Regression and error analysis for a saturating-exponential-plus-linear model

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Introduction

One tool helpful in attempts to attain accurate TL dates of both unheated sediments and heated material is the use of accurate extrapolation methods for laboratory TL dose-response curves. Berger and others (1987) have described a rapid and accurate (Berger and Huntley, 1989) regression and error analysis method for the simple saturating exponential model of dose response. However, with an increasing effort to date accurately geological material older than about 50 ka, I have frequently encountered dose-response curves that do not show saturation at high applied doses. The simplest model that adequately describes the data and which has a physical basis seems to be a saturating exponential with an added linear term.

As pointed out recently by Levy (1989, equation 4), linear TL buildup beyond an apparent saturation stage is just one of several forms of high-dose response curves that have been observed in the color center and radiation damage literature over the past two decades. Examples of geological quartz that exhibit either this added linear or a more general added supralinear response have been summarized by Fleming (1979), for example. An added linear response may manifest creation of defect traps simultaneous with trap filling during laboratory irradiation.

To allow more accurate extrapolation from one such "multi-stage" dose-response curve, I outline here modifications to the equations of Berger and others (1987) (hereafter denoted BLK87) that allow their regression and rapid error analysis procedure to be applied to the simple exponential-plus-linear model. The use of these modifications is illustrated with an application of the additive-dose method to fine-grained volcanic glass about 170 ka old. These modifications can also be applied straightforwardly to the partial-bleach method used for unheated sediments.

Regression

Using the terminology of BLK87, the modified fitting function is

$$f(D, \theta) = a(1 + \exp[-b(d+D)]) + mD \qquad (1)$$

where D is applied dose (in units of irradiation time to avoid inclusion of systematic error from dose calibration factors), θ is a vector of four regression parameters (or coefficients), and a, b, d and m are these coefficients.

As outlined by BLK87, the Gauss-Newton algorithm for linearizing equation (1) and the quasi-likelihood method (e.g., Dobson, 1990; Seber and Wild, 1989) of regression are used to obtain best estimates of the four coefficients. As before, $w_j = f^{-2}(D_j,\theta)$ is a weighting element (for the j^{th} data point) of the function (1) in the quantity R to be minimized.

The weighted-residual function $R(\theta)$ (BLK87 equation 7)

$$R(\theta) = \sum_{j=1}^{n} w_j \, [Y_j - f - \sum_{k=1}^{4} \beta_k G_k (D_j)]^2 \qquad (2)$$

is modified by extending the parameter summation k from 3 to 4 so that $G_4(D_j) = \partial f/\partial m = D_j$ from (1) above. Thus the j^{th} row in the design matrix X (BLK87 equation 9) becomes simply

$$[1 - e_j, \; a_r (d_r + D_j) e_j, \; a_r b_r e_j, \; D_j] \qquad (3)$$

where $e_j = \exp[-b_r (d_r + D_j)]$ and the subscript r denotes the r^{th} iteration of BLK87 equation 9. Equations 9 and 8 of BLK87 can then be used as outlined there to update the parameter estimates and iterate equation 9 until the required degree of precision is obtained.

In the case of the additive-dose method dealt with here, the required equivalent-dose value (D_e) is not equal to the coefficient d in equation (1) above (as it is in the simple saturating exponential model) but must be obtained by numerical solution of f = 0. For this the standard Newton-Raphson procedure is used.

Error analysis

The variance in this additive-dose D_e is calculated from equation 17 of BLK87, with terms for the second growth curve (required for the partial bleach method) being dropped so that

$$\Delta^2 = \frac{V^t \psi V}{|\partial f/\partial D|^2}$$

Here the extended variance-covariance matrix ψ is related to the information matrix I (BLK87 equations 14 and 10) for which the elements are calculated with BLK87 equation 11. For the model in (1) I becomes a symmetric 4 x 4 matrix with added elements I_{am}, I_{bm}, I_{dm}, I_{mm}, and their symmetric counterparts (e.g., $I_{ma} = I_{am}$). Note that for the saturating exponential, subscript c of BLK87 has been replaced by subscript d, as explained in BLK87. Because of the form of (1) above, the original nine elements of I (Appendix C of BLK87) do not change here.

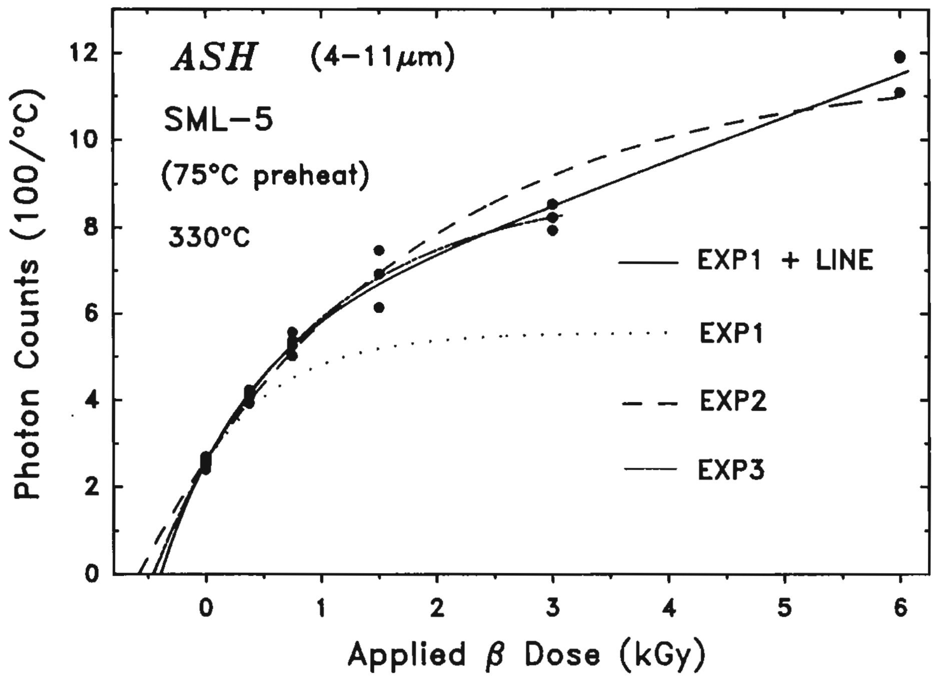

Figure 1.
Additive-dose data for purified volcanic glass from sample SML-5 at the 321-330 °C temperature zone of the glowcurves, preheated for 8 days to remove unstable TL. There are three weighted best-fit curves: EXP1+LINE (x-axis intercept 39151 Gy), EXP2 (intercept 582 ± 51 Gy), and EXP3 (intercept 456 ± 34 Gy). The intercept for the imbedded EXP1 curve is 443 Gy (error not computed).

Applying BLK87 equation 11 to (1) above we obtain for the additional matrix elements of I

$$I_{am} = a^{-1} \sum_{j=1}^{n} \frac{D_j}{f_j}, \qquad I_{bm} = \sum_{j=1}^{n} \frac{(d+D_j)D_j}{S_j f_j},$$

$$I_{dm} = \sum_{j=1}^{n} \frac{D_j}{S_j f_j} \quad \text{and} \quad I_{mm} = \sum_{j=1}^{n} \frac{D_j^2}{f_j^2}$$

where $S_j = \exp[b(d+D_j)] - 1$.

Similarly applying BLK87 equation 16 to (1) gives us the additional fourth element ($\partial f/\partial m$) of the transpose vector V^t, that is, D_e. The first three elements of V^t remain unchanged (Appendix D of BLK87). Finally, the partial derivative in the denominator of (4) above becomes $abe + m$, where $e = \exp[-b(d+D_e)]$.

Application

Data from the 321 - 330 °C glow-curve interval for a purified (by high-speed centrifugation using heavy liquids) volcanic ash sample of about 170 ka old are shown in Figure 1. The calculated D_e values define a plateau (over the interval 321 - 410 °C) only for the exponential-plus-linear fit in Figure 1. A plateau is not observed otherwise. Figure 1 also shows the poor fit of the saturating exponential model to the entire data set (EXP2), with a concomitant overestimate (582 ± 51 Gy at 330 °C) of the De value.

Discussion

The main motivation for using a large applied dose range in constructing dose-response curves is to minimize the range of extrapolation and therefore the error in the D_e value. However, for a fixed number of data points an increase in fitting parameters from 3 to 4 increases the error in the extrapolation. This effect is seen here in the somewhat larger error (± 51 Gy) for the preferred EXP1+LINE fit compared to the EXP3 fit (±34 Gy) in spite of the additional 3 data points (at 6 kGy). Nevertheless, had the new model been considered when these data were generated, then additional points in the 1.5 - 6 kGy range could have been produced to better constrain the linear term and thereby reduce the error in the D_e value. Thus for optimum use of the EXP1+LINE model, considerably more data may need to be generated than for the simple exponential model.

Alternatively, if the simple exponential model is applied to only a limited range of the applied dose values (e.g., EXP3 in Fig. 1) then unacceptably large extrapolations may be required for older samples than this example, and selection of these truncated data points may require unjustifiable subjectivity. Moreover, this use of truncated data may cause an artificial failure of the plateau test, as observed with the sample in Figure 1. The plateau test failed probably because truncation at a constant dose value for all temperature points was inappropriate for this sample. Even if truncated regression does yield a plateau, the resultant TL age is merely "a model age".

Is the EXP+LINE regression model "physically realistic" ? I have several data sets (for both glass-rich ash and feldspar-rich sediments) for which this model clearly produces better fits than does the simple exponential model. One of these data sets (for a feldspar-rich sediment) appears to require an even more complicated EXP+SUPRALINEAR model. This observation is consistent with the general emphasis of Levy (1989) that a range of high- dose-response behaviour may be expected, and that the EXP+LINE model is just one of several physically realistic models. As stated by Levy (1989), equation (1) above may represent continual creation of defects throughout the burial history.

Data such as in Figure 1 also suggest the need for reconsideration of empirical comparisons of natural and laboratory "saturation" levels of TL in feldspars for the purpose of making corrections for long-term fading (e.g. Mejdahl, 1989; Hütt and Jaek, 1989). The usual assumption that the "efficiency" of defect creation is insignificant except at very high doses may need reassessment. Such defect creation can give the appearance (e.g., EXP3 in Figure 1) of a higher "saturation" level than is appropriate for simple trap filling alone.

Finally, several (but not all) of my data sets for old samples suggest that equation (1) is a more realistic approximation to the underlying (undetermined) physical processes than is the simple saturating exponential. In the author's general dating applications (wherein final accuracy is assessed by comparison with at least one independent control age for a sample suite) the stage has not yet been reached where routine application of yet more complicated models (e.g. the sum of equations 6 and 7 of Levy, 1989) is justifiable.

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