to be more reliable than for the previous “bipolar” distribution of Fe in the BGW Zielona Góra rock models (see Table 3).

Table 8. Parameters of the multiple linear regression (correlation coefficient squares R^2 and standard deviations S_y) for correlations between the reference (*chem*) and simulated (*MCNP*) concentrations of H, Si, Ca, Fe, for N = 21 rock models.

Dependence (eq. 1+4)	Simulations	"MCNP"	N
	R^2	S_y (wt %)	
$Y = C_{Si}^{opt}(I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0.9812	2.827	21
$Y = C_{Ca}^{opt}(I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0.9707	2.802	21
$Y = C_{Fe}^{opt}(I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0.9879	0.208	21
$Y = C_H^{opt}(I_H^{opt}, I_{Si}^{opt}, I_{Ca}^{opt}, I_{Fe}^{opt})$	0.9345	0.133	21

5. Conclusions

The spectrometric Neutron-Gamma Logging (sNGL) - suitable for lithology identification - is one of the complementary geophysical techniques being used worldwide in oil and gas prospecting. The results of the real and simulated sNGL experiments have been compared in this paper.

The upgraded, borehole n-gamma spectrometer, SO-5-90-SN type, has been used for the sNGL experiment performed at the BGW Zielona Góra calibration station [Zorski et al., 2001] where the main lithology models show rather poor diversification of the Si, Ca and Fe concentrations. The Monte Carlo benchmark simulations (MCNP code) have been done for the above sNGL experiment which gave the satisfactory agreement with the measurements. Simulated and measured gamma-ray spectra were the base for quantitative elemental analyses which have been done using multiple linear regression method. The H, Ca and Fe concentrations obtained from the simulations ("MCNP") have been highly correlated with their reference ("chem") concentrations, R^2 amounted to 0.931, 0.969, 0.973, respectively. For the dependence $C_{Si}^{MCNP}(C_{Si}^{chem})$ slightly lower R^2 (0.972) has occurred than for $C_{Si}^{meas}(C_{Si}^{chem})$. This is mainly attributed to the unavailable B, Cl and REE contents, of the BGW Zielona Góra rock models and their geological inhomogeneities. Introducing into the MCNP the preliminary analyses for B, Cl and REE in the Mu 2 and Br 2 sandstones an improvement has been obtained for the correlation $C_{Si}^{MCNP}(C_{Si}^{chem})$ where $R^2 = 0.977$ and for $C_{Fe}^{MCNP}(C_{Fe}^{chem})$ with $R^2 = 0.995$. At present, the complete chemical analyses, including the REE, B and Cl contents, are being done for all BGW rock models.

The poorly diversified elemental concentrations of the BGW Zielona Góra rock models caused that the new, artificial rock models of required physical and chemical parameters have been simulated for accurate spectrometer calibration. Particularly models with the Fe content changing up to 5 wt % were of high importance as such concentrations were estimated for the shaly-sand of Miocene formations of the Carpathian Foredeep. Simulated artificial rocks were the homogeneous mixtures of silica SiO_2 (2.65 g/cm³) and hematite Fe_2O_3 (5.2 g/cm³). The Fe contents changed gradually from 0 to 5 wt% and porosities K_p were 0 % and 10 % for every model. To evaluate probe sensitivity to the changing Fe content, sensitivity parameter S_w has been introduced which is well correlated ($R^2 = 0.972$) with the ratio of γ -counts from the Fe and Si spectral windows. Sensitivity parameter of 22.3 % has been obtained for $w_0 = 2.5$ wt.% Fe.

As the MCNP simulations give the effective support for the calibration of the sNGL logging tool, this code will be used for an investigation of the disturbing effects influence (e.g. Cl in boreholes and in geological formations) on the logging tool response.

Acknowledgement – Scientific work, partly supported by the funds from the State Committee for Scientific Research KBN, during 2004-2007 years, as the research project No: 4 T12B 056 27.

References

- Briesmeister J. F., MCNP4C (CCC-700) – A General Monte Carlo N-Particle Transport Code, Los Alamos National Laboratory, Los Alamos, New Mexico, 2000.
- Cywicka-Jakiel T., Zorski T. (a): Monte-Carlo simulations of the spectrometric n-gamma well logging. Comparison of simulations and measurements for the SO-5-90 logging tool. INP Report No 1941/AP, Instytut Fizyki Jądrowej, Kraków, 2004. <http://www.ifj.edu.pl/reports/2004/1941.pdf>.
- Cywicka-Jakiel T., Zorski T. (b): Possibility of determination the Si, Ca and Fe concentrations in Miocene gas formations of the Carpathian Foredeep using borehole gamma spectrometry. Measurements and MCNP calculations. Transactions of the Scientific and Technical Conference “GEOPETROL 2004”, Zakopane 20-23 Sept. 2004, Research Reports No 130 of the Gas and Oil Institute Kraków, PL ISSN 0209-0724 (in Polish).
- Drabina A., Zorski T., Woźnicka U, Correlation Between Measurements and Monte-Carlo Calculations for the NNTE Logging-Tool, Report INP No 1926/AP, 2003.
- Harvey P.K., Lovell M.A., Lofts J.C., Pezard P.A., Bristow J.F., 1997: Petrophysical estimation from downhole mineralogy logs, Geological Society Special Publication No.122: Developments in Petrophysics, Geological Society of London, 1997.
- Herron S. L., Herron M.M., Quantitative Lithology: an Application for Open Cased Hole Spectroscopy, Transactions of SPWLA, Thirty-seventh Annual Logging Symposium, New Orleans, LA, June 16-19, Paper E, 1996.
- Hertzog R., Colson L., Seeman B., O'Brien M., Scott H., McKeon D., Wraight P., Grau J., Ellis D., Schweitzer J., Herron M., Geochemical Logging with Spectrometry Tools. SPE Paper 16792, 1987.
- Massalski T., Calibration Facility for the Nuclear Logging Tools Based on the Rock Standards, Transactions of the Fourth Scientific and Technical Conference on Well Logging, Drzonków near Zielona Góra, September 1988 (in Polish).
- Massalski T., Stadtmuller M., Ossowski A., Zorski T., Results of the Laboratory Analysis of the Rock Standards at the Zielona Góra Calibration Facility, Transactions of the Sixth Scientific and Technical Conference on Well Logging, Dobczyce, 28-30.09.1994 (in Polish).
- Pałka K.W., Zorski T., Set of the Nuclear Tools for the Shallow Well Logging, AGH Quarterly – Geology Vol.20, No 2, Kraków, 1994 (in Polish).
- Passey Q., Dahlberg K.E., Sullivan K.B., Yin H., Xiao Y.H., Guzman-Garcia A.G., Brackett R.A., 2004. A systematic approach to evaluate hydrocarbons in thinly bedded reservoirs, *Trans. of SPWLA 45th Annual Logging Symposium*, June 6-9, 2004, pap. NNN.
- Saxena K., Klimentos T., 2004. Field – study of integrated formation evaluation in thinly laminated reservoirs. *Trans. of SPWLA 45th Annual Logging Symposium*, June 6-9, 2004, pap. SSS.
- Schweitzer J. S. , Ellis D. V. , Grau , J. A. , Hertzog R. C. , Elemental Concentration from Gamma-ray Spectroscopy Logs, *Nucl. Geophys. 2 (3)*, 1988, pp. 175-181.
- Środoń J, Peveraro R., Kowalska S., 2004 . Correlation between different mineralogical and chemical parameters of the Miocene rocks from the Carpathian Foredeep and their use in the interpretation o the geophysical logging, Transactions of the Scientific and Technical Conference “GEOPETROL 2004”, Zakopane 20-23 Sept. 2004, Research Reports No 130 of the Gas and Oil Institute Kraków, PL ISSN 0209-0724 (in Polish).
- Tickner J, n-gamma cross sections for Ge - file jt2000, CSIRO Division of Mineral Engineering in Lucas Heights, Australia.
- Zorski T, Ossowski N. Górecka N., Description of the measurements performed, in July 2001, at the BGW Zielona Góra Calibration Station using SO-5-90-SN spectrometer - Supplement to the “Experimental Verification of the Possibility of the Elemental Composition Determination by Means of the Spectrometric Neutron-gamma Logging and Neutron Activation Logging”, Report on the Research Activity of the Well Logging Department (Faculty of Geology, Geophysics and Environmental Protection of the AGH University of Science and Technology) in 2000 year, Kraków, 2001 (in Polish).
- Zorski T., 2004. Metodyka interpretacji pomiarów geofizyki otworowej w cienkobarstowych utworach gazonośnych przedgórza Karpat, *Kwartalnik AGH, Geologia, Zeszyt 3 2004*.
- Zorski T., Massalski T., 1997. Empirical and semiempirical approach to the comprehensive calibration of nuclear logging tools, Extended Abstracts Volume 1 59th EAEG Conference & Exhibition, 26 – 30 May 1997, Geneva, Switzerland.
- Zorski T., Pałka K., Spectral neutron – gamma logging tool SO-5-90-SN 2004 and its application in Miocene gas formation, Carpathian Foredeep, Poland, Transactions of the Scientific and Technical Conference “GEOPETROL 2004”, Zakopane 20-23 Sept. 2004, Research Reports No 130 of the Gas and Oil Institute Kraków, PL ISSN 0209-0724 (in Polish).

APPENDIX

Table A1. The measured (“*meas*”), simulated (“*MCNP*” – tally24/-5) and standardized (“*stand*”) gross gamma counts from the selected spectral windows.

Symbol/name of standard-Nr/date of simulations	I_H^{MCNP}	I_{Si}^{MCNP}	I_{Ca}^{MCNP}	I_{Fe}^{MCNP}	I_H^{meas}	I_{Si}^{meas}	I_{Ca}^{meas}	I_{Fe}^{meas}	$I_H^{stand(*)}$	$I_{Si}^{stand(*)}$	$I_{Ca}^{stand(*)}$	$I_{Fe}^{stand(*)}$
	(cps)	(cps)	(cps)	(cps)	(cps)	(cps)	(cps)	(cps)	(cps)	(cps)	(cps)	(cps)
BM2_2/Biała Marianna2 - 45,54,93/ 2002	1302.4	786.1	466.2	163.9	659.2	710.75	276.4	110.3	621.2	594.0	252.5	83.3
MO2_2/Morawica2 - 48,64,94/2002	1216.3	790.3	480.9	153.0	601.6	638.9	248.6	91.1	589.2	596.3	259.0	79.5
JO2/Józefow2 - 49,98,100/ 04.07.2002	962.4	592.7	368.5	103.2	510.7	481.4	189.6	58.2	495.0	491.0	209.3	61.8
Li2_2/Libiąż2 - 47,97/2002	1023.8	583.5	316.8	109.3	535	490.7	183.2	67.8	517.8	486.1	186.4	64.0
Pi2_2/Pinczów2 - 46,92/2002	865.5	401.9	252.9	71.3	476.1	365.6	143	42.2	459.0	389.3	158.2	50.5
Mu2_2/Mucharz2 - 1,2,3,4,27,27a,27b,50,55/2002	1168.3	912.3	286.3	223.6	535.2	609.5	185.3	104.2	571.4	661.3	173.0	104.5
Br2_2/Brenna2 - 48,68,99/2002	1103.5	904.7	266.6	220.7	510.5	598.6	164.2	88.3	547.3	657.3	164.2	103.5
Ra2_2/Radków2 - 61,95/2002	1117.3	868.8	210.8	170.2	549.2	644.5	149	81.8	552.5	638.1	139.6	85.6
Ze2_2/Żerkowice2 - 47,69,70/2002	1058.6	680.8	159.4	141.4	506.1	511.7	119.7	64.1	530.7	538.0	116.9	75.4

(*) (“*stand*”) - from simulated counts (“*MCNP*”) using equations included in Figs. 5 – 8.

Table A2. The ratios of gross gamma counts from the selected spectral windows.

Symbol/name of standard-Nr/date of simulations	$(I_{Fe}/I_{Si})^{meas}$	$(I_{Fe}/I_{Si})^{stand}$
BM2_2/Biała Marianna2 - 45,54,93/ 2002	0.155	0.140
MO2_2/Morawica2 - 48,64,94/2002	0.143	0.133
JO2/Józefow2 - 49,98,100/ 04.07.2002	0.121	0.126
Li2_2/Libiąż2 - 47,97/2002	0.138	0.132
Pi2_2/Pinczów2 - 46,92/2002	0.115	0.130
Mu2_2/Mucharz2 - 1,2,3,4,27,27a,27b,50,55/2002	0.171	0.158
Br2_2/Brenna2 - 48,68,99/2002	0.148	0.157
Ra2_2/Radków2 - 61,95/2002	0.127	0.134
Ze2_2/Żerkowice2 - 47,69,70/2002	0.125	0.140

Table A3. Linear regression coefficients (equations 1÷4) for C_H^{opt} , C_{Si}^{opt} , C_{Ca}^{opt} , C_{Fe}^{opt} determination.
 (The BGW Zielona Góra rock models with borehole diameters from the range 215÷220 mm.)

	Coefficients (eq. 1÷4)	MCNP	meas	stand
C_H^{opt}	b_{11}^{opt}	3.4048	0.8213	4.4975
	b_{12}^{opt}	-0.0001	0.0086	-0.0003
	b_{13}^{opt}	-0.0021	-0.0045	-0.0039
	b_{14}^{opt}	-0.0034	-0.0111	-0.0077
	b_{15}^{opt}	-0.0001	-0.0028	-0.0004
C_{Si}^{opt}	b_{21}^{opt}	-4.7868	24.2458	-17.4588
	b_{22}^{opt}	0.0157	-0.0567	0.0423
	b_{23}^{opt}	0.0860	0.1471	0.1613
	b_{24}^{opt}	-0.1457	-0.4141	-0.3295
	b_{25}^{opt}	-0.0863	0.2097	-0.2435
C_{Ca}^{opt}	b_{31}^{opt}	19.8667	3.8537	24.2854
	b_{32}^{opt}	-0.0074	-0.0039	-0.0200
	b_{33}^{opt}	-0.0414	-0.0368	-0.0776
	b_{34}^{opt}	0.1367	0.4403	0.3090
	b_{35}^{opt}	-0.0337	-0.5455	-0.0950
C_{Fe}^{opt}	b_{41}^{opt}	1.9376	6.0196	2.2183
	b_{42}^{opt}	-0.0030	-0.0178	-0.0080
	b_{43}^{opt}	-0.0031	0.0015	-0.0058
	b_{44}^{opt}	0.0009	0.0039	0.0021
	b_{45}^{opt}	0.0244	0.0318	0.0687

Tabele A4. C_{Si}^{meas} and C_{Si}^{MCNP} concentrations^(*) obtained from the sNGL measurements and MCNP simulations using eqs. 1÷4. Reference (*chem*) values included.

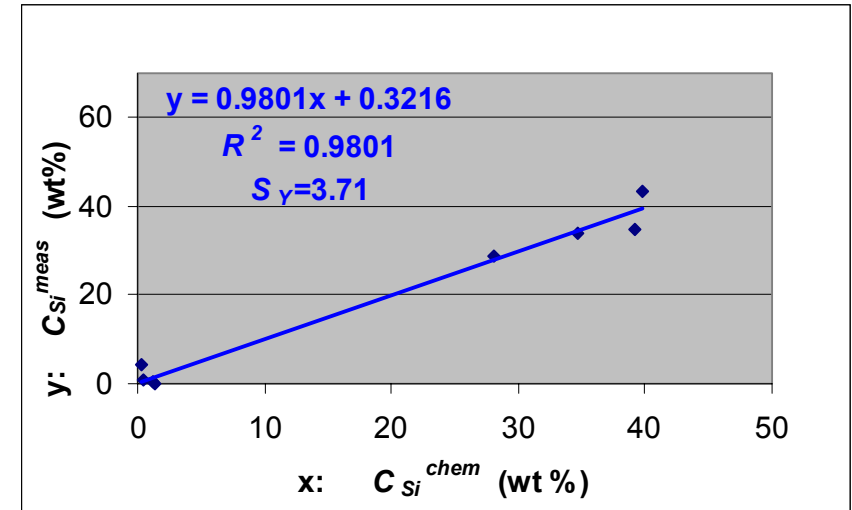
Rock model	C_{Si}^{chem} ·(wt %)	C_{Si}^{meas} ·(wt %)	C_{Si}^{MCNP} ·(wt %)
BM2 - Biała Marianna 2 - limestone	1.301	0.063	1.199
MO2 - Morawica 2 limestone	1.142	0.248	-0.983
JO2 - Józefów 2 - limestone	0.685	-0.227	-1.286
Pi2 - Pinczów 2 - limestone	0.446	4.426	5.886
Li2 - Libiąż 2 – dolomite	0.252	0.646	0.372
Mu2 - Mucharz 2 - sandstone	28.073	28.651	31.002
Br2 - Brenna 2 – sandstone	34.700	33.853	32.453
Ra2 - Radków 2 - sandstone	39.831	43.342	42.076
Ze2 - Żerkowice 2 – sandstone	39.250	34.675	34.958

(*)Negative concentrations resulting from statistical analysis are within standard deviations $S_y = 3.71$ wt.% for “*meas*” and $S_y = 4.39$ wt.% for “*MCNP*”.

Right: Figs. A1. Comparisons between the concentrations:

- (a) C_{Si}^{chem} and C_{Si}^{meas}
- (b) C_{Si}^{chem} and C_{Si}^{MCNP}

(a)



(b)

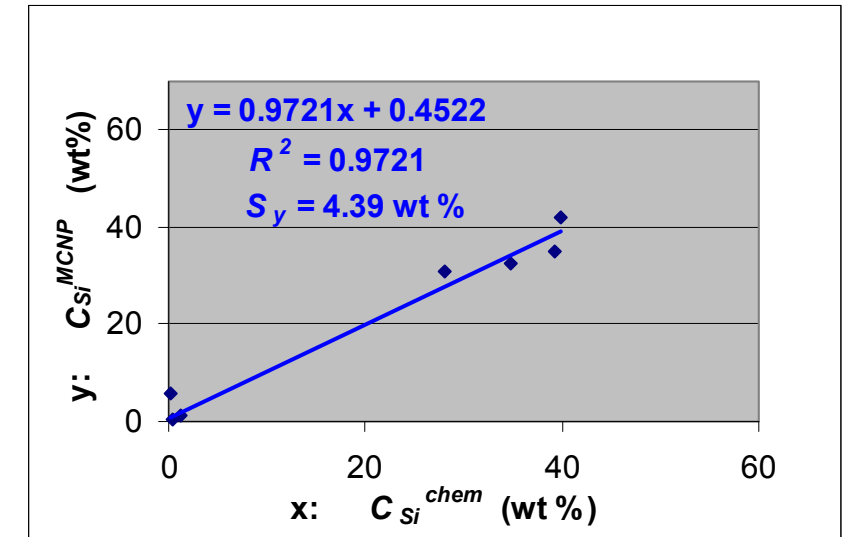


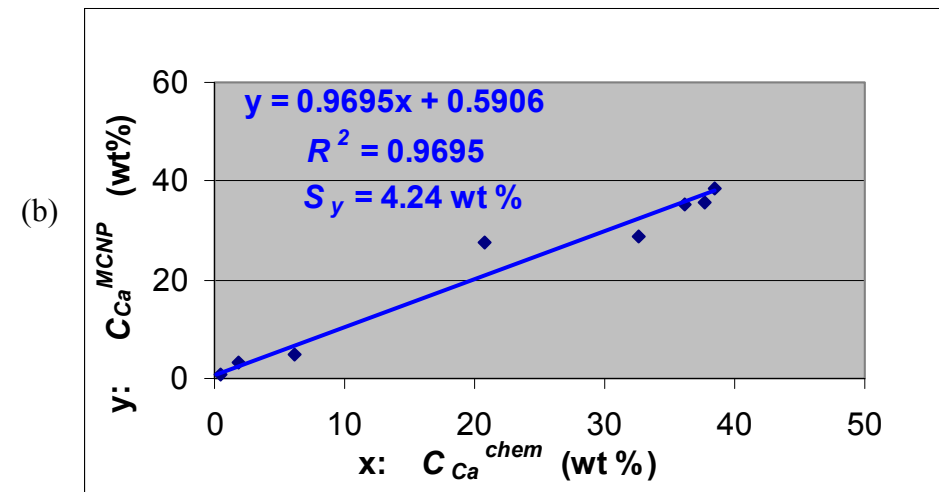
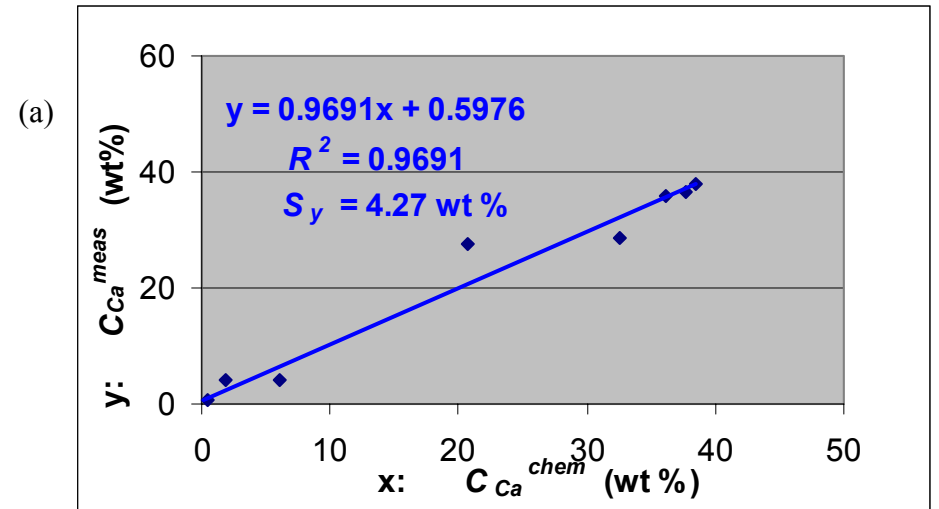
Table A5. C_{Ca}^{meas} and C_{Ca}^{MCNP} concentrations(*) obtained from the sNGL measurements and MCNP simulations using eqs. 1÷4. Reference (*chem*) values included.

Rock model	C_{Ca}^{chem} ·(wt %)	C_{Ca}^{meas} ·(wt %)	C_{Ca}^{MCNP} ·(wt %)
BM2 - Biała Marianna 2 - limestone	37.635	36.697	35.877
MO2 - Morawica 2 limestone	38.517	37.795	38.707
JO2 - Jozefów 2 - limestone	36.161	35.908	35.084
Pi2 - Pinczów 2 - limestone	32.546	27.418	27.743
Li2 - Libiąż 2 – dolomite	20.694	28.511	28.983
Mu2 - Mucharz 2 - sandstone	6.127	4.117	5.047
Br2 - Brenna 2 – sandstone	1.923	3.996	3.247
Ra2 - Radków 2 - sandstone	0.223	-0.989	-1.290
Ze2 - Żerkowice 2 – sandstone	0.442	0.816	0.869

(*)Negative concentrations resulting from statistical analysis are within standard deviations $S_y = 4.27$ wt.% for “*meas*” and $S_y = 4.24$ wt.% for “*MCNP*”.

Right: Figs. A2 Comparisons between the concentrations:

- (a) C_{Ca}^{meas} and C_{Ca}^{chem}
- (b) C_{Ca}^{meas} and C_{Ca}^{MCNP}



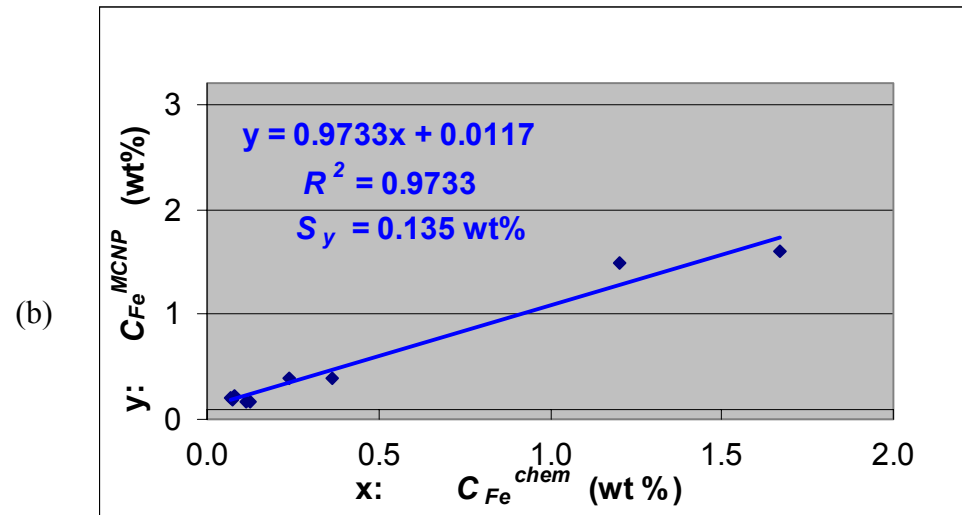
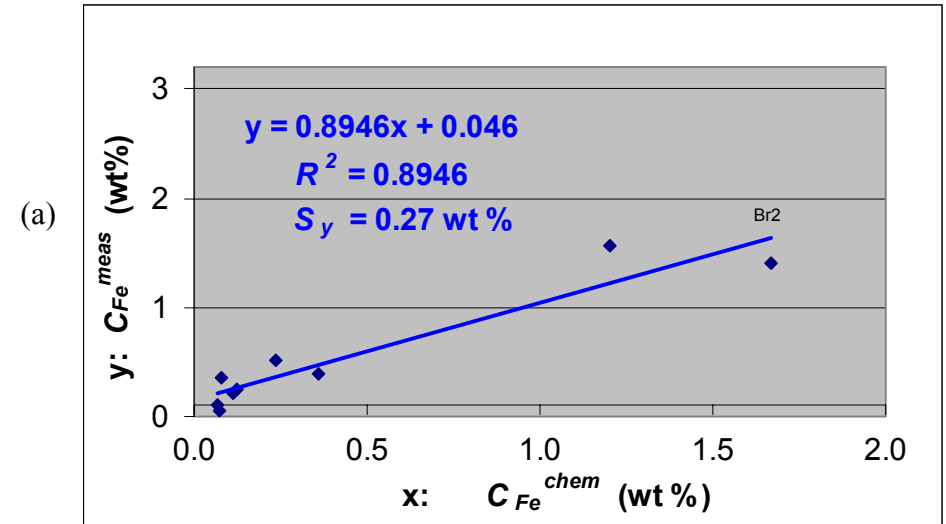
Tabele A6. C_{Fe}^{meas} and C_{Fe}^{MCNP} concentrations^(*) obtained from the sNGL measurements and MCNP simulations using eqs. 1÷4. Reference (*chem*) values included.

Rock model	C_{Fe}^{chem} (wt %)	C_{Fe}^{meas} (wt %)	C_{Fe}^{MCNP} (wt %)
BM2 - Biała Marianna 2 - limestone	0.075	-0.046	0.086
MO2 - Morawica 2 limestone	0.125	0.150	0.076
JO2 - Jozefów 2 - limestone	0.079	0.251	0.118
Pi2 - Pinczów 2 - limestone	0.068	0.113	0.066
Li2 - Libiąż 2 - dolomite	0.115	-0.001	0.110
Mu2 - Mucharz 2 - sandstone	1.202	1.460	1.379
Br2 - Brenna 2 - sandstone	1.667	1.296	1.505
Ra2 - Radków 2 - sandstone	0.238	0.412	0.292
Ze2 - Żerkowice 2 - sandstone	0.362	0.297	0.298

(*)Negative concentrations resulting from statistical analysis are within standard deviation $S_y = 0.27$ wt.%

Right: Figs. A3 Comparisons between the concentrations:

- (a) C_{Fe}^{meas} and C_{Fe}^{chem}
- (b) C_{Fe}^{MCNP} and C_{Fe}^{chem}



Tabele A7. C_H^{meas} and C_H^{MCNP} concentrations^(*) obtained from the sNGL measurements and MCNP simulations using eqs. 1÷4. Reference (*chem*) values included.

Rock model	C_H^{chem} (wt %)	C_H^{meas} (wt %)	C_H^{MCNP} (wt %)
BM2 - Biała Marianna 2 - limestone	0.004	-0.092	0.007
MO2 - Morawica 2 limestone	0.109	0.099	-0.041
JO2 - Jozefów 2 - limestone	0.704	0.773	0.790
Pi2 - Pinczów 2 - limestone	0.664	0.984	0.978
Li2 - Libiąż 2 - dolomite	1.813	1.558	1.597
Mu2 - Mucharz 2 - sandstone	0.326	0.325	0.368
Br2 - Brenna 2 - sandstone	0.484	0.441	0.459
Ra2 - Radków 2 - sandstone	0.784	0.752	0.730
Ze2 - Żerkowice 2 - sandstone	1.307	1.354	1.306

(*)Negative concentrations resulting from statistical analysis are within standard deviations $S_y = 0.22$ wt.% for “*meas*” and $S_y = 0.22$ wt.% for “*MCNP*”.

Right: Figs. A4 Comparisons between the concentrations:

- (a) C_H^{meas} and C_H^{chem}
- (b) C_H^{MCNP} and C_H^{chem}

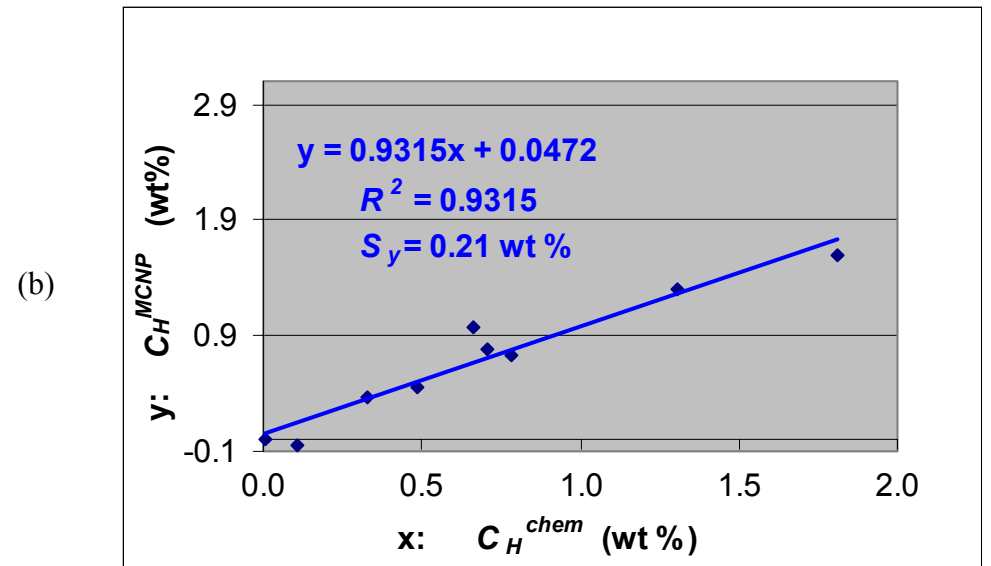
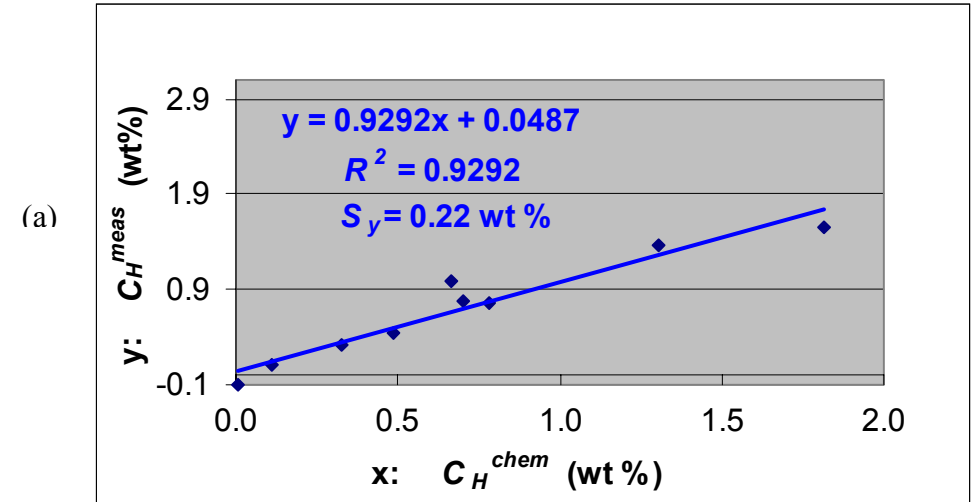


Table A8. The simulated “MCNP”(tally24/-5) and standardized (*stand*) gross gamma counts from the selected spectral windows for the artificial rocks.

Nr, name of MCNP run wg. Kalibr2.xls	I_H^{MCNP} cps	I_{Si}^{MCNP} cps	I_{Ca}^{MCNP} cps	I_{Fe}^{MCNP} cps	I_H^{stand} cps	I_{Si}^{stand} cps	I_{Ca}^{stand} cps	I_{Fe}^{stand} cps	$(I_{Fe}/I_{Si})^{stand}$
143/22.03.03.DFe0a	1729.7	1275.6	324.8	269.6	779.8	854.9	190.0	120.8	0.211
243/27.02.04.DFe1aa	1651.1	1234.4	339.7	292.8	750.7	832.9	196.6	129.1	0.237
145/24.03.03.DFe2a	1605.8	1173.4	327.2	303.3	733.9	800.4	191.1	132.8	0.258
146/25.03.03.DFe3a	1544.8	1146.9	322.7	336.3	711.2	786.4	189.1	144.5	0.293
147/26.03.03.DFe4a	1509.4	1115.5	331.6	350.4	698.1	769.6	193.0	149.5	0.314
148/27.03.03.DFe5a	1485.0	1058.2	310.5	366.8	689.0	739.1	183.7	155.3	0.347
149/27.03.03.DFe0_10a	1294.5	1070.0	244.5	200.4	618.3	745.4	154.5	96.3	0.187
244/28.02.04.DFe1_10b	1278.9	1047.7	255.0	231.4	612.5	733.5	159.1	107.3	0.221
151/29.03.03.DFe2_10a	1212.0	973.5	236.7	243.7	587.6	693.9	151.0	111.6	0.250
152/01.04.03.DFe3_10a	1161.0	954.2	241.9	274.8	568.7	683.6	153.3	122.7	0.288
153/02.04.03.DFe4_10a	1108.9	956.3	244.1	300.7	549.3	684.8	154.3	131.9	0.314
154/02.04.03.DFe5_10a	1104.5	915.2	250.3	304.6	547.7	662.8	157.0	133.2	0.333

