NMR data analysis

My task in the COMPASS polarized target group was to analyze the NMR signals from the year 2003. After learning the basics of Linux operating system, a bit of C++ programming language, a bit of the program Root, and the basics of Latex, I started analyzing the signals.

The process that leads to the analysis of NMR signals has been already explained in the previous section. This analysis was carried out with the aid of some C++ programs (disp_polfxc.C, mydisp_enh1.C). These programs basically work taking the raw NMR data files for a certain period of time as the input, and producing an output file that contains the time and the polarization (in %) for each of the 9 coils in the target cells. It must be pointed out that coil number 5 does not exist. These programs include the background subtraction, baseline fit, baseline subtraction and area calculation mentioned in the previous section. Several modifications were introduced to this programs in order to improve their performance. They will be discussed in the following paragraphs.

Correction with calibration constants was introduced in order to get the correct value for the polarization. The polarization,(Pol), is obtained from the integrated area, ($Area$), of the NMR signal:

$$Pol = \frac{Area \times gain \times tepol}{au \times ff} \tag{1}$$

where $gain$ is the gain factor corresponding to the ratio of DC amplification of the TE signal measurement to that of the enhanced signal measurement, $tepol = 0.0524078\%$ is the thermal equilibrium polarization at 1K, au is the calibration constant measured at positive field (area unit), and ff is the field correction factor used to calibrate negative field measurements. The values of these parameters are characteristic of each NMR channel and are given in table 1.

The program was modified so that the magnet current could be read from the input NMR data files, and corrections could be introduced to the value of the polarization in case the magnet current was found to be negative. It was checked that it is the negative magnetic field data that should be corrected with the field factor and not the positive magnetic field data. It was also checked that the correction by the field factor should be done dividing by it, and not multiplying by it. The program was made to write a $'+'/'-'$ flag to the end of each line after calculating the polarization to distinguish between positive and negative magnetic field polarization data.

The calculation of the Unix time in seconds from the input files was corrected, since writing: $date--date='2003-4-30-23:00:00CET'$ in the command line gives: Thu May 1 00:00:00 CEST 2003, writing: $date--date='2003-4-30-23:00:00CET'+\%s$ gives: 1051740000 (unix time in seconds), and writing: $date--date='2003-5-0100:$

$00:00 CET'$ gives: Thu May 1 01:00:00 CEST 2003. (See program disp_polfxc.C)

The NMR signal has its resonant frequency at 16381800 Hz. The frequency window of the NMR signal is 100000 Hz (from 16330000 Hz to 16430000 Hz). The baseline is obtained by fitting a straight line to the off-resonance region of the signal. It was found that the optimum width of the off-resonance region selected for the baseline fit was from 16330000 Hz to 16341800 Hz, to the left of the resonant peak, and from 16421800 Hz to 16430000 Hz, to the right of the resonant peak. Making this selected region wider makes things worse, as it can be seen in figure 1.

Once the programs were ready, the data analysis started. Five cdroms containing NMR data from 2003 were provided. This NMR data was taken as the input for the programs, producing output files with the time and polarization for each coil. Some of the data points in these files had to be eliminated manually, the reason being that their value was far too high or too low, (caused by PAR error), meaning that they would interfere with any fit performed on all the data points.

First of all the polarization for the 2003 **pre-run** period is plotted in figure 2. The pre-run period starts on 2003-May-13$^{\text{th}}$ and goes on until 2003-June-10$^{\text{th}}$.
The polarization for the 2003 **run** period is shown in figure 3. This period goes from 2003-June-11$^{\text{th}}$ to 2003-July-16$^{\text{th}}$.
In figures 2 and 3, the upstream average polarization for coils 1 to 4 is shown in red, while the downstream average polarization for coils 6 to 10 is shown in blue. Upstream and downstream polarizations were calculated from the average value of the polarization for coils 1 to 4 and from that of coils 6 to 10, respectively. (Programs averagepol.C and plotaverage.C were written to calculate and plot the average polarization values.) The polarization points in both figures contain data from several cdroms, as detailed in the following paragraphs.

The first cdrom contained NMR data from 2003-June-24$^{\text{th}}$ to 2003-July-10$^{\text{th}}$ (data files from 030624_025111.bgr to 030710_120145.sig). The list-file containing only the names of these files is 'nmrlist'. After the program disp_polfxc.C was run using 'nmrlist' as the input file, the file 'nmrlistk2' was produced containing one column with the time in Unix seconds, and ten more columns with the polarization of each of the 10 NMR coils. (Data removed manually from this file were: from 1056590063 to 1056591808; 1057453986; 1057594342; from 1057821509 to 1057823484; all in Unix time seconds). The data points in the resulting file 'nmrlistk2' were plotted with the program mydisp-polpm.C. This program plots both the positive and negative magnet current data. The resulting graph can be seen in figure 4.

The second cdrom contained NMR data from 2003-May-13$^{\text{th}}$ to 2003-May-23$^{\text{rd}}$ (files from

030513_185400.bgr to 030523_155043.sig). The list-file containing only the names of these files is 'nmrlistcd2'. After the program disp_polfxc.C was run using 'nmrlistcd2' as the input file, the produced output file giving the polarization was 'nmrlistcd2bisbis' (Files 030514_001119.sig (2003-May-14th; 00:11:19 CET) and 030515_185418.sig (2003-May-15th; 18:54:18 CET) were not used because they had no magnet current value written at the end of the file. Data deleted manually from this file were: the beginning and end of the file; 1053000805; 1053001526; from 1053011351 to 1053016933; 1052930495; 1052982920; 1052986227; all in Unix time seconds). The data points in the resulting file 'nmrlistcd2bisbis' were plotted with the program mydisppolpm.C. The resulting graph can be seen in figure 5.
Exponential fits were performed on these data in order to calculate the polarization build-up time. The exponential functions were: $p2 + exp(p0 + p1 \cdot x)$ for coils 1 to 4, and $p2 - exp(p0 + p1 \cdot x)$ for coils 6 to 10. The resulting parameters p0, p1 and p2 from the fits are given in table 2. Figure 6 shows the fits graphically. The calculated polarization build-up time for May 2003 data (from 2003-May-13 to 2003-May-23) is given in table 3. It can be seen that negative polarization has a shorter build-up time than positive polarization. Also, the difference in build-up time among all positive coils (1 to 4) and among all negative coils (6 to 10) is not high. For the positive coils the average build-up time is 54.7 hours, and the highest deviation from this mean value is of 5%. For the negative coils, the average build-up time is 47.5, and the highest deviation from it is 4%.

The third cdrom contained NMR data from 2003-June-14th to 2003-June-20th(files from 030614_000003.sig to 030620_235805.sig). The list-file containing only the names of these files is 'nmrlistcd3'. The background file 030616_102828.bgr (2003-June-16th; 10:28:28 CET) was added to the beginning of this list-file. (Data point 1056032629 in Unix time seconds was manually removed). The program disp_polfxc.C was run entering 'nmrlistcd3' as the input file, and the produced output file giving the polarization was 'nmrlistcd3bis'. A plot of these data points can be seen on figure 7.

The fourth cdrom contained data from 2003-June-21st to 2003-July-16th (files from 030621_000006.sig to 030716_235911.sig). The corresponding list-file is 'nmrlistcd4', and the polarization file that the program disp_polfxc.C outputs is 'nmrlistcd4bis'. The background file 030620_185505.bgr (2003-June-20th; 18:55:05 CET) from the previous cdrom was added to the beginning of this list-file. (Data points manually removed were: 1056318288; from 1056348336 to 1056350159; from 1056590063 to 1056591808; from 1057821509 to 1057823484; 1056386693; 1057594342; 1058249538; all in Unix time seconds). A plot of the polarization during this period can be seen on figure 8. Note that this period includes that on the first cdrom.

The beginning of 'nmrlistcd4bis' was put together with the end of 'nmrlistcd3bis' in order to study the polarization build-up in June 2003. Figure 9 shows this graphically.

Exponential fits were made in the same way as for the polarization build-up for May 2003 data, and the results can be seen in table 4. Note that negative polarization has again shorter build-up time than positive polarization. Also polarization build-up is faster for June 2003 data than from May 2003 data. The difference in build-up time among all positive coils (1 to 4) and among all negative coils (6 to 10) is not high. For the positive coils the average build-up time is 44.7 hours, and the highest deviation from this mean value is of 3%. For all the negative coils except coil 6, the average build-up time is 41.8 hours, and the highest deviation from this value is 2%. From the inverse of the fitting parameter p1, the polarization build-up time was calculated for each coil. Results of these calculations are shown in table 5.

Most of the polarization points in 'nmrlistcd4bis' except some at the beginning and at the end of the file were used to study the nuclear polarization decay in time. This made a period about 450 hours long, nearly 19 days long. It is illustrating as an example to mention that at the beginning of this period, the polarization for coil 1 was around 57.5%, while that at the end of the period was around 56.5%. Also for the negative coil 7, the polarization was around -48% at the beginning of the period, and around -47% at the end of the period.
The data corresponding to each coil were fitted to an exponential line. Exponential functions were: exp(p0+p1.x) for coils 1 to 4, and -exp(p0+p1.x) for coils 6 to 10. From the inverse of the parameter p1, the polarization decay time and its error were calculated. This calculations were first done using all polarization data points: those corresponding to positive magnet current as well as those corresponding to negative current. Then the same fits and calculations were carried out using exclusively positive magnet current data or negative current data. The resulting parameters from these fittings are shown in table 6. Table 7 shows the results of the polarization decay time calculations. Note that negative polarization decays faster than positive polarization. Also note that for coil 6 the decay time is shorter than for the rest of the negative coils. Coil 6 is placed inside the target material, while the rest of the coils are placed outside. Figure 10 shows some graphs where the exponential decay of nuclear polarization can be seen, including the exponential fits.

The fifth cdrom contained NMR data from 2003-May-26$^{\text{th}}$ to 2003-June-13$^{\text{th}}$. The list-files containing only the names of these files are 'quinto' and 'sexta'. The program disp_polfxc.C was run entering both list-files as the input file, and the produced output files giving the polarization were 'quintobis' and 'sextabis', respectively.