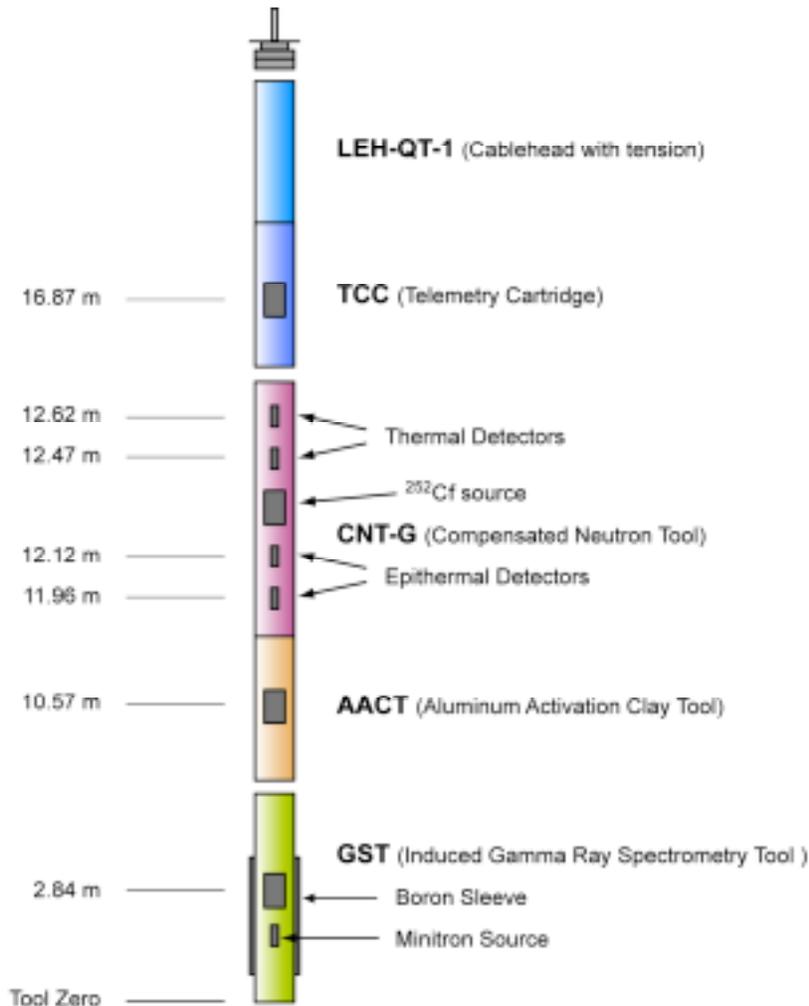


Leg 144: Geochemical Processing Report

(based on: Bristow, J. F. et al. (1993). Onshore geochemical processing. NOTE: the paper was erroneously omitted from both the Initial Reports volume and the CD-ROM (Premoli-Silva, I., Haggerty, J., Rack, F. et al., Proc. ODP, Init. Reports, 144: College Station, TX (Ocean Drilling Program)).

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 tool below subtracts out the aluminum activation background radiation 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 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 not implemented in this leg; the results of the Mg+Na calculation have been found to be erroneous in many ODP logging environments (Bristow et al., 1992; Pratson et al., 1993). The inclusion of this unreliable Mg + Na curve in the normalization with the other elements would have induced noise into all the other elements.

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.

The elemental standards (Si, Ca, Fe, Ti, Gd, K, Cl, and H) were used in the spectral analysis step of Holes 801C, 871C, 873A, 874B, and 878A. The spectral standard for S was not used at each of the logged sites, because this element existed in concentrations below the resolution of the tool and including them was found to increase significantly the noise level of all the other yields. The spectral standard for K was also omitted at Hole 873A as it was found to represent noise. A straight, seven-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 ten-point (5 ft, 1.524 m) smoothing filter was applied to further reduce the noise level in the normalization factor (explained in Step 5), which affects the output elemental yields.

The processed yields are in the files
801C-yields.dat

871C-yields.dat
873A-yields.dat
874B-yields.dat
878A-yields.dat.

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). The geochemical tool string was chosen as the reference run in Hole 801C, 871C, and 878A; the first pass of the FMS run was chosen as the reference run in Hole 873A and 874B.

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). 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 Th, U, and K. 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
801C-ngt.dat
871C-ngt.dat
873A-ngt.dat.
874B-ngt.dat
878A-ngt.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. A porosity log is recorded on the geochemical tool string; however, it can only be used as a quantitative measurement, since it carries a ^{252}Cf source rather than the americium-beryllium source needed to make a quantitative measurement. A porosity curve was derived from the resistivity curve in Holes 801C, 871C, and 874B, from the density curve in Hole 878A and from a combination of resistivity and neutron in Hole 873A (resistivity-derived porosity was used in the basalt and limestone section, neutron-derived porosity was used in clays). These porosity curves were chosen in each case because of their close agreement with core.

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 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: $CaCO_3$ or CaO (Table 1). In order to convert the measured yields to elements, a dominant oxide factor must be assumed at each depth level: $CaCO_3$ is used in carbonate sediments, CaO is used in the basement.

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.

The oxide weight percentages are loaded in the files

- 801C-oxides.dat
- 871C-oxides.dat
- 873A-oxides.dat
- 874B-oxides.dat
- 878A-oxides.dat.

The statistical uncertainties are loaded in the files

801C-oxierr.dat
871C-oxierr.dat
873A-oxierr.dat
874B-oxierr.dat
878A-oxierr.dat
801C-elerr.dat
871C-elerr.dat
873A-elerr.dat
874B-elerr.dat
878A-elerr.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	1.399
Ca	CaCO ₃	2.497
Fe	FeO*	1.358
K	K ₂ O	1.205
Ti	TiO ₂	1.668
Al	Al ₂ O ₃	1.889

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