The first NMR experiment

August 23, 2011

1 Relaxation time calculation results

During the results processing the following relaxation times were calculated: T_1, T_2, T_2^* moreover gyromagnetic ratio constant γ. We will cover up shortly the calculation process for each one of them:

- firstly, the gyromagnetic ratio was calculated out of the given experiment data, after ω_o (the Larmor percession frequency) was found by the following formula: $\gamma = \frac{\omega_0}{B_0}$
- then, out of FID decay slope (after single $\frac{\pi}{2}$ pulse) T_2^*value was evaluated, by detecting the FID peak and fitting the exponential curve
- next, T_1 was calculated by fitting the results of inversion recovery experiment into the curve of $M_{\perp}(T_I) = \left|M_0\left(1 - 2e^{-T_I/T_1}\right)\right|$ and ignoring the T_2^* influence
- at last T_2 was found out of two experiment datasets (CP and CPMG) by finding the points on the signal envelope, calculating the logarithm and fitting them into the linear model

Figure 1: Gyromagnetic ratio calculation results

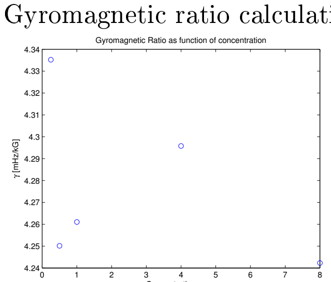
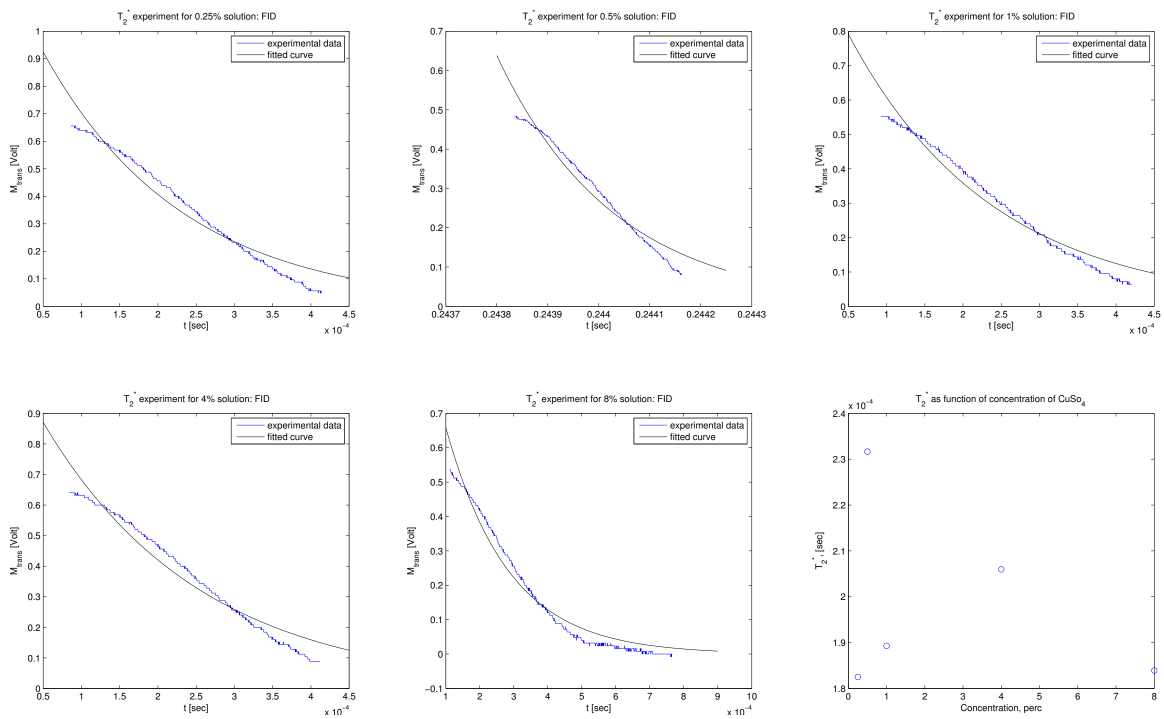


Figure 2: T_2^* calculation results



2 Noise

As the following results predict there is no actual way to model the noise distribution due to low sensitivity of oscilloscope comparing with the noise levels. No autocorrelation is observed as well. Thus the only use of the raw noise data could be by evaluating the zero-offset of the data by calculating the mean noise level, when $t \to \infty$ and attenuating our data accordingly. The one could suppose that the application of low-pass filter (such as for example moving average filter) could improve the SNR, yet in this case one may think the resulting values are affected as well. Interestingly as it could be seen in the results, while applying moving average filter on the CPMG results, as the filter length grows and its smoothing features being emphasized and the fit goodness is improved significantly only the tiniest change in T_2 values could be observed.

In the same time the usage of MA-filter (LP FIR) has an another effect on the T_2^* experiment results. Here both the fit goodness and the measured values remained almost intact. The possible cause for this is the error source in this experiment, which does not probably find its source in the oscilloscope noises and sampling errors.

Figure 3: T_1 calculation results

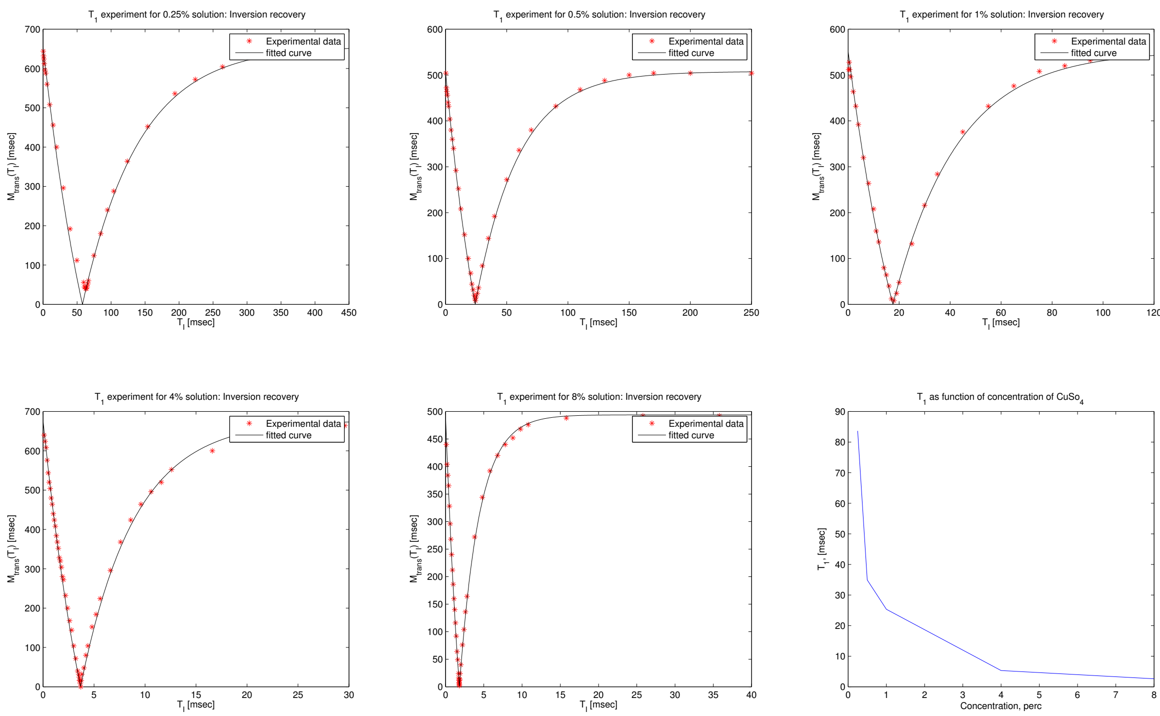


Figure 4: T_2 calculation results using CP sequence

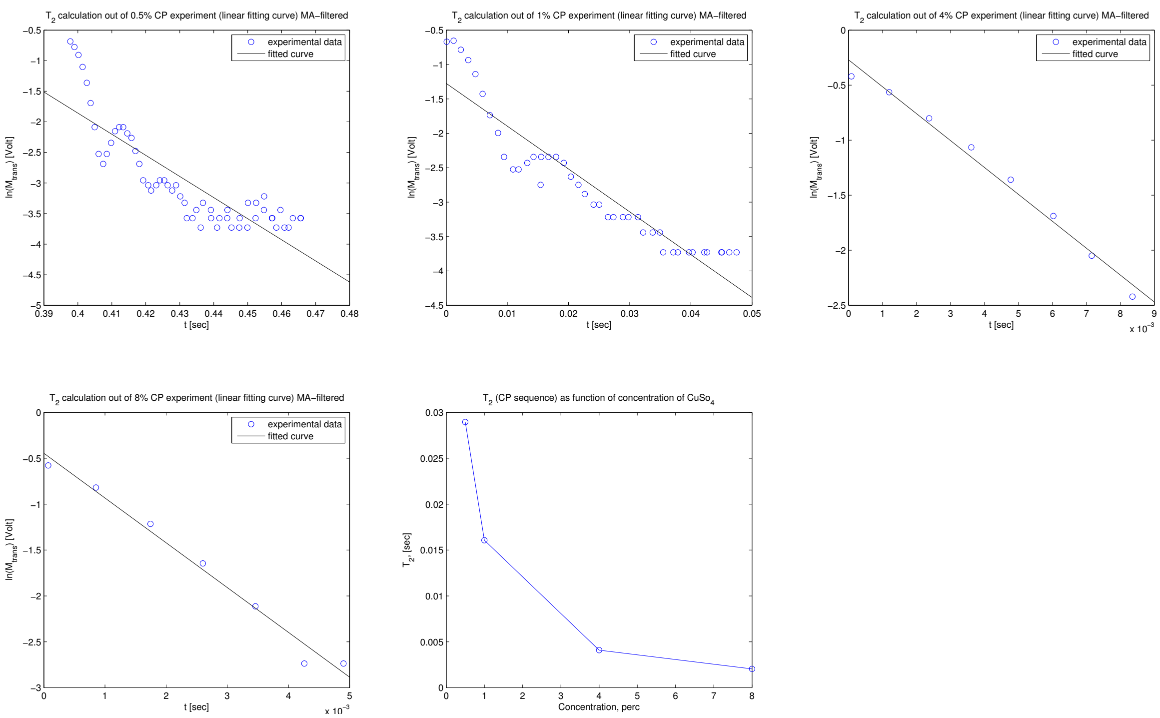


Figure 5: T_2 calculation results using CPMG sequence

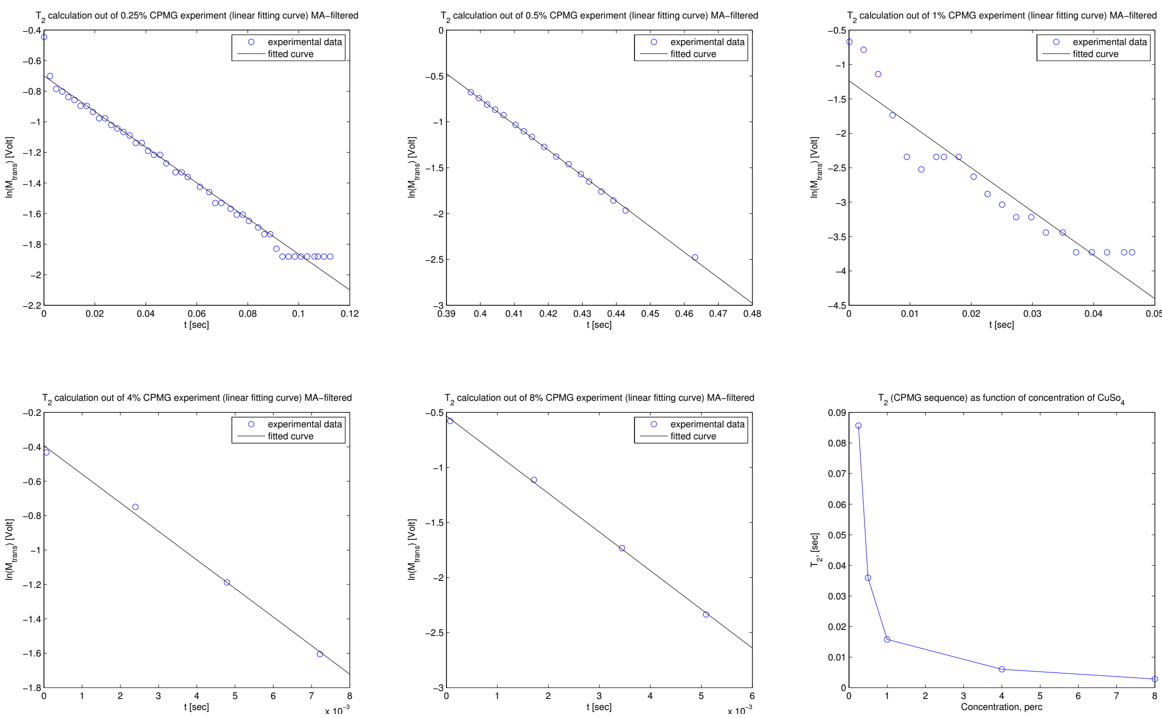


Figure 6: T_2 CPMG experiment results after 3 points MA-filter

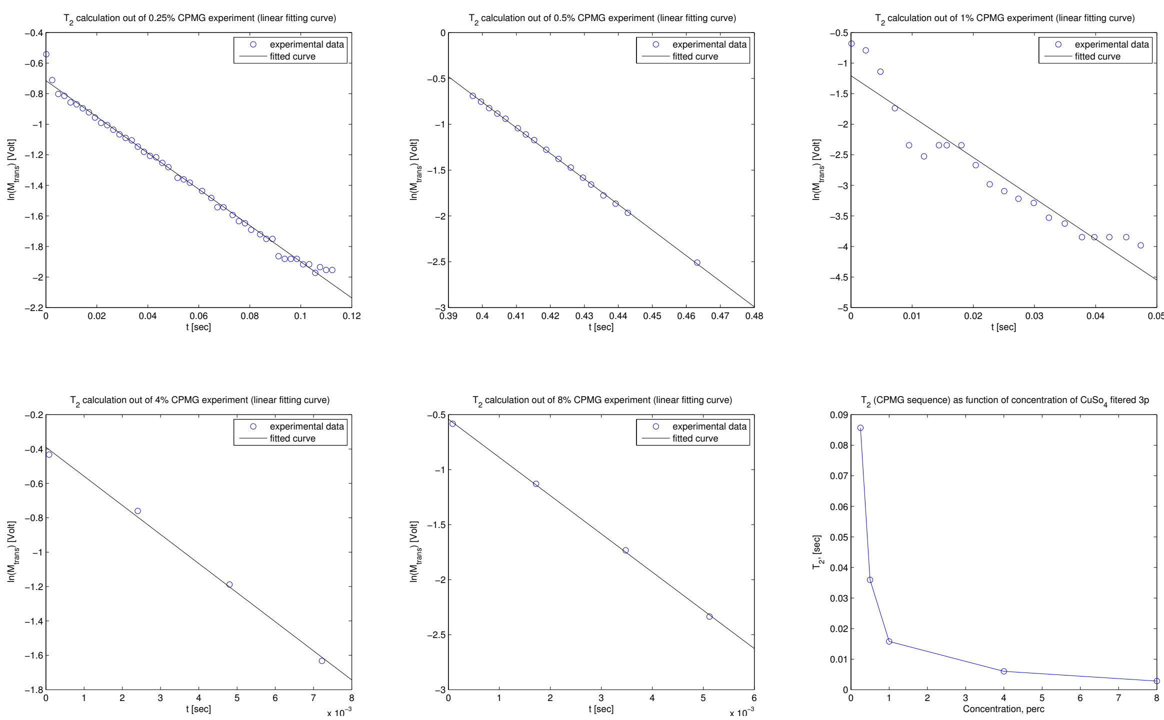


Figure 7: T_2 CPMG experiment results after 5 points MA-filter

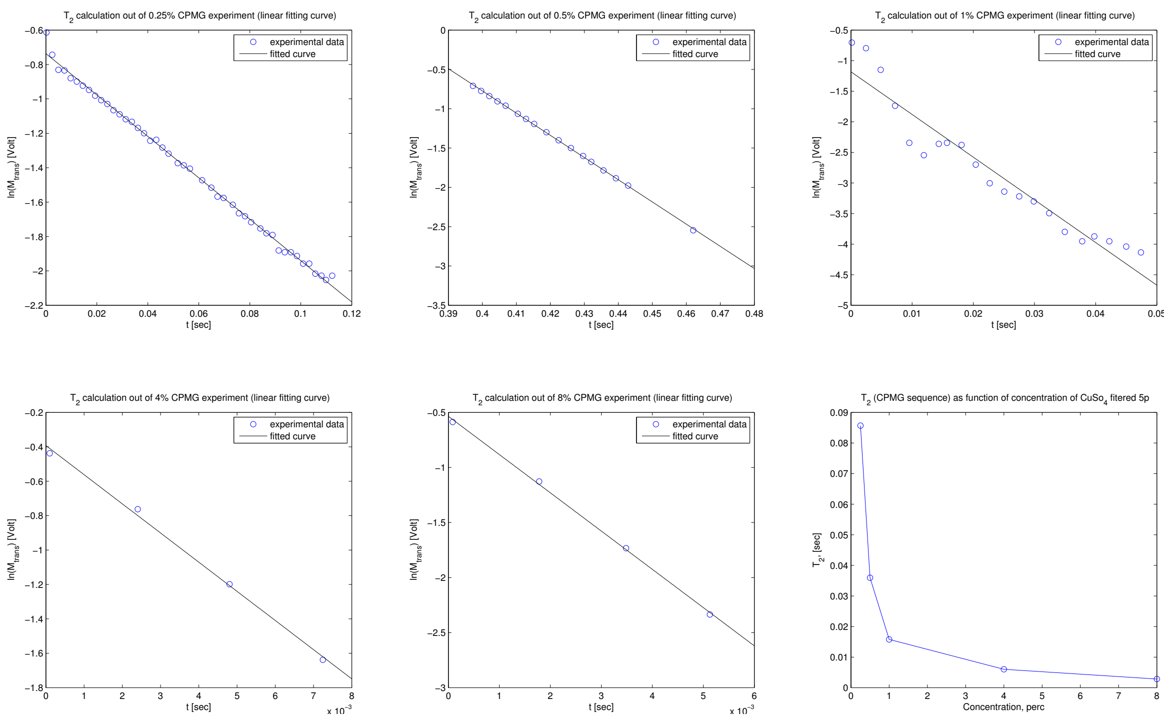


Figure 8: T_2 as function of concentration and filter length

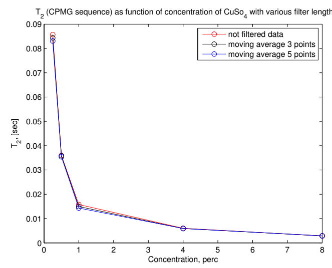
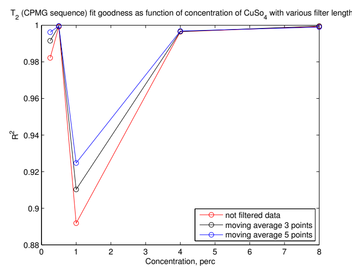


Figure 9: T_2 fit goodness as function of concentration and filter length



3 Errors

The errors during the gyromagnetic ratio calculation are as could be seen in the table.

4 Conclusions & Discussion

As we have seen as the concentration of $CuSO_4$increases the values of T_1 and T_2 decrease. It could be explained by the fact that the increase in the number and the strength of hydrogen bonds decreases the relaxation constants. The atom that is involved in the hydrogen bond lacks mobility and thus tends to transfer its energy in somewhat slower rate. As well no relation has been found between

Table 1: Gyromagnetic ratio errors evaluation

C [%]	$\Delta\omega_0$ [mHz]	B_0 [kG]	$\Delta\gamma \left[\frac{\text{mHz}}{\text{kG}}\right]$
8	$5.9e^{-4}$	0.0260	0.1103
4	$1.4e^{-4}$	0.09	0.3866
1	0.00104	0.03	0.1278
0.5	$9.5e^{-4}$	0.022	0.0935
0.25	0.0013	0.05	0.2168

Table 2: Goodness of fit and error for T_1

C [%]	$\Delta V(\Delta T_1)$ [mV]	R^2
8	2	0.995090479788588
4	8	0.998373866290817
1	8	0.997606683891853
0.5	4	0.997373659484487
0.25	4	0.998523365234285

Table 3: Goodness of fit and error for T_2^*

C [%]	$\Delta V(\Delta T_1)$ [mV]	R^2
8	8	0.947153769510568
4	8	0.954733389385057
1	8	0.962159888407492
0.5	4	0.950465317124662
0.25	8	0.971028338239175

Table 4: Goodness of fit and error for T_2 (CP)

C [%]	$\Delta V(\Delta T_1)$ [mV]	R^2
8	8	0.727050183648995
4	8	0.880960532707183
1	8	0.986442306447831
0.5	4	0.982985382999466

Table 5: Goodness of fit and error for T_2 (CPMG)

C [%]	$\Delta V(\Delta T_1)$ [mV]	R^2
8	8	0.982205667211536
4	8	0.999220823241915
1	8	0.891864392054010
0.5	4	0.996526977690483
0.25	8	0.999281421640704

Figure 10: T_2^* as function of concentration and filter length

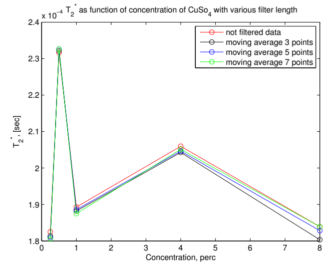
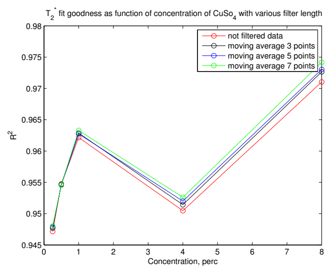


Figure 11: T_2^* fit goodness as function of concentration and filter length



the values of γ and T_2^* and the solution concentration. The result is obvious due to the facts that gyromagnetic ratio is constant for each imaged atom (Hg in our case). As well T_2^* is solely related to the magnet inhomogenity defined by its properties. Yet it could be seen that there is a connection between these 2 values, the fact that remains to be explained.