

Leg 129: Geochemical Processing Report

(based on: Pratson, E. L. et al. (1992). Data Report: Geochemical well logs through Cenozoic and Mesozoic sediments from Sites 800, 801, and 802. In Larson, R. L., Lancelot, Y. et al., Proc. ODP, Sci. Results, 129: College Station, TX (Ocean Drilling Program), 635-652.)

Note: A complete revision of all of the processed data from this leg was performed before putting the data online. This may have resulted in minor depth discrepancies between the published geochemical data and the online database version, particularly before Leg 128. The revision of Hole 801B revealed that the data had not been properly depth matched. Due a technical problem with the processing program, however, the new depth shifts could not be applied to the final results. For this reason, though the data of Hole 801B is available online, it should be used with caution when compared to the other logs.

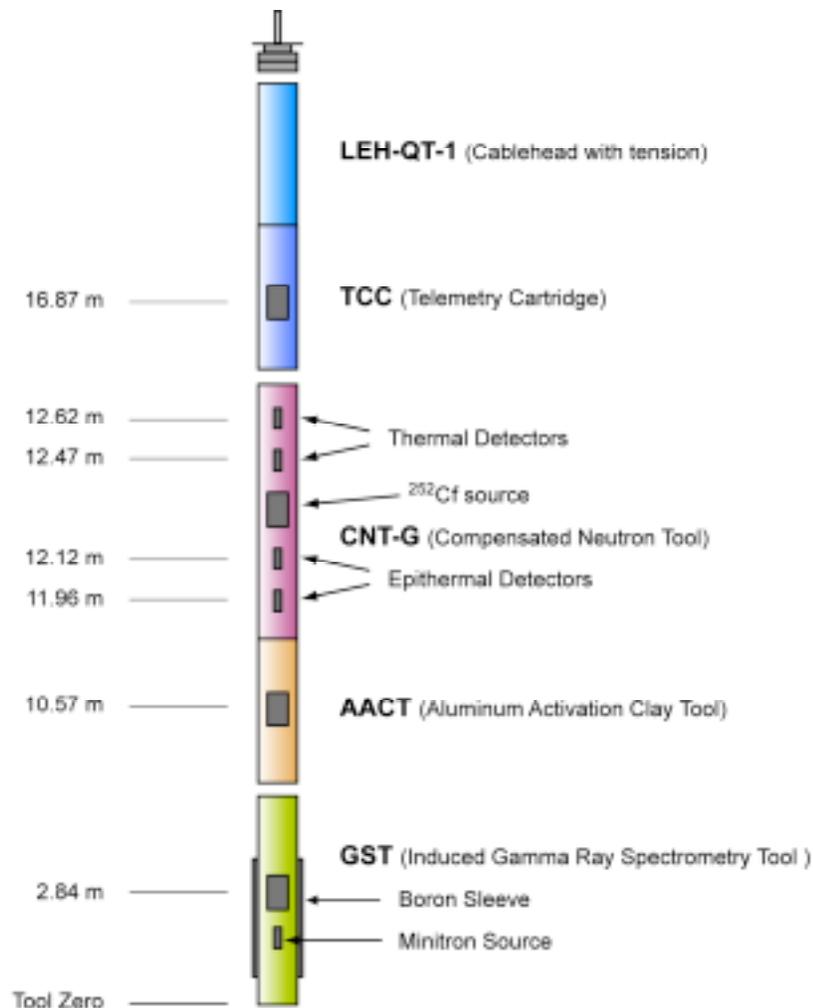
Geochemical Tool String

The Schlumberger geochemical tool string consists of four logging tools: the natural gamma-ray tool (NGT) the compensated neutron tool (CNT), the aluminum activation clay tool (AACT), and the gamma-ray spectrometry tool (see figure below). The natural gamma-ray tool is located at the top of the tool string, so that it can measure the naturally occurring radio nuclides, Th, U, and K, before the formation is irradiated by the nuclear sources contained in the other tools below. The compensated neutron tool, located below the natural gamma-ray tool, carries a low-energy californium source (^{252}Cf) to activate the Al atoms in the formation. The aluminum activation clay background radiation is subtracted out by the aluminum activation clay tool below 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 bombard the borehole and formation and an NaI(Tl) scintillation detector, which measures the spectrum of gamma-rays generated by neutron-capture reactions. Because each of the elements measured (silicon, iron, calcium, titanium, sulfur, gadolinium, and potassium) is characterized by a unique spectral signature, it is possible to derive the contribution (or yield) of each of them to the measured spectrum and, in turn, to estimate their abundance in the formation. The GST also measures the hydrogen and chlorine in the borehole and formation, but the signal for these elements is almost entirely due to seawater in the borehole, and they are hence of little value.

The only major rock-forming elements not measured by the geochemical tool string are magnesium and sodium; the neutron-capture cross-sections of these elements are too small relative to their typical abundance for the tool string to detect them. A rough estimate of Mg+Na can be made by using the photoelectric factor (PEF) measured by the lithodensity tool. This measured PEF is compared with a calculated of PEF (a summation of the PEF from all of the measured elements). The separation between the measured and calculated PEF is, in theory, attributable to any element left over in the formation (i.e., Mg, and Na). Further explanation of this technique is found in Hertzog et al. (1989). This calculation was attempted, but it yielded an unlikely straight zero Na+Mg curve with scattered spikes. The inclusion of this unreliable curve in the normalization with the other elements would have induced noise; therefore, it was not included.

Data Reduction

The well log data from the Schlumberger tools have been transmitted digitally up a wireline and recorded on the JOIDES Resolution in the Schlumberger Cyber Service Unit (CSU). The results from the CSU have been processed to correct for the effects of drilling fluids, logging speed, and 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 modified to account for the lithologies and hole conditions encountered in ODP holes. The processing steps are summarized below:



Step 1: Reconstruction of relative elemental yields from recorded spectral data

The first processing step uses a weighted least-squares method to compare the measured spectra from the geochemical spectrometry tool with a series of standard spectra in order to determine the relative contribution (or yield) of each element. Whereas six elemental standards (Si, Fe, Ca, S, Cl, and H) are used to produce the shipboard yields, three additional standards (Ti, Gd, and K) can be included in the shore-based processing to improve the fit of the spectral standards to the measured spectra (Grau and Schweitzer, 1989). Although these additional elements often appear in the formation in very low concentrations, they can make a large contribution to the measured spectra, because they have large neutron-capture cross-sections. For example, the capture cross-section of Gd is 49,000 barns, that of Si 0.16 barns (Hertzog et al., 1989). Gd is, therefore, included in the calculation of a best fit between the measured and the standard spectra.

This best-fit analysis was performed to include spectral standards for Si, Ca, Fe, Ti, Gd, H, and Cl. The spectral standard for K and S were not used because these two elements existed in concentrations below the resolution of the GST tool, and including them would significantly increase the noise level of all the other yields. A straight, seven-point smoothing filter was applied to all the yields in each of the holes to reduce the noise in the data. The Ca yield was divide by two to correct for chlorine interference, a routine typically done when logging in saline fluids (J. A. Grau, pers. comm., 1988).

The recomputed yields are loaded in the files
800A-yields.dat
802A-yieldsm.dat
802A-yieldsr.dat
No recomputed yields are available online for Hole 801B.

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. A total gamma-ray curve (from the gamma-ray tool, which is run on each tool string) is usually chosen as a reference curve, based on cable tension (the logging run with the least amount of cable sticking) and cable speed (tools run at faster speeds are less likely to stick).

In both Holes 800A and 801B, the NGT was incorrectly mounted on the quad-combo tool string, which includes gamma ray, resistivity, sonic, and density tools. The NGT is ordinarily located at the top of the string, in order to measure the natural gamma rays before the formation has been activated by any nuclear source. In these two holes, however, the NGT was positioned below the density tool carrying a Cesium source, which emits gamma rays. This would activate the formation and cause the gamma ray readings to be too high. Despite this, the NGT logs could be used qualitatively for depth matching. The quad-combo tool string was chosen as the reference run in Hole 800A. The FMS tool string was chosen as the reference run in Hole 801B, as this was the only run during which the wireline heave compensator was working. The geochemical tool string was used as the reference run in Hole 802A, because the WHC was not working on the other runs.

Step 3: Calculation of total radioactivity and Th, U, and K concentrations

The third processing routine calculates the total natural gamma radiation in the formation as well as concentrations of Th, U, and K, using the counts in five spectral windows from the natural gamma-ray tool (Lock and Hoyer, 1971). This resembles shipboard processing, except that corrections for hole-size changes are made in the shore-based processing of these curves. A Kalman filter (Ruckebusch, 1983) is applied to minimize the statistical uncertainties in the logs, which would otherwise create erroneous negative readings and anti-correlation (especially between Th and U). At each depth level calculations and corrections also were performed for K contained in the mud. This K correction is particularly useful where KCl is routinely added to the hole: because of dispersion, however, it is difficult to know exactly how much K is in the borehole. The outputs of this program are: K (wet wt %), U (ppm), and Th (ppm), along with a total gamma-ray curve and a computed gamma-ray curve (total gamma-ray minus U contribution).

The processed gamma-ray data are loaded in the files
800A-ngt.dat
801B-ngt.dat
802A-ngtm.dat

Step 4: Calculation of Al concentration

The fourth processing routine calculates an Al curve using four energy windows, while concurrently correct for natural activity, borehole fluid neutron-capture cross-section, formation neutron-capture cross-section, formation slowing-down length, and borehole size. Porosity and density logs are needed in this routine to convert the wet weight percent K and Al curves to dry weight percent.

Because the density logs in all three holes compared well with shipboard core measurements, and because no porosity logs were recorded, a porosity curve was calculated from the density logs using the following equation:

$$\rho_f = (\rho_m - \rho_b) / (\rho_m - \rho_f)$$

where:

ρ_f = percentage of porosity,

ρ_m = matrix density

(a constant value or log matrix density can be used in g/cm^3),

ρ_b = bulk density from the log in g/cm^3 , and

ρ_f = density of fluid = 1.05 g/cm^3 .

A correction is also made for Si interference with Al; the ^{252}Cf source activates the Si, producing the aluminum isotope, ^{28}Al (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 in the calculation and normalization of the remaining elements.

Step 5: Normalization of elemental yields from the GST to calculate the elemental weight fractions

This routine combines the dry weight percentages of Al and K with the reconstructed yields to obtain dry weight percentages of the GST elements using the relationship:

$$W_i = F Y_i / S_i$$

where

W_i = dry weight percentage of the i-th element

F = normalization factor determined at each depth interval

Y_i = relative elemental yield for the i-th element

S_i = relative weight percentage (spectral) sensitivity of the i-th element

The normalization factor, F , is a calibration factor determined at each depth from a closure argument to account for the number of neutrons captured by a specific concentration of rock elements. Because the sum of oxides in a rock is 100%, F is given by

$$F (\sum X_i Y_i / S_i) + X_K W_K + X_{Al} W_{Al} = 100$$

where

X_i = factor for the element to oxide (or carbonate) conversion

X_K = factor for the conversion of K to K_2O (1.205)

X_{Al} = factor for the conversion of Al to Al_2O_3 (1.889)

W_K = dry weight percentage of K determined from natural activity

W_{Al} = dry weight percentage of Al determined from the activation measurement

The sensitivity factor, S_i , is a tool constant measured in the laboratory, which depends on the capture cross-section, gamma-ray production, and detection probabilities of each element measured by the GST (Hertzog et al., 1989).

The factors X_i are simply element to oxide (or carbonate, sulfate) conversion coefficients and effectively include the O, C or S bound with each element. In processing the GLT data the correct choice of X_i is important in the closure algorithm described above and requires geological input. In

most lithologies the elements measured by the tool occur in silicates where the compositions can be expressed completely as oxides.

With carbonate or carbonate-rich lithologies the measured calcium is more likely to be present as CaCO_3 (XCa: 2.497) than as the oxide (CaO ; XCa: 1.399). A good indication of the choice of calcium conversion factors can often be gained from shipboard X-ray diffraction (XRD) and CaCO_3 measurements, which estimate acid-liberated CaCO_3 . In Hole 800A, CaO was assumed to be the dominant fraction from 48.5 to 81 mbsf and from 219.4 to 317 mbsf; CaCO_3 was assumed to be dominant from 81 to 219.5 mbsf. A dominant CaO was assumed throughout Hole 801B. In Hole 802A, CaO and CaCO_3 were assumed as dominant above and below 218 mbsf, respectively.

Steps 6-7: Calculation of oxide percentages and statistical uncertainty

These routines convert the elemental weight percentages into oxide percentages by multiplying each by its associated oxide factor (Table 1); finally the statistical uncertainty of each element is calculated, using methods described by Grau et al. (1990) and Schweitzer et al. (1988). This error is strongly related to the normalization factor, F, which is calculated at each depth level. A lower normalization factor represents better counting statistics and therefore higher quality data. Note that these statistical uncertainties were not presented in the data paper on which this document is based, as the routine that calculates them was not available at the time of publication. They were added a few years later, when the revision of the data was performed.

The oxide weight percentages are loaded in the files

800A-oxides.dat

801B-oxides.dat

802A-oxidesspl.dat

The statistical uncertainties are loaded in the files

800A-oxierr.dat

801B-oxierr.dat

802A-oxierrspl.dat

800A-elerr.dat

801B-elerr.dat

802A-elerrspl.dat

Core data are loaded in the files

800A-core.dat

801B-core.dat

802A-core.dat

Table 1. Oxide/carbonate factors used in normalizing elements to 100% and converting elements to oxides/carbonates.

Element	Oxide/carbonate	Conversion factor
Si	SiO_2	2.139
Ca	CaO	2.339
Ca	CaCO_3	2.497
Fe	FeO^*	1.358
K	K_2O	1.205
Ti	TiO_2	1.668
Al	Al_2O_3	1.889

References

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