Comment on: A cautionary note: apparent sensitivity change resulting from curve fitting†

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In both TL and ESR dating studies the artificial growth curves are described commonly by a saturation function of the form $Y(D) = Y_{MAX}[1-\exp(-\gamma D)]$, where Y_{MAX} is the saturation value of the TL (or ESR) intensity, γ is the dose sensitivity and D is the irradiation dose. As Li (1991) has noted that trying to describe a growth curve composed of more than one exponential saturation functions with a simple one exponential model, leads to an ED value which differs from the true ED value. He has tried to show this by applying a curve fitting method employing a simple exponential function to a computer generated data set composed of two exponential saturation functions. This can easily be shown analytically with less effort by using only elementary calculus. In this note the analytical verification of existence of the above mentioned difference is done by obtaining the analytical expression of calculated ED as a a function of true ED.

Calculations

The growth curve composed of two exponential terms is expressed as

$$I = I_{MAX_1}[\,1 - e^{-\alpha(ED+D_i)}\,] + I_{MAX_2}[\,1 - e^{-\alpha(ED+D_i)}\,] \qquad (1)$$

where I_{MAX_1} and I_{MAX_2} are saturation values, α and β ($\alpha \neq \beta$) are dose sensitivities of the two components, respectively. D_i are the dose values for irradiation steps and ED is the equivalent dose. In the curve fitting procedure equation 1 is forced to be equal to a simple exponential saturation function for each irradiation step D_i.

$$I_{MAX_1}[1 - e^{-\alpha(ED+D_i)}\,] + I_{MAX_2}[\,1 - e^{-\beta(ED+D_i)}\,] = Y_{MAX}[\,1 - e^{-\gamma(ED'+D_i)}\,] \qquad (2)$$

where Y_{MAX} is the saturation value ($Y_{MAX} = I_{MAX_1} + I_{MAX_2}$), γ is the dose sensitivity and ED' is the equivalent dose obtained from curve fitting. The result of this can be investigated for three special values of $(ED+D_i)$:

i) For small values of $(ED+D_i)$ equation 2 reduces to

$$Y_{MAX}[1 - e^{-\gamma(ED'+D_i)}] \simeq [I_{MAX_1}\alpha + I_{MAX_2}\beta\,](ED+D_i) \qquad (3)$$

and then $(ED'+D_i)$ is expressed as

$$(ED'+D_i) \simeq -\frac{1}{\gamma}\ln\left[1 - \frac{(I_{MAX_1}\alpha + I_{MAX_2}\beta)\,(ED+D_i)}{Y_{MAX}}\right] \qquad (4)$$

For small values of x, ln(1-x) reduces to -x, so

$$(ED' + D_i) \simeq \frac{1}{\gamma}\frac{[I_{MAX_1}\alpha + I_{MAX_2}\beta]}{Y_{MAX}}(ED+D_i) \qquad (5)$$

In order to have $(ED'+D_i)$ to be equal to $(ED+D_i)$ it is apparent that

$$\gamma Y_{MAX} \simeq I_{MAX_1}\alpha + I_{MAX_2}\beta \qquad (6)$$

must be satisfied. This can be obtained for any α, β and γ for fixed Y_{MAX}, I_{MAX_1} and I_{MAX_2}; so it is always possible to find ED' values very close to true ED values.

ii) If $(ED+D_i)$ is not so small then one should take into account higher order terms in the expansion of exponential terms in equation 2, ie

$$\sum_n Y_{MAX}\frac{(-\gamma)^n}{n!}(ED'+D_i)^n = \sum_n \left[I_{MAX_1}\frac{(-\alpha)^n}{n!} + I_{MAX_2}\frac{(-\beta)^n}{n!}\right](ED'+D_i)^n \qquad (7)$$

According to the uniqueness theorem for power series to have $(ED'+D_i)$ to be equal to $(ED+D_i)$ the coefficients in equation 7 must be equal to each other for all n, ie

$$\sum_n Y_{MAX}\frac{(-\gamma)^n}{n!} = \sum_n \left[I_{MAX_1}\frac{(-\alpha)^n}{n!} + I_{MAX_2}\frac{(-\beta)^n}{n!}\right] \qquad (8)$$

Now it can easily be deduced that the above set of equations can only be satisfied if and only if $\alpha=\beta$. But

† Li, Sheng-Hua (1991) A Cautionary note: apparent sensitivity change resulting from curve fitting. *Ancient TL* 9(1), 12-13.

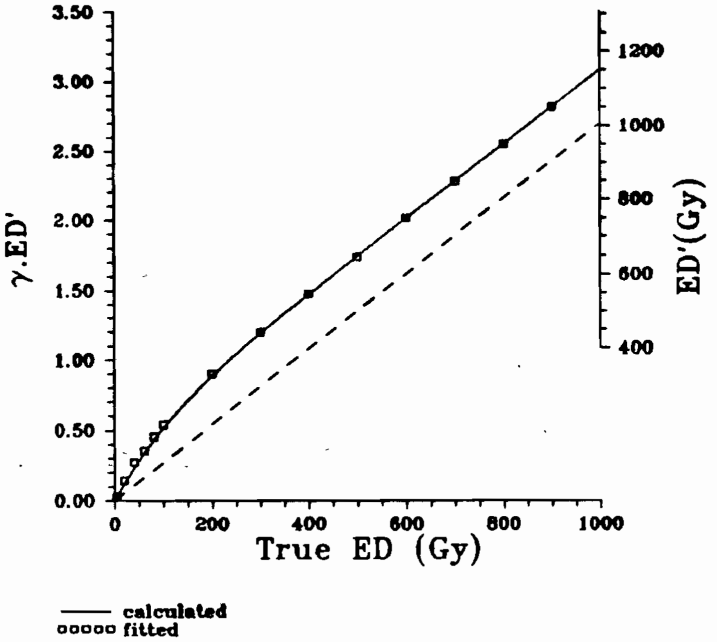

Figure 1.
The graph of γED' vs. true ED. The solid line refers to the calculated value, dashed line refers to the true ED value and boxes are the data points obtained by curve fitting.

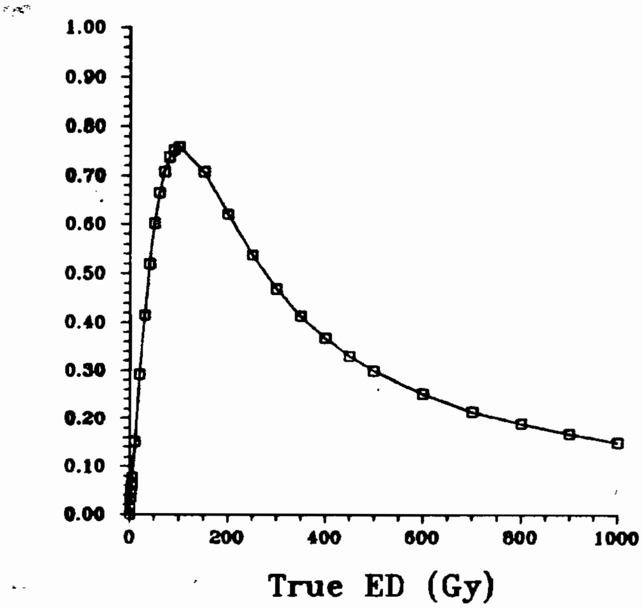

Figure 2.
Fractional error in ED as a function of true ED.

it was stated earlier that $\alpha \neq \beta$ so it is impossible to have ED' = ED.

iii) For very large ED values one of the terms in left hand side of Eqn.2 saturates (say $\beta > \alpha$), ie

$$I_{MAX_1}[1 - e^{-\alpha(ED+D_i)}] + I_{MAX_2} = Y_{MAX}[1 - e^{-\gamma(ED'+D_i)}] \tag{9}$$

In this case the growth curve is described by a single exponential saturation function plus a constant. By using a curve fitting technique one can express this curve with a simple exponential saturation function. In the fitting procedure the value for γ is obtained equal to α and ED' is expressed as

$$ED' = ED + \frac{1}{\alpha} \ln(\frac{Y_{MAX}}{I_{MAX_1}}) \tag{10}$$

by setting $D_i = 0$ for clarity. As it is seen the ED' value can be found in the experiment with a constant shift, after the point at which one of the exponential terms is saturated.

Three special cases mentioned above result in different errors in obtaining the ED value. In order to show this, the hypothetical data given by Li (1991) was used. For each case a data set generated by computer is obtained and fitted to a single exponential model by fixing the saturation value Y_{MAX}. Results are summarized in figure 1. In the figure calculated (γ ED') values are plotted against ED due to dose dependent behaviour of γ for small and medium doses. The expression for (γ ED') is obtained from equation 2,

$$(\gamma ED') = - \ln \left\{ 1 - \frac{(I_{MAX_1}[1 - e^{-\alpha(ED+D_i)}] + I_{MAX_2}[1 - e^{-\beta(ED+D_i)}])}{Y_{MAX}} \right\} \tag{11}$$

In the second y axis (right hand side of the graph) ED' values are used since after a certain dose ED dependence of γ disappears so that ED' can be obtained directly from the ED value with a constant shift. As can be seen from the graph for small values of ED, the discrepancy of calculated values from the true value (dashed line) is small and increases logarithmically as the ED value increases. After a certain point the discrepancy remains constant, implying that one of the exponential terms is saturated. For the data given in Li (1991) this difference is 150 Gy after the ED reaches about 500 Gy.

Conclusion

In this note analytical verification of the difference between true ED and calculated ED values, when a double exponential growth curve is fitted to a single exponential model, has been performed. As a result it was found that the absolute error in obtaining the ED value for such a system, having two exponential components with different dose sensitivities, does not increase as the ED increases but remains constant after the point at which one of the exponentials is saturated. For ED values near to saturation of the growth curve the relative error becomes smaller, as is the case for small ED values (figure 2).

Reference

Li, Sheng-Hua (1991) A Cautionary note: apparent sensitivity change resulting from curve fitting. *Ancient TL* 9, 12-13.

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The major point of the original paper by Li (1991) was to draw attention to the fact that if one has overlapping TL or ESR signals, then errors in ED will result by proceeding to analyze the growth curve using the assumption that only one component is present. The simulation presented by Li to illustrate this was itself a simplification - perhaps an oversimplification - of a real situation, ie only 2 components were assumed, and each signal was assumed to follow perfect saturating exponentials as functions of dose. In reality, aside from the fact that there may well be more than two components contributing to the measured signal, none of the components being monitored may actually follow saturating exponentials. Indeed, I believe that a saturating exponential is such a special case that it is unlikely to be observed in most cases. (The latter statement is especially true for TL signals for which, in many if not most real samples, the final measured signal is the result of charge exchange interactions between several different defects. The resulting growth curve - signal versus dose - can be quite complex.) In view of this I believe that in some respects an analytical treatment of the situation discussed by Li, as presented in the present paper, is not necessary. It is true that some insights are gained from the analysis - eg the behaviour of the relative error as a function of actual ED - but readers should be cautioned not to assume that such behaviour will be typical of all situations in which overlapping signals are suspected. It is the opinion of this reviewer that the case presented is as unlikely as any other situation.