2004 DATA ANALYSIS FOR COMPASS POLARIZED TARGET

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Contents

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1 INTRODUCTION ABOUT TE CALIBRATION

Thermal Equilibrium (TE) calibration of the Nuclear Magnetic Resonance (NMR) system for COMPASS experiment was carried out using five different temperatures around 1K during the months of May and June 2004.

This report includes many different methods and results so that the best possible ones can be chosen by the experts.

Nine coils that surround the target material were used to acquire the NMR signals. The coils are connected to Liverpool Q-meters. Yale cards compensate the DC voltage and amplify the detected NMR signals (see Ref. [1]).

The polarization of the target is proportional to the area of the NMR signal:

$$Pol = B \times Area \tag{1}$$

$$B = \frac{Pol_{TE}}{Area_{TE}} \tag{2}$$

$$Pol_{enhanced} = \frac{Pol_{TE}}{Area_{TE}} \times Area_{enhanced} \tag{3}$$

B is obtained measuring $Area_{TE}$ and calculating the TE-Polarization, Pol_{TE}, analytically from the Brillouin function at a known temperature.
The TE-Area also depends on the temperature used. To avoid repeating the process each time the temperature is changed, Curie Law is used for calibration:

$$Area_{TE} = \frac{C}{T} \tag{4}$$

where C is the Curie constant.
Five different temperatures were used for calibration in 2004.

2 GENERAL PROCEDURE FOR TE CALIBRATION

The following steps were taken for each group of measured NMR signal files corresponding to one TE-temperature:

Step 1. Each signal was analyzed in the following way:

- the background was subtracted from the signal
- selected points in the off-resonance region were fitted to a straight line to obtain the baseline
- the baseline was subtracted
- the TE area was calculated by integration of the resulting points (signal minus background minus baseline).

Step 2. All the TE areas calculated in the previous way from all the files corresponding to one TE temperature were plotted against time to check their stability. This graph was fitted to a constant to find the final area for the given temperature. This was done for each of the NMR coils.

Step 3. Five different temperatures were used, and their final area values were plotted against the inverse of temperature. Since the TE polarization is proportional to the TE area, the points could be fitted to a Curie law.

3 TE CALIBRATION ANALYSIS

In 2004 the analysis was carried out for Deuterons and for positive magnet current.

Coil number 5 did not exist and coil 6 was not working properly, so that only coils 1 to 4 and 7 to 10 were considered for the analysis.

It was seen that there was an offset between the measured background and its corresponding signal for many coils and for different signals (see Fig.1). This is due to the function of Yale Cards to subtract DC contribution to signals. In the end, this had no effect on the analysis of the TE calibration, since, this DC voltage difference could be canceled out by baseline fitting and subtraction.

Files corresponding to approximately 15 hours after each reset of the TE temperature (as found in the Log Book) were not considered in the analysis since there is a transition time after each change of temperature during which the spin system is not yet in thermal equilibrium with the lattice.

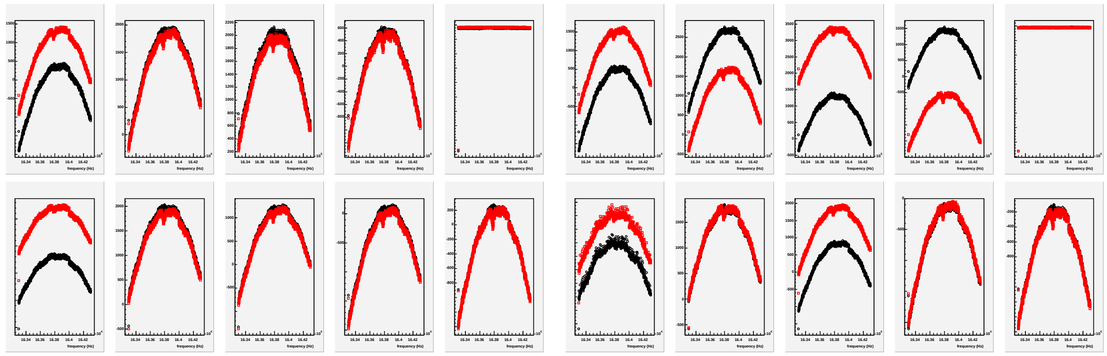

Figure 1: Examples of signal and background offset. Signal is shown in red and background is shown in black. *Left*: temperature was 1.17 K. *Right*: temperature was 1.51 K. Coils 1 to 10 are shown from top to bottom and left to right on both graphs.

Files	No. of TE signals	TE temperature (K)
From 040505_111843.sig to 040507_140350.sig	201	1.5065 ± 0.0037
From 040508_051420.sig to 040509_161035.sig	162	1.2802 ± 0.0011
From 040510_083355.sig to 040512_135344.sig	249	1.1713 ± 0.0020
From 040610_125645.sig to 040612_151551.sig	216	0.9994 ± 0.0023
From 040613_061839.sig to 040614_101322.sig	131	1.3157 ± 0.0018

Table 1: Analyzed files for 2004 TE calibration. From top to bottom group files were called TE1K5, TE1K2, TE1K, TE2_1K, TE2_1K3. The names of the files are given in the way YYMMDD_HHMMSS, where Y is the year, M is the month, D is the day, H the hour, M the minutes and S the seconds. See Ref. [3] for the temperatures.

The files considered in the analysis and their corresponding TE temperatures can be seen in Table 1. Each group of files corresponding to one TE temperature was named TE1K5, TE1K2, TE1K, TE2_1K and TE2_1K3, in chronological order.

At thermal equilibrium the NMR signal is very small and this makes it difficult to calculate the TE area. The integrated area value from the signal depends on the baseline used for fitting the off-resonant region. This is the reason why the choice of the fitting region for the baseline plays an important role in the analysis of the TE signals.
A program was written in ROOT (C++) (MINUIT package) so that a hight number of baselines, each one corresponding to a different width of the region selected for the baseline fit, could be calculated for each signal file. Several methods were tested to try and calculate the TE area as precisely as possible:

1. The "Average Method".

2. The "Histogram Method":

    - Histogram of all areas.

- Histogram of selected areas (Chi-square selection).
- The area coming from the baseline fit with the minimum Chi-square.

They will be discussed in the following sections.

Since the NMR signals at thermal equilibrium are very small compared to the background noise, no signal processing was needed, (such as correction due to the left-to-right asymmetry of the signal), and raw signals were used.

It was checked that the baseline fits were appropriate by plotting them. An example of 8 different fitting regions for the baseline fit, for coil number 4 can be seen in figure 2. The first selected fitting region is wide, while the last one is narrow. The baseline is plotted and it can be seen that the fits look quite good. The fit parameters p0, p1 and p2 for all fits agree with each other within their errors. The same figure shows the final signal after subtraction of the background and the baseline, and it can be seen that for all the different fits for coil 4 the points in the off-resonance region take a value around zero, meaning that the baseline fit was correct.

3.1 The fit of all areas corresponding to one temperature against time.

Step number 2 of the general procedure was studied in detail to try and improve the final results. The evolution in time of the obtained area values at one constant temperature was observed to check their stability.
A program (areatimerobust.C) was written for plotting all the areas for one temperature against time, and for fitting the resulting points to a constant to find the final TE area at that temperature. Some satellite points having an area value much lower or higher than the others could be seen nearly in all cases. It was thought that the use of some χ^2 selection for the baseline fits, which will be described later in the "Histogram Method" section, would improve the results and get rid of some of the satellite points mentioned. However, this did not happen and not much difference was observed in the plots of the areas against time. (The χ^2 selection consisted on considering only the baselines that came from the fits with the lower χ^2 values).

For this reason it was seen that robust fitting (see Ref. [2]) would be needed to improve the results of the fits of those plots to a constant. In this robust fitting method the constant that we were looking for was simply the median of the points to fit. This is the value that minimizes the sum of the absolute deviations.

As well as robust fitting, quantiles were used as a way to select the areas. The quantile q(p), $0 \leqslant p \leqslant 1$, of our normalized distribution of all areas, f(area), is the value of the

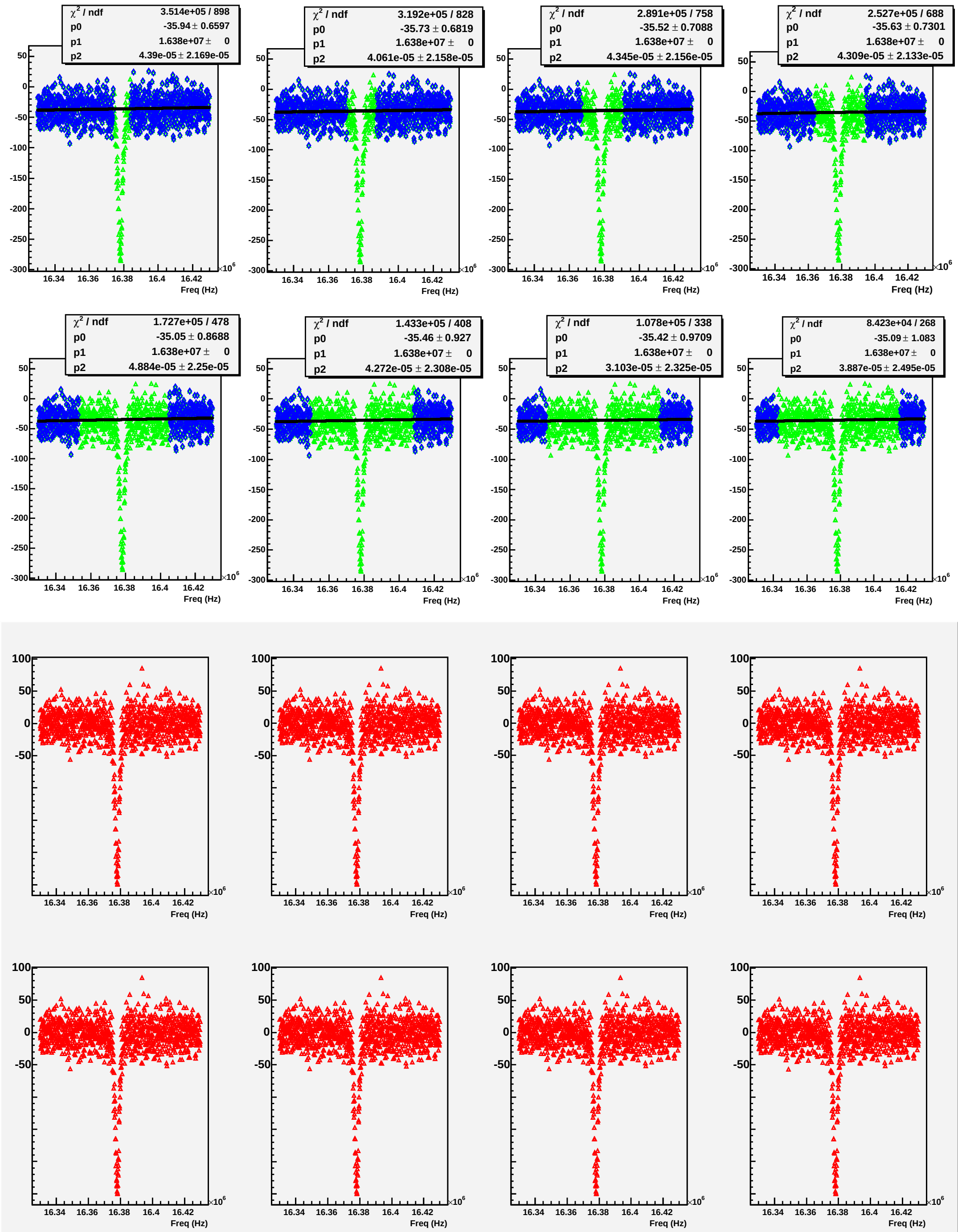

Figure 2: Example of 8 different baseline fits for coil 4 for file 'prueba' (040510_001455.sig). *Top*: the TE signal minus the background is shown in green, while the selected points for the baseline fit are shown in blue. The fitted baseline is shown in black (baseline equation $y = p0 + p2.(x - p1)$), and the fitting parameters are written in each graph. *Bottom*: The final signal after subtraction of the background and baseline is shown in red for each of the 8 different baseline fits performed before. All plots correspond to coil 4. It can be seen that the baseline fits look correct.

area so that the integral of the distribution between $-\infty$ and q(p), is equal to p:

$$\int_{-\infty}^{q(p)} f(area)d(area) = p;$$

$$0 \leqslant p \leqslant 1;$$

For example, the median is calculated as the 0.5 quantile.

All area values were entered in a histogram and the 0.07 and 0.93 probability quantiles of the distribution of all areas were calculated. Only areas having a value between those quantiles were selected to be fitted to the final constant, which was the median of the selected areas. This proved to be a good way of eliminating the satellite points mentioned above.
The histograms of all areas were fitted to a gaussian, and it was seen that they were not so far from such distribution. Figure 3 shows an example of this method. Histograms of all areas can be seen at the top while histograms of selected areas between the quantiles can be seen at the bottom. It is clear that area points with low probability are cut off. Figure 4 shows an example of the plots of all the areas against time (top), and the same plot for only the selected areas between quantiles (bottom). It can be seen that satellite points have been eliminated.

Table 2 shows the values of the median area, the mean area, and the constant coming from the fits performed by ROOT for all the TE areas corresponding to the temperature 1.5065 ± 0.0036 K (TE1K5), for comparison. These values correspond to ALL areas, no quantile selection is applied yet. The difference between the mean and the median is between 0.2% (for coil 4) and 2.0% (for coil 2), and the difference between the fit constant and the median is between 0.4% (for coil 4) and 2.8% (for coil 2).
All the differences (in %) coming from comparison between the values in most of the tables in this report can be found in the attached appendix.
Table 3 shows exactly the same as table 2 but instead of using all areas, only selected areas between the 0.07 and 0.93 probability quantiles were used. The difference between the mean and the median is between 0.02% (for coil 9) and 2.1% (for coil 2), and the difference between the fit constant and the median is between 0.1% (for coil 10) and 2.5% (for coil 2).

The median value of the selected areas between the mentioned quantiles would be used in the rest of the analysis when calculating the final TE area for a given TE temperature. The error of the median was estimated as the half width of the area interval containing 68% probability inside it. This was done because 68% of the total probability in a gaussian distribution is contained in the interval $mean \pm stdev$. After calculating the median of the distribution of TE areas, the 0.16 and 0.84 probability quantiles were calculated, so that 68% of the total probability would be contained between their values.

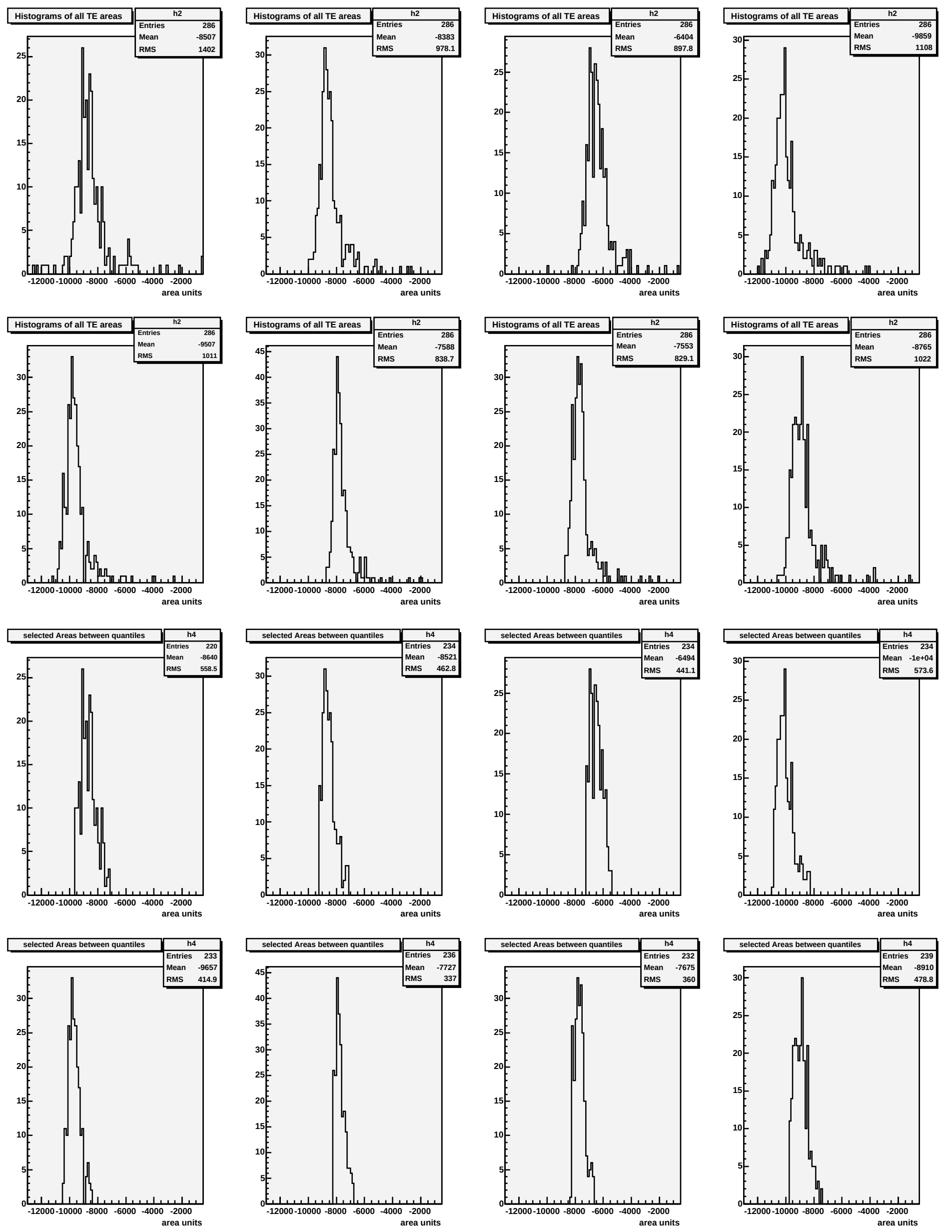

Figure 3: Example of TE area histograms from all files in TE2_1K (TE temperature = 0.9994 K). The top half figure shows the histograms of all areas while the bottom half shows the histograms of areas selected between the quantiles. Both figures show coils 1 to 4 from left to right at the top and coils 7 to 10 from left to right at the bottom. The selection eliminates the area values that have a low probability. (The method used for the baseline fits is the 'average method' (case 2)).

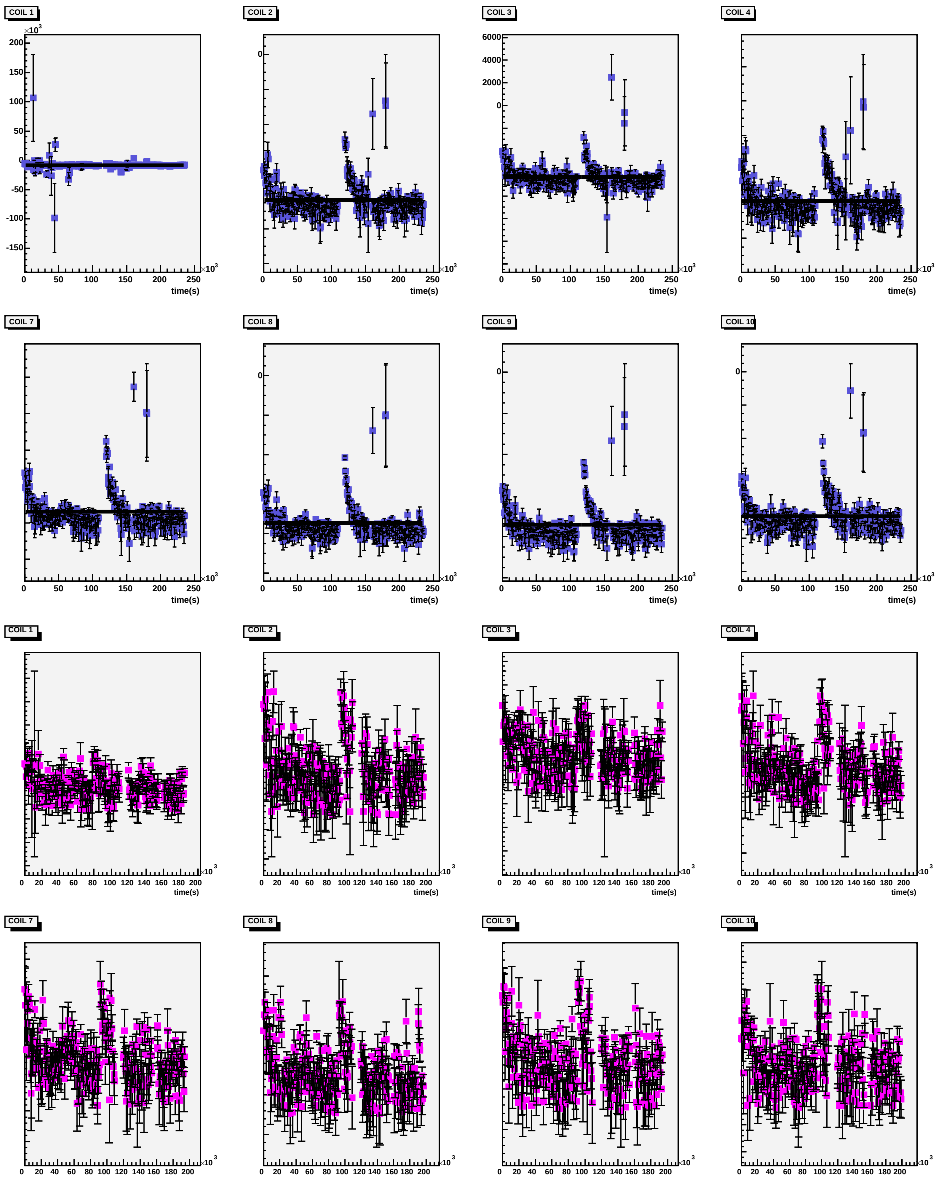

Figure 4: Example of plots of TE area values against time for one TE temperature (0.994 K), for all files in TE2_1K. Both figures show, from left to right, coils 1 to 4 at the top and coils 7 to 10 at the bottom. In the top figure all areas are plotted against time, and satellite points can be clearly seen. In the bottom figure, only selected areas between quantiles are plotted, and it can be seen that satellite points have disappeared. The fitted method used for the baseline fits is the 'average method' (case 2).

For ALL areas						
coil no.	Median	Mean	fit const.	% Differences		
	A	B	C	A-B	B-C	A-C
1	-5833	-5773	-5762	1.0	0.2	1.2
2	-5406	-5514	-5558	2.0	0.8	2.8
3	-4354	-4424	-4386	1.6	0.9	0.7
4	-6573	-6589	-6550	0.2	0.6	0.3
7	-6298	-6336	-6360	0.6	0.4	1.0
8	-4993	-5036	-5021	0.9	0.3	0.6
9	-5097	-5125	-5154	0.5	0.6	1.1
10	-5919	-5957	-5959	0.6	0.0	0.7

Table 2: Final TE areas for 1.5065 ± 0.0036 K (TE1K5). All areas were used (for all times), and no quantile selection was applied. These areas came from the "Average Method" with narrow fitting regions (case 1 in section 3.2.). The median, mean and constant coming from their fit are shown.

For SELECTED areas						
coil no.	Median	Mean	fit const.	% Differences		
	A	B	C	A-B	B-C	A-C
1	-5844	-5817	-5809	0.5	0.1	0.6
2	-5406	-5521	-5540	2.1	0.3	2.5
3	-4359	-4424	-4385	1.5	0.9	0.6
4	-6568	-6582	-6547	0.2	0.5	0.3
7	-6284	-6305	-6329	0.3	0.4	0.7
8	-4989	-5006	-5021	0.3	0.3	0.6
9	-5097	-5096	-5127	0.0	0.6	0.6
10	-5969	-5950	-5963	0.3	0.2	0.1

Table 3: Example of final TE areas for 1.5065 ± 0.0036 K (TE1K5). Only selected areas between the 0.07 and 0.93 quantiles were used.These areas came from the "Average Method" with narrow fitting regions (Case 1 in section 3.2). The median, mean and constant coming from their fit are shown.

3.2 The "Average method".

One hundred different baselines were calculated using different fitting regions, and all the obtained areas were simply averaged to calculate the final TE area for each file.

The total frequency window of each NMR signal always goes from 1633×10^4 Hz to 1643×10^4 Hz, with the resonant NMR peak corresponding to 1637.91×10^4 Hz.
TE signals were analyzed twice with this method:

Case 1 Program 'do-te.C' (fwin=24000Hz) performed 100 fits for each file and coil, making the fitting region narrower as it went from fit number 1 to fit number 100. The fitting region for the first fit was from 1633×10^4 Hz to 1635.51×10^4 Hz, to the left of the NMR peak, and from 1640.31×10^4 Hz to 1643×10^4 Hz, to the right of the peak. The last fitting region was from 1633×10^4 Hz to 1633.11×10^4 Hz, to the left of the NMR peak, and from 1642.71×10^4 Hz to 1643×10^4 Hz, to the right of the peak.

Case 2 Program 'do-tebis.C' (fwin=5000Hz) also performed 100 fits, but starting with a much wider fitting region than before. The fitting region for the first fit was from 1633×10^4 Hz to 1637.41×10^4 Hz, to the left of the NMR peak, and from 1638.41×10^4 Hz to 1643×10^4 Hz, to the right of the peak. The last fitting region was from 1633×10^4 Hz to 1633.945×10^4 Hz, to the left of the NMR peak, and from 1641.875×10^4 Hz to 1643×10^4 Hz, to the right of the peak.

Comparison between these two cases was carried out first for two different single files, for 'prueba' and for 'prueba3', and results can be seen in table 4. Comparison was also carried out for each group of all files corresponding to one May TE temperature (TE1K5, TE1K2 and TE1K), and results are shown in tables 5, 6 and 7. It can be seen that the different ranges of fitting regions (Case 1 and Case 2) certainly produced different values of the TE areas. For the single files 'prueba' and 'prueba3' (table 4), the difference can be large (File 'prueba': from 0.7% for coil 8 to 9.3% for coil 3; File 'prueba3': from 1.2% for coil 9 to 16.3% for coil 3;), but still both values overlap if we take their errors into account. For tables 5, 6 and 7, the differences are smaller, ranging between 0.1% and 3.6% for TE1K5, between 0.2% and 3.2% for TE1K2, and between 0.6% and 2.7% for TE1K.

3.3 The "Histogram method".

3.3.1 Histograms of all areas:

All the area values obtained from each of the different fitting regions considered (100 fits were calculated), were entered into a histogram and plotted. The histograms were fitted to a gaussian and it was seen that they clearly did not follow such distribution. The

	Area for file 'prueba'		Area for file 'prueba3'	
Coil no.	Area. Case 1.	Area. Case 2.	Area. Case 1.	Area. Case 2.
1	-8645 ± 397	$-8213 \pm 410.$	-9572 ± 850	-8130 ± 998
2	-7242 ± 676	-7311 ± 333	-5290 ± 668	-6029 ± 429
3	-6628 ± 837	-6011 ± 258	-7625 ± 889	-6383.30 ± 803
4	-8155 ± 870	-8399 ± 242	-6502 ± 1074	-7423.32 ± 453
7	-8588 ± 200	-8512 ± 277	-7908 ± 314	-7788.58 ± 310
8	-6663 ± 103	-6615 ± 166	-5590 ± 322	-5840.68 ± 137
9	-7053 ± 197	-6936 ± 277	-6138 ± 202	-6064.92 ± 157
10	-6786 ± 394	-7380 ± 412	-6261 ± 548	-6835.21 ± 279

Table 4: The 'Average method' for file 'prueba' (040510_001455.sig), and for file 'prueba3' (040508_225039.sig), for Cases 1 and 2.

For all files in TE1K5		
Coil no.	Area. Case 1.	Area. Case 2.
1	-5843.75 ± 1178.75	-5630.68 ± 662.97
2	-5406.25 ± 895.98	-5562.50 ± 581.60
3	-4359.38 ± 990.00	-4244.05 ± 593.23
4	-6567.71 ± 1100.94	-6562.50 ± 621.56
7	-6283.65 ± 658.66	-6274.04 ± 403.69
8	-4988.97 ± 565.91	-5002.23 ± 377.80
9	-5097.22 ± 520.14	-5052.88 ± 360.45
10	-5968.75 ± 692.08	-5904.17 ± 428.67

Table 5: The 'Average method' for all files in TE1K5 (1.5065 K), for Cases 1 and 2.

For all files in TE1K2		
Coil no.	Area. Case 1.	Area. Case 2.
1	-7000.00 ± 961.34	-6826.92 ± 577.08
2	-7046.88 ± 786.11	-6819.44 ± 494.78
3	-5173.61 ± 962.92	-5163.46 ± 594.17
4	-8229.17 ± 955.08	-8048.61 ± 533.54
7	-7882.81 ± 665.42	-7636.72 ± 386.46
8	-6347.22 ± 605.45	-6150.74 ± 349.55
9	-6265.62 ± 474.69	-6099.14 ± 308.39
10	-7075.00 ± 753.44	-7019.23 ± 474.00

Table 6: The 'Average method' for all files in TE1K2 (1.2802 K), for Cases 1 and 2.

For all files in TE1K		
Coil no.	Area. Case 1.	Area. Case 2.
1	-7363.64 ± 852.19	-7475.00 ± 605.04
2	-7538.46 ± 887.08	-7422.79 ± 488.99
3	-5671.88 ± 872.92	-5592.26 ± 574.58
4	-8820.31 ± 1024.54	-8733.55 ± 581.19
7	-8450.66 ± 638.12	-8361.11 ± 340.18
8	-6706.25 ± 604.33	-6666.67 ± 334.96
9	-6812.50 ± 535.27	-6743.53 ± 298.47
10	-8019.74 ± 731.94	-7802.08 ± 464.53

Table 7: The 'Average method' for all files in TE1K (1.1713 K), for Cases 1 and 2.

	First fit (no.1). Freq region ($\times 10^4$ Hz).				Last fit (no.100). Freq region ($\times 10^4$ Hz).			
	Left of peak		Right of peak		Left of peak		Right of peak	
Choice	From	to	From	to	From	to	From	to
1	1633	1635.51	1640.31	1643	1633	1633.11	1642.71	1643
2	1633	1635.91	1639.91	1643	1633	1633.91	1641.91	1643
3	1633	1636.41	1639.41	1643	1633	1634.91	1640.91	1643
4	1633	1636.91	1638.91	1643	1633	1635.91	1639.91	1643
5	1633	1637.41	1638.41	1643	1633	1633.95	1641.88	1643

Table 8: The different choices for fitting regions in the 'histogram method'.

histograms were adjusted to have a small number of bars so that the final TE area could be calculated as the center of the highest bar in the histogram (most probable area), with its error being estimated as the whole width of the histogram bar (histograms with 40 bins, between -12500 and 500 area units were used, and hence the error in the TE area for each file was 325 area units).

This method was tested for one signal file and its corresponding background, for 100 baseline fits, for different widths of the first and last fitting regions. Table 8 summarizes the different choices of fitting regions. Table 9 shows results for the different choices for file 'prueba' (040510_001455.sig), and table 10 shows results for file 'prueba3' (040508_225039.sig). From those tables it can be seen that the values of the calculated TE areas could differ a lot, and, therefore, the histogram method was quite sensitive to the choice of fitting regions for the 100 fits that were done. In table 9 the maximum difference between the values is 14.3%, and the minimum is 0%; whereas in table 10, the maximum difference is 26.7% and the minimum is 0%. Refer to the appendix of % differences to see calculations for all coils.

Tables 9 and 10 also show (on their 3rd and 8th columns) that for most coils there

'Histogram of all areas method' for file 'prueba'							
Coil no.	choice 1 100 fits	choice 1 500 fits	choice 2 100 fits	choice 3 100 fits	choice 4 100 fits	choice 5 100 fits	choice 5 500 fits
1	-8437.5	-8437.5	-8437.5	-8437.5	-7787.5	-8437.5	-8437.5
2	-7462.5	-7462.5	-7462.5	-7462.5	-7137.5	-7462.5	-7462.5
3	-6162.5	-6162.5	-6162.5	-6162.5	-6162.5	-6162.5	-6162.5
4	-8437.5	-8437.5	-8437.5	-8437.5	-8437.5	-8437.5	-8437.5
7	-8762.5	-8762.5	-8762.5	-8762.5	-8437.5	-8762.5	-8762.5
8	-6812.5	-6812.5	-6812.5	-6812.5	-6487.5	-6812.5	-6812.5
9	-7137.5	-7137.5	-7137.5	-7137.5	-6812.5	-7137.5	-7137.5
10	-6812.5	-6812.5	-6812.5	-7787.5	-7787.5	-7787.5	-7787.5

Table 9: Results for the single file 'prueba' (040510_001455.sig) with the 'histogram of all areas' method. The error is 325 area units for all areas. Different choices for fitting regions are used. These choices can be seen in table 8.

'Histogram of all areas method' for file 'prueba3'							
Coil no.	choice 1 100 fits	choice 1 500 fits	choice 2 100 fits	choice 3 100 fits	choice 4 100 fits	choice 5 100 fits	choice 5 500 fits
1	-9737.5	-9737.5	-9087.5	-7462.5	-7137.5	-9087.5	-7137.5
2	-5837.5	-5837.5	-5837.5	-6162.5	-6487.5	-6487.5	-6487.5
3	-7462.5	-7462.5	-6487.5	-6162.5	-5512.5	-5512.5	-6162.5
4	-7137.5	-6487.5	-7462.5	-7462.5	-7787.5	-7787.5	-7787.5
7	-7787.5	-7787.5	-7787.5	-7787.5	-7462.5	-7787.5	-7787.5
8	-5837.5	-5837.5	-5837.5	-5837.5	-5837.5	-5837.5	-5837.5
9	-6162.5	-6162.5	-6162.5	-6162.5	-6162.5	-6162.5	-6162.5
10	-6812.5	-6812.5	-6812.5	-7137.5	-7137.5	-7137.5	-7137.5

Table 10: Results for the single file 'prueba3' (040508_225039.sig) with the 'histogram of all areas' method. The error is 325 area units for all areas. Different choices for fitting regions are used. These choices can be seen in table 8.

	Final TE Area (area units)		
Coil	All files in TE1K5	All files in TE1K2	All files in TE1K
1	-5607.81 ± 532.56	-6800.78 ± 507.17	-7413.27 ± 602.97
2	-5575.00 ± 362.38	-6805.74 ± 515.00	-7406.98 ± 490.55
3	-4196.93 ± 461.36	-5161.64 ± 430.92	-5582.69 ± 508.33
4	-6463.66 ± 674.37	-8009.77 ± 483.65	-8791.67 ± 501.74
7	-6226.29 ± 475.63	-7807.57 ± 330.25	-8409.25 ± 406.05
8	-4869.52 ± 315.49	-6190.48 ± 334.25	-6761.79 ± 370.30
9	-5135.74 ± 240.14	-6186.22 ± 326.54	-6781.67 ± 362.09
10	-5829.55 ± 330.79	-7132.62 ± 478.31	-7832.95 ± 478.56

Table 11: Final TE area results for the groups of files TE1K5, TE1K2 and TE1K, for choice number 5 of the fitting regions, for the 'Histogram of all areas' method.

was hardly any difference between calculating 100 fits and 500 fits, and therefore, since calculating 500 fits would take much longer, 100 fits were always used for the rest of the analysis in this section.

After testing all those choices for the fitting regions on a single file, it was decided to use choice number 5 for the analysis of the grouped files on TE1K5, TE1K2 and TE1K, each corresponding to a different TE temperature. Since we were using histograms it seemed more logical to cover the widest possible range of fitting regions for the baseline, so that the fitting region for fit number 1 would be wide and very close to the resonant peak, and the fitting region for fit number 100 would be narrow and as far as possible from it (similar to figure 2 (top graph) but with 100 fits instead of 8).
Therefore, all files for the different TE temperatures were analyzed in this way producing the final TE area results shown in table 11. The final TE area for each temperature was obtained after plotting all the TE areas calculated for each file against time, and obtaining the median of all the selected areas between the 7% and 93% probability quantiles (refer to section 3.1.).

3.3.2 Histograms of selected areas (χ^2 selection):

For each of the baseline fits performed in the previous method, the Chi-square (χ^2) parameter was calculated and divided by the number of degrees of freedom (ndf), which was equal to the number of data points to be fitted minus one. This χ^2/ndf fit parameter could be used as an indicator of how good the linear fit was. For a perfect fit, it would take the value zero.
After calculation of χ^2/ndf for all fits, the minimum, $(\chi^2/ndf)_{min}$, that in principle corresponded to the best fit, was found. Only baseline fits having a χ^2/ndf value within the range $(\chi^2/ndf)_{min} \pm \alpha$ were accepted, so that the worse fits could be eliminated from the analysis. Hence, only the areas resulting from those selected fits were entered in the

Chi-square selection method for file 'prueba'								
	$\alpha = 4$		$\alpha = 7$		$\alpha = 9$		$\alpha = 11$	
coil	N	TE area	N	TE area	N	TE area	N	TE area
1	3	-8437.5	4	-8437.5	9	-8437.5	13	-8762.5
2	12	-7787.5	19	-7462.5	26	-7462.5	27	-7462.5
3	3	-6487.5	6	-6487.5	7	-6487.5	8	-6487.5
4	2	-8437.5	4	-8762.5	4	-8762.5	5	-8762.5
7	26	-8437.5	40	-8762.5	56	-8762.5	70	-8762.5
8	12	-6812.5	26	-6812.5	38	-6812.5	68	-6812.5
9	41	-7137.5	96	-7137.5	100	-7137.5	100	-7137.5
10	25	-6812.5	36	-6812.5	59	-6812.5	96	-7787.5

Table 12: Results for file 'prueba' using the 'Histogram method' with different Chi-square confidence regions. 100 baseline fits were calculated for each coil. N is the number of accepted fits (or area values) within the confidence limits $(\chi^2/ndf)_{min} \pm \alpha$. All errors are $\pm$325 area units.

new histograms of the TE areas. The final TE area and its error were calculated from the most probable value (highest bar) in the histogram of selected areas, in the same way as in method 3.3.1.

The single files 'prueba' and 'prueba3' were analyzed with this method (program dotechi.C), using different confidence regions for the χ^2/ndf parameter, that is, different values of α. Results for file 'prueba' and 'prueba3' are shown in tables 12 and 13 respectively. The different TE area values are quite close to each other (4% difference at the most), only for coil 10 the differences can be up to 16%.

Attached to the end of this report are the complete results of the Chi-square selection for file 'prueba3', for $\alpha = 4$ and $\alpha = 7$, where, for all coils, the calculated area and χ^2/ndf fit parameter are shown for each of the 100 fits, and also the accepted areas coming from fits with a χ^2/ndf within the range $(\chi^2/ndf)_{min} \pm \alpha$ can be seen. In most cases the values of the accepted areas are very close to each other and come from the last fits performed, i.e. from fits with a small number of fitted points. It is also clear that χ^2/ndf decreases from fit number 1 to fit number 100, and that it takes much higher values for coils 1 to 4 than for coils 7 to 10.

- Study of the (χ^2/ndf) fit parameter:

It was not so clear whether the Chi-square selection would be a valid method, since it compared fits of different regions, i.e., different points (even if the Chi-square parameter was divided by ndf). The fact that a certain baseline fit would produce the minimum Chi-square/ndf would not necessarily mean that was the best possible baseline, since it

Chi-square selection method for file 'prueba3'								
	$\alpha = 4$		$\alpha = 7$		$\alpha = 9$		$\alpha = 11$	
coil	N	TE area	N	TE area	N	TE area	N	TE area
1	5	-9087.5	6	-9087.5	13	-9087.5	16	-9087.5
2	5	-5187.5	7	-5187.5	9	-5187.5	10	-5187.5
3	4	-6812.5	6	-6812.5	8	-6812.5	12	-6812.5
4	3	-7787.5	8	-7462.5	8	-7462.5	11	-7462.5
7	10	-8112.5	41	-8112.5	58	-7787.5	99	-7787.5
8	29	-5837.5	79	-5837.5	99	-5837.5	100	-5837.5
9	49	-6162.5	100	-6162.5	100	-6162.5	100	-6162.5
10	9	-6162.5	58	-6812.5	96	-7137.5	100	-7137.5

Table 13: Results for file 'prueba3' using the 'Histogram method' with different Chi-square confidence regions. 100 baseline fits were calculated for each coil. N is the number of accepted fits (or area values) within the confidence limits $(\chi^2/ndf)_{min} \pm \alpha$. All errors are ±325 area units.

would also depend on the fitting region and on the shape of the signal. It was also seen that using the Chi-square selection did not help to get rid of the satellite points in the plots of the TE areas against time. Hence, Chi-square selection could be used with a much broader acceptance band just to control very bad fits and eliminate them from the analysis. For all these reasons, a study of the Chi-square/ndf fit parameter was carried out.

The values of the Chi-square/ndf fit parameter were plotted against the fit number (the fit number went from 1 to 100, making the fitting region for the baseline narrower for each fit). This was helpful to check any dependence of the parameter on the fitting region for the baseline and on the number of points that were fitted.
Seeing figure 5 it is clear that such a dependence existed, since, for all coils, the Chi-square/ndf got clearly smaller as the fitting region was made narrower and the number of fitted points decreased (fit number increased) . It should be pointed out that this happened even after dividing by the number of fitted points (ndf).
It can be seen as well that coil 9 had the lowest value of (χ^2/ndf), while coil 4 had the highest one.

The histograms of the Chi-square/ndf values from each of the 100 different baseline fits, for each coil, can be seen in figure 6. It can be observed that the range of Chi-square/ndf values was much wider for coils 1 to 4, and also that the parameter values themselves were much higher than for coils 7 to 10. Hence, the baseline fits were much better for coils 7 to 10, since the points in the off-resonance region would be normally more compact, leading to smaller values of the Chi-square/ndf parameter (see figure 7).

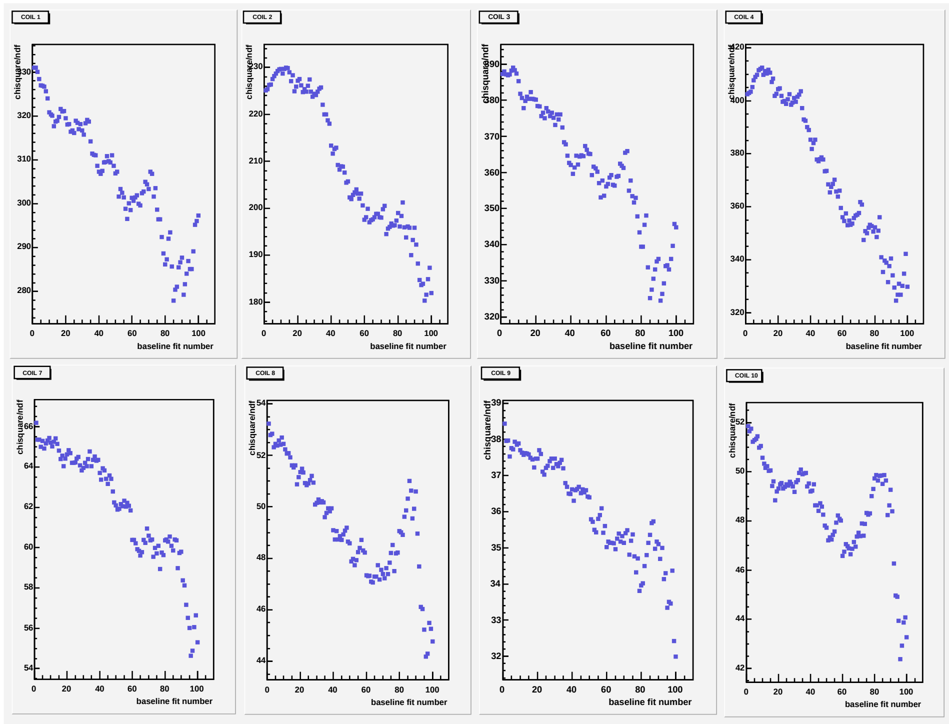

Figure 5: Example of plots of Chi-square/ndf against the fit number. From left to right: top: coils 1 to 4; Bottom: coils 7 to 10.

3.3.3 The area corresponding to the minimum χ^2/ndf

A program (tebestarea.C) was used to calculate the TE area for each file as the area corresponding to the baseline fit having the minimum value of the χ^2/ndf parameter.
It was checked if using more than 100 fits would improve the results. For example, using 400 fits for file 'prueba3' led to a difference in TE areas of 0.4%, 0.1%, 1.4%, 2.3%, 0.3%, 0.5%, 0.4%, and 0%, respectively for each coil, in comparison to those TE areas obtained using 100 fits. The χ^2/ndf parameters, however, were very similar in most cases, and differed in 1.2 at the most. Using 1000 fits produced exactly the same results as for 400 fits, so finally, 400 fits were used for all the calculations in this section.
The results of the analysis of the single files 'prueba' and 'prueba3' can be seen in table 14.

The groups of files TE1K5, TE1K2 and TE1K were also analyzed with this program (400 fits were calculated), and the final TE area for each temperature was obtained after plotting all the TE areas calculated from each file against time, and obtaining the median of all the selected areas between the 7% and 93% probability quantiles. Table 15 shows results of these calculations.
The plots of the TE areas for one temperature against time were not improved by the use of this method, and satellite points appeared in a similar way as before.

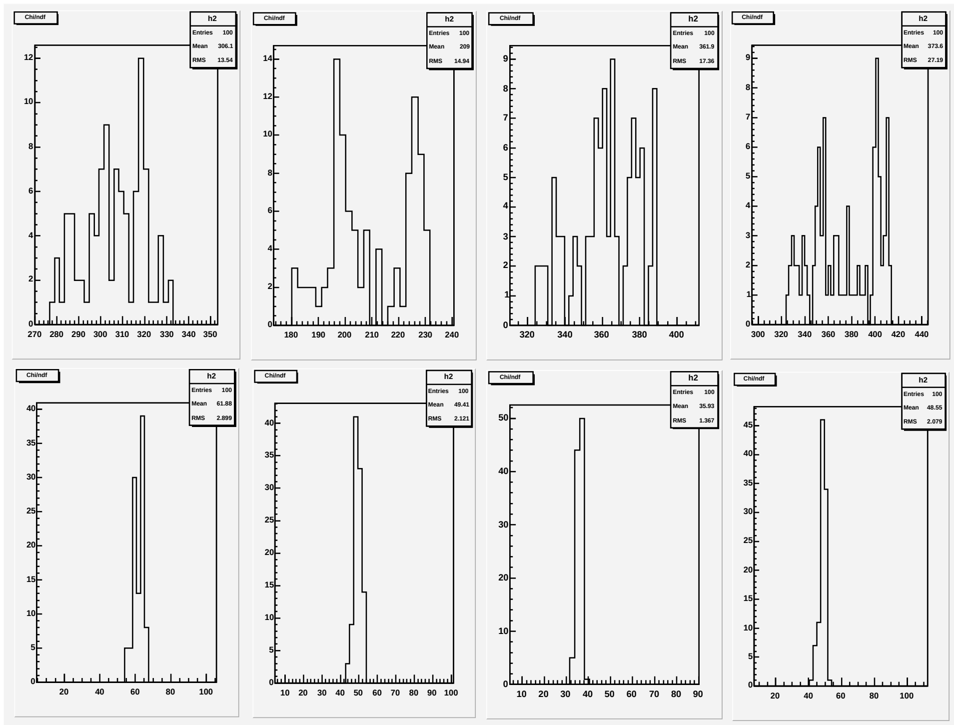

Figure 6: Example of histograms of the Chi-square/ndf values for fits 1 to 100. From left to right: top: coils 1 to 4; Bottom: coils 7 to 10.

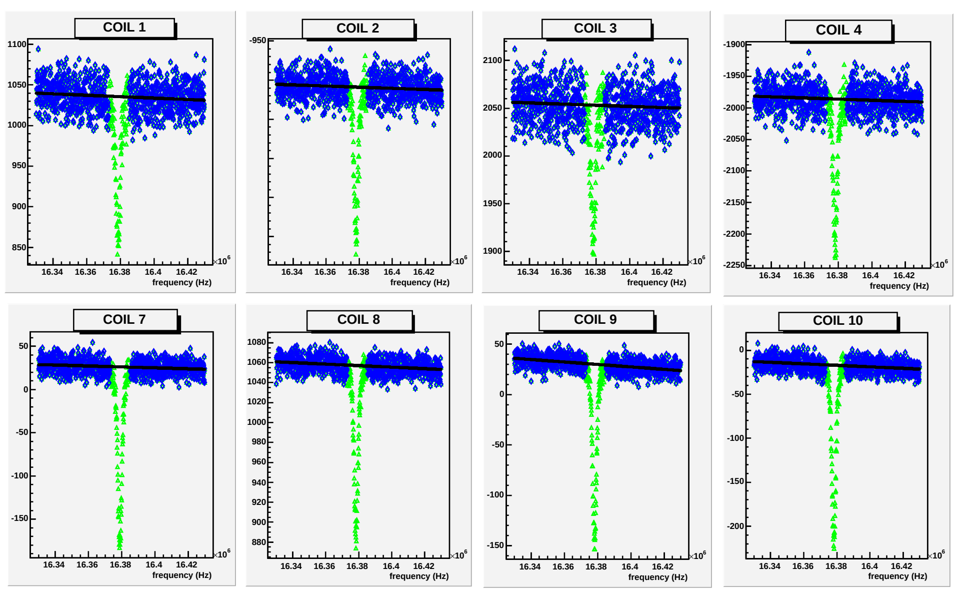

Figure 7: Selected fitting regions (blue points) and baseline fits (black line). From left to right: *Top*: coils 1 to 4; *Bottom*: coils 7 to 10. Note that for coils 1 to 4 the points in the off-resonance region are more dispersed, while those for coils 7 to 10 are more compact.

coil	For file 'prueba'	For file 'prueba3'
1	-8335.11	-9404.71
2	-7880.28	-5248.20
3	-6314.81	-6757.73
4	-8576.57	-7460.50
7	-8581.58	-8198.92
8	-6630.27	-5714.59
9	-7139.22	-6344.60
10	-6562.31	-6174.12

Table 14: Area coming from the baseline fit that produces the lowest value of the χ^2/ndf parameter among 400 fits. Results for single files 'prueba' and 'prueba3'.

coil	For all files in TE1K5	For all files in TE1K2	For all files in TE1K
1	-5743.06 ± 1083.00	-6828.12 ± 935.62	-7361.61 ± 1014.28
2	-5489.58 ± 829.50	-6959.82 ± 730.62	-7483.33 ± 716.75
3	-4287.50 ± 873.75	-5196.43 ± 841.67	-5607.14 ± 918.06
4	-6443.18 ± 1045.44	-8145.83 ± 820.83	-8857.14 ± 876.75
7	-6227.27 ± 656.70	-7681.82 ± 591.18	-8410.71 ± 596.72
8	-5040.18 ± 482.00	-6112.50 ± 535.66	-6710.00 ± 481.19
9	-5062.50 ± 419.21	-6191.41 ± 402.96	-6697.50 ± 436.71
10	-5930.15 ± 643.56	-7033.65 ± 627.80	-7835.53 ± 604.11

Table 15: For each file corresponding to one TE temperature, the TE area was obtained as that coming from the baseline fit that produced the lowest value of the χ^2/ndf parameter among 400 fits. Among all those TE areas only the ones between the 7% and 93% probability quantiles were selected, and the median of those was the final TE area for that temperature.

Due to the small dependence of χ^2/ndf on the fit number, I would say this was not a very reliable method, since the TE area corresponding to the lowest χ^2/ndf value would systematically correspond to a fit number close to 400, i.e., it would correspond to a baseline fit calculated from a few points, far from the resonant peak.

3.4 Comparison between different methods.

The results from three different methods were compared first for the single files 'prueba' and 'prueba3', and then for the groups of files TE1K5, TE1K2 and TE1K. Results are presented in tables 16 to 20 respectively. All these tables show three columns that correspond to the following methods:

- Column 1: the 'average method', Case 2 (refer to section 3.2, Case 2).
- Column 2: the 'histogram of all areas method', choice 5 for the fitting regions, (refer to section 3.3.1).
- Column 3: the method of the area corresponding to $(\chi^2/ndf)_{min}$, (400 fits), (refer to section 3.3.3).

All these three methods used the same range of fitting regions for the baseline, which corresponds to choice 5 (last row) in table 8.
All the differences (in %) coming from comparison between the area values for each of these three methods can be seen in tables 16 to 20 of the appendix, where the relative differences between columns 1 and 2, between columns 2 and 3, and between columns 1 and 3, are given in percentages for each coil. For the groups of files TE1K5, TE1K2 and TE1K, the differences are not too large, and can go up to 3.5%.
Note that the errors for Column 2 tend to be lower than for the rest of the columns in most cases.

3.5 Curie plots. Final results.

Finally June 2004 data was also analyzed as well as May data. The quantile selection for the distribution of all areas for different times corresponding to one TE temperature was changed to the 9% and 91% quantiles.

Only two methods were chosen. Recapping, they were the following:

- A) The 'average method': for each file the average of all the areas obtained from the 100 baseline fits was calculated. After that, all those average areas from all files corresponding to one TE temperature were entered into a histogram, and only

Comparison for file 'prueba'			
coil	1	2	3
1	-8212.71	-8437.50	-8335.11
2	-7311.37	-7462.50	-7880.28
3	-6010.90	-6162.50	-6314.81
4	-8398.70	-8437.50	-8576.57
7	-8511.87	-8762.50	-8581.58
8	-6615.20	-6812.50	-6630.27
9	-6935.82	-7137.50	-7139.22
10	-7380.31	-7787.50	-6562.31

Table 16: Comparison between results from different methods for file 'prueba'. Column 1: the 'average method', Case 2. Column 2: the 'Histogram of all areas method'. Column 3: the minimum chi-square area method.

Comparison for file 'prueba3'			
coil	1	2	3
1	-8130.39	-9087.50	-9404.71
2	-6028.99	-6487.50	-5248.20
3	-6383.30	-5512.50	-6757.73
4	-7423.32	-7787.50	-7460.50
7	-7788.58	-7787.50	-8198.92
8	-5840.68	-5837.50	-5714.59
9	-6064.92	-6162.50	-6344.60
10	-6835.21	-7137.50	-6174.12

Table 17: Comparison between results from different methods for file 'prueba3'. Column 1: the 'average method', Case 2. Column 2: the 'Histogram of all areas method'. Column 3: the minimum chi-square area method.

Comparison for all files in TE1K5			
coil	1	2	3
1	-5630.68 ± 662.97	-5607.81 ± 532.56	-5743.06 ± 1083.00
2	-5562.50 ± 581.60	-5575.00 ± 362.38	-5489.58 ± 829.50
3	-4244.05 ± 593.23	-4196.93 ± 461.36	-4287.50 ± 873.75
4	-6562.50 ± 621.56	-6463.66 ± 674.37	-6443.18 ± 1045.44
7	-6274.04 ± 403.69	-6226.29 ± 475.63	-6227.27 ± 656.70
8	-5002.23 ± 377.80	-4869.52 ± 315.49	-5040.18 ± 482.00
9	-5052.88 ± 360.45	-5135.74 ± 240.14	-5062.50 ± 419.21
10	-5904.17 ± 428.67	-5829.55 ± 330.79	-5930.15 ± 643.56

Table 18: Comparison between results from different methods for all files in TE1K5. Column 1: the 'average method', Case 2. Column 2: the 'Histogram of all areas method'. Column 3: the minimum chi-square area method.

Comparison for all files in TE1K2			
coil	1	2	3
1	-6826.92 ± 577.08	-6800.78 ± 507.17	-6828.12 ± 935.62
2	-6819.44 ± 494.78	-6805.74 ± 515.00	-6959.82 ± 730.62
3	-5163.46 ± 594.17	-5161.64 ± 430.92	-5196.43 ± 841.67
4	-8048.61 ± 533.54	-8009.77 ± 483.65	-8145.83 ± 820.83
7	-7636.72 ± 386.46	-7807.57 ± 330.25	-7681.82 ± 591.18
8	-6150.74 ± 349.55	-6190.48 ± 334.25	-6112.50 ± 535.66
9	-6099.14 ± 308.39	-6186.22 ± 326.54	-6191.41 ± 402.96
10	-7019.23 ± 474.00	-7132.62 ± 478.31	-7033.65 ± 627.80

Table 19: Comparison between results from different methods for all files in TE1K2. Column 1: the 'average method', Case 2. Column 2: the 'Histogram of all areas method'. Column 3: the minimum chi-square area method.

Comparison for all files in TE1K			
coil	1	2	3
1	-7475.00 ± 605.04	-7413.27 ± 602.97	-7361.61 ± 1014.28
2	-7422.79 ± 488.99	-7406.98 ± 490.55	-7483.33 ± 716.75
3	-5592.26 ± 574.58	-5582.69 ± 508.33	-5607.14 ± 918.06
4	-8733.55 ± 581.19	-8791.67 ± 501.74	-8857.14 ± 876.75
7	-8361.11 ± 340.18	-8409.25 ± 406.05	-8410.71 ± 596.72
8	-6666.67 ± 334.96	-6761.79 ± 370.30	-6710.00 ± 481.19
9	-6743.53 ± 298.47	-6781.67 ± 362.09	-6697.50 ± 436.71
10	-7802.08 ± 464.53	-7832.95 ± 478.56	-7835.53 ± 604.11

Table 20: Comparison between results from different methods for all files in TE1K. Column 1: the 'average method', Case 2. Column 2: the 'Histogram of all areas method'. Column 3: the minimum chi-square area method.

those between the 9% and 91% quantiles were selected. The final TE area was obtained as the median of all those selected areas for each coil.

- B) The 'histogram method' with less restrictive Chi-square selection: since, as explained before, the Chi-square selection in this method was not very reliable, it was decided to use $\alpha = 85$, so that, for each file, only baseline fits producing a χ^2/ndf within $(\chi^2/ndf)_{min} \pm 85$ would be accepted. This wider range of selection would help to get rid of very bad fits only. In the histograms of those selected areas, the most probable one was found for each file. Its error was estimated as ± 352 area units. After that, all areas from all files corresponding to one TE temperature were entered into a histogram and only those between the 9% and 91% quantiles were selected. The final TE area for that temperature was calculated as the median of those selected areas for each coil.

Both these methods used the same range of fitting regions for the baseline, which corresponds to choice 5 (last row) in table 8.

Since the TE polarization is proportional to the TE area under the signal, Curie fits could be performed. The values of the final TE area corresponding to each TE temperature were plotted against the inverse of temperature for each coil. These points were fitted to a line with equation $y = p0 + p1.x$. Parameter $p0$ was forced to be equal to zero. Results for the Curie fits for each of the two methods explained before are shown in tables 21 and 22. The errors in the fit parameter $p1$ are between 2.0% and 4.2% (see Tables 21 and 22 from the appendix).
See the attached appendix for the differences (in %), in the parameter $p1$ of the Curie fits, between both methods. The differences between the two methods range between 0.2% and 1.0%. The values of the parameter $p1$ for both methods agree within their

Curie fits. A): 'Average method'.				
Coil no.	χ^2/ndf	$p0$	$p1$	% Error in $p1$
1	0.0817 / 4	0 ± 0	-8746 ± 285	3.3
2	0.1602 / 4	0 ± 0	-8663 ± 235	2.7
3	0.1009 / 4	0 ± 0	-6593 ± 275	4.2
4	0.2031 / 4	0 ± 0	-10210 ± 286	2.8
7	0.3241 / 4	0 ± 0	-9752 ± 196	2.0
8	0.3368 / 4	0 ± 0	-7812 ± 171	2.2
9	0.2963 / 4	0 ± 0	-7803 ± 167	2.1
10	0.1014 / 4	0 ± 0	-9004 ± 239	2.7

Table 21: Results from the Curie fits for A), the 'Average method' (Case 2). The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$, where $p0$ was forced to be zero.

Curie fits. B): 'Histogram method'.				
Coil no.	χ^2/ndf	$p0$	$p1$	% Error in $p1$
1	0.2419 / 4	0 ± 0	-8669 ± 283	3.3
2	0.3129 / 4	0 ± 0	-8632 ± 250	2.9
3	0.3483 / 4	0 ± 0	-6536 ± 227	3.5
4	0.3161 / 4	0 ± 0	-10190 ± 280	2.7
7	0.6411 / 4	0 ± 0	-9813 ± 192	2.0
8	1.749 / 4	0 ± 0	-7879 ± 167	2.1
9	0.4314 / 4	0 ± 0	-7879 ± 168	2.1
10	0.3775 / 4	0 ± 0	-9027 ± 224	2.5

Table 22: Results from the Curie fits for B) the 'histogram method' with Chi-square ± 85 selection. The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$, where $p0$ was forced to be zero.

errors.

Figures 30 to 35 show the plots of the calculated areas against time for TE1K5, TE1K2, TE1K, TE2_1K and TE2_1K3, at the end of this report.

The Curie Law is only a 'good approximation' of the Brillouin function in the limit of high temperature. Nuclear NMR thermometry equations (see Ref. [4]) include also a temperature independent term in the equation for the Curie fit, so that $p0$ can be different from zero. No strong arguments were found by Jaakko to give a good reason why $p0$ should be forced to zero even for insulators without conduction electrons. This is why the Curie fits were calculated again, this time without forcing $p0$ to zero. The resulting parameters are given in tables 23 and 24 , for both methods, A) and B) respectively. In

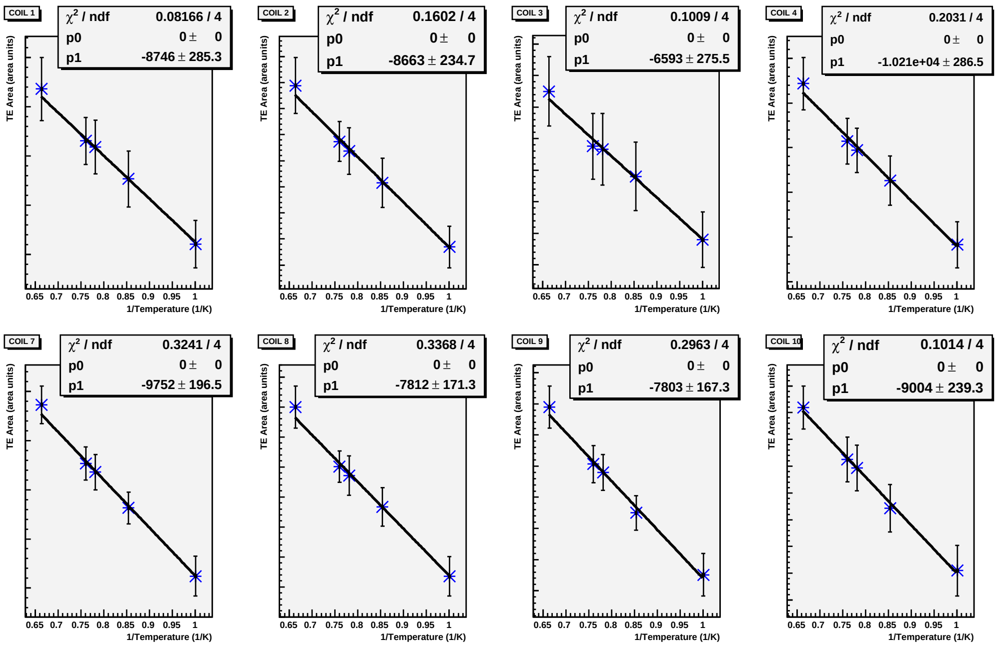

Figure 8: Curie fits for A), the 'average method' (Case 2). The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$, where $p0$ was forced to be zero. Top: coils 1 to 4; Bottom: coils 7 to 10.

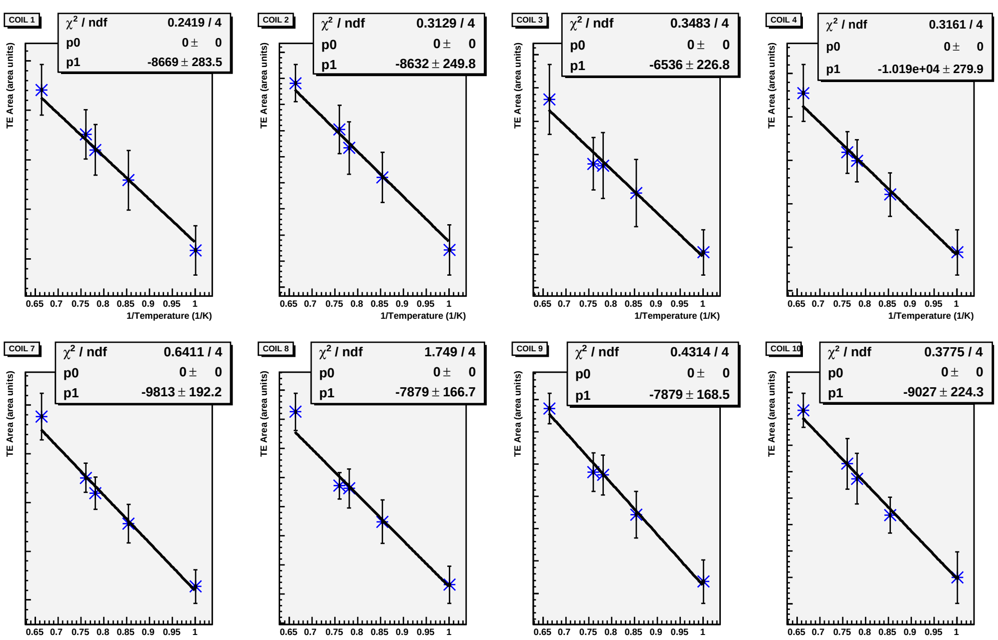

Figure 9: Curie fit for B), the 'histogram method' with Chi-square ±85 selection. The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$, where $p0$ was forced to be zero. Top: coils 1 to 4; Bottom: coils 7 to 10.

Curie fits. A): 'Average method'. $p0$ not forced to 0.			
Coil no.	χ^2/ndf	p0	p1
1	0.0525 / 3	$(0.30 \pm 1.76) \times 10^3$	-9100 ± 2103
2	0.1470 / 3	$(0.17 \pm 1.45) \times 10^3$	-8861 ± 1743
3	0.0943 / 3	$(0.13 \pm 1.61) \times 10^3$	-6748 ± 1921
4	0.1982 / 3	$(0.12 \pm 1.76) \times 10^3$	-10360 ± 2142
7	0.2387 / 3	$(0.37 \pm 1.27) \times 10^3$	-10200 ± 1556
8	0.2854 / 3	$(0.24 \pm 1.08) \times 10^3$	-8110 ± 1322
9	0.2824 / 3	$(0.13 \pm 1.09) \times 10^3$	-7959 ± 1334
10	0.0990 / 3	$(0.07 \pm 1.43) \times 10^3$	-9090 ± 1775

Table 23: Results from the Curie fits for A), the 'Average method' (Case 2). The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$. The fit parameter $p0$ was not forced to zero in this case.

Curie fits. B): 'Histogram method'. $p0$ not forced to 0.			
Coil no.	χ^2/ndf	p0	p1
1	0.0269 / 3	$(0.76 \pm 1.65) \times 10^3$	-9591 ± 2010
2	0.0611 / 3	$(0.69 \pm 1.37) \times 10^3$	-9483 ± 1714
3	0.3252 / 3	$(-0.21 \pm 1.35) \times 10^3$	-6295 ± 1591
4	0.3052 / 3	$(0.19 \pm 1.83) \times 10^3$	-10410 ± 2215
7	0.6407 / 3	$(-0.03 \pm 1.24) \times 10^3$	-9782 ± 1505
8	1.6120 / 3	$(0.38 \pm 1.02) \times 10^3$	-8342 ± 1261
9	0.4255 / 3	$(0.72 \pm 9.36) \times 10^2$	-7969 ± 1182
10	0.2418 / 3	$(0.48 \pm 1.31) \times 10^3$	-9623 ± 1633

Table 24: Results from the Curie fits for B) the 'Histogram method' with Chi-square ± 85 selection. The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$. The fit parameter $p0$ was not forced to zero in this case.

all cases, the χ^2 of the fit is smaller if $p0$ is not forced to zero, but the errors in $p0$ and $p1$ are much larger than in the case when $p0$ is forced to zero. Since, in tables 23 and 24, parameter $p0$ is close to zero anyway and the errors are so large, forcing $p0$ to zero is probably a better choice.

3.6 Errors

For case A) of the final results the main errors were the following:

- the error coming from each of the baseline fits for one file (not estimated).
- the error coming from the average of 100 areas for each file (calculated as the standard deviation).

- the error from the median of the quantile-selected average areas coming from all files (calculated as the 68% confidence region in the histogram.).
- the error of the TE temperature (given, see Ref. [3]).
- the error of the Curie fits to a line (calculated by MINUIT).

For case B) of the final results the main errors were the following:

- the error coming from each of the baseline fits for one file (not estimated).
- the error coming from finding the most probable area in the histogram of Chi-square selected areas for each file (estimated as ±325 area units, which was the width of the histogram bars).
- the error from the median of the quantile-selected most probable areas coming from all files (calculated as the 68% confidence region in the histogram.)
- the error of the TE temperature (given, see Ref. [3]).
- the error of the Curie fits to a line (calculated by MINUIT).

The MINUIT fitting package gives different fit parameters and errors for different considered points and their error bars. If the error bars of the points to be fitted are changed, the fit parameters and their errors also change. For this reason, it was assumed that the errors are propagated to the last stage of the analysis.

3.7 One Other Method

From the Curie law we have:

$$Area_{TE} = \frac{C}{Temperature_{TE}} \tag{5}$$

where C is the Curie constant that should not depend on the temperature.
Hence, the previous equation can be re-written as:

$$Area_{TE} \times Temperature_{TE} = C \tag{6}$$

This means that for all the calculated areas from all files and for all temperatures, the products ($Area_{TE} \times Temperature_{TE}$) can be plotted against time and fitted to find the final value of the Curie constant C.
Program todo.C used all 2004 TE calibration files to plot all values of the ($Area_{TE} \times Temperature_{TE}$) against time. Hence values coming from TE1K5, TE1K2, TE1K, TE2_1K and TE2_1K3 were plotted one after the other on the same graph. All those

values were entered into a histogram and only the ones between the 9% and 91% probability quantiles were selected. This was done to remove satellite points. The final Curie constant, C, was initially calculated in two ways: first fitting the selected points to a constant with ROOT, and second, calculating the median of all the selected values of $(Area_{TE} \times Temperature_{TE})$.

Apart from that, the histograms of ALL values of $(Area_{TE} \times Temperature_{TE})$ were fitted to a gaussian and it was seen that the fits were extremely good for the 'Average Method', and a bit worse for the 'Histogram method' (See figure 10). Hence it was seen that the Curie constant C could also be obtained from the 'mean' and the 'sigma' of the fitted gaussian function, for comparison.

These three ways of calculating the Curie constant C were used for both methods, (A):the 'Average method', and B): the 'Histogram Method') explained in section 2.5. Results can be seen in table 25 for the 'Average method', and in table 26 for the 'Histogram method'. These tables show, for each coil: in the first column the constants from the fits of the selected values to a line; in the second column the median of the selected values; and in the third column the mean from the fit of all values to a gaussian. Note that, for the 'Average method', the median of the selected values between the quantiles is in all cases closer to the mean value from the fitted gaussian than the constant from the fit of selected values to a line is. For the 'Histogram method the fits of all values to a gaussian are not that good, but, still, the values of C obtained from those fits are very similar to those from the median of selected areas.

For the 'Average method' (see table 25) the errors of the median of all selected values of $(Area_{TE} \times Temperature_{TE})$ are between 4.8% and 9.4%, while those for the mean of the gaussian fit of the histogram of all values are between 6.1% and 12.0%. The difference between both is between 0.03% and 0.49% (refer to table 25 of the appendix).
The results for the Curie constant C coming from the Curie fits of the final TE Areas against the inverse of temperature for this method (table 21) where compared with the values of C obtained using the values of the product $(Area_{TE} \times Temperature_{TE})$ (table 25). The difference between table 21 and the median of selected values was between 0.09% and 0.45%, while the difference between table 21 and the mean of the gaussian fit was between 0.04% and 0.67% (see appendix).

For the 'Histogram method' (see table 26) the errors of the median of all selected values of $(Area_{TE} \times Temperature_{TE})$ are between 5.0% and 8.4%, while those for the mean of the gaussian fit of all values are between 5.0% and 9.5%. The difference between both is between 0.04% and 1.82% (refer to table 26 of the appendix).
The results for the Curie constant C coming from the Curie fits of the final TE Areas against the inverse of temperature for this method (table 22) where compared with the

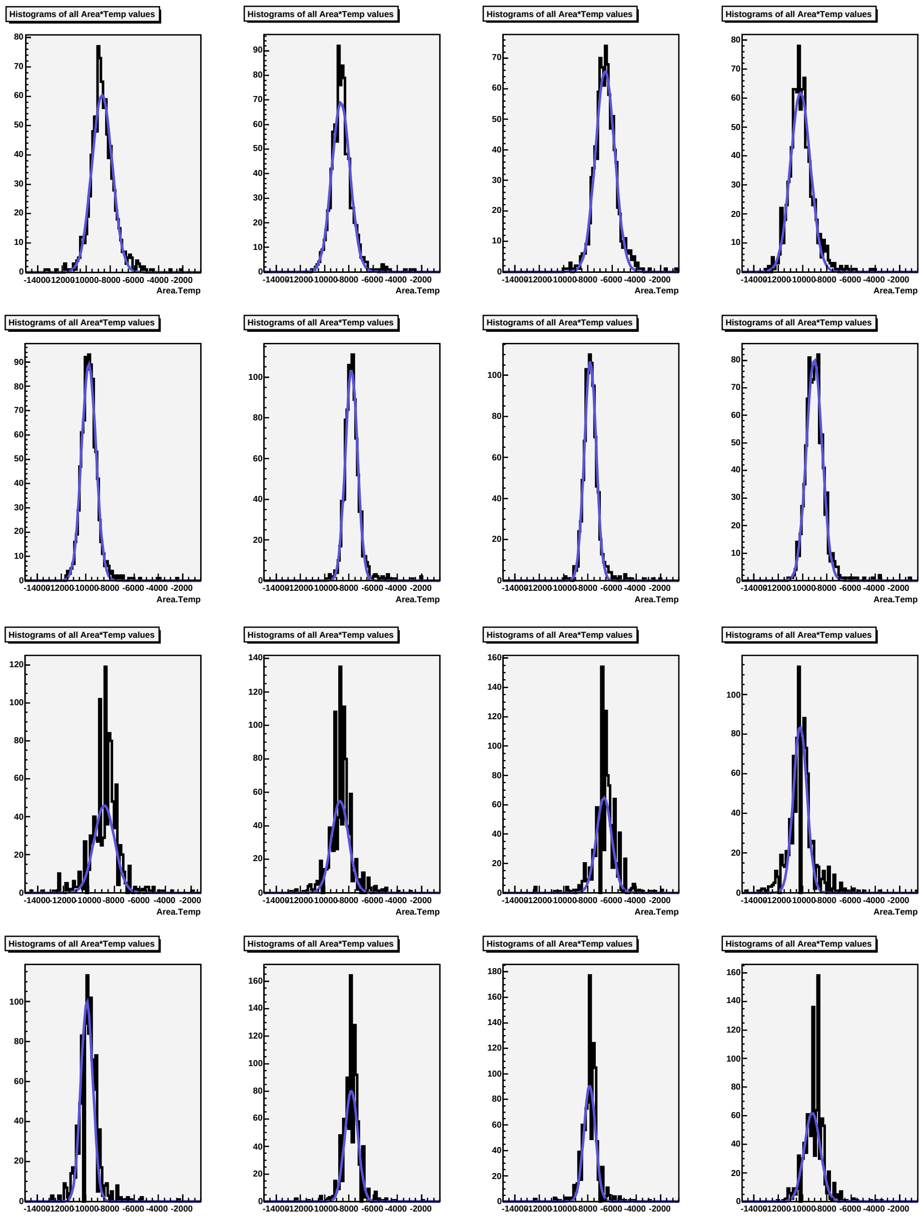

Figure 10: The top half figure shows the gaussian fits for the histograms of all ($Area_{TE} \times Temperature_{TE}$) values, for the 'Average method'. The bottom half shows gaussian fits for the histograms of all ($Area_{TE} \times Temperature_{TE}$) values, for the 'Histogram method'. Both figures show, from left to right, coils 1 to 4 at the top and coils 7 to 10 at the bottom. Note how the gaussian fits for the 'Average method' are extremely good.

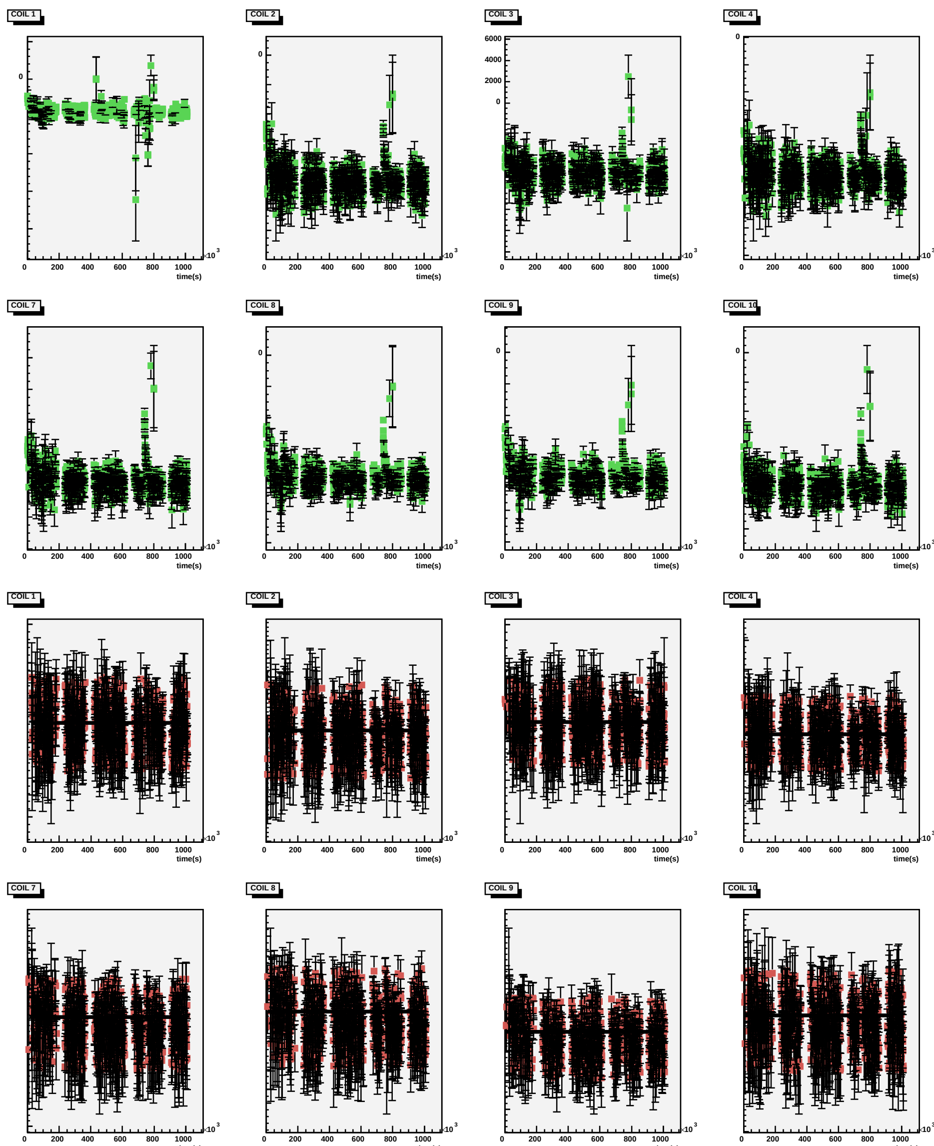

Figure 11: The top half figure shows the plots of all values of $(Area_{TE} \times Temperature_{TE})$ against temperature. The bottom half shows the plots of the selected values of $(Area_{TE} \times Temperature_{TE})$ between quantiles, against time. Both figures show, from left to right, coils 1 to 4 at the top and coils 7 to 10 at the bottom.

Using $Area \times Temperature$ for the 'Average method'					
coil	constant from fit of selected values to a line	Median of selected values	← % error	mean ± sigma from gaussian fit of all values	← % error
1	-8560 ± 15	-8730 ± 662	7.6	-8688 ± 846	9.7
2	-8517 ± 11	-8651 ± 561	6.5	-8655 ± 756	8.7
3	-6503 ± 14	-6573 ± 617	9.4	-6575 ± 790	12.0
4	-10070 ± 14	-10196 ± 647	6.3	-10171 ± 826	8.1
7	-9549 ± 9	-9721 ± 467	4.8	-9738 ± 592	6.1
8	-7629 ± 7	-7776 ± 401	5.2	-7785 ± 503	6.5
9	-7655 ± 6	-7796 ± 383	4.9	-7799 ± 488	6.3
10	-8858 ± 3	-9020 ± 522	5.8	-9030 ± 653	7.2

Table 25: Curie constant C calculated from the values of $Area \times Temperature$ for the 'Average method'.

values of C obtained using the values of the product $(Area_{TE} \times Temperature_{TE})$ (table 26). The difference between table 22 and the median of selected values was between 0.01% and 1.05%, while the difference between table 22 and the mean of the gaussian fit was between 0.08% and 1.95% (see appendix).

Comparison between table 25 and table 26 was also carried out (see appendix). For the median of selected values of $(Area_{TE} \times Temperature_{TE})$, the difference between the 'Average method' (table 25) and the 'Histogram method' (table 26) was between 0.08% and 0.71%. For the mean of the gaussian fit of the histogram of all values of $(Area_{TE} \times Temperature_{TE})$ the difference between the 'Average method' (table 25) and the 'Histogram method' (table 26) was between 0.11% and 1.78%.

Using $Area \times Temperature$ for the 'Histogram method'					
coil	constant from fit of selected values to a line	Median of selected values	← % error	mean ± sigma from gaussian fit of all values	← % error
1	-8729 ± 14	-8668 ± 646	7.5	-8787 ± 801	9.1
2	-8653 ± 14	-8644 ± 507	5.9	-8722 ± 704	8.1
3	-6563 ± 14	-6542 ± 550	8.4	-6663 ± 631	9.5
4	-10170 ± 14	-10233 ± 570	5.6	-10198 ± 564	5.5
7	-9810 ± 14	-9776 ± 500	5.1	-9895 ± 494	5.0
8	-7806 ± 14	-7796 ± 402	5.2	-7794 ± 536	6.9
9	-7822 ± 14	-7806 ± 390	5.0	-7850 ± 476	6.1
10	-9025 ± 14	-9046 ± 502	5.5	-9194 ± 667	7.3

Table 26: Curie constant C calculated from the values of $Area \times Temperature$ for the 'Histogram method'.

4 TE CALIBRATION: FURTHER ANALYSIS

4.1 Construction of a 'super-TE-signal'.

The idea was to construct a 'supersignal' by averaging all the signals from the 2004 TE calibration. This would be useful to clarify if there was any residual baseline or dispersion part in the NMR signal.

After subtraction of the background and calculated linear baseline, all the signals were scaled with their corresponding temperature.
The average of all the values of *(signal minus background minus baseline)*$\times$*Temperature* was calculated for each of the 1000 frequency channels measured for each signal. The resulting 'supersignal' can be seen in Fig.12.

The off-resonance region of the 'supersignal' was fitted to a parabola to check if there was any remaining parabolic baseline.
The fitting parabolic function was $y = p0 + p2 \times (x - p1)^2$, were the coefficients, $p2$, of the second order term were found to be of the order of 10^{-10} for all coils. This result meant that the second order contribution to the equation of the baseline was negligible, and therefore, linear fits could be safely used instead of parabolic fits.

No files were eliminated at all to construct the 'supersignal'. The average 'supersignal' was calculated from all files at thermal equilibrium from 2004, using no selection at all.

The small residual parabolic baseline was subtracted from the 'supersignal', which was then fitted to the so-called Memory function (see Ref.[6]) in order to obtain relevant parameters of the NMR line shape, and to compare different coils. An example of this fit can be seen in figure 13, for coil number 8.
Table 27 contains the resonant frequency *f0*, the second moment *M2*, the fourth moment *M4* of the dipole interaction, and the scaling factor A, obtained from the fit for each coil.
Table 28 shows the area calculated from the raw supersignal, the area calculated from its fit to the Memory function, the ratio of them, and the percentage difference between them. This was done in order to check if there was any coupling between coils, to see if upstream and downstream coils provided different results (see Ref.[7]). The ratio of the areas from both calculations were between 0.95% and 0.96% for all coils, with no difference between upstream and downstream coils.

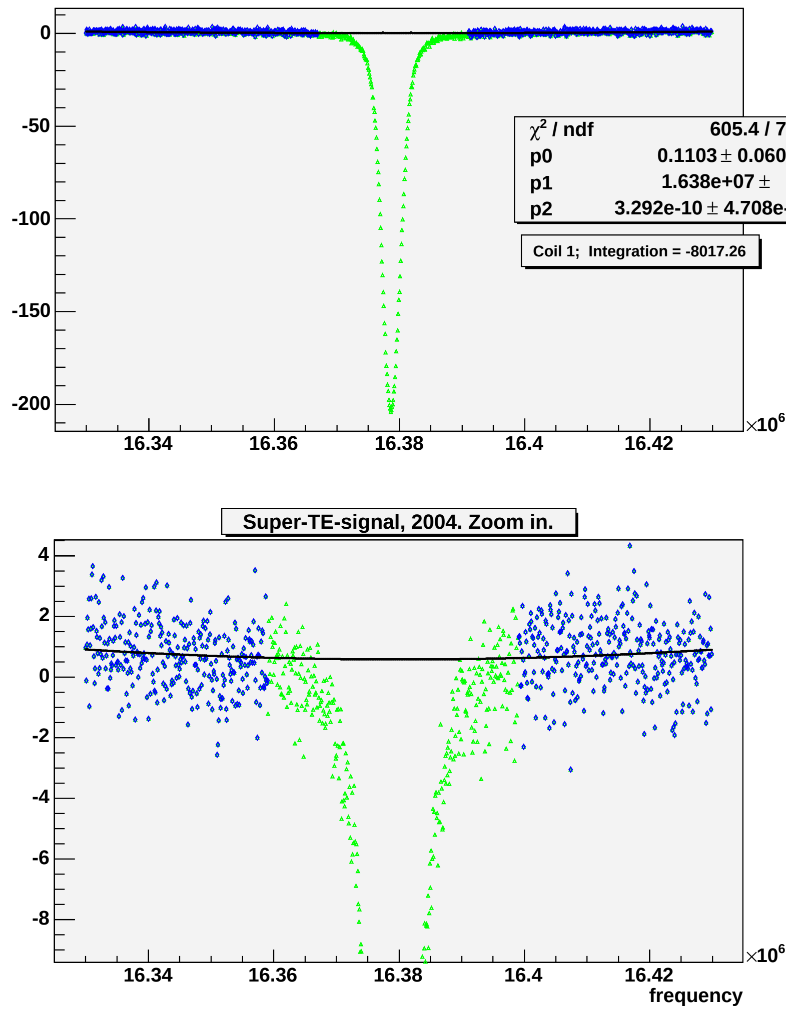

Figure 12: *Top:* Supersignal calculated from the average of all TE signals from 2004 scaled with their corresponding temperatures. The fit of the off-resonance region to a parabola is shown. The second order coefficient of this fit, $p2$, is of the order of 10^{-10}. *Bottom:* zoom in. Note that the supersignal is slightly shifted upward from zero. This is because the average of all $(signal \times Temperature)$ values is plotted, and not the average of all $signals$. Most temperatures were close to 1K, but slightly larger (see table 1).

coil	*f0* (Hz)	*M2* (Hz^2)	*M4* (Hz^4)	*A*
1	1.63791×10^7	3.81197×10^6	6.84867×10^{13}	1.64891×10^6
2	1.63787×10^7	3.40898×10^6	5.01521×10^{13}	1.63726×10^6
3	1.63789×10^7	3.21252×10^6	4.17704×10^{13}	1.24531×10^6
4	1.63788×10^7	3.33439×10^6	4.83815×10^{13}	1.93287×10^6
7	1.63792×10^7	3.43471×10^6	5.83418×10^{13}	1.83949×10^6
8	1.63789×10^7	3.36093×10^6	5.10102×10^{13}	1.47490×10^6
9	1.63789×10^7	3.34103×10^6	4.68944×10^{13}	1.47994×10^6
10	1.63788×10^7	3.46570×10^6	4.97415×10^{13}	1.71228×10^6

Table 27: Results from the fit of the supersignal to the Memory function. $f0$ is the resonant frequency, $M2$ and $M4$ are the second and fourth moments, and A is the scaling factor.

coil	a	b	b/a	$100 \times (b-a)/a$
1	-8659.19	-8244.57	0.95	4.8%
2	-8514.51	-8186.31	0.96	3.9%
3	-6526.17	-6226.57	0.95	4.6%
4	-10015.3	-9664.34	0.96	3.5%
7	-9607.38	-9197.43	0.96	4.3%
8	-7690.72	-7374.48	0.96	4.1%
9	-7708.37	-7399.70	0.96	4.0%
10	-8910.81	-8561.42	0.96	3.9%

Table 28: Results from the fit of the supersignal to a Memory function. The first column shows the area (a) obtained from integration of the raw supersignal. The second column shows the area (b) obtained from the fit to the Memory function. The third column shows the ration of the previous two columns, and the last column shows their percentage difference.

4.2 Selection of the off-resonance region.

One NMR signal with its background was chosen among all the TE calibration signals measured in 2004. This signal could be fitted to a gaussian using the equation:

$$F(f) = A \times exp\Big(-\frac{(f-f_0)^2}{2M_2}\Big) \tag{7}$$

were A is the maximum amplitude of the NMR signal after subtraction of the background, f is the frequency, f_0 is the resonant frequency, and M_2 is the second moment.

In the off-resonance region the signal should be zero, but instead of that, noise is measured. In this region there is no information about the signal, only noise. It can be assumed that the baseline should be fitted using the points in that region in which there

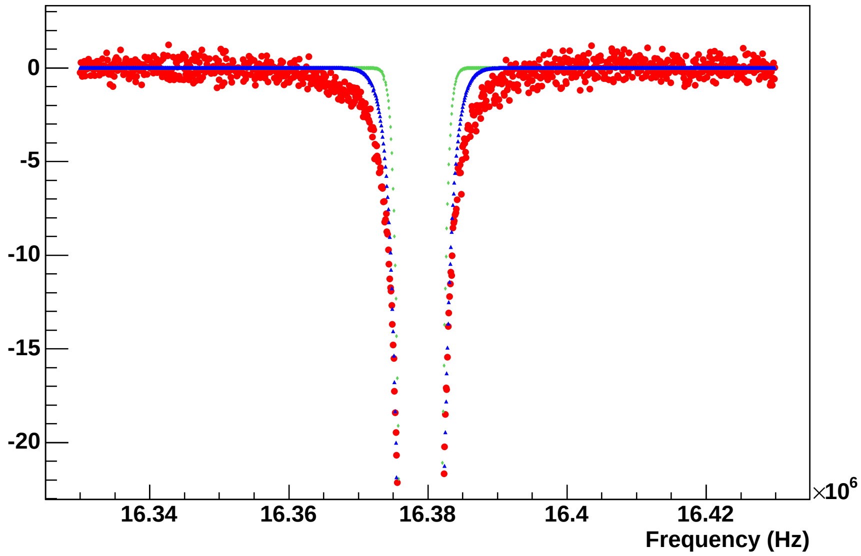

Figure 13: Fit of the supersignal to the Memory function. Zoom in. The supersignal is shown in red. An initial fit to a gaussian is shown in green, and the fit to the Memory function is shown in blue.

is no information about the signal. To determine the limits of this region, the criteria was to assume that when the amplitude of the NMR signal was the same as the amplitude of its noise, there would be no information about the signal anymore, since the noise would be comparable to it.
Therefore, we need to find the frequency, f_1, for which:

$$A \times exp\Big(-\frac{(f_1 - f_0)^2}{2M_2}\Big) = noise \tag{8}$$

Solving this equation for $(f_1 - f_0)$ we obtain:

$$(f_1 - f_0) = \sqrt{2 \times M_2 \times ln\Big(\frac{A}{noise}\Big)} \tag{9}$$

For a quick estimation of $(f_1 - f_0)$ the following values from the chosen NMR signal were used:
$A = 200$;
$noise = 30$;
$M_2 = 1.7 \times 10^6$, (obtained from the gaussian fit);

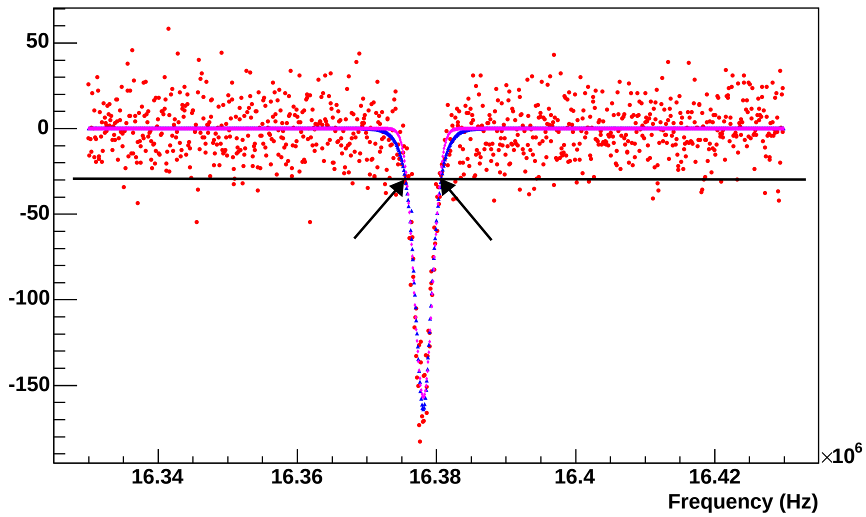

Figure 14: Fit of one TE signal to a gaussian (*pink colour*), and to a Memory function (*blue colour*). The horizontal line indicates when the amplitude of the signal is similar to that of the noise. The arrows indicate the estimated limits of the fitting region for the baseline.

The result was

$(f_1 - f_0) \backsimeq 2540 Hz$

Figure 14 shows the fit of the chosen signal to a gaussian in pink (coil 2 was used). The horizontal black line tries to show when the amplitude of the signal is similar to that of the noise. The arrows indicate where the obtained value of f_1 would be.

This estimation of $(f_1 - f_0)$ could be taken as the maximum limit of the fitting region for the baseline, though it should be pointed out that this was only a rough calculation. In the analysis described in section 3, the value of $(f_1 - f_0)$ used was 5000 Hz or larger, being well away from that limit.

In the case of the 'supersignal', calculated from the average of around 1000 signals, the *noise* factor should be substituted by $\frac{noise}{\sqrt{1000}}$, leading to a value of $(f_1 - f_0) \backsimeq 4265 Hz$. The value of $(f_1 - f_0)$ used in section 4.1 for the fitting of the off-resonance region of the supersignal was 20000 Hz.

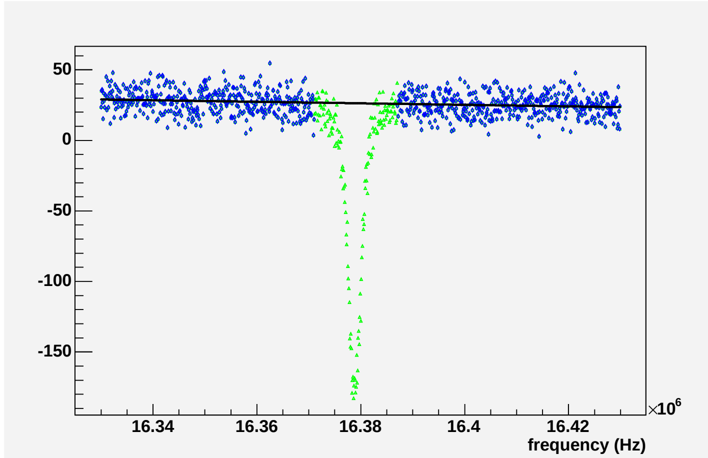

Figure 15: Fitting region for the analysis in section 4.3.1 (*blue points*).

4.3 Analysis of all the 2004 TE calibration data using 1 baseline fit per signal file, instead of 100 baseline fits.

All the signals from the 2004 TE calibration period were analyzed again, but this time only one baseline was calculated per signal file, instead of 100. The analysis methods were those explained in section 3.5.(A), using Curie fits, and in section 3.7., using the products of ($Area \times Temperature$).

4.3.1 The fitting region for the baseline including all the first and last frequency channels.

All points in the signal except the ones around the resonant peak, inside the frequency interval $f_0 \pm 8000Hz$, were used for the baseline fit performed for each signal file. The points corresponding to the first and last frequency channels were also fitted. The fitting region for the only baseline calculated for each file is shown in blue in figure 15.

Results for TE1K2, TE1K and TE2_1K3, (refer to table 1), showed good and narrow histograms of the calculated area values coming from all files (see Fig.16, for files in TE1K2). For these groups of files, no points were eliminated at all via quantile selection, since it was not needed.
For TE1K5 a few points were removed manually, and for TE2_1K the zone showing a spike due to a problem with the magnet (see Fig.4), was eliminated.

Results for the Curie constant, C, for each coil, coming from Curie fits are shown in table 29. Results for C, using the values of ($Area \times Temperature$) (see section 3.7.) are shown in table 30.

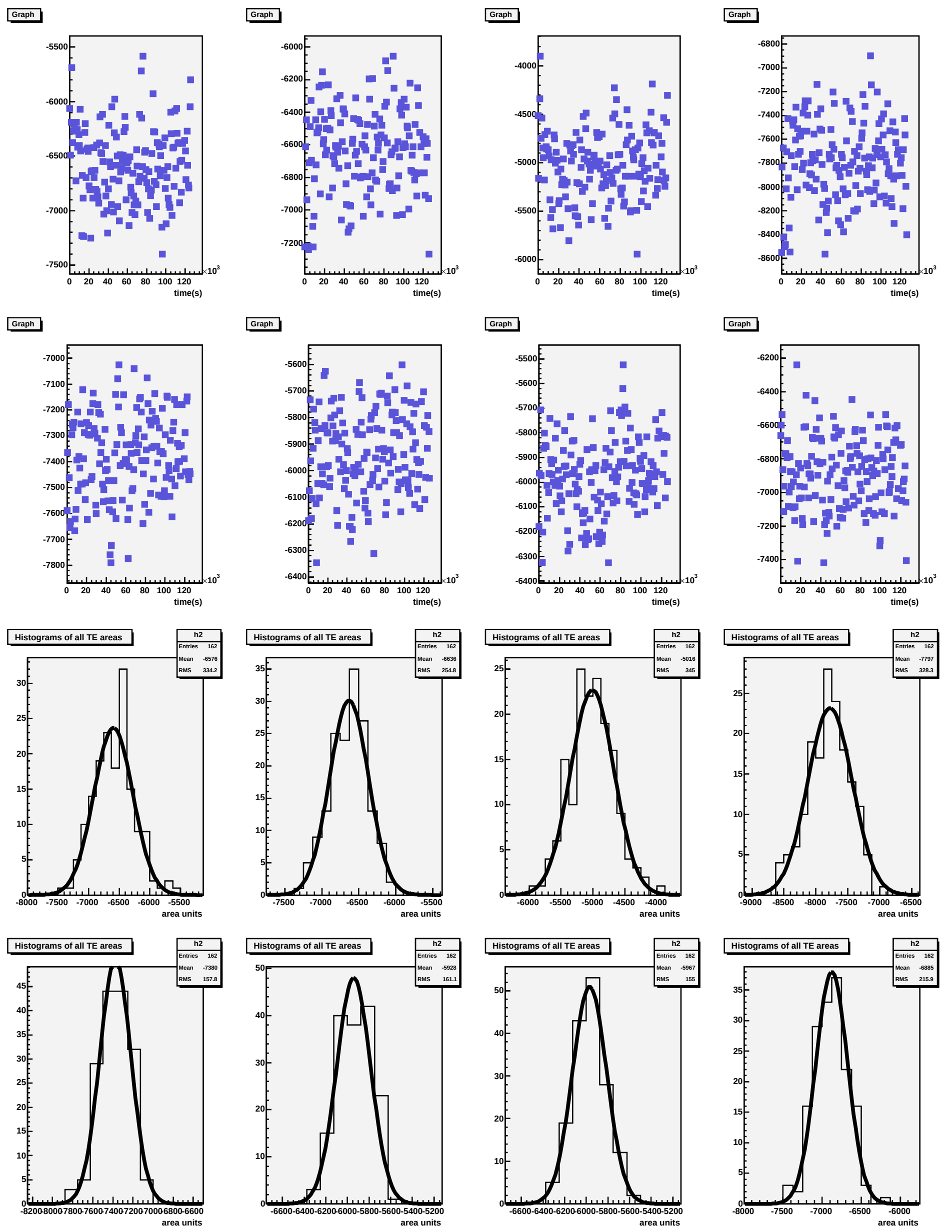

Figure 16: *Top*: Example of plots of calculated area values against time for all files in TE1K2. Only one baseline was calculated for each file. *Bottom*: Histograms of all areas. Both figures show, from left to right, coils 1 to 4 at the top and coils 7 to 10 at the bottom.

Coil no.	χ^2/ndf	$p0$	$p1$	% Error in $p1$
1	0.2007 / 4	0 ± 0	-8444 ± 169	2.0
2	0.3398 / 4	0 ± 0	-8456 ± 131	1.6
3	0.1598 / 4	0 ± 0	-6454 ± 162	2.5
4	0.2248 / 4	0 ± 0	-9986 ± 168	1.7
7	0.3961 / 4	0 ± 0	-9468 ± 101	1.1
8	0.3482 / 4	0 ± 0	-7598 ± 92	1.2
9	0.08055 / 4	0 ± 0	-7631 ± 86	1.1
10	0.09725 / 4	0 ± 0	-8804 ± 120	1.4

Table 29: Results from the Curie fits using only one baseline fit per signal. The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$, where $p0$ was forced to be zero.

coil	Median of all values	← % error	mean ± sigma from gaussian fit of all values	← % error
1	-8423 ± 543	5.3	-8429 ± 396	4.7
2	-8434 ± 559	6.6	-8440 ± 325	3.8
3	-6424 ± 437	6.8	-6429 ± 413	6.4
4	-9962 ± 553	5.6	-9948 ± 390	3.9
7	-9452 ± 535	5.7	-9449 ± 238	2.5
8	-7585 ± 325	4.3	-7584 ± 203	2.7
9	-7628 ± 282	3.7	-7627 ± 195	2.6
10	-8799 ± 269	3.1	-8809 ± 259	2.9

Table 30: Curie constant C calculated from the values of $(Area \times Temperature)$, using only one baseline fit per signal file.

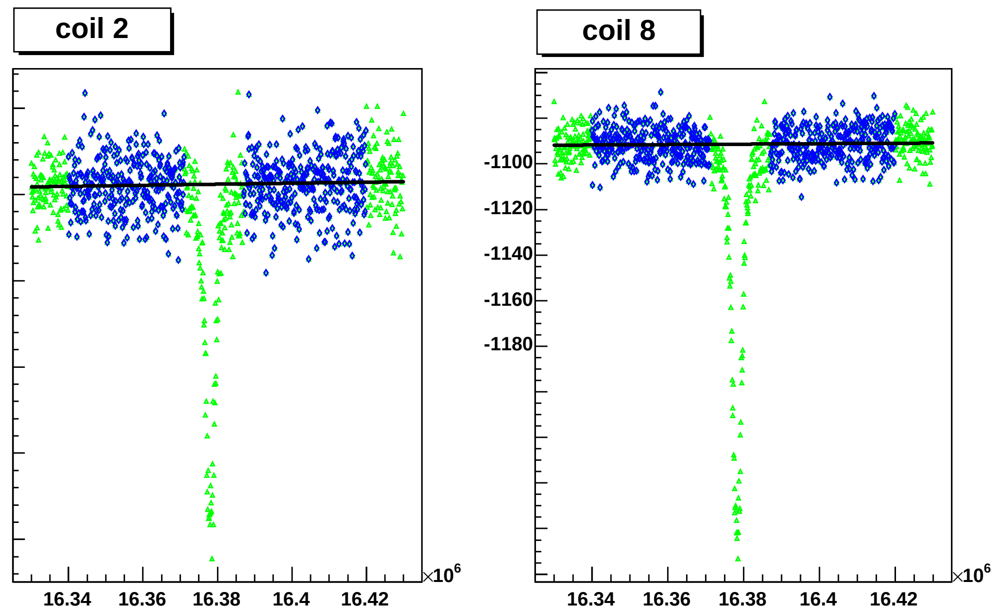

Figure 17: Fitting region for the analysis in section 4.3.2 (*blue points*).

4.3.2 The fitting region for the baseline excluding the first and last frequency channels.

All points in the signal except the ones around the resonant peak, inside the frequency interval $f_0 \pm 8000Hz$, and except those corresponding to the first 100 and last 100 frequency channels were used for the only baseline fit performed for each signal file. The fitting region for this section is shown in figure 17 (*blue points*).

Again, no points were eliminated from TE1K2, TE1K and TE2_1K3, via quantile selection, since it was not needed; for TE1K5 a few points were removed manually; for TE2_1K the zone showing a spike due to a problem with the magnet was eliminated.

Results for the Curie constant, C, for each coil, coming from Curie fits are shown in table 31. Results for C, using the values of $(Area \times Temperature)$ (see section 3.7.) are shown in table 32.

Figure 18 shows the plots of all the values of $(Area \times Temperature)$ against time, as well as the histograms of all these values, and their fit to a gaussian curve.

Note that, for all coils, the value of the Curie constant C obtained from baseline fits that exclude the first and last frequency channels is lower than the value of C calculated from baseline fits that include those channels.

Coil no.	χ^2/ndf	$p0$	$p1$	% Error in $p1$
1	0.2441 / 4	0 ± 0	-8321 ± 257	3.1
2	0.1092 / 4	0 ± 0	-8313 ± 195	2.3
3	0.1605 / 4	0 ± 0	-6374 ± 238	3.7
4	0.1044 / 4	0 ± 0	-9839 ± 251	2.5
7	0.1781 / 4	0 ± 0	-9292 ± 135	1.4
8	0.1164 / 4	0 ± 0	-7463 ± 113	1.5
9	0.1179 / 4	0 ± 0	-7518 ± 102	1.4
10	0.1516 / 4	0 ± 0	-8691 ± 161	1.8

Table 31: Results from the Curie fits using only one baseline fit per signal, and excluding the first and last frequency channels of the signal. The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$, where $p0$ was forced to be zero.

coil	Median of all values	← % error	mean ± sigma from gaussian fit of all values	← % error
1	-8293 ± 728	8.8	-8308 ± 588	7.1
2	-8292 ± 833	10.0	-8298 ± 455	5.5
3	-6354 ± 615	9.7	-6347 ± 585	9.2
4	-9807 ± 807	8.2	-9804 ± 606	6.2
7	-9276 ± 837	9.0	-9279 ± 314	3.4
8	-7458 ± 439	5.9	-7460 ± 256	3.4
9	-7518 ± 357	4.7	-7516 ± 227	3.0
10	-8679 ± 316	3.6	-8672 ± 365	4.2

Table 32: Curie constant C calculated from the values of $(Area \times Temperature)$, using only one fit per signal file, and excluding the first and last frequency channels of the signal.

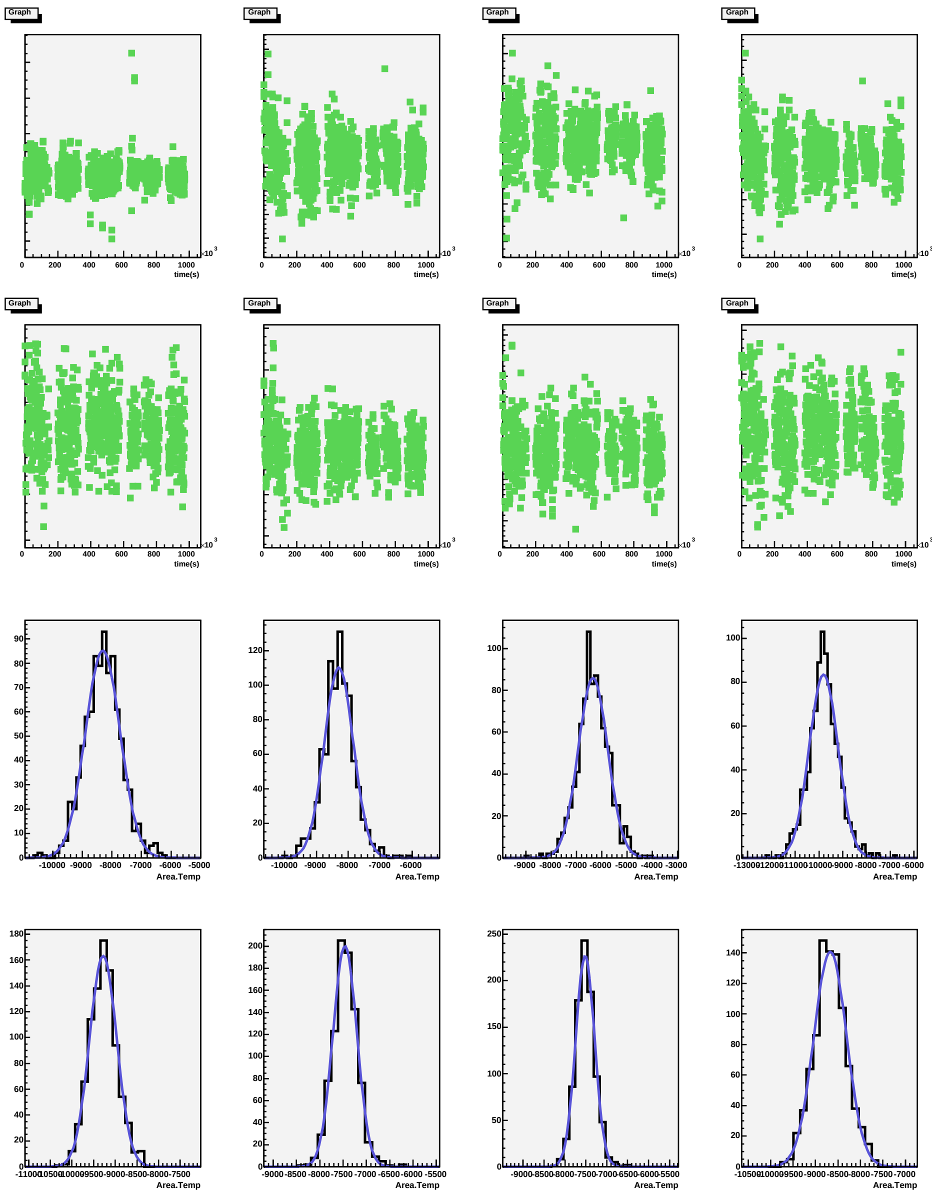

Figure 18: *Top*: Example of plots of calculated values of $(Area \times Temperature)$ against time for all files and all temperatures. Only one baseline was calculated for each file, excluding the first and last frequency channels. *Bottom*: Histograms of all values of $(Area \times Temperature)$. Both figures show, from left to right, coils 1 to 4 at the top and coils 7 to 10 at the bottom.

4.4 Another check for the linear baseline.

If the signal points (after subtraction of the background) that are inside the selected region for the baseline fit are named $selected(j)$, and the fitted linear baseline in that region is named $baseline(j)$, with j being those selected frequency channels, the following calculations can be done:

- the area under the selected points for the baseline fit, $Area_1$, can be obtained from raw integration of the points:

$$Area_1 = \sum_{j}^{fitting\,region} selected(j)$$

- the area under the fitted baseline in the region selected for the baseline fit, $Area_2$:

$$Area_2 = \sum_{j}^{fitting\,region} baseline(j)$$

- the difference between the previous areas, which should be close to zero area units:

$$Area_1 - Area_2$$

- the area under the points in the fitting region after subtraction of the linear baseline, $Area_3$:

$$Area_3 = \sum_{j}^{fitting\,region} [selected(j) - baseline(j)]$$

For the fitting region that excludes only the central frequency channels inside $f_0 \pm 5000Hz$, (see Fig.7), the plots of the values of $(Area_1 - Area_2)$ and $Area_3$ versus time are shown in figure 19. It can be seen that most values of $(Area_1 - Area_2)$ go up to around 2 area units at the most, while the values of $Area_3$ can go up to around 0.005 area units.

For the fitting region that excludes the central frequency channels inside $f_0 \pm 8000Hz$, as well as the first 100 and last 100 channels (see Fig.17), the plots of the values of $(Area_1 - Area_2)$ and $Area_3$ versus time are shown in figure 20. It can be seen that most values of $(Area_1 - Area_2)$ go up to around 1 area unit at the most, while the values of $Area_3$ can go up to approximately 0.003 area units.

In all cases, both areas, $(Area_1 - Area_2)$ and $Area_3$, are very close to zero area units, indicating that after subtraction of the linear baseline, the contribution of the off-resonance region to the total area of the TE signal is negligible.

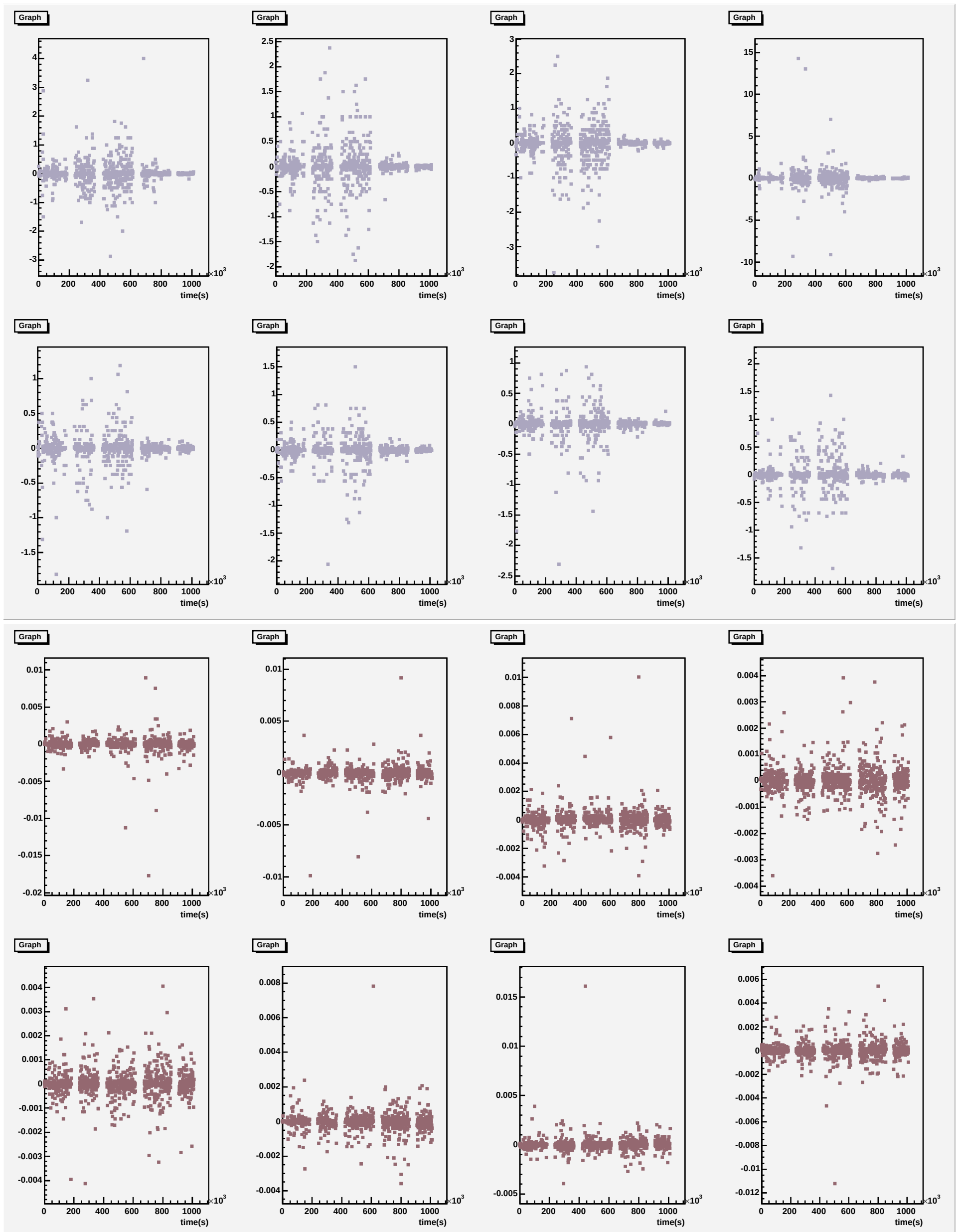

Figure 19: *Top*: Plots of $(Area_1 - Area_2)$ against time for all files and all temperatures, for the fitting region shown in Fig.7. *Bottom*: Plots of $Area_3$ against time for all files and all temperatures, for the same fitting region. Both figures show, from left to right, coils 1 to 4 at the top and coils 7 to 10 at the bottom.

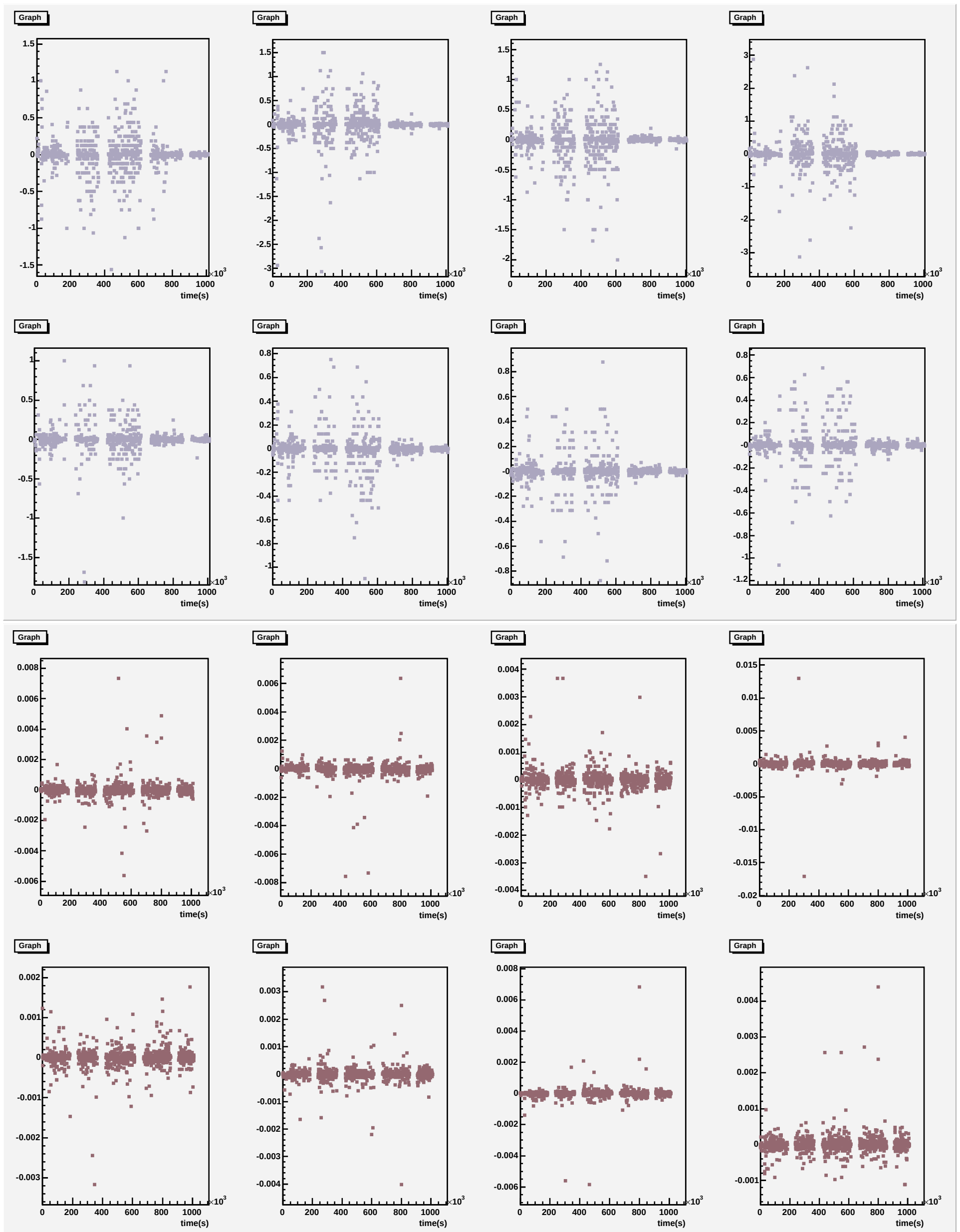

Figure 20: *Top*: Plots of $(Area_1 - Area_2)$ against time for all files and all temperatures, for the fitting region shown in Fig.17. *Bottom*: Plots of $Area_3$ against time for all files and all temperatures, for the same fitting region. Both figures show, from left to right, coils 1 to 4 at the top and coils 7 to 10 at the bottom.

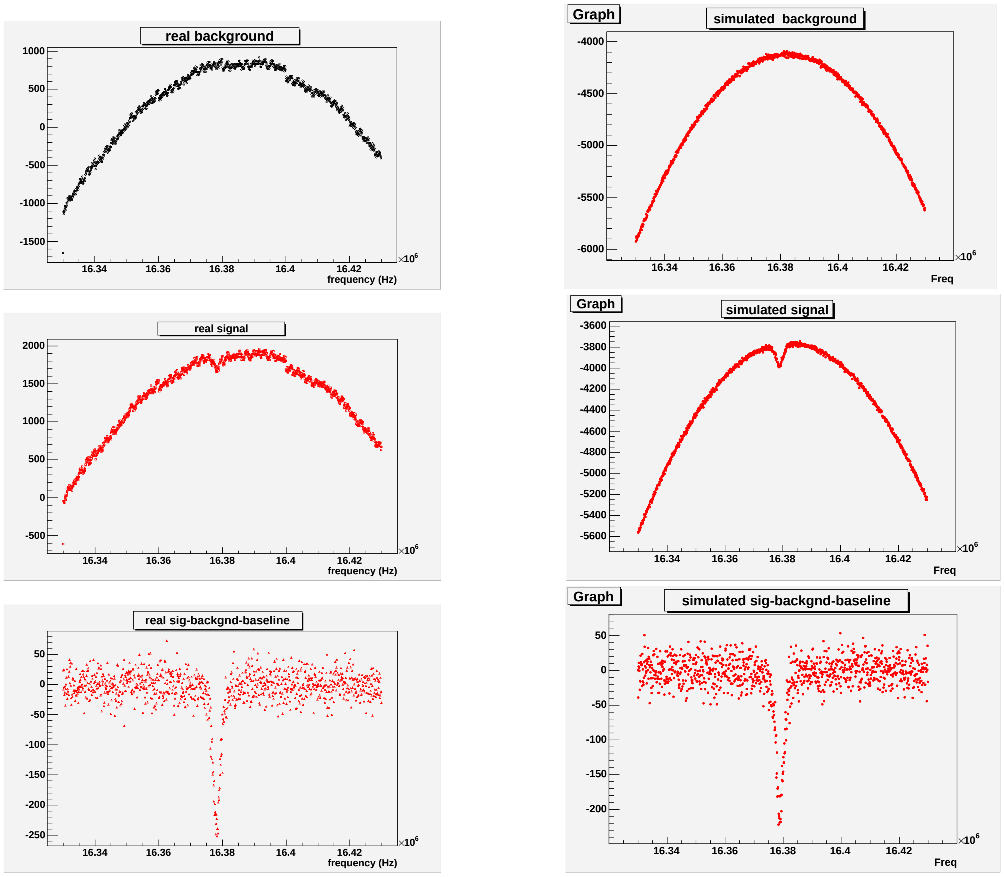

Figure 21: Comparison between real (*left*) and simulated (*right*) backgrounds, signals, and signal after subtraction of the background and baseline.

4.5 Simulation of the TE calibration analysis

Monte Carlo simulations can be useful to characterize the errors of parameter estimation in a very precise way. The idea was to use this to obtain an estimate of the error of the parameter C, the Curie constant. The process of simulating our set of TE signals, analyzing them and calculating the Curie constant from them, could be repeated many times to obtain a distribution of values of C. From this distribution, the error of our parameter C could be estimated considering a certain confidence region, i.e., a region that contains a certain percentage of the total probability distribution of Curie constants (see Ref. [2]).

A Monte Carlo random simulation was used to produce the TE signals and their backgrounds. The values of the parameters entered in the simulation were obtained from the real (measured) Q curves and signals. Figure 21 shows examples of some simulated signals, compared to the real ones.

Program simulTEsigs.C allowed to perform a certain number of simulations. In each simulation a number of signals where generated, and these were analyzed in the same way as if they were the real set of measured TE signals. The analysis method was that in section 3.7., using the values of the product ($Area \times Temperature$). One hundred baseline fits were calculated per signal file.

In each simulation, 201, 162, 249, 216, and 131 signals were generated respectively for each of the 5 calibration temperatures used in 2004. Each simulation took approximately 4 minutes and provided a value of the Curie constant with its error.

The Curie constants obtained from all simulations were entered into a histogram and plotted. A large number of simulations was needed in order for the histogram to follow a gaussian distribution. This histogram was fitted and an estimate of the error in the Curie constant was obtained from the sigma of the fitted gaussian curve, and also from the half width of the 68% confidence region.

A histogram of the Curie constants obtained from these simulations can be seen in Fig. 22. 345 full simulations were carried out using the following values of the parameters:

Parameters for the Q curve :

A $= -4.4 \times 10^7$;

Q $= 22.613$;

f0 $= 1.63821 \times 10^7$;

offset $= 82283.4$;

noise $= 13$;

Parameters for the NMR signal :

M2 $= 3 \times 10^6$;

M4 $= 4.5 \times 10^{13}$;

phase $= 0$;

f $= 1.63789 \times 10^7$;

h $= 1.5 \times 10^6$;

The estimated error of the Curie constant obtained from the 68% confidence region in the histogram was 0.27%, while that obtained from the fit to a gaussian was 0.26%.

Another program (simul1fit.C) was used for the simulations, that would calculate only one baseline fit per signal file, instead of calculating 100 fits. The fitting region used for these fits was that shown in figure 17.
The same parameters as before were used for the simulation. The results were similar to the ones obtained for 100 fits per file. For 500 simulations, the estimated error of

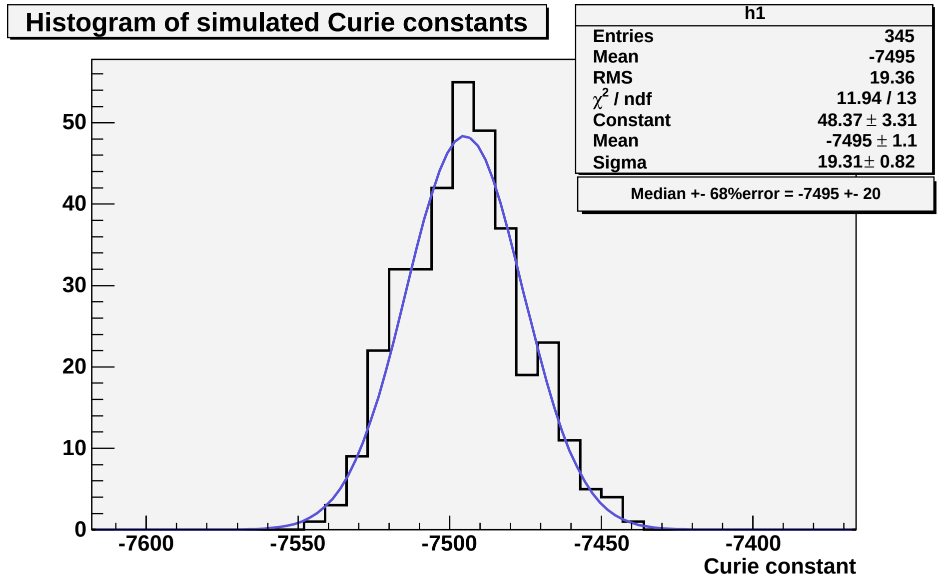

Figure 22: Histogram of all the values of the Curie constant obtained from the simulations. The fit to a gaussian is shown in blue. One hundred baseline fits were calculated for each generated signal.

the Curie constant obtained from the 68% confidence region in the histogram of all the simulated Curie constants was 0.24%, while that obtained from the fit to a gaussian was 0.23%. The histogram for this case can be seen in Fig. 23.

After this, the parameters of the simulation were changed to the following:

Parameters for the Q curve :

A $= -4.1875 \times 10^7$;

Q $= 22.613$;

f0 $= 1.63821 \times 10^7$;

offset $= 82283.4$;

noise $= 15$;

Parameters for the NMR signal :

M2 $= 2.5 \times 10^6$;

M4 $= 3.1 \times 10^{13}$;

phase $= 0$;

f $= 1.63791 \times 10^7$;

h $= 1.7 \times 10^6$;

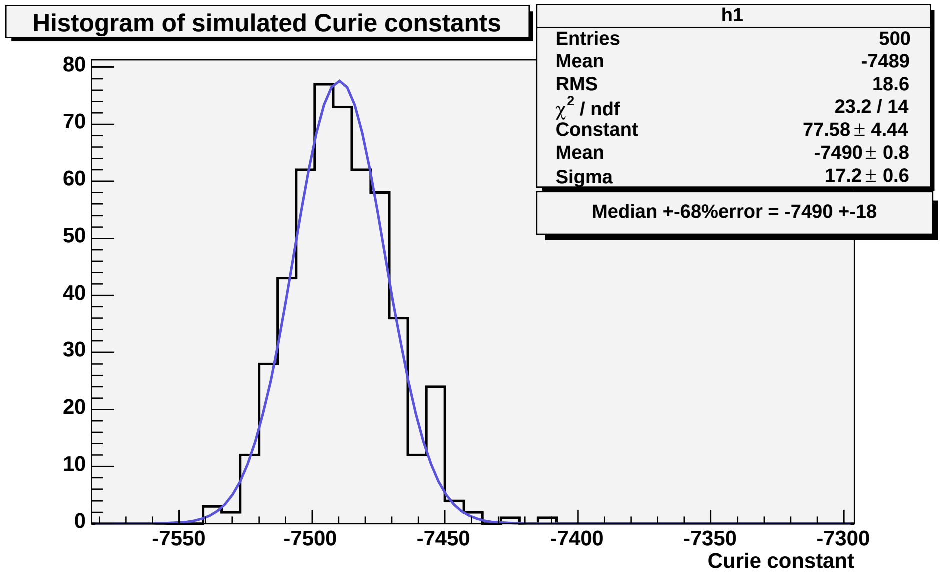

Figure 23: Histogram of all the values of the Curie constant obtained from the simulations. The fit to a gaussian is shown. Only one baseline fit was calculated for each generated signal.

500 simulations were carried out using only one baseline fit per generated signal. Results are shown in Fig. 24. The estimated error for the Curie constant was 0.26% from the half width of the 68% confidence region in the histogram of all simulated values of C, and 0.25% from the sigma of the gaussian fit.

Therefore, it can be said that the error estimated from the Monte Carlo simulation of the TE calibration analysis is between 0.23% and 0.27%.

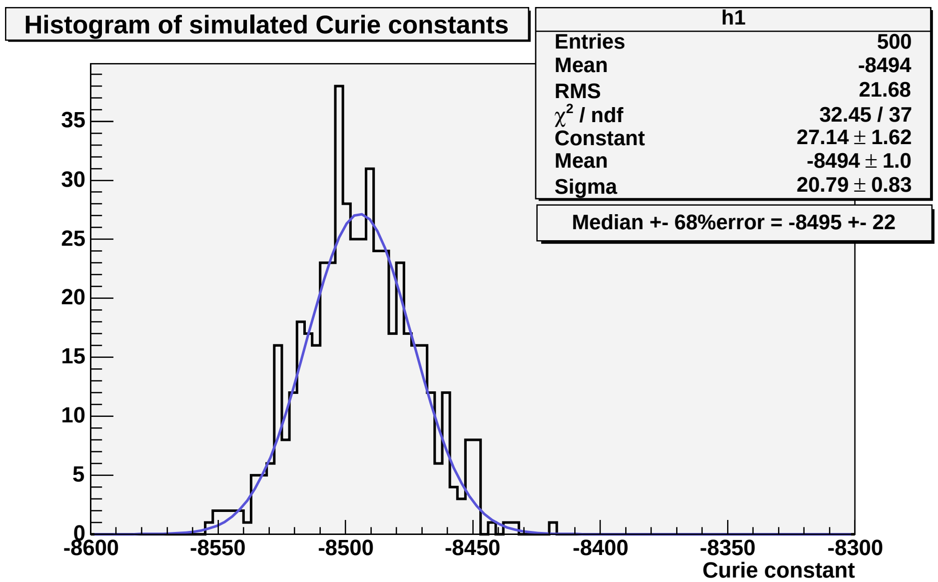

Figure 24: Histogram of all the values of the Curie constant obtained from the simulations (second set of parameters). The fit to a gaussian is shown. Only one baseline fit was calculated for each generated signal.

5 TE CALIBRATION RESULTS FOR THE NEW TEMPERATURES

The TE temperatures used in the previous sections were corrected by Jaakko, that provided the following new temperatures (see Ref. [8]):

$1.5068 \pm 0.0046K$
$1.2801 \pm 0.0025K$
$1.1716 \pm 0.0032K$
$0.9992 \pm 0.0053K$
$1.3159 \pm 0.0030K$

The analysis of all the 2004 TE signals was repeated using these new temperatures with their new uncertainties.
The data points that in the group of files TE2_1K produced a 'spike' in the plot of the areas against time were removed. This 'spike' was due to a problem with the magnet.

The new results calculated in the same way as in section 3.5, (using Curie fits, and 100 baseline fits per file), are shown in tables 33 and 34, for the 'Average method' and the 'Histogram method' respectively.
Results obtained using the new temperatures and the method described in section 3.7, (using the values of $Area \times Temperature$ and 100 baseline fits per file), can be seen in tables 35 and 36, for the 'Average method' and the 'Histogram method' respectively.

Results calculated using the procedure explained in section 4.3.2, (only one baseline fit per file), and the new temperatures are shown in tables 37 and 38, for calculations obtained from the Curie fits and for calculations using the values of $(Area \times Temperature)$, respectively.

New temperatures. Curie fits: 'Average method'.				
Coil no.	χ^2/ndf	$p0$	$p1$	% Error in $p1$
1	0.1090 / 4	0 ± 0	-8770 ± 276	3.1
2	0.1767 / 4	0 ± 0	-8698 ± 220	2.5
3	0.1579 / 4	0 ± 0	-6650 ± 255	3.8
4	0.1950 / 4	0 ± 0	-10250 ± 269	2.6
7	0.3525 / 4	0 ± 0	-9773 ± 191	2.0
8	0.3760 / 4	0 ± 0	-7837 ± 157	2.0
9	0.2508 / 4	0 ± 0	-7821 ± 162	2.1
10	0.08522 / 4	0 ± 0	-9036 ± 223	2.5

Table 33: Results from the Curie fits for the 'Average method'. The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$, where $p0$ was forced to be zero. The new temperatures were used.

New temperatures. Curie fits: 'Histogram method'.				
Coil no.	χ^2/ndf	$p0$	$p1$	% Error in $p1$
1	0.2539 / 4	0 ± 0	-8672 ± 288	3.3
2	0.3864 / 4	0 ± 0	-8664 ± 223	2.6
3	0.3357 / 4	0 ± 0	-6540 ± 232	3.5
4	0.3560 / 4	0 ± 0	-10270 ± 276	2.7
7	0.6348 / 4	0 ± 0	-9813 ± 189	1.9
8	1.741 / 4	0 ± 0	-7881 ± 166	2.1
9	0.4315 / 4	0 ± 0	-7880 ± 168	2.1
10	0.3742 / 4	0 ± 0	-9042 ± 202	2.2

Table 34: Results from the Curie fits for the 'histogram method' with Chi-square ± 85 selection. The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$, where $p0$ was forced to be zero. The new temperatures were used.

New temp. Using $Area \times Temperature$, Average method.				
coil	Median of selected values	← % error	mean ± sigma from gaussian fit of all values	← % error
1	-8742 ± 656	7.5	-8699 ± 836	9.6
2	-8676 ± 541	6.2	-8688 ± 727	8.4
3	-6598 ± 615	9.3	-6595 ± 783	11.9
4	-10224 ± 619	6.1	-10201 ± 803	7.9
7	-9747 ± 440	4.5	-9756 ± 574	5.9
8	-7797 ± 388	5.0	-7801 ± 490	6.3
9	-7816 ± 366	4.7	-7815 ± 474	6.1
10	-9042 ± 501	5.5	-9054 ± 636	7.0

Table 35: Curie constant C calculated from the values of *(Area.Temperature)* for the 'Average method'. The new temperatures were used.

New temp. Using $Area \times Temperature$, 'Histogram method'.				
coil	Median of selected values	← % error	mean ± sigma from gaussian fit of all values	← % error
1	-8664 ± 633	7.3	-8857 ± 848	9.6
2	-8653 ± 494	5.7	-8725 ± 687	7.9
3	-6551 ± 539	8.2	-6666 ± 638	9.6
4	-10247 ± 571	5.6	-10202 ± 561	5.5
7	-9783 ± 491	5.0	-9896 ± 491	5.0
8	-7803 ± 395	5.1	-7804 ± 533	6.8
9	-7818 ± 379	4.8	-7859 ± 468	6.0
10	-9055 ± 494	5.5	-9199 ± 663	7.2

Table 36: Curie constant C calculated from the values of $Area \times Temperature$ for the 'Histogram method'. The new temperatures were used.

New temperatures. 1 baseline. Curie fits.				
Coil no.	χ^2/ndf	$p0$	$p1$	% Error in $p1$
1	0.2459 / 4	0 ± 0	-8322 ± 257	3.1
2	0.1049 / 4	0 ± 0	-8313 ± 195	2.3
3	0.1598 / 4	0 ± 0	-6374 ± 238	3.7
4	0.1021 / 4	0 ± 0	-9840 ± 252	2.6
7	0.1728 / 4	0 ± 0	-9293 ± 135	1.5
8	0.1130 / 4	0 ± 0	-7463 ± 113	1.5
9	0.1192 / 4	0 ± 0	-7519 ± 102	1.4
10	0.1471 / 4	0 ± 0	-8692 ± 161	1.9

Table 37: Results from the Curie fits for the new temperatures. The TE area versus the inverse of the TE temperature was fitted to a line: $y = p0 + p1.x$, where $p0$ was forced to be zero. Only one baseline fit was calculated per signal file.

New temperatures. 1 baseline. Using $Area \times Temperature$.				
coil	Median of selected values	← % error	mean ± sigma from gaussian fit of all values	← % error
1	-8294 ± 470	5.7	-8307 ± 587	7.1
2	-8293 ± 335	4.0	-8299 ± 455	5.5
3	-6349 ± 446	7.0	-6343 ± 589	9.3
4	-9809 ± 447	4.6	-9805 ± 608	6.2
7	-9274 ± 245	2.6	-9280 ± 314	3.4
8	-7455 ± 207	2.8	-7461 ± 257	3.4
9	-7521 ± 177	2.4	-7517 ± 227	3.0
10	-8682 ± 277	3.2	-8673 ± 366	4.2

Table 38: Curie constant C calculated from the values of $Area \times Temperature$ for the new temperatures. Only one baseline fit per signal file was calculated.

6 POLARIZATION CALCULATION FOR 2004

6.1 Polarization plots

The dynamic polarization of the target can be obtained from the enhanced signals using the following equation:

$$Pol_{dyn} = Area_{dyn} \times \frac{gain \times tepol}{au \times ff} \tag{10}$$

where $Area_{dyn}$ can be obtained from integration of the dynamic signals, $gain$ is the gain factor used to amplify the TE signals, $tepol$ is the thermal equilibrium polarization at 1K, au is the calibration constant at positive field, and ff is the field factor that needs to be used in order to correct for negative magnetic field.

The gain factors should not be very different to the ones used in 2003, so the 2003 gain factors from Jaakko were used to produce this preliminary polarization plots.
The value of $tepol$ can be calculated analytically from the Brillouin function and corresponds to $Pol_{TE}(1K) = 0.0524078\%$.
The area unit, au, is obtained from the TE area at 1K, using the values of the Curie constants obtained from the TE calibration which are given in table 25 (third column). The following expression is used:

$$au = \frac{C}{T} \tag{11}$$

where C is the calculated Curie calibration constant for each coil and T is set to 1K.
The field correction factor ff was calculated by Kaori in 2004. Only when the magnetic field is negative the polarization is divided by this factor.
For the calculation of $Area_{dyn}$ only one baseline fit was calculated per signal file, with the fitting region excluding the first 5 and last 5 frequency channels and also the central frequency channels around the resonant peak, inside $f_0 \pm 40000Hz$. The fitting region chosen for the dynamic signals can be seen in figure 25.

Table 39 shows the values of $gain$, au and ff used to calculate the polarization for each coil.

The polarization for each coil from 18-May to 13-August 2004 is shown in figure 26, while the average polarization during the same period for upstream coils and downstream coils

coil	ff	au	$gain$
1	1.048503834	8687.5	212.80
2	0.973520494	8654.9	212.09
3	1.054143658	6575.2	211.33
4	0.972206203	10171.4	213.19
7	1.007100898	9737.9	213.33
8	1.006414195	7785.1	212.18
9	1.011273171	7799.5	211.61
10	1.006484725	9030.1	211.63

Table 39: Factors used to calculate the 2004 polarization.

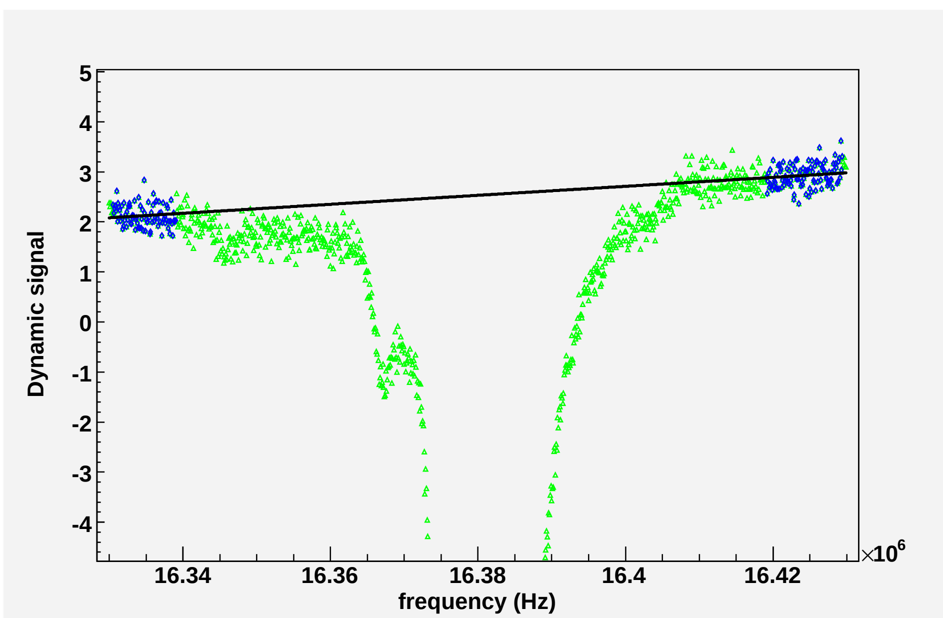

Figure 25: Selected fitting region for the only baseline calculated for each dynamic signal. The signal after subtraction of the background is shown in green while the selected points for the baseline fit are highlighted in blue. The first 5 and last 5 frequency channels are excluded.

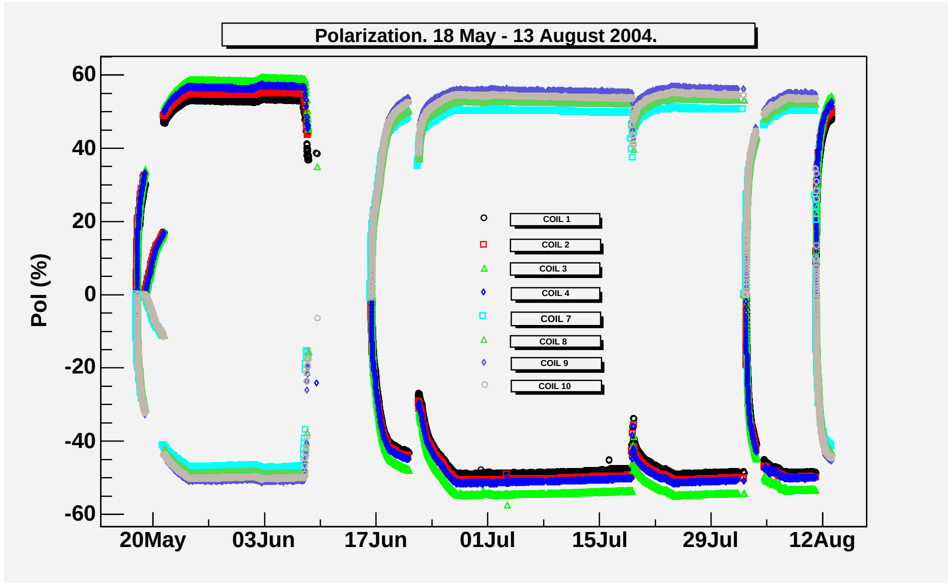

Figure 26: Polarization for each coil during the 2004 run: from 18 May to 13 August 2004. Upstream coils 1 to 4 are shown in black, red, green and blue, while downstream coils 7 to 10 are shown in turquoise, green, blue and grey.

respectively is shown in figure 27.

The average positive polarization during this period went up to around 56.2%, while the average negative polarization reached a maximum value of around 51.5%.

6.2 Test for the fitting region used for dynamic signals

Forty nine dynamic signals were chosen among a group of them showing a constant polarization value (frozen mode). These 49 signals were from 040628_000912.sig to 040628_125251.sig.

The value of the polarization for each of those files was calculated using two different procedures to obtain $Area_{dyn}$:

a) Calculating only one baseline fit per signal file, using a very narrow fitting region that excludes the first 5 and last 5 frequency channels as well as the region around the resonant peak, $f_0 \pm 40000Hz$. This fitting region is shown in Fig.25.

b) Calculating 100 baseline fits per signal, decreasing the width of the fitting region each time, the same way it was done for the TE signals (Histogram Method). The final value of the area was calculated from the most probable value in the histogram of

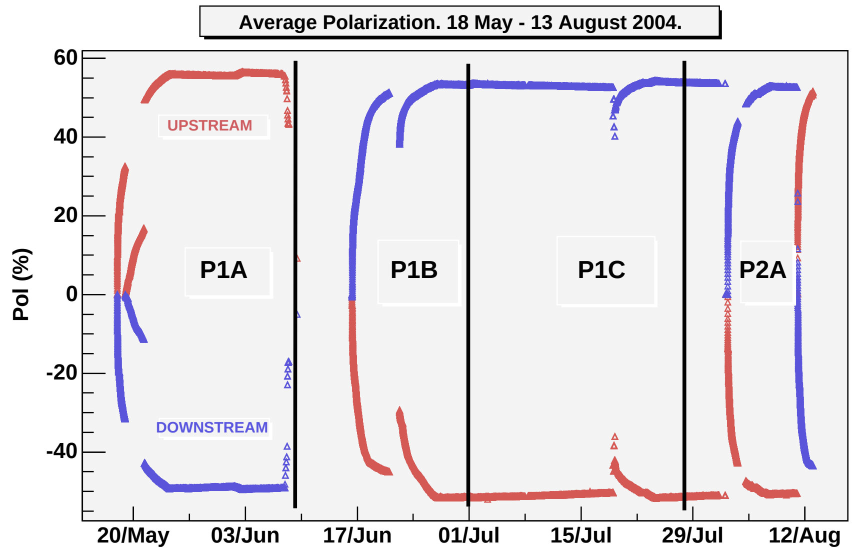

Figure 27: Average polarization during the 2004 run: from 18 May to 13 August 2004. The average of upstream coils is shown in red, while that of the downstream coils is shown in blue.

all the 100 areas calculated from each of the 100 baseline fits.

The values of the polarization obtained from these two procedures were plotted against time and fitted to a constant coil by coil, in order to compare results from **a)** and **b)**. Figure 28 shows the fits of the polarization for the **upstream** coils 1 to 4 for method **a)**, (1 fit, narrow region), on the left, while the graph on the right shows the same for method **b)**, (100 fits).
Figure 29 shows the fits of the polarization for the **downstream** coils 7 to 10 for method **a)**, (1 fit, narrow region), on the left, while the graph on the right shows the same for method **b)**, (100 fits).
Table 40 shows the results of those fits to a constant and the ration between the constants obtained from **b)** and **a)**. In principle, the selected region for the baseline fit should be the same for TE signals and for dynamic signals. These ratios could be used to calibrate the results obtained for the enhanced signals using only one baseline fit. However, it can be seen that the difference between both procedures is around 0.2%, which is quite small.

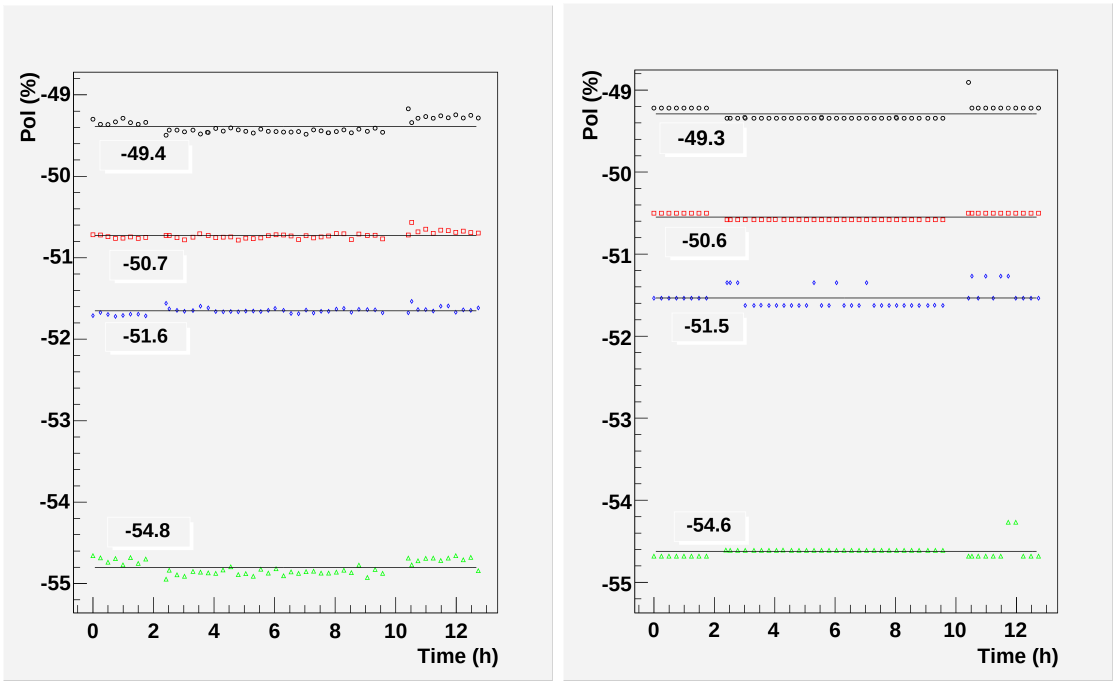

Figure 28: *Left*: Polarization against time for **upstream** coils, for procedure **a)**, that calculates only one baseline with the fitting region shown in Fig.25. *Right*: Polarization vs. time for **upstream** coils calculating 100 fits per file, as in the Histogram method for the TE analysis (procedure **b)**). Coils 1 to 4 are shown in black, red, green and blue respectively. The fits of the polarization to a constant are shown (black line).

coil	**a** (1 narrow fit)	**b** (100 fits)	**ratio b/a**
1	-49.4	-49.3	0.99798
2	-50.7	-50.6	0.99803
3	-54.8	-54.6	0.99635
4	-51.6	-51.5	0.99806
7	50.5	50.4	0.99802
8	52.9	52.7	0.99622
9	55.7	55.6	0.99820
10	54.5	54.3	0.99633

Table 40: Results of the fits of the polarization to a constant for both procedures **a)** and **b)**. The last column gives the ratio of both values.

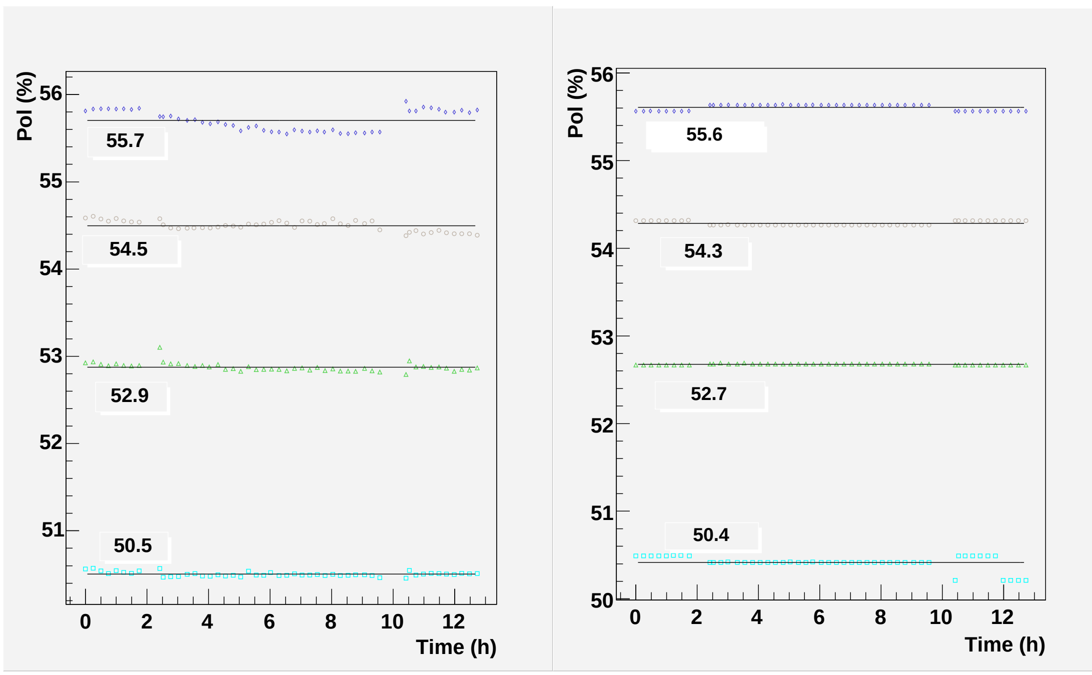

Figure 29: *Left*: Polarization against time for **downstream** coils, for procedure **a)**, that calculates only one baseline with the fitting region shown in Fig.25. *Right*: Polarization vs. time for **downstream** coils calculating 100 fits per file, as in the Histogram method for the TE analysis (procedure **b)**). Coils 7 to 10 are shown in turquoise, green, blue and brown respectively. The fits of the polarization to a constant are shown (black line).

7 LIST OF PROGRAMS USED

do-te.C Automatic TE calibration program with n different baselines. Raw integration to calculate area. Final area calculated from the average of all areas. Fitting regions: section 3.2., Case 1.

do-tebis.C Automatic TE calibration program with n different baselines. Raw integration to calculate area. Final area calculated from the average of all areas. Fitting regions: section 3.2., Case 2.

do-teHist.C Automatic TE calibration program with n different baselines. Raw integration to calculate area. Final area calculated from the most probable value in the histogram of ALL areas. Plots the histograms if enabled to do it. Fitting regions can be modified by input. (Refer to section 3.3.1.).

do-techi.C Automatic TE calibration program with n different baselines. Raw integration to calculate area. Area value rejected if it comes from a baseline fit with a Chi-square/ndf too high (outside the confidence limits). Final area calculated from the most probable value in the histogram of all ACCEPTED areas. Produces 3 canvas: c1: histograms of selected areas, c2: histograms of chisquare/ndf values, and c3: chisq/ndf vs fitnumber. (Refer to section 3.3.2.).

tebestarea.C Automatic TE calibration program with n different baselines. Raw integration to calculate area. Final area is the one coming from the fit having the lowest Chi-square/ndf. No histograms used. (Refer to section 3.3.3.).

areatimerobust.C Generates 4 canvases. Plots TE area vs time for each coil to check stability (canvas c1). Fits the resulting graphs to a constant to find final area (optional). Outputs the final area and its error from those fits (optional). Plots the histogram of ALL areas (canvas c2). Performs robust fitting to try and ignore bad points. Median is the constant: finds the median of ALL areas and outputs it (optional). In histogram of all areas, only areas between certain quantiles are selected: Plots SELECTED TE areas vs time for each coil (canvas c3). Fits the resulting graphs to a constant to find new final area (optional). Outputs new area and new error for those fits (optional). Plots histograms of SELECTED areas between quantiles (canvas c4). Finds the new median and outputs it. Output file can contain for each coil (what you chose from): coil number, area coming from the fits of all areas to a constant, its error, median for all areas, area coming from the fits of selected areas, its error, median for selected areas only. (Refer to section 3.1).

curie.C Fits to Curie Law. TE Area is proportional to TE polarization. Outputs no file. Plots the final TE area corresponding to each TE temperature against the inverse of temperature, and fits the points to a line. (Refer to section 3.5).

tegraf.C Plots signal, background, signal minus background, region selected for baseline fit, baseline, and signal minus background minus baseline FOR EACH COIL. No output file. You enter what to plot as input.

tegraf2.C Plots different baseline fits, to compare them, for one coil only. Plots signal, background, signal minus background, region selected for baseline fit, baseline, and signal minus background minus baseline FOR ONE COIL ONLY. No output file. You choose what to plot (enter as input).

todo.C Plots the values of the product $Area \times Temperature$ for all files and all temperature from 2004. Enters them into a histogram, selects the ones between the 9% and 91% probability quantiles, and then finds the median of the selected ones. Error is given as the half width of the 68% probability region. Also gives mean +- sigma from fit to a gaussian.

simulTEsigs.C Simulates TE signals (background and signal)(Monte Carlo), and performs the same analysis that was done for the real signals.Calculates the Curie constant for each simulation, using the values of Area.Temp. Parameters for the simulation are in MCTE04params. 100 baseline fits are calculated for each signal file.

simul1fit.C The same as the previous program but only 1 baseline fit is calculated for each signal file.

allc.C Plots all the simulated Curie constants, C, in a histogram, to calculate error and final value. It gives mean and sigma from fit to a gaussian and the median and 68% error.

super.C Makes a super TE signal by averaging all the Area.Temp values for all files and temperatures. Outputs the supersignal in a file, for each coil and frequency.

superplot.C Plots the supersignal (or signal) and fits the off-resonance region to a line and to a parabola.

plotTEsig.C Takes a supersignal (or signal) (with background and baseline already subtracted), fits the off-resonance region to a parabola and subtracts it, and finally fits the result to the memory function to obtain the central frequency f0, the moments M2, M4, and the scaling factor A. Finds the area from the raw signal and from the fit to the memory function.

disp_baseline.C Allows to check the parameters of the Q curve: A, Q, f0, offset, and noise.

areatimerobust2.C Finds the median of ALL the calculated TE areas, without selecting or removing any points.

do-tebis2.C Same as do-tebis.C but excludes the first 100 channels and the last 100 channels from the baseline fits. Therefore, the edges are never used for the baseline fits.

calculos.C Finds the area under the selected points in the fitting region for the baseline. Finds the area under the fitted baseline in that region. Outputs the difference of both areas. Outputs also the area under the selected points after the baseline has been subtracted. The fitting region for the baseline excludes the fist 100 and last 100 frequency channels.

calculos2.C Calculates the same as calculos.C but the fitting region for the baseline includes all the first and last frequency channels.

plotcalculos.C Plots the results of calculos.C or calculos2.C in two canvasses.

curie2003.C Same as curie.C but for TE calibration data from 2003.

curienew.C Same as curie.C but using the corrected new temperatures given by Jaakko, and having removed the spike from TE2_1K.

todonew.C Same as todo.C but using the corrected new temperatures given by Jaakko, and having removed the spike from TE2_1K.

disp_polfxc04.C Calculates the polarization (in %) for the dynamic signals in 2004. Calculates only one baseline per file, excluding the first 5 and last 5 frequency channels and using fwin = 40000 Hz. Uses gain factors from 2003, ff from kaori 2004, au from TE calibration 2004. Input is a listfile. Output is a file with the polarization for each coil.

mydisppolpm04.C Plots the polarization calculated by disp_polfxc04.C for each coil.

averagepol04.C Calculates the average polarization (for 2004) from upstream coils 1 to 4, and the same for downstream coils 7 to 10. Input is a file with the polarization from each coil. Output is a file with the average polarization for up and downstream.

plotaverage04.C Plots the average polarization for upstream and downstream coils, for 2004.

do-tebisenhanced.C The same as do-tebis.C but excluding the first 5 and last 5 frequency channels.

polkaori.C Calculates the polarization using 100 baseline fits per dynamic signal (including first and last channels), and selecting the most probable area in the histogram of all the areas obtained from each baseline. The polarization is then obtained correcting with ff, au, tepol, and gain. It basically does the same as the histogram method did with the TE signals, and then calculates the polarization. Inputs a listfile, outputs a file with the polarization for each coil.

testparabolefit.C TE calibration program with only ONE baseline fit. First performs linear fit to get baseline and calculates area from it. Then performs parabolic fit to get baseline and calculates area. Raw integration to calculate area. Compares area obtained using linear and parabolic baseline, and plots their percentage difference.

References

[1] K. Kondo et al. *Polarization measurement in the COMPASS polarized target.* Nucl. Instr. and Meth. In Phys. Rev. A. **526** (2004) 70-75.

[2] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery. *Numerical Recipes in C++. The art of scientific computing. Chapter 15.7. Robust Estimation; Chapter 15.6. Monte Carlo simulations and confidence limits.*

[3] Jaakko Koivuniemi provided these temperatures from his calculations.

[4] F. Pobell, *Matter and methods at low temperatures*, Springer-Verlag Berlin Heidelberg (1996).

[5] Root User's Guide 3.05. June 2003.

[6] M. Mehring and V. A. Weberuub. *Object-Oriented Magnetic Resonance. Chapter 7. Section 7.2.3.3. IV. The memory function approach.*

[7] J. Koivuniemi et al. *NMR line shapes in highly polarized large* $^6Litargetat2.5T.$. Nucl. Instr. and Meth. In Phys. Rev. A. **526** (2004) 100-104.

[8] J. Koivuniemi et al. *Thermal equilibrium temperature 2004.* COMPASS Note 2004-X, 17 August 2004. (http://wwwcompass.cern.ch/compass/notes/2004-X/2004-X.ps).

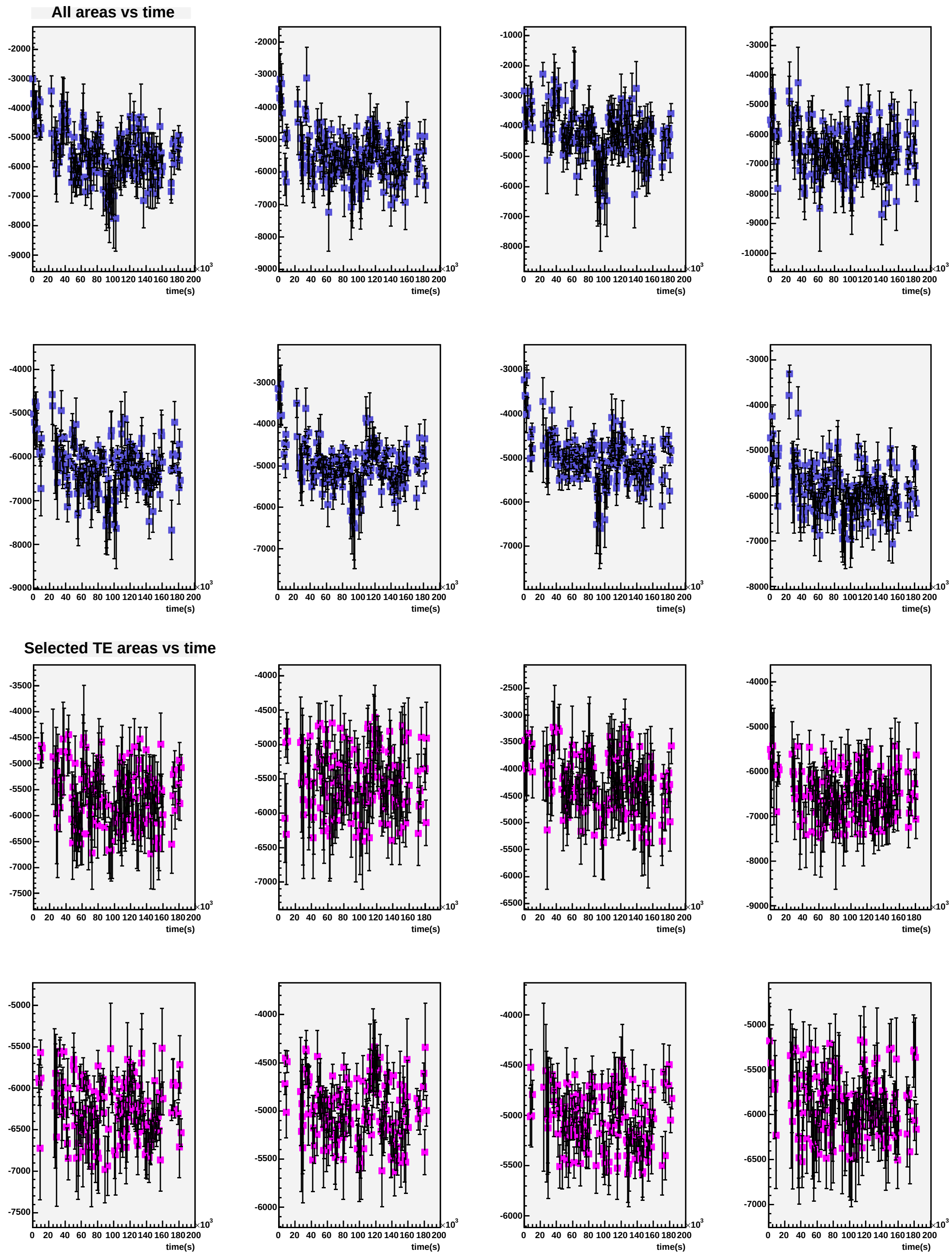

Figure 30: For the group of files TE1K5. *Top*: plots of all the calculated TE areas against time for the 'Average method' in section 3.5. *Bottom*: selected areas against time. Each graph shows coil 1 to 4 at the top and coils 7 to 10 at the bottom.

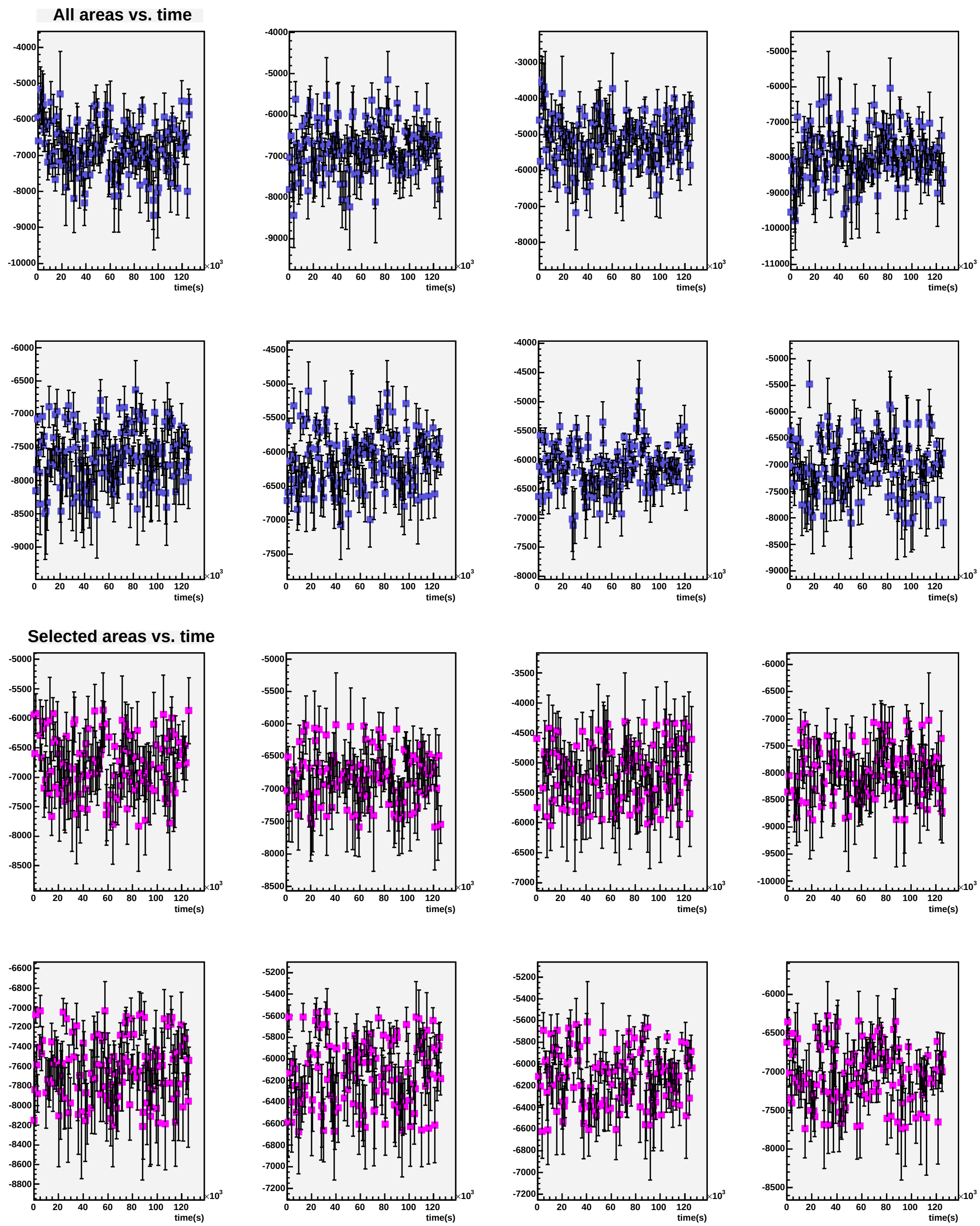

Figure 31: For the group of files TE1K2. *Top*: plots of all the calculated TE areas against time for the 'Average method' in section 3.5. *Bottom*: selected areas against time. Each graph shows coil 1 to 4 at the top and coils 7 to 10 at the bottom.

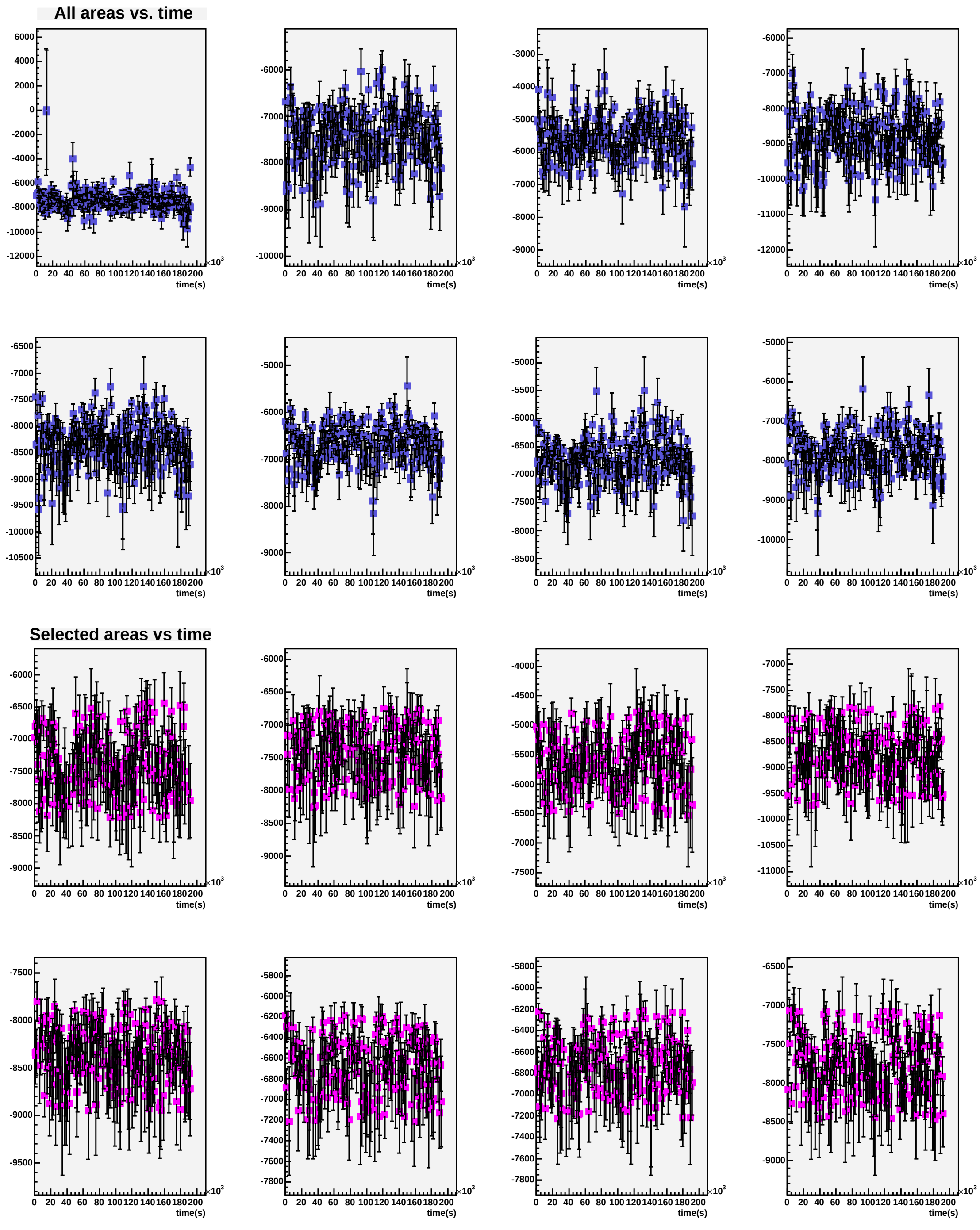

Figure 32: For the group of files TE1K. *Top*: plots of all the calculated TE areas against time for the 'Average method' in section 3.5. *Bottom*: selected areas against time. Each graph shows coil 1 to 4 at the top and coils 7 to 10 at the bottom.

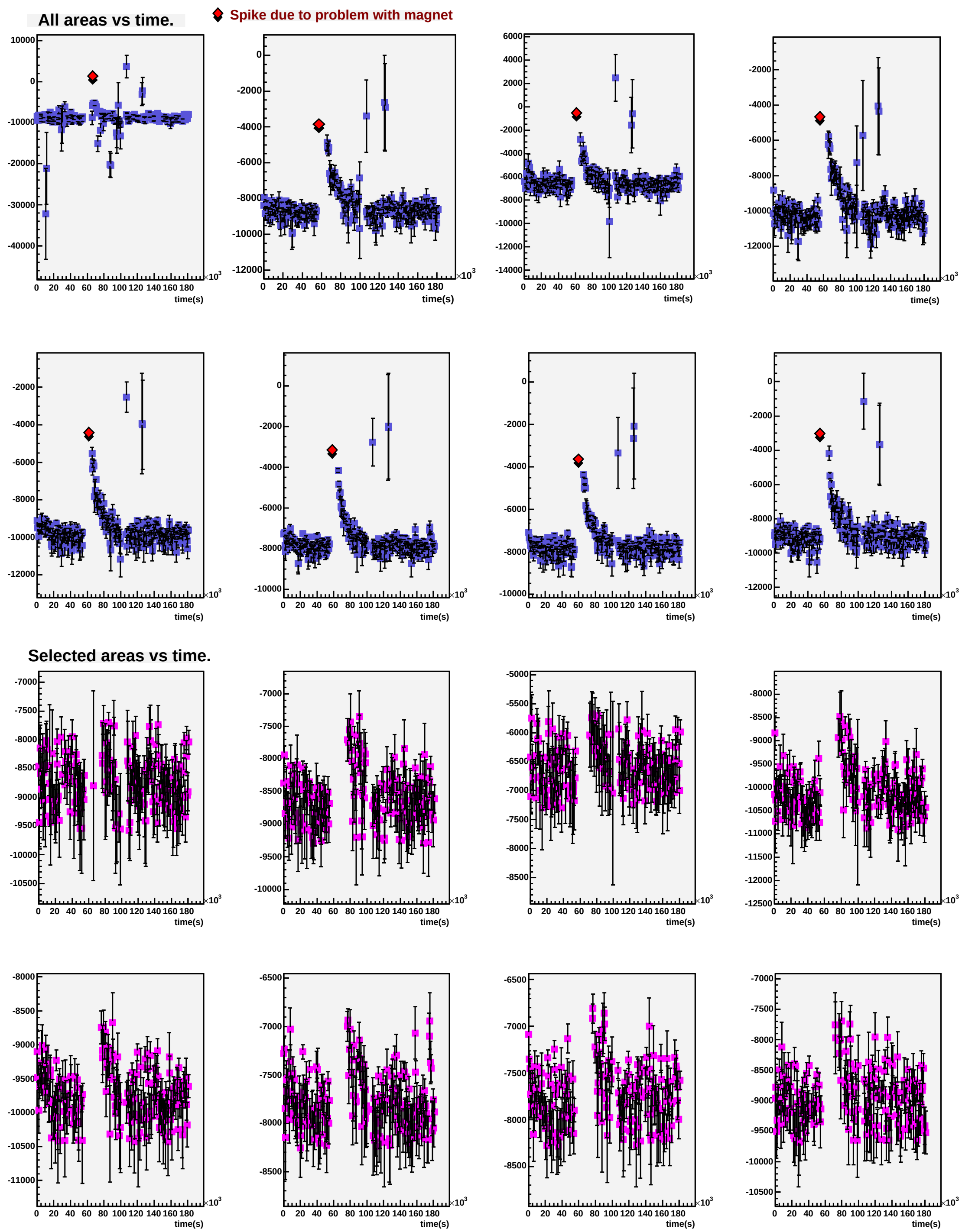

Figure 33: For the group of files TE2_1K. Note the spike due to a problem with the magnet. *Top*: plots of all the calculated TE areas against time for the 'Average method' in section 3.5. *Bottom*: selected areas against time. Each graph shows coil 1 to 4 at the top and coils 7 to 10 at the bottom.

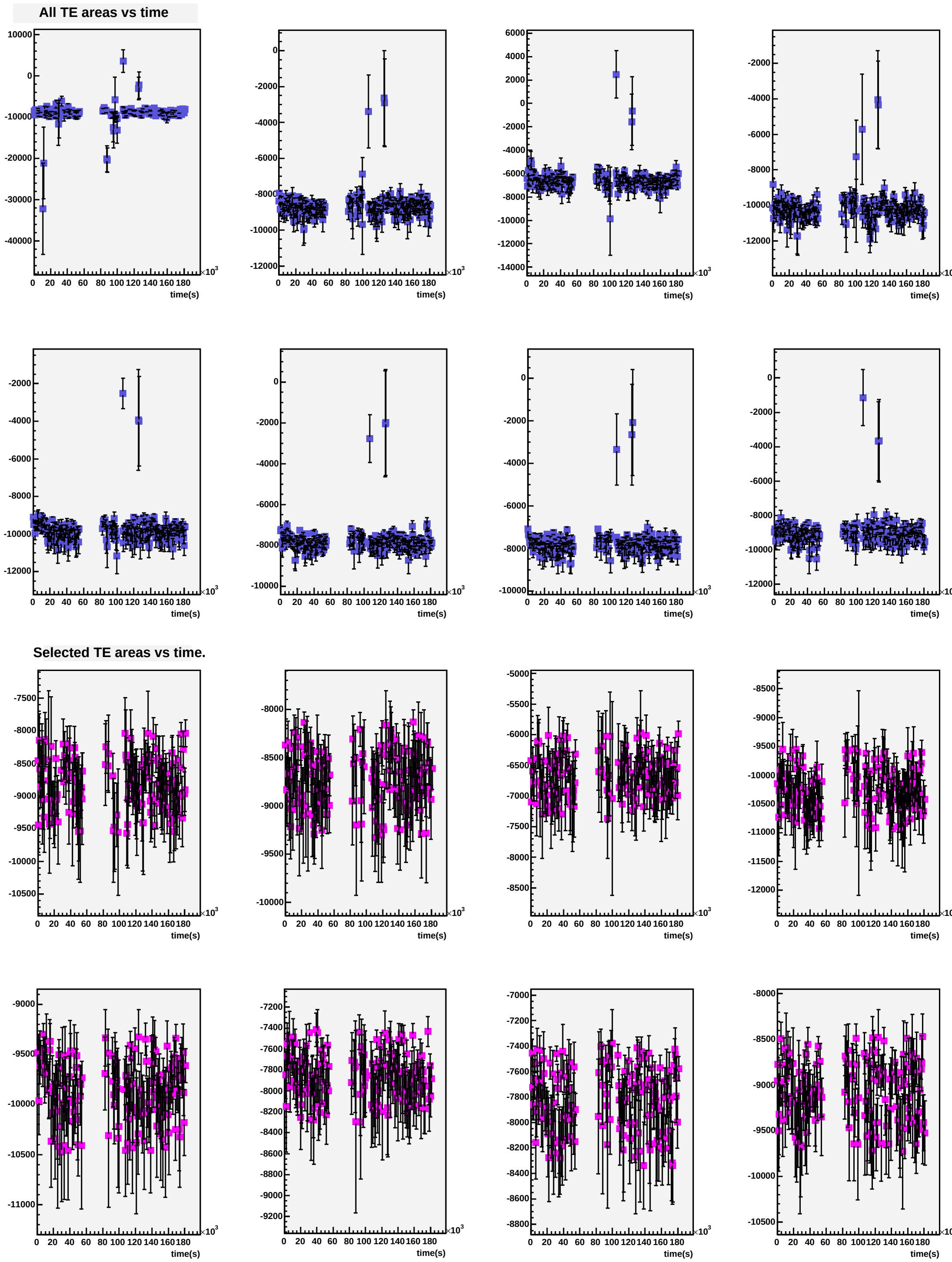

Figure 34: For the group of files TE2_1K. The spike seen in Fig. 33 has been removed. *Top*: plots of all the calculated TE areas against time for the 'Average method' in section 3.5. *Bottom*: selected areas against time. Each graph shows coil 1 to 4 at the top and coils 7 to 10 at the bottom.

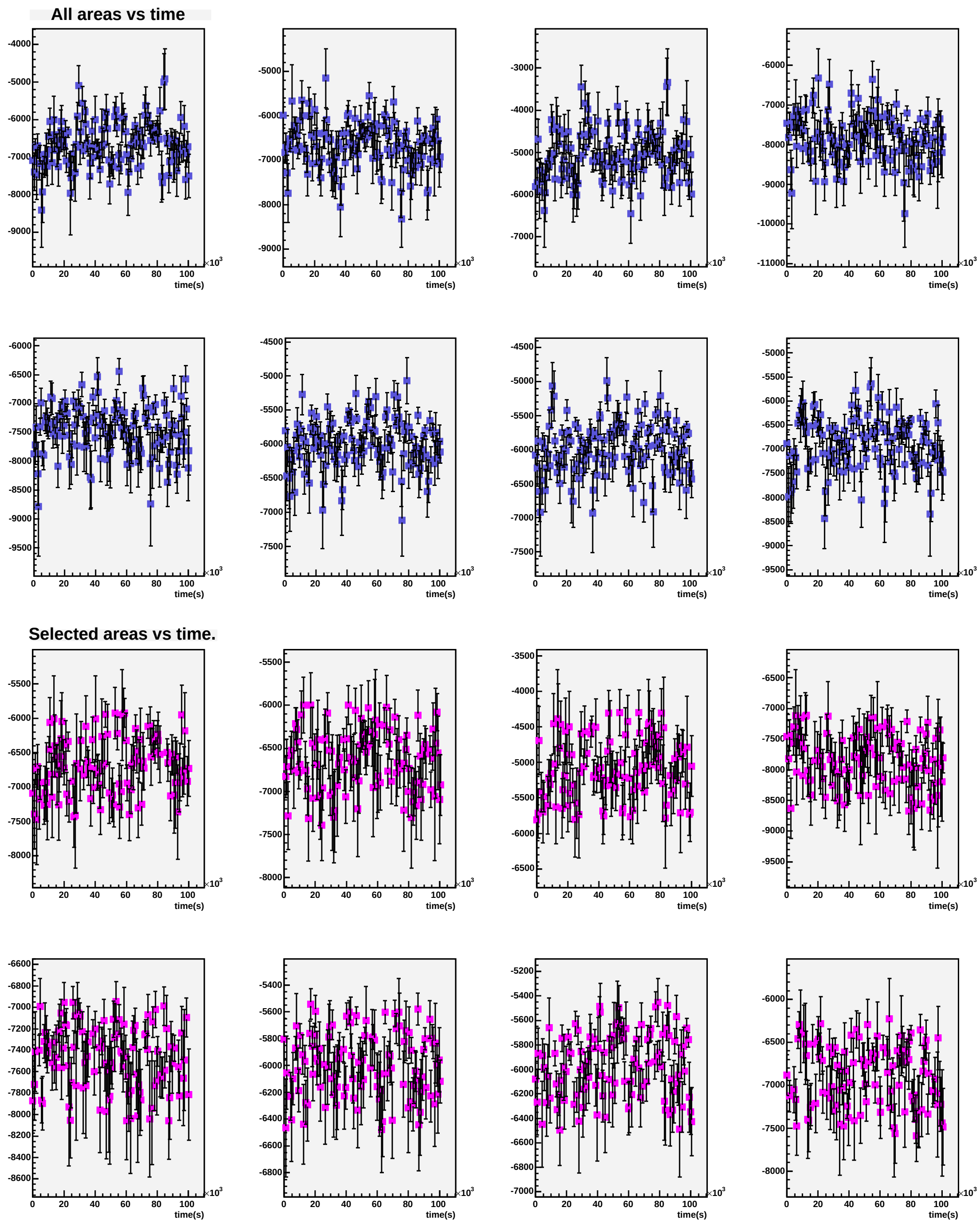

Figure 35: For the group of files TE2_1K3. *Top*: plots of all the calculated TE areas against time for the 'Average method' in section 3.5. *Bottom*: selected areas against time. Each graph shows coil 1 to 4 at the top and coils 7 to 10 at the bottom.