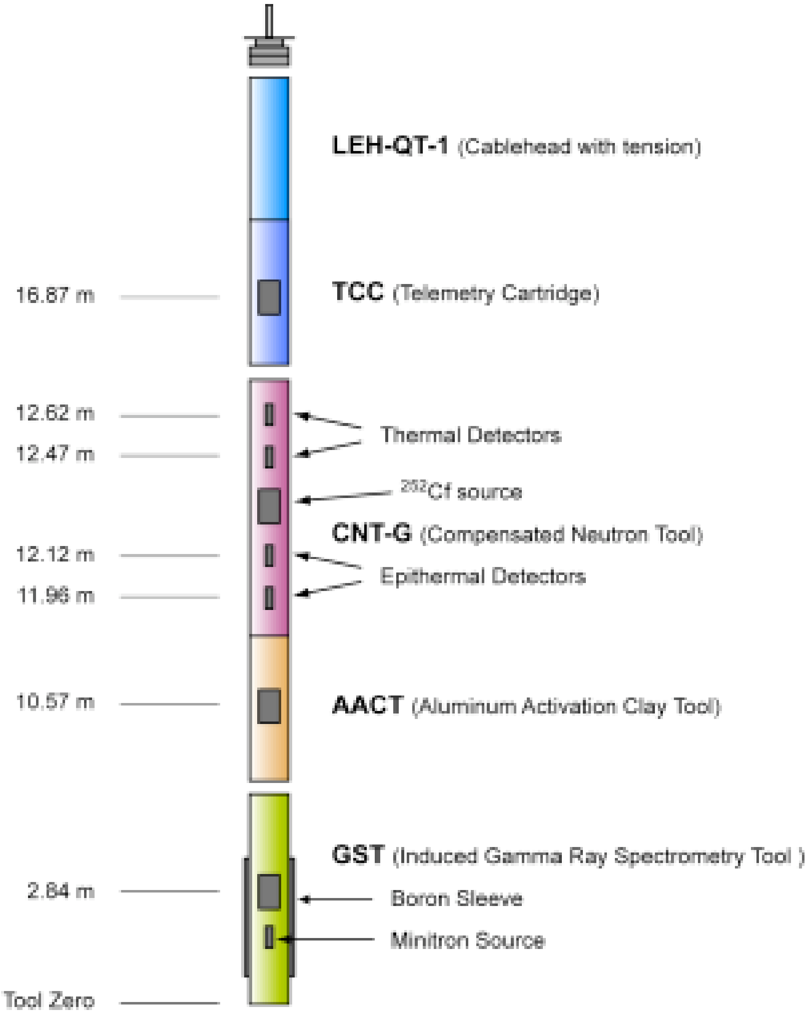
Leg 141: Geochemical Processing Report

(based on: Pratson, E.L. et al. (1995). Data Report: Geochemical logging through an accretionary prism: Chile Triple Junction. In Lewis, S.D., Berhmann, J.H., Musgrave, R.J. et al., Proc. ODP, Sci. Results, 141: College Station, TX (Ocean Drilling Program), 427-444.)

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 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 not attempted on this leg, because including it in the normalization with the other elements often induces noise into all other elements (Pratson et al., 1993). $MgO+Na_2O+MnO$ values from core data are included in the normalization step of the processing. This is explained further in Step 5 of the data-reduction section below.

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 spectral analysis was performed using the spectral standards for H, Si, Ca, Cl, Fe, Ti, S and Gd. The spectral standards for K was not used, because this element exist in concentrations below the resolution of the tool, and the inclusion of K was found to significantly increase the noise level of all the other yields. A straight, five-point (2.5 ft, 0.762 m) smoothing filter was applied to all the yields to reduce the noise in the data during this reconstruction step. An additional 10-point (7 ft, 2.13 m) smoothing filter was applied to the hole to further reduce the noise level in the normalization factor (explained in step 5), which affects the overall character of the final elemental yields.

The recomputed yields are loaded in the files 859B-yields.dat and 863B-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 859B; the third pass of the Formation MicroScanner tool string was the reference for Hole 863B.

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 the Th, U, and K. The outputs of this program are K (wet wt %), U (ppm), and Th (ppm), as well as total gamma-ray and computed gamma-ray (total gamma-rayminus U contribution) curves.

The processed gamma-raydata are loaded in the files 859B-ngt.dat and 863B-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. The neutron porosity curve was used in both Holes 859B and 863B. In Hole 859B, this curve had to be rescaled to match cores using the formula:

$$\underline{\varnothing_t} = (\underline{\square_n} - 35) * 0.54$$

where:

$\underline{\varnothing_t}$= percentage porosity

$\underline{\square_n}$= neutron density

The reason for this large rescaling of porosity is the fact that the neutron source in this tool is a ^{252}Cf, instead of an Americium-Beryllium (AmBe) source, which the tool was originally calibrated for.

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:

$$Wi = F\ Yi/Si)$$

where
Wi = dry weight percentage of the i-th element
F = normalization factor determined at each depth interval
Yi = relative elemental yield for the i-th element
Si = 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

$$F\ (\sum Xi\ Yi\ /\ Si) + XK\ WK + XAl\ WAl = 100$$

where
Xi = factor for the element to oxide (or carbonate) conversion
XK = factor for the conversion of K to K_2O (1.205)
XAl = factor for the conversion of Al to Al_2O_3 (1.889)
WK = dry weight percentage of K determined from natural activity
WAl = dry weight percentage of Al determined from the activation measurement

The sensitivity factor, Si, 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 Xi 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 Xi 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 the absence of suitable shipboard data a rough rule of thumb is generally used such that if elemental Ca is below 6% then all Ca is assumed to be in silicate, above 12%, in carbonate. Ca concentrations between these figures are converted using linear interpolation.

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%, therefore $CaCO_3$ is a logical assumption in these instances. When Ca is less than 6%, even if $CaCO_3$ was incorrectly assumed, the error would be very small when 1.39 is used as the oxide factor instead of 2.49. The linear interpolation is done in order to provide a smooth transition and avoid invoking any erroneous chemical changes on the final processed logs. This procedure for Ca gives the best model in most cases and minimizes the error when the model is not exactly correct.

The Mg- and Na-content curves cannot be calculated from the logs, because the neutron-capture cross sections of these elements are too small relative to their typical abundance for detection by the tool string; therefore, available core information is included. A constant value of 6.38% $MgO+Na_2O+MnO$ was used in the normalization of Hole 863B. This value was derived from the average measured core values. No re-normalization was performed in Hole 859B to account for these oxides, due to lack of representative XRF data at the time of processing.

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 859B-oxides.dat and 863B-oxides.dat.
The statistical uncertainties are loaded in the files
859B-oxierr.dat
859B-elerr.dat
863B-oxierr.dat
863B-elerr.dat.
Core data are in the files 859B-core.dat and 863B-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<6%	CaO	1.399
6%>Ca<12%	CaO & $CaCO_3$	1.399-2.49 linearly interpolated
Ca>12%	$CaCO_3$	2.49
Fe	Fe_2O_3	1.43
K	K_2O	1.205
Ti	TiO_2	1.668
Al	Al_2O_3	1.889

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