4. ONSHORE GEOCHEMICAL PROCESSING¹

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GEOCHEMICAL TOOL STRING

The geochemical logging tool string consists of four separate logging tools: the natural gamma-ray tool (NGT), the compensated neutron tool (CNTG), the aluminum activation clay tool (AACT), and the gamma-ray spectrometry tool (NGT, CNT, AACT, and GST are trademarks of Schlumberger; Fig. 1). These four tools use three separate modes of gamma-ray spectroscopy for a comprehensive elemental analysis of a formation. The NGT is located at the top of the tool string so that it can measure the naturally occurring radionuclides, thorium (Th), uranium (U), and potassium (K), before the formation is irradiated by the nuclear sources contained in the lower tools. The CNTG, located below the NGT, carries a low-energy californium-252 (252Cf) neutron source to activate the alumunum (Al) atoms in the formation. The AACT, a modified NGT, is located below the 252Cf source, and measures the activated gamma rays in the formation. By combining the AACT measurement with the previous NGT measurement, the background radiation is subtracted out and a reading of formation Al is obtained (Scott and Smith, 1973). The gamma-ray spectrometry tool, at the base of the string, carries a pulsed neutron generator to induce prompt-capture gamma-ray reactions in the borehole and formation and an NaI (T1) scintillation detector to measure the energy spectrum of gamma rays generated by the neutron-capture reactions. Because each of the elements in the formation is characterized by a unique spectral signature, it is possible to derive the contribution (or yield) of each of the major elements silicon (Si), iron (Fe), calcium (Ca), titanium (Ti), sulfur (S), gadolinium (Gd), and potassium (K) from the measured spectrum and, in turn, to estimate the relative abundance of each in the formation when combined with the elemental concentrations from the NGT and AACT. The GST also measures the hydrogen (H) and chlorine (Cl) in the borehole and formation, but these elements are not used for determining rock geochemistry.

The only major rock-forming elements not measured by the geochemical tool string are magnesium (Mg) and sodium (Na); the neutron-capture cross sections of these elements are too small relative to their typical abundances for the tool string to detect them. In some instances, a rough estimate of Mg + Na can be made by using the photoelectric factor (PEF), measured by the lithodensity tool. An explanation of this technique is found in Hertzog et al. (1989). This calculation has been found to give erroneous estimates in ODP holes (Pratson et al., in press), resulting in an unreliable Mg + Na curve that induces noise into all the other elemental yields in the normalization process. Consequently, this processing step was not attempted.

DATA REDUCTION

The well-log data from the Schlumberger tools are transmitted digitally up a wireline and are recorded and processed on board the *JOIDES Resolution* in the Schlumberger Cyber service unit (CSU). The results from the CSU are made available as "field logs" for initial shipboard interpretation. Subsequent reprocessing is necessary to correct these data for the effects of drilling fluids added to the well, logging speed, and drill-pipe interference. Processing of the spectrometry data is required to transform the relative elemental yields into oxide weight fractions.

The processing is performed with a set of log-interpretation programs written by Schlumberger that have been slightly modified to account for the lithologies and hole conditions encountered in ODP holes. The steps are summarized as follows.

Step 1: Reconstruction of Relative Elemental Yields from Recorded Spectral Data

The first processing step compares the measured spectra from the GST with a series of "standard" spectra to determine the relative contribution (or yield) of each element. These standards approximate the spectrum of each element. Using a weighted, least- squares inversion method, the relative elemental yields are calculated at each depth.

Six elemental standards (Si, Fe, Ca, S, Cl, and H) are used to produce the shipboard yields, but three additional standards (Ti, Gd, and K) can be included in the post-cruise processing to improve the fit of the spectral standards to the measured spectra (Grau and Schweitzer, 1989). Although Ti, Gd, and K often appear in the formation in very low concentrations, they can contribute greatly to the measured spectra because they have large neutron-capture cross sections. For example, the capture cross section of Gd is 49,000 barns, whereas that of Si is 0.16 barns (Hertzog et al., 1989). Therefore, including Gd is necessary when calculating the best-fit of the standard spectra to the measured spectrum.

The spectral analysis was performed using only the spectral standards for Si, Ca, Fe, Ti, Gd, H, and Cl in each of the processed holes. The spectral standards for K and S were not used (1) because these two elements existed in concentrations below the resolution of the tool and (2) we found that including them increased the noise level significantly of all the other yields. A straight, 10-point (3.5-ft, 1.067-m) smoothing filter was applied to all the yields in each of the holes to reduce the noise in the data during this reconstruction step. An additional 10-point (5-ft, 1.524-m) smoothing filter was applied to reduce the noise level further in the normalization factor (explained in Step 5), which affects the output elemental yields.

Step 2: Depth-shifting

Geochemical processing involves the integration of data from the different tool strings; consequently, it is important that all the data are depth-correlated to one reference logging run. The NGT, run on each of the logging tool strings, provides a spectral gamma-ray curve with which to correlate each of the logging runs. A reference run is chosen on the bases of constant, low cable tension and high cable speed (tools run at faster speeds are less likely to stick and are less susceptible to data degradation caused by ship-heave). The depth-shifting procedure involves selecting a number of reference points, based on similar log character, and then invoking a program that stretches and squeezes the matching logging run to fit the reference logging run. The geophysical tool string was chosen as the reference run in Hole 869B.

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Figure 1. Schematic drawing of the Schlumberger geochemical logging tool string.

Step 3: Calculation of Total Radioactivity and Th, U, and K Concentrations

The third processing routine calculates the total natural gamma-ray radiation in the formation, as well as concentrations of Th, U, and K, using the counts in five spectral windows from the NGT (Lock and Hoyer, 1971). This routine resembles shipboard processing; however, the results are improved during post-cruise processing by including corrections for hole-size changes and temperature variations. A Kalman filtering (Ruckebusch, 1983) is used in the CSU processing at sea to minimize the statistical uncertainties in the logs, which can otherwise create erroneous negative values and anti-correlations (especially between Th and U). An alpha filter has been introduced more recently and is now recommended by Schlumberger for shore-based processing. This filter strongly smooths the raw spectral counts, but keeps the total gamma-ray curve unsmoothed before calculating out the Th, U, and K (Charles Flaum, pers. comm., 1988). The outputs of this program are K (wet wt%), U (ppm), and Th (ppm), as well as total and computed gamma rays (total gamma rays minus U contribution) (Fig. 2).

Step 4: Calculation of Al Concentration

The fourth processing routine calculates the concentration of Al in the formation using the four energy windows recorded by the AACT. During this step, corrections are made for natural radioactivity, borehole-fluid neutron-capture cross section, formation neutroncapture cross section, formation slowing-down length, and borehole size. Porosity and density logs are needed as inputs into this routine to convert the wet-weight percentages of K and Al curves to dryweight percentages. A porosity log is recorded on the geochemical tool string; however, it can only be used as a qualitative measurement, because it carries a ²⁵²Cf source, rather than the americium-beryllium source needed to perform a quantitative measurement. Because the density logs in each of the three holes compared well with shipboard core measurements, a porosity curve was derived from the density log using the following equation:

$$\phi_{\tau} = (\rho_m - \rho_b)/(\rho_m - \rho_f), \tag{1}$$

where

$$\begin{split} \varphi_t &= \text{percentage porosity,} \\ \rho_m &= \text{matrix density (from core measurements),} \\ \rho_b &= \text{bulk density from the log in g/cm}^3, \text{ and} \\ \rho_f &= \text{density of fluid} = 1.05 \text{ g/cm}^3. \end{split}$$

These calculated porosities showed excellent agreement with core measurements.

A correction has also been made for Si interference with Al; the ²⁵²Cf source activates the Si, producing the aluminum isotope, ²⁸Al (Hertzog et al., 1989). The program uses the Si yield from the gamma-ray spectrometry tool to determine the Si background correction. The program outputs dry-weight percentages of Al and K, which are used for calculating and normalizing the remaining elements.

Step 5: Normalization of Elemental Yields from the GST To Calculate the Elemental Weight Fractions

Relative concentrations of the GST-derived elemental yields can be determined by dividing each elemental yield by a relative spectral sensitivity factor (S_i). This factor is principally related to the thermal neutron-capture cross sections and also to its gamma-ray production and detection probability of each element (Hertzog, 1989). The relative elemental concentrations are related to the desired absolute concentrations by a depth-dependent normalization factor (F), as defined by the relationship:

$$Wt_i = FY_i / S_i, \tag{2}$$

where

 Wt_i = absolute elemental concentration,

 Y_i = relative elemental yield, and

 S_i = spectral sensitivity factor.

The normalization factor is calculated on the basis that the sum of all the elemental weight fractions is unity (100%). The closure model handles the absence of carbon and oxygen, which are not measured by this tool string, with the approximation that each of the measurable elements combines with a known oxide or carbonate. The dry weight percentage of Al and K are normalized with the reconstructed elemental yields to determine the normalization factor at each depth interval from the following equation:

$$F(\sum_{i} X_{i} Y_{i}/S_{i}) + X_{k}Wt_{k} + X_{Al}Wt_{Al} = 100,$$
(3)

where

 X_i = oxide factor; atomic weight of the associated oxide or carbonate of element *i*/atomic weight of element *i*,

 X_k = oxide factor; atomic weight K₂O/atomic wt of K,

 $Wt_k = dry wt\%$ of K, as determined from the NGT,

 X_{Al} = oxide factor; atomic weight of Al₂O₃/atomic weight of Al, and

 $Wt_{Al} = dry wt\%$ of Al, as determined from the AACT.

The value X_i accounts for the C and O associated with each element. Table 1 lists the oxide factors used in this calculation. All the measured elements associate with C and O in a constant ratio in these lithologies, except for Ca, which associates with C and O in one of two ways: CaCO₃ or CaO (Table 1). To convert the measured yields

to elements, a dominant oxide factor must be assumed at each depth level. A routine that combines both these oxide factors is implemented here, as suggested by Jim Grau at Schlumberger-Doll Research (pers. comm., 1992). When the elemental form of Ca is less than 6%, CaO is assumed and an oxide factor of 1.39 is used. When the elemental form of Ca is greater than 12%, CaCO₃ is assumed and an oxide factor of 2.49 is used. When the elemental form of Ca is between 6% and 12%, both forms are assumed to be present and the oxide factor is linearly interpolated between 1.39 and 2.49.

The parameters 6% and 12% were chosen according to observations of how Ca occurs in nature. CaO is not likely to occur in quantities greater than 12%. When Ca is less than 6%, even if it is CaCO₃, the error will be small when 1.39 is used as the oxide factor instead of 2.49. The linear interpolation is done to provide a smooth transition and to avoid invoking any erroneous chemical changes in the final processed logs. In most cases, this procedure for Ca gives the best model and minimizes the error when the model is not exactly correct.

Step 6: Calculation of Oxide Percentages

The final routine converts the elemental weight percentages into oxide/carbonate percentages by multiplying each by its associated oxide factor, as shown in Table 1.

Step 7: Calculation of Error Logs

The statistical uncertainty of each element is calculated for each of the elements measured with the GST and NGT (Grau et al., 1990; Schweitzer et al., 1988). This error is strongly related to the normalization factor, which is calculated at each depth (Eq. 3). The normalization factor is displayed to the right of the logs (Fig. 3). A lower normalization factor represents better counting statistics and higher quality data.

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* Abbreviations for names of organizations and publication titles in ODP reference lists follow the style given in *Chemical Abstracts Service Source Index* (published by American Chemical Society).

Table 1. Oxide factors used for normalizing elements to 100% and for converting elements to oxides.

Element	Oxide/carbonate	Conversion factor
Si	SiO ₂	2.139
Ca<6%	CaŐ	1.399
6%>Ca<12%	CaO and CaCO ₃	1.399-2.49 linearly interpolated
Ca>12%	CaCO ₃	2.49
Fe	FeO*	1.358
K	K ₂ O	1.205
Ti	TiO ₂	1.668
A1	$A1_2O_3$	1.889



Figure 2. Processed natural gamma-ray data, Hole 869B.



Figure 2 (continued).



Figure 3. Estimates of calcium carbonate and major oxide-weight fractions from geochemical logs, Hole 869B. Solid circles represent carbonate values from core measurements. The normalization factor is displayed to the right of the logs. A lower normalization factor represents better counting statistics and higher quality data. A log of the Ca oxide factor used is displayed to the right of the normalization factor.



Figure 3 (continued).