Tutorial on Using Excel Solver to Analyze Spin-Lattice Relaxation Time Data

In the measurement of the Spin-Lattice Relaxation time T_1, a 180° pulse is followed after a delay time of t with a 90° pulse, and at each delay time the magnetization M_z is measured by measuring the voltage level of the signal that is detected. According to the theory, the magnetization M_z is given by

$$M_z = M_0 \left[1 - 2e^{-t/T_1} \right], \tag{0.1}$$

where M_0 is the initial magnetization following the 180° pulse, t is the delay time, and T_1 is the spin-lattice relaxation time. There are 2 unknowns in this equation, M_0 and T_1. Frequently with exponentially decaying quantities, the equation can be manipulated and the logarithm of both sides of the equation taken so that the natural exponential is removed. This usually results in a linear equation of dependence with the time t and a direct relationship between the slope of the linear graph and the decay rate constant, $1/T_1$. However, in this case, this is not possible so that a non-linear least squares fitting procedure is needed. Excel provides a method of doing this called "Solver."

In this application the measurements results in a N data pairs, t_i and V_i, where V_i is the voltage measurement representative of the magnetization M_z at each time t_i. Since the voltage V is proportional to the magnetization M_z, Equation (0.1) becomes

$$V_z = V_0 \left[1 - 2e^{-t/T_1} \right] \tag{0.2}$$

and this is the equation we wish to fit to the data to find V_0 and T_1. In least squares fitting, the value of each measured value of V_i is compared to a calculated value $V_{zi}(t_i)$. Their difference is measured, squared, and summed for all measurement values. This sum is

$$Sum = \sum_{i=1}^{N} \left[V_i - V_{zi} \right]^2 \tag{0.3}$$

The parameters V_0 and T_1 that provide the best fit are the values that make the sum a minimum value. Solver requires good estimates of these values to begin the fitting process.

The procedure to find the parameters V_0 and T_1 with Excel solver is then as follows:

1. First open a blank Excel worksheet and label the first row of columns A through G as i, t_i, V_i, $V_{zi}(t_i)$, Difference^2, Sum, V_0, and T_1 as in Figure 1.1.

Microsoft Excel - NMR Example of Solver.xls

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	A	B	C	D	E	F	G	H
1	i	t	V	Fit Value	Difference	Sum	V_0	T_1
2	1	2	-1.5	-1.461185596	0.001506558	0.048531603	1.730696	24.67302
3	2	4	-1.24	-1.212659923	0.00074748			
4	3	6	-1	-0.983484909	0.000272748			
5	4	8	-0.78	-0.772153877	6.15617E-05			
6	5	10	-0.56	-0.577277462	0.000298511			
7	6	12	-0.32	-0.397574478	0.0060178			
8	7	14	-0.12	-0.231863494	0.012513441			
9	8	16	0.016	-0.079055068	0.009035466			
10	9	18	0.056	0.061855417	3.42859E-05			
11	10	20	0.144	0.191794356	0.0022843			
12	11	22	0.264	0.311616014	0.002267286			

2. Enter the pairs of t_i and V_i measurements into columns B and C of a blank Excel worksheet.

3. Fill in the values of i in column A. Note: Column A could have been eliminated, but is used here for clarity of explanation of the technique.

4. Prepare a xy scatter plot of the data in columns B and C as illustrated in Figure 1.2.

Relaxation Time Graph of Mineral Oil
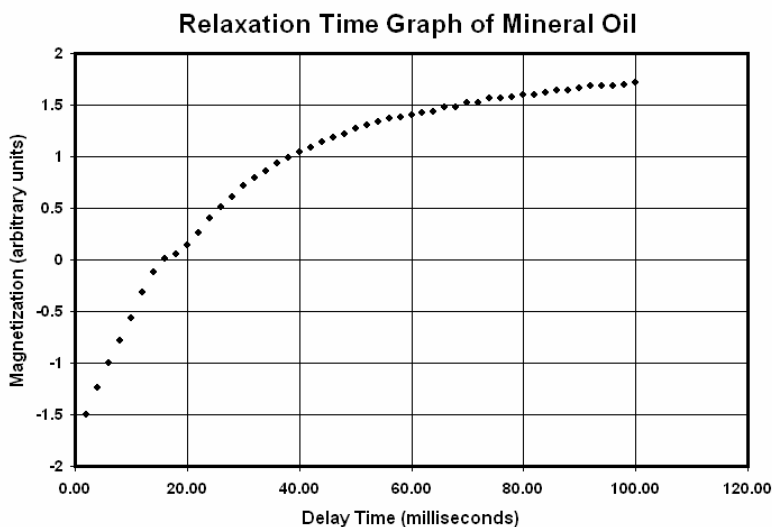
5. From the graph, estimate the values of V_0 and T_1 and enter them into cells G2 and H2 respectively. Remember that from Equation (0.2), V_0 is the value of V at long time delays, i.e. the asymptotic value, and T_1 would be the time that a value decreases to 1/e of some initial value.

6. In cell D2, calculate the value of $V_{z1}(t_1)$ using Equation (0.2), the time for the first value of time, t_1, and the parameters for V_0 and T_1 in cells G2 and H2. Remember

to lock the values of G2 and H2 by using the $ sign so that they are written as
$G$2 and $H$2.

$$=\$G\$2*\left(1\text{-}2*\exp\left(\text{-}B2/\$H\$2\right)\right). \tag{0.4}$$

7. Copy the formula contents of cell D2 to the remaining cells corresponding to the measurements through cell D"N".

8. In cell E2 calculate the square of the difference between the measured value V_1 and the calculated value V_{z1}, i.e.

$$=\left(C2\text{-}D2\right)\wedge 2. \tag{0.5}$$

9. Copy the formula contents of cell E2 to the remaining cells corresponding to the measurements through cell E"N".

10. In cell F2 compute the sum of all the values in column E.

$$=SUM(E2:E"N") \tag{0.6}$$

11. Under Tools of the main menu, select Solver. This brings up a text selection box as shown in Figure 1.2
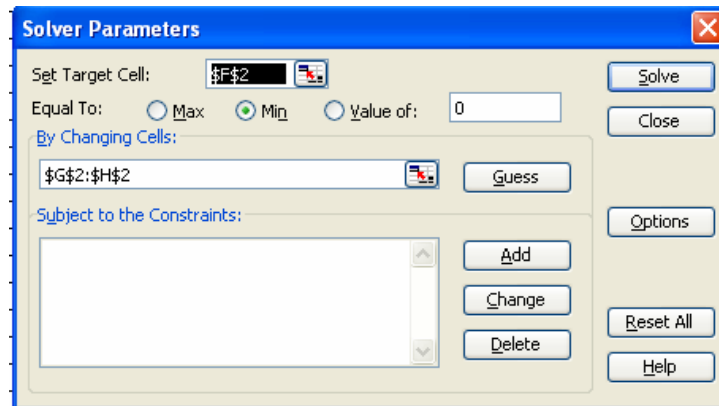
12. In the box labeled "Set Target Cell:" choose the cell that you wish to minimize and that is the cell with the sum of the squares of the differences, cell $F$2.

13. In the "Equal To:" section, choose the Min option, since you want to minimize the target cell, the sum of the squares of the differences between the actual values and the fitted values.

14. In the text box labeled "By Changing Cells:" choose $G$2 and $H$2 or type $G$2:$H$2.

15. Click on Solve and the values for minimizing the sum in the target cell should be calculated and should appear in their respective cells, $G$2 and $H$2. The minimum value for the sum should also appear as an updated value.

16. Add the fitted or calculated values to your graph and compare your fit to the measured values.