



A method for improving the evaluation of elemental concentrations measured by geochemical well logging

Juntao Liu¹ · Shucai Liu¹ · Feng Zhang² · Bin Miao¹ · Chao Yuan³ · Bo Su⁴

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Abstract

The increasing complexity of oil and gas reservoirs demands an accurate understanding of formation composition and mineralogy. Geochemical well logging based on prompt gamma neutron activation analysis technique (PGNAA) plays a crucial role in determining elemental concentrations, identifying lithology and improving the evaluation of matrix properties. The accuracy of elemental concentrations dictates the accuracy of other derived parameters. Elemental standard gamma ray spectra, which are predetermined for each instrument in the research and development phase, can be obtained by experimental measurements. These standards are the foundation of the processing of the neutron induced gamma ray spectroscopy and are considered to be fixed for each instrument. By using Monte Carlo numerical modelling, the standard gamma ray spectra of individual elements under different conditions are calculated. The results show that variation of borehole size, drilling mud types and other logging conditions have impacts on the shapes of the standard libraries. Therefore, if only one set of fixed standard spectra is utilized in processing measured spectra, the accuracy of elemental concentrations is affected. To address this problem, a model for compensating for the effect of logging conditions on the shapes of standard spectra is proposed. A field example is illustrated to validate the proposed method and result shows that the agreement between computed elemental weight fractions and XRF core analysis results is improved by using the introduced method.

Keywords Geochemical well logging · Monte Carlo simulation · Elemental weight fractions · PGNAA · XRF analysis

Introduction

The determination of elemental concentrations, mineralogy and lithology is essential for the evaluation of unconventional plays [1–3]. Geochemical well logging based on

PGNAA technique have been widely used to evaluate mineral composition, matrix density and total organic content of unconventional reservoirs [4–8]. For the early generation of geochemical well logging, Am–Be neutron sources are adopted [9, 10]. However, due to the regulatory and safety issues of Am–Be neutron sources, pulsed neutron sources, such as D–T generators, are being gradually utilized in geochemical logging instruments. Neutrons are emitted from the neutron source and interact with surrounding medium. They quickly lose energies because of inelastic and elastic scattering. Inelastic gamma rays are emitted from the inelastic scatterings. Eventually, the neutrons are absorbed by nuclei of formation elements due to neutron capture interaction and capture gamma rays are generated from the absorption [11–15]. Inelastic and capture gamma ray energy spectra can be measured by the design of time sequence of pulsed neutron generator.

The measured gamma ray energy spectrum can be approximated by a linear combination of the standard

✉ Juntao Liu
liujt@cumt.edu.cn

✉ Shucai Liu
liushucai@cumt.edu.cn

¹ School of Resources and Geosciences, China University of Mining and Technology, Xuzhou 221116, Jiangsu Province, China

² School of Geosciences, China University of Petroleum, Qingdao 266580, Shandong Province, China

³ Research Institute of Petroleum Exploration and Development, PetroChina, Beijing 100083, China

⁴ Tarim Business Division, CNPC Logging Company, Xinjiang, Korla 841001, China

spectra of individual elements. Each geochemical well logging instrument has its unique set of elemental standard spectra, which can be obtained by experimental approaches [2, 16]. For example, the standard gamma ray spectra of silicon be measured by placing the instrument in a clean sandstone calibration tank or rock formation [16–18]. If the “borehole” of the tank or rock is filled with water, the effect of hydrogen on the standard spectrum of the element of interest needs to be deducted.

For a specific pulsed neutron spectroscopy logging instrument, the standard spectra used in processing measured spectra are considered to be fixed. A decomposition of measured spectrum is carried out based on the elemental standard spectra to determine the relative elemental yields, which represent the contribution of gamma rays emitted by each element to the total spectrum. Then the elemental yields can be converted to elemental weight fractions by using oxide closure model [19, 20]. Another method of converting yields to concentrations is to use the calibration relationships between them. The calibration depends on formation and borehole conditions [11, 16]. The key to identification of elements within measured spectra is that characteristic energies of individual elements are unique. Accurate definitions of the elemental standard spectra are critical to the accurate determination of elemental concentrations.

In this paper, the effects of logging conditions such borehole size and drilling muds on the shapes of standard gamma ray spectra is analyzed using Monte Carlo simulation methods. A model for compensating for those effects is proposed. At last, the field measurement data of a pulsed neutron gamma ray spectroscopy instrument from a well, in which barite mud is used, is processed using the proposed method. The calculated elemental concentrations show a good agreement with the core analysis results.

Calculation of elemental yields and simulation of elemental standard spectra

As mentioned above, the measured spectrum is assumed to be the linear superposition of elemental standard spectra. Weighted least squares technique is used to calculate the yields of different elements [21, 22]. The recorded counting rate c_i in channel i can be described as:

$$c_i = \sum_{j=1}^m a_{ij}y_j, \quad i = 1, 2, \dots, n \quad (1)$$

where, a_{ij} is the elemental standard spectrum counting rate of channel i of element j ; y_j is the elemental yield of j .

The yields of different elements are calculated by minimizing the following Chi square (E^2) objective function [21, 23]:

$$E^2 = \sum_i \frac{(\hat{c}_i - c_i)^2}{u_i} \quad (2)$$

where, \hat{c}_i is fitting count rate of channel i ; u_i is the counting variance of channel i .

Elemental standard spectra can be derived from the measurements carried out in the formations or tanks of which composition is well known. However, studying the effects of logging conditions, such as borehole size and drilling mud, on the shapes of elemental standard spectra is impractical, because it is extremely expensive and time consuming. Fortunately, numerical simulation method has been validated as an effective alternative to some experiments. Monte Carlo simulation method has been widely used in the study of responses of nuclear well logging under different conditions [24–26]. The Monte Carlo method can duplicate theoretically a statistical process, such as the interaction of nuclear particles with materials. It is particularly useful for the complex problems, which is difficult to be simulated accurately by deterministic methods [27]. In particle transport, the Monte Carlo technique is pre-eminently realistic (a theoretical experiment). It consists of actually following each of many particles from a source throughout its life to its death in some terminal category. Monte Carlo N-Particle code (MCNP) developed by Los Alamos National Lab is one of the most popular code used in nuclear well logging simulation in the oil and gas industry and in nuclear spectroscopy analysis [21, 28]. A new patch is developed, which allows the MCNP code to flag the production reactions and positions of the detected gamma rays. It is used to model the response of a specific pulsed neutron well logging instrument under different conditions as shown in Fig. 1. In practice, the geochemical well logging instrument is designed to be run decentralized against the borehole wall

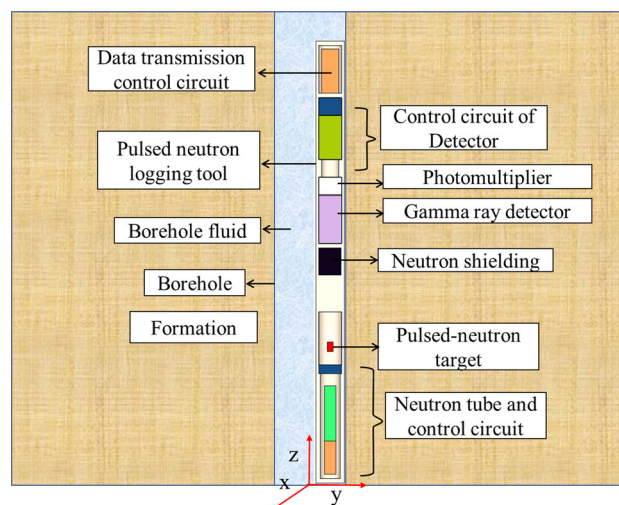


Fig. 1 Numerical simulation model

to avoid the impact of the instrument's shaking inside the wellbore on the measurement. The decentralization can be achieved by the placement of a bow spring. The model used the following specifications:

- D-T neutron source and LaBr_3 gamma ray detector are utilized. Diameter of the instrument is 9 cm.
- The spacing of the gamma ray detector to neutron source is 46 cm. The length and diameter of the gamma ray detector is 15 and 5 cm, respectively.
- The outer radius of the formation is 90 cm, and the instrument is placed against the sidewall. Borehole is filled with fresh water and diameter of the borehole is 24 cm.

In the simulation, neutrons emitted by the neutron source continue to slow down through inelastic and elastic scatterings until they are absorbed by nuclei of the surrounding mediums. The energy spectra of inelastic and capture gamma rays can be calculated at the detector position. Due to the extremely low neutron capture cross sections of oxygen and carbon, their contribution to capture spectra can be neglected. Therefore, oxides and carbonate minerals are usually selected as the filling materials of the artificial formation to obtain capture standard spectra of individual elements. The model formation is set to SiO_2 , Fe_2O_3 , CaCO_3 , TiO_2 , K_2O and H_2O , respectively. The capture standards of the corresponding elements that are commonly found in the earth formations are calculated. Several standard spectra under the “standard” conditions in which borehole is filled with fresh water and its radius is 12 cm, are calculated as shown in Fig. 2. It can be seen that the shape of the standard spectrum for each element is different, which is the basis for elemental analysis.

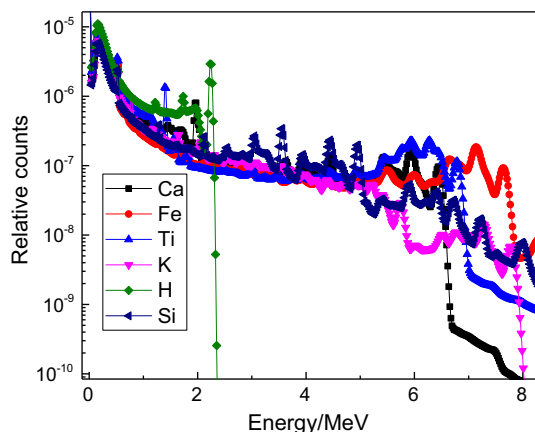


Fig. 2 Part of the standard spectrum of individual elements

Effect of element distribution on standard spectra

The capture standard of hydrogen is usually acquired by placing a pulsed neutron logging instrument in a water tank. However, in practice, when the porosity formation is extremely low, most hydrogen exists within borehole. To study if the hydrogen standard changes, formation matrix of the model is set to sandstone. The pores of the formation are filled with fresh water with a density of 1.0 g/cm^3 , and multiple porosities between 0 and 30 p.u. are calculated. In addition, the standard of hydrogen is also calculated when all around the instrument is fresh water.

The source of 2.23 MeV gamma rays emitted from hydrogen can be divided into two parts, one from the borehole and the other from the formation zone. It is easy to understand that when formation porosity is 0 p.u., hydrogen only exists in borehole. All the hydrogen capture gamma rays are only generated from interaction between neutron and borehole water. When porosity is 0 and 30 p.u., the origins of the gammas generated from hydrogen are recorded as shown in Fig. 3. Evidently, the origins of the capture gammas are different, which will affect the path of gamma rays arriving at the gamma ray detector.

Cumulative distribution functions (CDF) of the hydrogen capture gammas as a function of the distance to the central axis of the borehole are calculated as illustrated in Fig. 4.

Figure 4 shows that when porosity is 0 p.u., all the gamma rays from hydrogen are emitted in the borehole whose radius is 10 cm. When porosity is 5 p.u., water content in the formation increases. The relative proportion of the gamma rays produced in the wellbore reduces to about 75% due to the increased content of hydrogen in formation. With the increasing of hydrogen in formation,

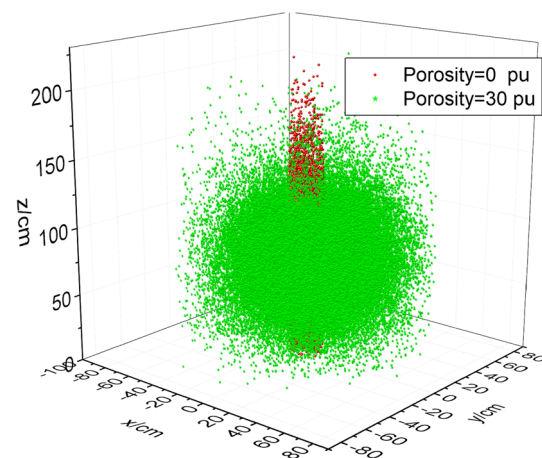


Fig. 3 The locations of the generated gamma rays from hydrogen when formation porosity is different

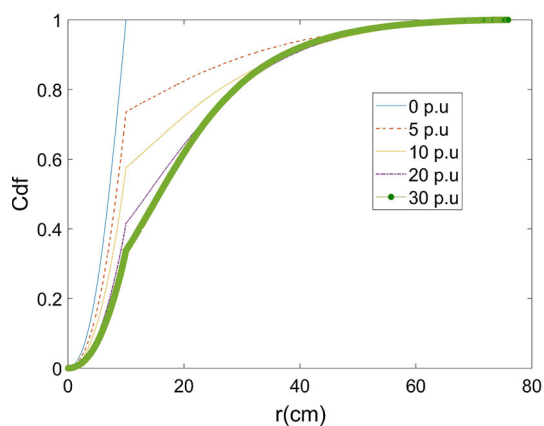


Fig. 4 Cumulative distribution function (CDF) of the locations of gamma rays generated from hydrogen

the relative contribution of the gamma rays from borehole to the total counts decreases. When porosity is 30 p.u., gamma rays from hydrogen in borehole only account for about 30% of all the emitted characteristic gamma rays. If more gamma rays are generated in the vicinity of the instrument, more characteristic gamma rays (2.23 MeV) will arrive at detector without collisions. If so, the full energy peak will be more pronounced in the energy spectrum., the standard spectra of hydrogen are compared when porosity is 0, 5 and 30 p.u., respectively as shown in Fig. 5.

It can be seen that the standard spectrum of hydrogen varies when the origins of gamma rays are different. After the normalization at position of the full-energy peak of hydrogen, the spectrum under low porosity conditions has a lower continuum as shown in Fig. 5 and the hydrogen spectrum exhibits a much different shape from that acquired in water tank. The gamma rays generated by the H element usually account for a large proportion of the total measured capture spectrum. The variation of hydrogen standard would affect the calculation of other elemental

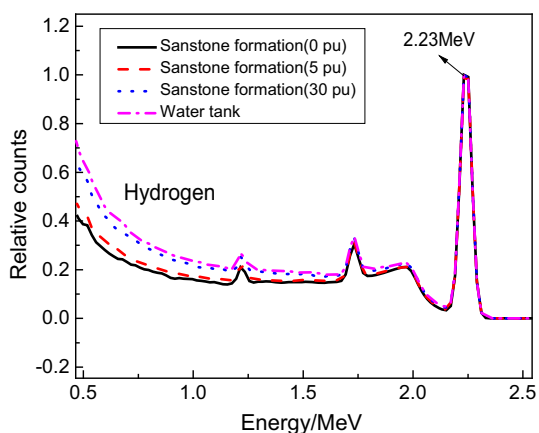


Fig. 5 Comparison of the standard capture spectra of hydrogen under different conditions

yields. When the standard derived from water tanks is used to process the spectrum acquired under low porosity conditions, inaccurate results are inevitably obtained due to the change of hydrogen standard.

The effect of drilling mud on standard spectra

For high formation pressure, mud density should be increased to balance pressure between borehole and formation zone to keep the wellbore stable. The commonly used weighting materials is barite. We assume the borehole of the calculation model is filled with barite mud, whose component includes water, bentonite and barite. The weight fraction of those three components are changed to study the effect of drilling mud on the energy spectrum. The radius of the borehole is 12 cm. Formation is pure sandstone and the standard spectra of silicon is calculated. It is compared with the spectrum acquired in fresh water borehole as illustrated in Fig. 6.

Figure 6 shows the silicon standard changes when formations are same and drilling muds are different. After normalization of the two spectra at 8 MeV position, the low energy part of the spectrum acquired under barite mud conditions has higher counts. It is because barite mud has a stronger ability to attenuate gamma rays compared with fresh water. More gamma rays interact with borehole materials and lose energy before they arrive at the gamma ray detector. The counts of the gamma rays with low energy increase. After the normalization, the spectrum obtained in fresh water borehole shows a lower value in low energy part. Again, if the fixed elemental standards obtained in experimental conditions are used to deconvolve the measured spectrum, it will produce inaccurate results.

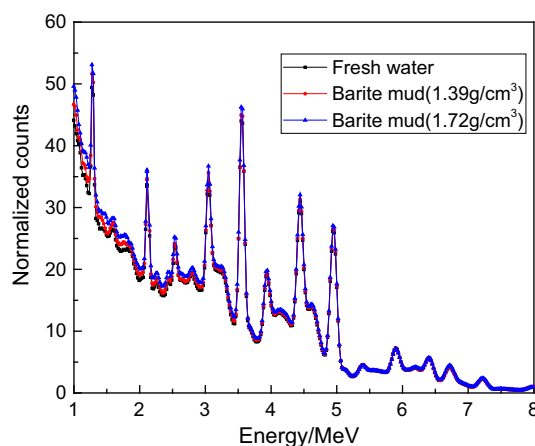


Fig. 6 Comparison of the standard spectrum of silicon under different conditions

The effect of borehole size on standard spectra

The size of the borehole shown in Fig. 1 is set to 8, 12 and 16 cm, respectively. Other simulation conditions keep the same. Matrix of the formation is SiO_2 with a density of 2.65 g/cm^3 . The gamma response of the pulsed neutron instrument is simulated and the calculated capture standard spectra of silicon after normalization at 8 MeV position are shown in Fig. 7.

It can be seen that the standard spectrum of silicon acquired under the condition of a large borehole displays a higher low-energy part. The variation of borehole sizes affects the flux distribution of thermal neutrons and also impacts the origins of the generated gamma rays. When borehole size becomes larger, the average path of gamma rays arriving at the detector become longer and more gamma rays lose their energy, and the spectrum shows a higher continuum compared with that obtained in small borehole.

A model for compensating for the effects on shapes of elemental standards and a field example

The attenuation of gamma rays in formation can be approximated by:

$$N(L) = N_0 e^{-\frac{\mu}{\rho} L} \quad (3)$$

where N_0 is the generated gamma ray flux, $N(L)$ is the detected gamma ray flux, ρ is medium density, μ is mass attenuation coefficient, which consists of the photoelectric effect, Compton scattering and pair production, L is the moving distance. The mass attenuation of different medium in formation and borehole is shown in Fig. 8.

The energy range of the measured spectrum to be processed is generally from 1 to 8 MeV. It can be seen that the

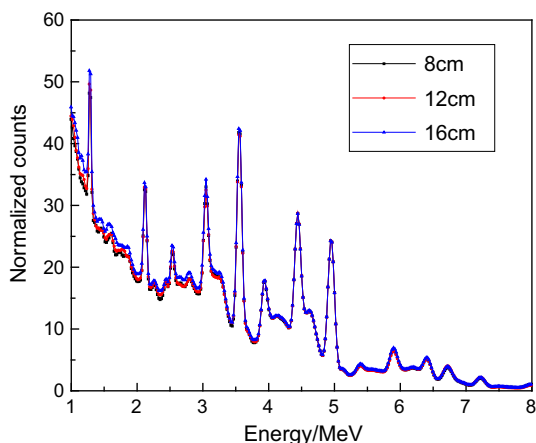


Fig. 7 Standard spectra of silicon under different conditions

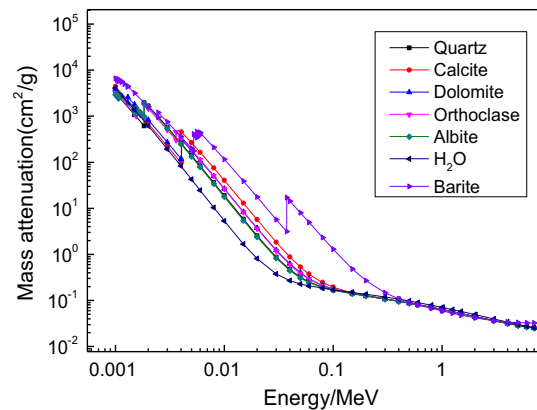


Fig. 8 Mass attenuation coefficient of different minerals

mass attenuation coefficients of media shown in Fig. 8 are very close in the energy interval of interest. The mass attenuation coefficient in general, decreases as the gamma energy increases. It means low-energy gamma rays are more likely to lose energy. The attenuation of the neutron induced gamma rays is a function of energy. A simple empirical model is proposed to compensate for the variation of the shape of elemental standard spectra under different conditions:

$$DST_i = OST_i \times e^{-(a \cdot E_i)} \quad (4)$$

where DST_i is the gamma count in channel i of the derived standard spectra, OST_i is the gamma count in channel i of the original standard spectrum obtained by experimental approaches, a is the fitting parameter which can either be negative or positive, E_i is the energy of gamma ray corresponding to channel i . The model is used to process the spectra shown in Fig. 6. The comparison of the spectra before and after the processing is shown in Fig. 9. The spectra are normalized at the 8 MeV position.

The spectrum of silicon acquired with borehole filled with fresh water is processed by the proposed method and

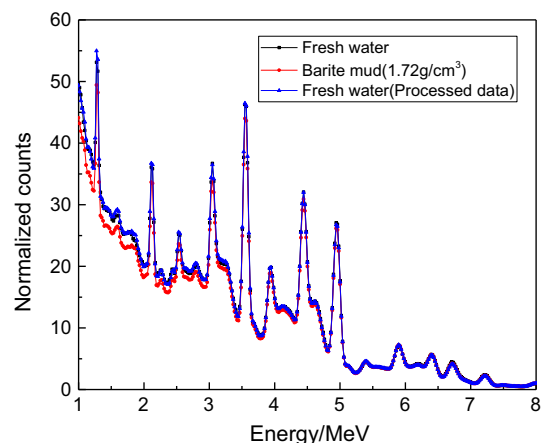


Fig. 9 Standard spectra of silicon before and after processing

shape of the processed spectrum agrees very well with the standard spectrum obtained in barite-mud filled borehole as shown in Fig. 9. The standard spectrum of hydrogen simulated with instrument placed in water tank is processed and the derived standard is compared with spectrum of hydrogen when porosity of the sandstone formation is 0 p.u. as shown in Fig. 10.

When formation porosity is 0 p.u. and borehole is filled with water, all hydrogen capture gammas are emitted within borehole, and the average path of them reaching the detector are short. Those gamma rays have the higher chance to be recorded by the detector without interactions with elemental nucleus compared those gamma rays generated outside the borehole range. The low energy part of those two spectra presents a difference as shown in Fig. 10. The hydrogen standard obtained in water tank exhibits a higher continuum. It is processed to derive a new hydrogen standard. The consistency between the new one and the spectrum acquired with porosity is 0 p.u. improved significantly, indicating the feasibility and accuracy of the introduced model. If a set of standard spectra of individual elements were acquired by experimental measurements, specific elemental standards under different conditions can be obtained.

Based on the standard spectra obtained in benchmarking conditions, new sets of standard libraries can be generated using the introduced model. In practice, the optimized fitting parameter in the model can be readily determined by an iteration algorithm as shown in Fig. 11. The final optimal fitting parameter is the average value of the fitting parameters for a number of selected depth. The final parameter is used to generate a new set of elemental standards, which is utilized to process the field data. We also can calculate elemental yields of each depth using the corresponding optimal set of standard spectra. However, if the logging section is long, it is very time consuming.

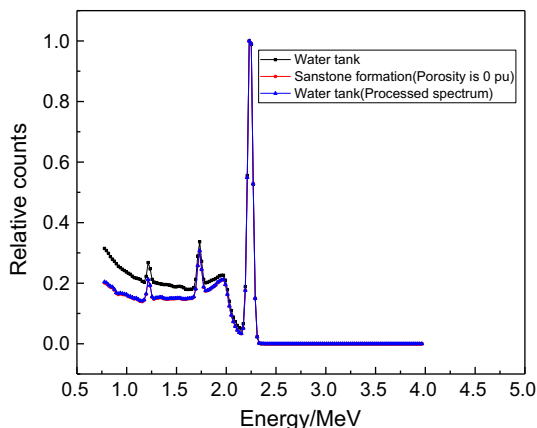


Fig. 10 Standard spectra of hydrogen before and after processing

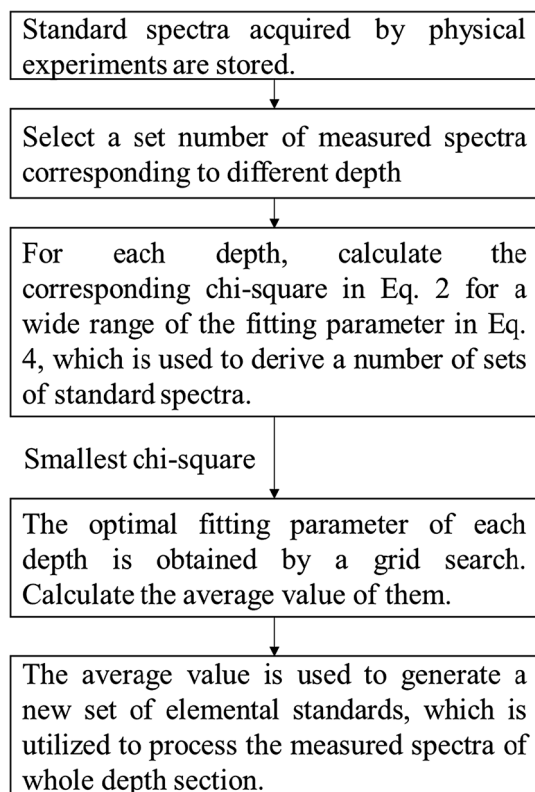


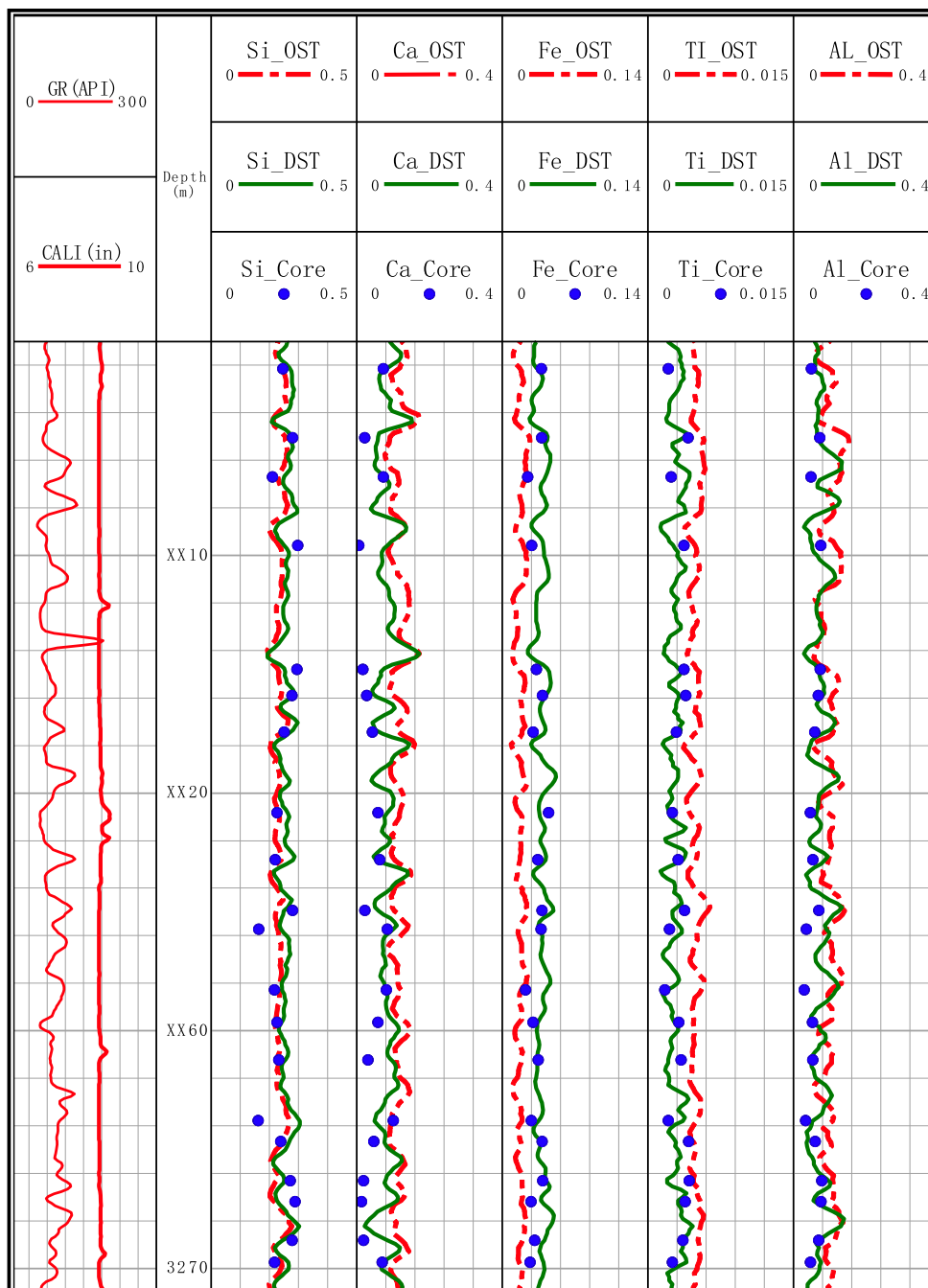
Fig. 11 Workflow for choosing the optimal fitting parameter and elemental standards

The proposed method is used to process the data of a pulsed neutron spectroscopy instrument in a well from Shengli oilfields of China. Picture of the instrument is shown in Fig. 12. D-T neutron source is adopted in the instrument, which can emit 14 MeV neutrons. When the instrument is running in borehole, the emitted neutrons would interact with the surrounding media. Spacing between neutron source target and detector is 46 cm. Neutron shielding material with a length of 10 cm is placed between source and detector. Original standard spectra of



Fig. 12 Picture of the pulsed neutron well logging instrument

Fig. 13 Comparison of the calculated elemental dry weights



the instrument are obtained from the oilfield services company and instrument manufacturer.

The case example is a tight oil and gas well. The average porosity of the interested interval is about 10% and hydraulic fracturing is needed to achieve the effective production. Lithology of the interval is relatively complex. Sandstone, limestone and mudstone coexist. The geochemical well logging is used to provide supports for determining mineral compositions and identify lithology, which is extremely important for finding favorable

reservoirs and providing guidance for fracturing. The accurately determination of elemental fractions dictates all the other derivative evaluations. The proposed method focuses on the improvement of the evaluation of elemental compositions. To validate the effectiveness of the method, elemental yields from capture spectra are calculated by using the original standard spectra and the newly derived standards, respectively. The yields are converted to dry weights [2, 29].

As shown in Fig. 13, the first track includes natural gamma ray and caliper curves. The curves with OST (Original standard spectra) as the suffix represent the weight fractions computed by using the original standards acquired by experimental measurements. The curves with DST (Derived standard spectra) as the suffix represent the calculated results based on the new derived standard spectra. The discrete data are core analysis results from XRF experiments. From Fig. 13, it can be seen that the calculated Si concentrations from two sets of standard spectra have good agreements with the experimental results. The results of Si and Al calculated with the derived standard spectra used shows a little higher sensitivity to the variations of their contents. When the original standard spectra are used, the calculated content of Ca shows higher values compared with the core data, and weight fractions of Fe are lower than the core experimental data. In addition, the dry weights of Ti is slightly higher the core points with the original standard spectra used. It can be seen that since variation of elemental standard spectra is considered, the consistency between computed elemental weight fractions and core data is improved when the new derived standard spectra are used.

Conclusion

Due to the difference between log conditions and the benchmarking condition of elemental standard spectra, the neutron flux around the instrument and moving path of the detected gamma rays arriving at the detector changed, which would affect the shape of the elemental standard spectra. A method is introduced to compensate for the variation of the standard spectra. Numerical calculations are made to validate the effectiveness of the method. The processing results of a field example shows the agreement between the calculated elemental weight fraction and XRF analysis results is improved by using the introduced method.

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