Fitting supralinear dose responses using non-empirical expressions; optimization using two computing environments.

K. Prevezanou[1,*], G. Kioselaki[1], P.G. Konstantinidis[1], E. Tsoutsoumanos[2, 3], G.S. Polymeris[3], V. Pagonis[4], G. Kitis[1]

[1] Nuclear Physics and Elementary Particles Physics Section, Physics Department, Aristotle University of Thessaloniki, GR-54124, Thessaloniki, Greece
[2] Condensed Matter Physics Laboratory, Physics Department, University of Thessaly, GR-35100, Lamia, Greece
[3] Institute of Nanoscience and Nanotechnology, NCSR "Demokritos", GR-15310, Ag. Paraskevi (Athens), Greece
[4] Physics Department, McDaniel College, MD-21157, Westminster, USA
*Corresponding Author e-mail: kpreveza@physics.auth.gr

Introduction

The key experimental finding in all applications of Thermoluminescence (TL), Optically stimulated luminescence (OSL), and Electron spin resonance dosimetry (ESR) is the response as a function of radiation dose. The aim of this study is to create three analysis routines to fit the dose response curves, (a) one using the superlinearity index (f(D)), (b) one using the initial analytical solution of the irradiation stage (I(D)), and (c) one that fits both simultaneously.

Methodology

By numerically integrating the differential equations of the one trap one recombination (OTOR) and two trap one recombination (TTOR) center models, Pagonis et al. (2020a, 2020b) developed two analytical solutions of the irradiation stage based on the Lambert W function.

OTOR model	$\frac{n(D)}{N} = 1 + \frac{W[(R-1)\,exp(R-1-\frac{R}{D_c})]}{1-R} = \frac{I(D)}{I_0}$
TTOR model	$\frac{n_2}{N_2} = 1 - \left(\frac{1}{B}\, W\left[B\, exp\,(B) exp\left(-\frac{D}{Dc}\right)\right]\right)^a$

Table 1. Dose response analytical expressions.

OTOR model	$f(D) = \frac{1}{kD}\left(1-\frac{W[Z_1]}{R-1}\right)$, $k = \frac{1}{(R-1)Dc}\frac{W[Z_R]}{1+W[Z_R]}$
TTOR model	$f(D) = \frac{1}{kD}\left[1-\left(\frac{W[Z_2]}{B}\right)^a\right]$, $k = \left(\frac{1}{B}\right)^a \frac{a}{Dc}\frac{W[z_B]^a}{1+W[z_B]}$.

Table 2. The supralinearity index f(D).

For dose response: retrapping ratio $R = A_n/Am$, saturation dose Dc=N/R. For the supralinearity index:
$B = -c = \frac{N_1(A_1-A_m)}{A_2N_2+A_mN_1}$, $Dc = \frac{A_2N_2+A_mN_1}{A_1}$.

For the dose response fitting analysis, two different approaches were adopted: at first, the dose response and the f(D) datasets were fitted independently, using similar initial values for the fitting parameters, indicating for the majority of the cases different final values for the same fitting parameters. In the framework of the second approach, both datasets for the dose response and the f(D) were fitted simultaneously, using a unique set of values corresponding to the fitting parameters. Fitting analysis was performed using both the Microsoft Excel commercial package as well as in Python, with all required libraries used to generate the relevant scripts for each task.

Results

The equation of the OTOR model includes three fitting parameters, among which two are common for the equation for the f(D); these are R and Dc parameters. For the corresponding case of TTOR, the equation of the dose response includes four fitting parameters, among which three are common with the corresponding equation for the f(D); these are the parameters R, B and a. Normally, for the case of independent fitting of the dose response and f(D) data sets, one expects that the common fitting parameters for each model get similar values, if not the same. In many cases of independent fitting, the case was not like that; common fitting parameters indicate values that in same cases differ over one order of magnitude. This problem is more prominent for the case of the TTOR model, as the specific model involves one fitting parameter more. On the contrary, the simultaneous fitting approach indicates low FOM values and a unique value set for the common fitting parameters. In many cases of the OTOR model, the results of the simultaneous fitting, in terms of values of fitting parameters, stand in moderate agreement with the corresponding results of the dose response data sets solely. It is quite important to note that for the case of the simultaneous fitting, the unique FOM value is independent on whether the dose response curve is normalised over the maximum intensity. The results of the present analysis are independent on the software applied.

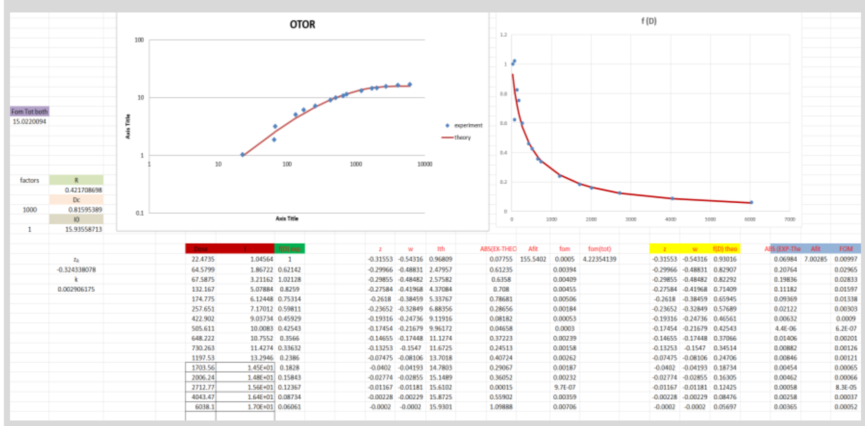

Figure 1. Snapshot from the excel spread-sheet.

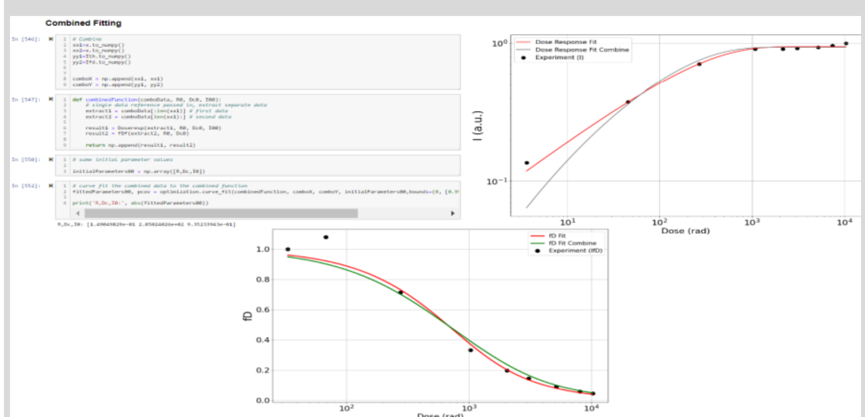

Figure 2. Snapshot from the python script.

Conclusions

When using non-empirical expressions to fit the dose response data, the Lambert W function is considered as the most physically meaningful equation. The results of the present study suggest that while using this function in the framework of the OTOR and TTOR models, simultaneous fitting of both dose response and supralinearity index data sets can guarantee both correctness and accuracy of the results. Simultaneous fitting could be easily achieved using either the Python computing environment or the Microsoft Excel commercial package using the solver add-in. The Python scripts of the present study are available in *https://github.com/GeorgiaKiose/Dose-response-stimulated-luminescence.*

References

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