Monte Carlo simulations of the spectrometric n-gamma well logging. Comparison of simulations and measurements for the SO-5-90 logging tool

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Abstract

The results of the Monte Carlo simulations (MCNP code) of the spectrometric neutron-gamma well logging (sNGL) are presented. The sNGL can be very useful for the precise lithology determination, what is especially important for oil and gas prospecting in shally-sand formations. Possibility of determination of the Si, Ca and Fe content in rocks by means of the analysis of gamma ray spectra induced by the captured neutrons is well known for 40 years at least [Larionov, 1969]. Preliminary sNGL experiments performed at the Polish Calibration Station in Zielona Góra, using a simple borehole spectrometer equipped with the isotopic Am-Be neutron source and the BGO detector, fully confirmed this possibility.

MCNP simulations of the sNGL experiments have been done for the SO-5-90 neutron-gamma spectrometer and for the lithology models (standards) of the Calibration Station. The concentrations of H, Si, Ca and Fe in these models have been determined from the real and simulated experiments using the simulated (“MCNP”) and measured (“meas”) spectra of gamma-rays from neutron interactions with the rock nuclei.

The H, Si and Ca concentrations obtained from the simulated experiment are well correlated with their reference values, known from the chemical (“chem”) analyses - regarded as true values. Squares of the correlation coefficients ($R^2$) amount to 0.992, 0.988 and 0.984, respectively. For Fe, a lower $R^2$ has occurred for the linear dependence $F_{\text{MCNP}}(Fe_{\text{chem}})$ than for $F_{\text{meas}}(Fe_{\text{chem}})$ amounting to 0.834 and 0.923 respectively.

Although the established correlations between results of the real and simulated sNGL experiments show the high values of correlation coefficients, the noticeable improvement of these correlations is expected for the fully verified chemical composition of the Zielona Góra standards and for improved parameters of the n-gamma spectrometer.
The usefulness of the MCNP code for modeling the spectrometric neutron-gamma logging tool responses is confirmed. The possibility of the fast and accurate computer simulations opens a new field for development of the spectrometric n-gamma logging. Especially the influence of such disturbing factors as borehole conditions, borehole and formation salinities or presence of the additional rock elements (like B, S, K, Gd) must be precisely known when the quantitative determination of Si, Ca and Fe is required.

1. Introduction

The spectrometric neutron-gamma well logging (sNGL) plays an important role in the quantitative analysis of the elements, Si, Ca, Fe and H, which are the main constituents of numerous minerals. In the sNGL experiments the characteristic energies and intensities of gamma-rays arising from neutron interactions are applied for identifying and quantifying the elements of geological formations. The Geochemical Logging Tool [Hertzog et al., 1987, Schweitzer et al., 1988] developed by Schlumberger allows quantification of the elements: K, U, Th, Al, Si, Ca, Fe, S, Gd and Ti by measuring the natural radioactivity, prompt gamma-rays following neutron capture and delayed gamma-rays from the Al activation. An attempts to use a less expensive spectroscopy device for determining Si, Ca and Fe concentrations were also reported [Heron and Heron, 1996], where the Am-Be source and BGO detector were used.

For calibration of the neutron-gamma spectrometer, numerous rock models of different lithology are necessary. Calibration facility in Zielona Góra Well Logging Base of Geofizyka Kraków Ltd. was established in 1988 [Massalski, 1988], where relatively wide range of the experiments can be performed [Zorski, Massalski, 1997]. The primary goal of the facility creation was calibration of the neutronic tools for the porosity measurements, like CNT (Halliburton) or PKNN (Geofizyka Kraków Ltd.). It soon became clear, that gathered rocks are a very good set of models for the experiments with different nuclear tools, including the sNGL [Zorski, Stadtmüller, 1991]. However, the calibration of the sNGL tools is much more complicated process than the calibration of the simple neutronic tools for the porosity measurements. Much more of the elements (Si, Ca, Fe, H) and disturbing factors (borehole, salinity of the borehole and formation, presence of the additional elements like S, K, Gd) must be taken into consideration in this case.

The possibility of the fast and accurate computer simulations, using a Monte Carlo code, opens the new field for development of the spectrometric n-gamma logging. Nevertheless the full success of this kind of the simulations is determined by a reliable benchmark. Particularly, the complete and precise chemical analyses including B and Rare Earth Elements are necessary for the standards.

The presented report gives the description of the first comparisons of the experimental measurements with the numerical simulations using the MCNP code for the SO-5-90 borehole spectrometer.

2. Spectrometric neutron-gamma well logging sNGL at the Zielona Góra Calibration Station.

The sNGL experiment for determining H, Si, Ca and Fe content in different rock models was performed at the Polish Calibration Station in Zielona Góra [Zorski et al., 2000, 2001]. The SO-5-90 neutron-gamma spectrometer was used [Palka, Zorski, 1994], which consisted of an isotopic neutron source (Am-Be) and the highly efficient scintillation detector (BGO) which registered gamma-rays following the neutron interactions with nuclei of the rock elements.

Lithology models i.e. sandstones, limestones and dolomites of variable porosities were used for the measurements. Models were put into the basin of water (100 cm layer of water above the rock) and placed on a 50 cm thick concrete floor. Water filled boreholes, drilled vertically in the centre of the every rock model had typical diameters amounted to 220 mm (215 and 216 mm appeared sporadically). The porosity, density and chemical compositions of the rock matrices were analysed by several laboratories. No analyses for B and Rare Earth Elements were done (the neutron absorption cross-section Σa of rock matrix is available only). An average elemental composition was established
for the every rock model [Massalski et al., 1994]. In Table 1 the concentrations of the main rock elements, i.e. \( Si, Ca, Fe \) and \( H \), are listed together with the porosities and matrix densities \( \rho_{\text{matrix}} \).

Table 1. Parameters of the Zielona Góra lithology models (standards) used for calibration of the SO-5-90 spectrometer – concentrations of \( H, Si, Ca, Fe \) elements, porosity and rock matrix density.

<table>
<thead>
<tr>
<th>The name and lithology of calibration standard</th>
<th>( H ) (wt%)</th>
<th>( Si ) (wt%)</th>
<th>( Ca ) (wt%)</th>
<th>( Fe ) (wt%)</th>
<th>porosity (%)</th>
<th>( \rho_{\text{matrix}} ) g/cm(^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BM2 - Biala Marianna 2 - limestone</td>
<td>0.004</td>
<td>1.301</td>
<td>37.635</td>
<td>0.075</td>
<td>0.100</td>
<td>2.714</td>
</tr>
<tr>
<td>MO2 - Morawica 2 - limestone</td>
<td>0.109</td>
<td>1.142</td>
<td>38.517</td>
<td>0.125</td>
<td>2.570</td>
<td>2.674</td>
</tr>
<tr>
<td>JO2 - Jozefow 2 - limestone</td>
<td>0.704</td>
<td>0.685</td>
<td>36.161</td>
<td>0.079</td>
<td>15.240</td>
<td>2.659</td>
</tr>
<tr>
<td>Pi2 - Pinczow 2 - limestone</td>
<td>1.813</td>
<td>0.446</td>
<td>32.546</td>
<td>0.068</td>
<td>34.460</td>
<td>2.828</td>
</tr>
<tr>
<td>Li2 - Libiaz 2 - dolomite</td>
<td>0.664</td>
<td>0.252</td>
<td>20.694</td>
<td>0.115</td>
<td>15.240</td>
<td>2.697</td>
</tr>
<tr>
<td>Mu2 - Mucharz 2 - sandstone</td>
<td>0.326</td>
<td>28.073</td>
<td>6.127</td>
<td>1.202</td>
<td>2.600</td>
<td>2.710</td>
</tr>
<tr>
<td>Br2 - Brenna 2 - sandstone</td>
<td>0.484</td>
<td>34.700</td>
<td>1.923</td>
<td>1.667</td>
<td>7.670</td>
<td>2.648</td>
</tr>
<tr>
<td>Ra2 - Radkow 2 - sandstone</td>
<td>0.784</td>
<td>39.831</td>
<td>0.223</td>
<td>0.238</td>
<td>14.700</td>
<td>2.620</td>
</tr>
<tr>
<td>Ze2 - Zerkowice 2 - sandstone</td>
<td>1.307</td>
<td>39.250</td>
<td>0.442</td>
<td>0.362</td>
<td>24.870</td>
<td>2.640</td>
</tr>
</tbody>
</table>

Hydrogen present in the borehole fluids and in the rock pores dominates the neutron moderation process. Therefore the gamma-rays from thermal neutron capture contribute predominantly to the gamma-rays spectra. Gamma-rays following the neutron interactions were detected using an efficient bismuth germanate (BGO) detector which is the main element of the borehole spectrometer SO-5-90 possessed by the Faculty of Geology, Geophysics and Environmental Protection of the University of Science and Technology in Kraków, Poland. The entire spectrometer was inserted into the aluminium pipe and consisted of the Am-Be source (inside a special steel source-housing), the scintillation detector with the BGO crystal (\( \Phi \) 40x60 mm), photomultiplier, electronic setup and a set of lead shields which protected the detector against direct 4.43 MeV gamma-rays from the source. Am-Be source (3 Ci) used in the experiments gave total \( 6.6 \times 10^6 \) n/s. The gamma-rays spectra were measured for all rock models in 100 energy channels (107 keV/channel). The source-to-detector distance was 37 cm.

Gamma peaks in the spectra from the BGO detector were not well-resolved (the energy resolution for the BGO crystal was about 23 % for photons of energy 0.662 MeV from the \( ^{137}Cs \) source). Thus the gross gamma counts from the appropriate energy windows \( \Delta E \gamma \) around the major peaks were used for the quantitative analyses. The measured spectra for two sandstones and limestone are presented in Fig.1. The energies of the major gamma lines and selected energy windows \( \Delta E \gamma \) are listed in Table 2.

![Gamma-rays spectra for different lithology models](image)

Fig.1. The measured gamma-rays spectra from n-gamma spectrometer (SO-5-90 type), for different rock models.
Table 2. The major gamma lines from the \((n, \gamma)\) interactions with H, Si, Ca, Fe and the selected energy windows \(\Delta E_\gamma\).

<table>
<thead>
<tr>
<th>Element</th>
<th>(E_\gamma) (MeV)</th>
<th>(\Delta E_\gamma) (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>2.22</td>
<td>1.71 (\div) 2.35</td>
</tr>
<tr>
<td>Si</td>
<td>3.54; 4.93</td>
<td>2.67 (\div) 5.03</td>
</tr>
<tr>
<td>Ca</td>
<td>6.42</td>
<td>5.25 (\div) 6.64</td>
</tr>
<tr>
<td>Fe</td>
<td>7.631; 7.645</td>
<td>6.85 (\div) 10.0</td>
</tr>
</tbody>
</table>

Experimental configuration of the borehole and surrounding rock model has approximately \(4\pi\) geometry and therefore the measured \(\gamma\)-rays spectra are dominated by the significant background including many multiple scattered gamma-rays. The side surface of the BGO crystal had no protection against low energy photons and no special shields of BGO were used against thermal neutrons. Therefore, the remarkable increase of the arising detector background and worsening of the spectra qualities appeared. Also existed disturbing contribution of the gamma peaks (of energy 7.631 MeV and 7.645 MeV from \(Fe(n, \gamma)Fe\) and interfering with them 7.72 MeV peak from \(Al(n, \gamma)Al\) due to iron and aluminium materials used for gauge construction. Furthermore the energy stabilization was not satisfied during the measurements as the photomultiplier quality was low.

3. Simulations of the neutron-gamma experiment using the Monte Carlo method.

The neutron and gamma-rays transport through matter, particularly when a complicated geometry occurs, can be successfully simulated using the Monte Carlo method. Furthermore, the availability of the accurate cross-section data enables the simulation of chemically complex geological media to be done. MCNP4c – a general-purpose Monte Carlo N-Particle code [Briesmeister, 2000] has been used. This code can be used for the simulation of neutron, photon, electron, or coupled neutron/photon/electron transport in a complex three-dimensional geometry of materials situated in the geometric cells.

For the simulations of the Zielona Góra sNGL experiment the average chemical compositions of the rock models and their average porosities have been assumed according to [Massalski et al., 1994]. Some elements were analyzed chemically with high uncertainty, furthermore no trace elements of the high neutron absorption cross sections were analyzed. The presence of \(B\) and Rare Earth Elements was expected especially for the sandstones Mucharz and Brenna. For these rock models the significant discrepancy between thermal neutron absorption cross sections, both measured and calculated from the average elemental compositions, was observed [Drabina et al., 2003]. Also porosities of the rock models showed high uncertainty. Generally, geological heterogeneities causing the above uncertainties have affected the simulated thermal neutron flux and the photon production and in consequence have been the significant source of discrepancies between results of the real and simulated experiments.

A general assumption has been established, which concerns geometry of the simulated standards - all of them have been considered as the regular cylinders of diameters amounted to 160 cm and height of 150 cm. Actual diameters of the boreholes amounted to 220 mm, 215 and 216 mm have been used. Source-to-detector distance was 37 cm. In the first stage of calculations the main effort has been focused on modelling the complex SO-5-90 tool situated in a borehole, surrounded by a rock model. In Fig. 2 a simplified scheme of the experimental arrangement used for the MCNP input, is presented.
MCNP simulations have run on the computers: HP Beta (Institute of Nuclear Physics), HP Maria (Cyfronet AGH) and on a PC computer with the AMD Athlon 1.33 GHz processor. Neutron and photon cross-sections libraries taken from the MCNP4c package are based mainly on the ENDF/B-VI, ENDF/B-V and MCPLIB02 data. The cross sections for $H$, $C$, $O$, $Na$, $Si$, $Ca$, $Mg$, $Al$, $K$, $Mn$, $Fe$, $Rh$, $Cd$ have been introduced. In the case of $H$ element in water, thermal neutrons scatterings have been described by the $S(\alpha,\beta)$ model (distinct from the free-gas treatment). The cross sections data for $Ge$ are not included into the MCNP4c package. They have been kindly obtained from CSIRO Division of Mineral Engineering in Lucas Heights, Australia.

The bismuth germanate – Bi$_4$Ge$_3$O$_{12}$ - scintillator of density 7.13 g/cm$^3$, diameter 4 cm and length of 6 cm has been surrounded by the aluminium casing and the layer of teflon (3 mm). The photomultiplier and electronic setup have been simulated by a “diluted” aluminium having the density of 1.35 g/cm$^3$. As in the experiment, the simulated detector has been separated from the source by the lead, aluminium and water shields.

The volume distributed $^{241}\text{Am-Be}$ source has been simulated. Neutrons from the source have been picked with the same probability. Neutrons have been emitted isotropically.

As the results of the simulations the track length estimate of the average $\gamma$-flux (tally F4), resulting from the neutron interactions, has been used as a function of $\gamma$-rays energy from four energy windows (see Table 1). The gamma flux averaged over the detector volume are as follows:

$$\bar{\phi}_\gamma = \frac{1}{V} \int \int \Phi(E, \mathbf{r}, t) dEdtdV \rightleftharpoons \frac{1}{V} \sum WT_i\quad (1)$$

where $\Phi(E, \mathbf{r}, t)$ is the $\gamma$-flux in a cell (BGO) of volume $V$, $W$ is the photon weight and $T_i$ is the track length.

The MCNP code estimates $\bar{\phi}_\gamma$ by summing $WT/V$ for all particle (gamma-ray) tracks in a chosen cell. The track length estimator is quite reliable because of many tracks in a cell and thus many contributions to tally F4. Tally F4 as other tallies in MCNP is normalized to be per starting particle.
For comparison with the experimental spectra the simulated reaction rates are more suitable. To obtain the photon rates in the BGO cell (in photons/cm$^3$ per one source neutron), which correspond to measurable $\gamma$-count rates, the Fm4 card has been introduced which gives the number of $K$ photon collisions in a detector volume:

$$K = C \int \phi(E) R_m(E) dE$$

(2)

where $\phi(E)$ is the energy-dependent $\gamma$ flux (in photons/(MeV-cm$^2$)), $R_m$ is the microscopic reaction cross section (in barns) for the $m$ type reaction taken from the MCNP libraries and $C$ constant is used for normalization ($C = -1$ was used for atomic density in atoms/(b·cm)).

The number of histories (nps) equal to 20 millions has been taken to obtain relative errors of photon rates in the range from 1 to 5%.

4. Evaluation of the correlation between sNGI measurements and simulations.

The $K$ photon rates in BGO, obtained by the use of the Fm4 card, have the units of photons/cm$^3$ per one source neutron and per energy bin. To obtain the results in counts (cps) per energy bin, the factor $N = 497.62812 \cdot 10^6$ (cm$^3$·n/s) was used which is a product of the source strength equal to $6.6 \cdot 10^6$ n/s and the volume of the BGO crystal amounted to 75.3982 cm$^3$. The simulated photon spectra, obtained from the MCNP code, should be regarded as that for a perfect detector registering all photons (100% efficiency) at their primary energy. Such a spectrum for Mucharz 2 sandstone is presented in Fig. 3 together with the experimental one. Neither direct gamma-rays from Am-Be source (4.43 MeV) nor those from the natural radionuclides have been simulated. The simulated and experimental spectra have been correlated to obtain the relationships between experimental and simulated data. The gross gamma counts from the selected energy windows ($I_{H}, I_{Si}, I_{Ca}, I_{Fe}$), listed in Table 3, have been used. The obtained linear dependencies are presented in Figs. 4, 5, 6 and 7 where the correlation coefficient squares $R^2$ and standard deviations $S_y$ from the suitable regression lines are included.
Table 3. The measured (“meas”) and simulated (“MCNP”) gross gamma counts from the selected energy windows.

<table>
<thead>
<tr>
<th>Calibration standards</th>
<th>( I_H^{MCNP} ) (cps)</th>
<th>( I_{Si}^{MCNP} ) (cps)</th>
<th>( I_{Ca}^{MCNP} ) (cps)</th>
<th>( I_{Fe}^{MCNP} ) (cps)</th>
<th>( I_H^{meas} ) (cps)</th>
<th>( I_{Si}^{meas} ) (cps)</th>
<th>( I_{Ca}^{meas} ) (cps)</th>
<th>( I_{Fe}^{meas} ) (cps)</th>
<th>Numbers and symbols of simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>BM2</td>
<td>1663</td>
<td>659</td>
<td>380</td>
<td>148</td>
<td>1071</td>
<td>727</td>
<td>305</td>
<td>155</td>
<td>30.11.01.BM2_2(83),3.12.01.cBM2_2(85/30e+6), 25.04.02.BM2_3a(25)</td>
</tr>
<tr>
<td>Mo2</td>
<td>1614</td>
<td>666</td>
<td>398</td>
<td>142</td>
<td>1023</td>
<td>684</td>
<td>284</td>
<td>128</td>
<td>03.12.01.MO2_1(86),06.12.01.PMO2_1(86a)</td>
</tr>
<tr>
<td>Li2</td>
<td>1494</td>
<td>578</td>
<td>304</td>
<td>150</td>
<td>969</td>
<td>593</td>
<td>238</td>
<td>119</td>
<td>03.12.01.LI2_1(87),03.12.01.PLI2_1(87), 3.12.01.cPLI2_1(87a/30e+6)</td>
</tr>
<tr>
<td>Pi2</td>
<td>1364</td>
<td>438</td>
<td>270</td>
<td>104</td>
<td>870</td>
<td>463</td>
<td>194</td>
<td>91</td>
<td>05.12.01.PI2_1(88a),03.12.01.PPI2_1(88)</td>
</tr>
<tr>
<td>Mu2</td>
<td>1452</td>
<td>800</td>
<td>269</td>
<td>222</td>
<td>929</td>
<td>676</td>
<td>225</td>
<td>152</td>
<td>23.11.01.MU2_6(81),14.03.02.PMU2_6,15.03.02, cMU2_6a (100e+6),15.03.02.cMU2_6b (200e+6)</td>
</tr>
<tr>
<td>Br2</td>
<td>1387</td>
<td>808</td>
<td>246</td>
<td>224</td>
<td>886</td>
<td>659</td>
<td>201</td>
<td>136</td>
<td>23.11.01.BR2_2(79)</td>
</tr>
<tr>
<td>Ra2</td>
<td>1422</td>
<td>791</td>
<td>204</td>
<td>192</td>
<td>960</td>
<td>735</td>
<td>196</td>
<td>121</td>
<td>23.11.01.RA2_2(80)</td>
</tr>
<tr>
<td>Ze2</td>
<td>1436</td>
<td>659</td>
<td>173</td>
<td>152</td>
<td>920</td>
<td>577</td>
<td>163</td>
<td>109</td>
<td>23.11.01.ZE2_1e(78b)</td>
</tr>
</tbody>
</table>

(*) for the simulated spectra (Fm4 type) “cps” means \( K \) photon rates (eq. 2) from the perfect detector of 100 \% efficiency, registered at their primary energy.
Fig. 3. The simulated (F8 tally) and the measured γ-rays spectra for the Mucharz 2 (Mu2) sandstone.
Fig. 4  Correlation between the simulated and experimental $I_H$ gross counts for hydrogen.

Fig. 5  Correlation between the simulated and experimental $I_Si$ gross counts for silicon.

Fig. 6  Correlation between the simulated and experimental $I_Ca$ gross counts for calcium.

Fig. 7  Correlations between the simulated and experimental $I_Fe$ gross counts for iron.
Highly correlated photon rates were obtained for the \( Ca \) and \( H \) spectral windows, as can be seen from Figs. 3 and 5. Lower correlation coefficients visible in Figs. 5 and 7, for the linear dependences \( I_{Si}^{MCNP}(I_{Si}^{meas}) \) and \( I_{Fe}^{MCNP}(I_{Fe}^{meas}) \), have been predominantly caused by the Mucharz 2 and Brenna2 sandstones, simulated without \( B \) and Rare Earth Elements, having a significant thermal neutron absorption cross sections. Remarkable amounts of \( B \) and Rare Earth Elements were recently announced for these sandstones. From the experimental side, the energy stabilization was not satisfied during measurements.

To improve conformity of the simulated and experimental photon rates for the \( Si \) and \( Fe \) spectral windows, full chemical composition of the rock models have to be introduced to the MCNP input, including trace elements of high thermal neutron absorption cross sections. Also porosity values should be verified. For example, the relative error of Mucharz 2 porosity amounts to about 20%. Porosity analyses for Mucharz and Brenna sandstones are treated as being imperfect [Massalski et al., 1994] and should be accompanied by additional analyses.

5. Results

The calibration equations for determining the \( H, Si, Ca \) and \( Fe \) concentrations have been obtained for the real and simulated experiments. The multiple linear regression has been used for data being the gamma counts from the appropriate energy windows and the concentrations of \( Si, Ca, Fe \) and \( H \), known from the chemical analyses of the calibration standards. The obtained equations are of the form:

\[
C_i = a_{i1} + a_{i2}I_H + a_{i3}I_{Si} + a_{i4}I_{Ca} + a_{i5}I_{Fe}
\]  

(3)

where \( C_i \) are concentrations of the elements of interest, \( a_{i1}, a_{i2}, a_{i3}, a_{i4}, a_{i5} \) are coefficients determined by multiple linear regression, \( I_H, I_{Si}, I_{Ca}, I_{Fe} \) are the gross gamma counts (cps) from the spectral windows.

Using the multiple linear regression equations of type (3) the concentrations of \( H, Si, Ca \) and \( Fe \) in calibration standards have been calculated for the real (“meas”) and simulated (“MCNP”) experiments. The results have been compared with the reference (“chem”) \( H, Si, Ca \) and \( Fe \) concentrations – regarded as “true” concentrations. The results of the comparisons are presented in Figs. 8 to 11 and in Table 4. It also should be noted that the preliminary results for the SO-5-90 spectrometer were presented in [Cywicka T. et al., 2002] and [Woźnicka U. et al., 2002].

\begin{align*}
\text{Si}^{MCNP} vs \text{Si}^{chem} & \quad y = 0.9876x + 0.2247 & \quad R^2 = 0.9876 \\
\text{Si}^{meas} vs \text{Si}^{chem} & \quad y = 0.9754x + 0.4462 & \quad R^2 = 0.9754
\end{align*}

Fig. 8. Comparison of the \( Si \) concentrations with the reference \( \text{Si}^{chem} \) data for the real and simulated experiments.
As can be seen in the presented graphs, the elemental concentrations calculated on a base of the simulated data are in good conformity with the reference concentrations (“chem”). The correlation coefficient squares ($R^2$), which are a measure of goodness for the linear dependence between predicted and reference (“chem”) elemental concentrations, are high. However, for the dependence $Fe^{MCNP}(Fe^{chem})$ a lower $R^2$ has occurred than for $Fe^{meas}(Fe^{chem})$ which, as mentioned, is mainly attributed to the Mucharz2 and Brenna2 sandstones, simulated without the Rare Earth Elements and $B$ in the rock matrices. Moreover the $Fe$ concentrations in the rock models showed rather limited range (0.068–1.667 wt %).
Table 4. Parameters of the multiple linear regression (correlation coefficient squares $R^2$ and standard deviations $S$) for: (a) correlation between the simulated and reference concentrations of $H$, $Si$, $Ca$ and $Fe$ (b) correlation between the experimental and reference elemental concentrations. All data are for the configuration of $N=8$ calibration standards.

<table>
<thead>
<tr>
<th>Multiple linear regression (eq. 3)</th>
<th>Simulations</th>
<th>Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1 = H(I_{H}, I_{Si}, I_{Ca}, I_{Fe})$</td>
<td>$R^2 = 0.9922$, $S = 0.083$</td>
<td>$R^2 = 0.9390$, $S = 0.231$</td>
</tr>
<tr>
<td>$C_2 = Si(I_{H}, I_{Si}, I_{Ca}, I_{Fe})$</td>
<td>$R^2 = 0.9876$, $S = 3.211$</td>
<td>$R^2 = 0.9754$, $S = 4.524$</td>
</tr>
<tr>
<td>$C_3 = Ca(I_{H}, I_{Si}, I_{Ca}, I_{Fe})$</td>
<td>$R^2 = 0.9839$, $S = 3.316$</td>
<td>$R^2 = 0.9610$, $S = 5.156$</td>
</tr>
<tr>
<td>$C_4 = Fe(I_{H}, I_{Si}, I_{Ca}, I_{Fe})$</td>
<td>$R^2 = 0.8363$, $S = 0.376$</td>
<td>$R^2 = 0.9227$, $S = 0.259$</td>
</tr>
</tbody>
</table>

6. Conclusions

The preliminary modelling of the complex n-gamma spectrometer (SO-5-90 type), surrounded by a water-filled borehole and geological formation (in a form of lithology models – standards) shows suitability of the MCNP code for the numerical reproduction of the sNGL experiment and enables us to use this code to support experimental work, in that part where experiments meet technical and economical difficulties.

The simulated photon spectra (tally F4 type), regarded as that for a perfect detector registering all photons (100% efficiency) at their primary energy, were compared with the measured spectra. High correlation coefficient squares ($R^2$) have been obtained for the linear dependencies: $I_{H}^{MCNP}(I_{H}^{meas})$ and $I_{Ca}^{MCNP}(I_{Ca}^{meas})$ being 0.927 and 0.910 respectively. Lower values of $R^2$ have been obtained for: $I_{Si}^{MCNP}(I_{Si}^{meas})$ and $I_{Fe}^{MCNP}(I_{Fe}^{meas})$, amounted to 0.625 and 0.376 respectively. The main reason of the poorer correlations, for the last two dependencies, is that two sandstones: Mucharz 2 and Brenna 2 were simulated with $a$ priori incorrect chemical compositions – without $B$ and Rare Earth Elements, recently confirmed as having significant concentrations in the above rock models. From the experimental side electronic instabilities have caused the worsening of correlations.

The $H$, $Si$ and $Ca$ concentrations obtained from the simulated experiment have been highly correlated with their true (“chem”) concentrations, $R^2$ amounted to 0.992, 0.988, and 0.984 respectively. For the dependence $Fe^{MCNP}(Fe^{chem})$ a lower $R^2$ has occurred than for $Fe^{meas}(Fe^{chem})$, which is mainly attributed to the mentioned Mucharz 2 and Brenna 2 incomplete chemical composition used for simulations and to the high uncertainties of $Fe^{chem}$ in the sandstones standards (relative errors: from 7.7% to 30.4%). From the experimental side the electronic instabilities introduced additional errors. The heterogeneity of the natural rock standards must be treated as the significant source of the uncertainty in the statistical comparison of the measurements and simulations.

Complementary chemical analyses of the benchmark standards including the Rare Earth Elements and $B$ contents is necessary for more precise modeling calculations. As a new, improved version of the n-gamma spectrometer (SO-5-90SN) has become available, the next set of benchmark calculations will be presented soon for this version.

In spite of some weak points visible in comparison between measured and simulated data, the presented results are promising for the effective support - in the nearest future - for the sNGL tool calibration by the MCNP simulations.
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