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Corresponding Author: Dr. Christopher Burbidge,

Corresponding Author's Institution: ITN

First Author: Christopher Burbidge

Order of Authors: Christopher Burbidge

Abstract: The present study investigates basic geometric forms for dose (D) response characteristics based on saturating exponential functions, for un-normalised (I), dose normalised (to DT: IN = I/IT) and standardised (IS = DT .I/IT) signals. Algebraic functions are assembled to describe the effect of the size of the normalisation or test dose, and that of dose dependent changes in relative trapping and recombination probabilities, on the shapes of dose response characteristics based on single and multiple saturating signal components. Values calculated using these functions are fitted using single saturating exponential curves, to explore the applicability of this form and to illustrate deviations from it.

The strong dependence of normalised signal levels on the size of the normalisation or test dose, and the much reduced dependence of standardised signals in this respect, are illustrated and described analytically. It is demonstrated that these differences in signal level do not affect the rate at which the signal saturates, i.e. the mean-dose of trap filling (D0). The assumption of a fixed linear test dose response (implicit in many studies) is shown to produce a saturating exponential standardised dose response characteristic for which, by definition, the signal at saturation (ISMax) is approximately equal to D0, and the gradient ($\delta IS/\delta D$) at zero dose is approximately unity. Thus, deviations from this case can be used to identify occurrences of more complex behaviour, and the wider presentation of results in standardised form would facilitate this.

The presence of multiple saturating components is shown to produce minor variability in single component fits, but changes in trapping probability between D and DT, and particularly changes in recombination probability between I and IT, are found capable of producing major differences in such fits. It is demonstrated that these changes in fact undo the saturating exponential nature of the dose response characteristic: although the resultant form may be closely approximated by a saturating exponential or saturating exponential plus linear fit over a given dose range, the parameters of this fit will not provide accurate values with which to assess the dose response characteristic of the sample. Thus, a saturating exponential fit (whether simple, summed, or plus linear, etc.) may still function well as a tool for localised interpolation but, just as for supralinearity in non-normalised additively dosed data, it is not reliable for extrapolation.

Relationships with results from the present study, and consideration of assumptions underlying the physics of the saturating exponential dose response in luminescence measurements, indicate that the

changes in trapping and recombination probability investigated herein for dose normalised data are analogous to the processes that cause superlinearity in non-normalised data.

It is observed that most variants of the form of the dose normalised dose response characteristic can be described when the relative recombination probability for I and IT is assumed to be a function of the dose, D. In this case the shape of the dose response characteristic may vary, but absorbed dose evaluations are not made inaccurate except by complicating the data analysis. The present study has developed an analytical framework with which dose rate, predose and non-dose dependent effects, which do adversely affect absorbed dose evaluation when using dose normalised dose response characteristics, may also be explored.

Cover Letter

S. R.

MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E ENSINO SUPERIOR

INSTITUTO TECNOLÓGICO E NUCLEAR

Estrada Nacional 10 – Apartado 21, 2686-953 Sacavém Telef.: 351-219946000 Fax:351-219946185

Exmº Prof. Ian Bailiff,
Editor in Chief,
Radiation Measurements

19/12/11

Dear Ian,

I hope I find you well.

Please find attached the manuscript entitled “Dose normalised dose response characteristics” for submission to Radiation Measurements, plus seven figures in separate .tiff files. The paper explores the form of dose normalised dose responses using simple theory and with reference to experimental data. It is aimed at potentially tricky middle ground between those of a theoretical/mathematical bent and more applied practitioners. I would therefore ask you to select reviewers who will be able to verify the maths without effort (i.e. annoyance), while still having sufficient patience and interest in the applied aspects that they do not find irrelevant either the level of explantion or the details entered into with respect to the luminescence dating literature. I have made some suggestions, but if you can think of someone who better fits the above description then please send it to them.

Best regards,

Chris Burbidge

***Highlights**

- Dose normalised dose response characteristics are explored using simple theory
- Uniformity and deviations of dose responses are explained
- Magnitude depends strongly on the size of the test/normalisation dose
- Dose dependent changes can explain non-exponential forms
- The effects are analogous to superlinearity in non-normalised characteristics

Dose normalised dose response characteristics

C. I. Burbidge

Instituto Tecnológico e Nuclear, Sacavém, Portugal. christoph@itn.pt
GeoBioTec, Universidade de Aveiro, Portugal

Abstract

The present study investigates basic geometric forms for dose (D) response characteristics based on saturating exponential functions, for un-normalised (I), dose normalised (to D_T: $I_N = I/I_T$) and standardised ($I_S = D_T .I/I_T$) signals. Algebraic functions are assembled to describe the effect of the size of the normalisation or test dose, and that of dose dependent changes in relative trapping and recombination probabilities, on the shapes of dose response characteristics based on single and multiple saturating signal components. Values calculated using these functions are fitted using single saturating exponential curves, to explore the applicability of this form and to illustrate deviations from it.

The strong dependence of normalised signal levels on the size of the normalisation or test dose, and the much reduced dependence of standardised signals in this respect, are illustrated and described analytically. It is demonstrated that these differences in signal level do not affect the rate at which the signal saturates, *i.e.* the mean-dose of trap filling (D_0). The assumption of a fixed linear test dose response (implicit in many studies) is shown to produce a saturating exponential standardised dose response characteristic for which, by definition, the signal at saturation (I_{SMax}) is approximately equal to D_0, and the gradient ($\delta I_S/\delta D$) at zero dose is approximately unity. Thus, deviations from this case can be used to identify occurrences of more complex behaviour, and the wider presentation of results in standardised form would facilitate this.

The presence of multiple saturating components is shown to produce *minor* variability in single component fits, but changes in trapping probability between D and D_T, and particularly changes in recombination probability between I and I_T, are found capable of producing *major* differences in such fits. It is demonstrated that these changes in fact undo the saturating exponential nature of the dose response characteristic: although the resultant form may be closely approximated by a saturating exponential or saturating exponential plus linear fit over a given dose range, the parameters of this fit will not provide accurate values with which to assess the dose response characteristic of the sample. Thus, a saturating exponential fit (whether simple, summed, or plus linear, *etc.*) may still function well as a tool for localised interpolation but, just as for supralinearity in non-normalised additively dosed data, it is not reliable for extrapolation.

Relationships with results from the present study, and consideration of assumptions underlying the physics of the saturating exponential dose response in luminescence measurements, indicate that the changes in trapping and recombination probability investigated herein for dose normalised data are analogous to the processes that cause superlinearity in non-normalised data.

It is observed that most variants of the form of the dose normalised dose response characteristic can be described when the relative recombination probability for I and I_T is assumed to be a function of the dose, D. In this case the shape of the dose response characteristic may vary, but absorbed dose evaluations are not made inaccurate except by complicating the data analysis. The present study has developed an analytical framework with which dose rate, predose and non-dose dependent effects, which do adversely affect absorbed dose evaluation when using dose normalised dose response characteristics, may also be explored.

Keywords: saturating exponential; standardised; growth curve shape; luminescence

1. Introduction

A geometric analysis is a description of the implications of prior assumptions – it is not *in itself* concerned with exploring whether the prior assumptions are actually correct (summarised from Descartes, in Hampshire, 1956, p71-82).

The present study reviews, introduces, describes algebraically, and illustrates the basic geometric forms for dose response characteristics based on saturating exponential functions, in the following cases:
- un-normalised.
- dose normalised and standardised, assuming a fixed test response to a small fixed test dose
- standardised or dose normalised for any fixed test response.
- standardised, for test responses affected by dose dependent changes in recombination and/or trapping probability.

The equations used to describe each type of dose response characteristic are not derived directly at each stage from sets of rate equations set up to explore a physical model of the system under examination, though this is should be possible and represents a possible test of the conclusions of this study. Instead, the objects analysed are constructed by combining a finite number of discrete elements of the simplest generalised form of dose response that have been previously obtained from the simplest models of the physical system to which they relate, *i.e.* models based on a single trap and a single centre (McKeever, 1985. Ch 3.4). A combination of these functions is developed and its geometry explored using basic calculus and other algebraic manipulation (*e.g.* Bird, 1988).

The *a priori* assumptions of the present study are, therefore, that the chosen elements are sufficient to describe the system, that they are well described by the chosen forms, and that they in fact combine in the manner presented. If these assumptions are correct then the results of the present analysis are expected to represent the general, or underlying, behaviour of the physics of the dosimetric system examined.

This work has the objective of developing descriptions of each case described above, to illustrate how the form of dose normalised dose response characteristics varies:
- with normalisation or test dose, D_T.
- with dose dependent changes in trapping probability between the beginning of irradiation with a dose D, and the beginning of irradiation with a subsequent normalisation or test dose, D_T.
- with dose dependent changes in recombination probability between the beginning of measurement of the dose response I, and the beginning of measurement of a subsequent normalisation or test dose response, I_T.

It aims to demonstrate with relevant examples:
- how the presence of multiple saturating exponential components can produce *minor* apparent differences between what appear to be single component dose response characteristics.
- if the test dose is small relative to D_{T0} and the test response is unaffected by changes in trapping and recombination probability between dose and normalisation/test dose, dose normalised dose response characteristics, then the dose response characteristic follows a saturating exponential form with gradient at $D = 0$ of 1 and I_{Max} approximates D_0.
- if same applies but the test dose is no longer small, then the saturating exponential form is maintained and changes in test dose produce changes in normalised (and standardised) signal levels but not in saturation rates.
- that where changes in trapping and particularly in recombination probability occur between dose and normalisation/test dose, then the dose response characteristic no longer follows a saturating exponential. *Major* apparent differences in form between what appear to be single component saturating exponential dose response characteristics, and that the forms of these

variations can be used to explain why certain variations in dose response characteristic have been observed in the literature.
- limits of the applicability of this analysis for selected dose responses obtained for high doses.

2. Saturating exponential dose response characteristic

The dose response characteristic for a luminescence signal based on a single trap single centre model (McKeever, 1985, Ch 3.4) follows a single saturating exponential, *e.g.*:

$$(1) \qquad I = I_{Max}\left(1 - e^{-D/D_0}\right)$$

, where I = signal intensity, I_{Max} = signal intensity at saturation and D_0 is the mean-dose of trap filling (analogous to mean life in radioactive decay). For $D = \infty$, $I = I_{Max}$.

The first derivative of (1) is:

$$(2) \qquad dI/dD = (I_{Max}/D_0)\, e^{-D/D0}$$

, *i.e.* the gradient of the curve is a function of D, I_{Max} and D_0. For $D = 0$, $dI/dD = I_{Max}/D_0$.

Where the dose response characteristic is composed of more than one saturating exponential component, due to the contributions of different trap types, then:

$$(3) \qquad I = \sum\{I_{Maxi}\,(1-e^{-D/D0i})\}_{\,i=(1-n)}$$

$$(4) \qquad dI/dD = \sum\{(I_{Maxi}/D_{0i})\, e^{-D/D0i}\}_{\,i=(1-n)}$$

dI/dD at $D = 0$ is often approximated using a linear regression to the growth characteristic for low doses (Grün, R., 1996), in the range where saturation is not easily resolved statistically. If more than one saturating component is present, then as D approaches zero the regression will give:

$$(5) \qquad I \approx D\Delta I/\Delta D \approx D dI/dD\ (D = 0) = D\sum\{I_{Maxi}/D_{0i}\}_{\,i=(1-n)}$$

At slightly higher doses the saturating exponential form of data may be apparent, but different saturating exponential components may not be resolvable statistically, so that a multiple saturating exponential dose response characteristic may be approximated by a single saturating exponential fit. Examples are illustrated in Fig. 1 and Table 1. If this fit were accurate then in addition to (5), for $D = \infty$ it would give:

$$(6) \qquad I\,(D = \infty) = I_{Max} = \sum\{I_{Maxi}\}_{i=(1-n)}.$$

3. Normalised and standardised dose response characteristics for a small fixed test response (*i.e.* assuming test dose response is proportional to dose)

Where I is un-normalised, dI/dD at $D = 0$ is the sensitivity of the sample to dose excluding saturation effects, but I_{Max} and D_0 may vary as a function of trapping and recombination probability, and changes in these with repeated measurement. Where a "test dose monitor" is applied, as in equal predose-dose normalised multiple aliquot measurements (Aitken, 1985, p128) or the SAR protocol (Murray and Wintle, 2000), the signal (I) response to a given variable dose (D) is divided by the response (I_T) to a fixed "test dose" (D_T) delivered after measurement of I, to produce a normalised signal I_N:

(7) $I_N = I/I_T$

If I_T accurately monitors sensitivity with respect to I, then in the idealised case of an infinitely small test dose:

(8) $I_T/D_T \equiv dI/dD\ (D = 0)$

However, I_N is inversely proportional to I_T (7), and hence where D_T is low enough that (8) may be reasonably assumed to apply, then I_N is approximately inversely proportional to the finite test dose employed for real measurements (but see Fig. 2). Roberts and Duller (2004) "standardised" I_N by multiplying by the test dose ($I_S = D_T I_N$). They observed that following standardisation, fits using (1) often produce similar values of I_{SMax} and D_0, and that if I_{SMax} is set equal to D_0 then D_T $dI_N/dD = 1$. For the saturating exponential case, and making the approximation of a small but finite test dose, it is evident from (2) and (8) that:

(9) $dI_S/dD = (dI/dD)/(I_T/D_T) = (I_{Max}/D_0)\ e^{-D/D_0}/(I_T/D_T)$

(10) $I_T/D_T \approx dI/dD\ (D = 0) = I_{Max}/D_0$

, therefore:

(11) $dI_S/dD \approx e^{-D/D_0}$

(12) $\int dI_S/dD.dD = I_S \approx D_0\,(1 - e^{-D/D_0})$

Thus, for the approximation of a small but finite test dose the gradient of the standardised dose response characteristic (11) at $D = 0$ must approximate 1, and since for $D = \infty$, $I = I_{Max}$ in (1), I_{SMax} in (12), now in units of Gy, must be approximately equal to D_0.

Where the dose response characteristic is composed of more than one saturating exponential component, but each component (i) conforms with (11) and (12), then I_{SMax} and D_0 are the sums of the values for each component, and $\sum\{ I_{Maxi}\}_{i=(1\text{-}n)} = \sum\{D_{0i}\}_{i=(1\text{-}n)}$, such that:

(13) $dI_S/dD \approx \sum\{e^{-D/D_{0i}}\}_{i=(1\text{-}n)}$

and,

(14) $I_S \approx \sum\{D_{0i}\}_{i=(1\text{-}n)}\,(1\text{-}\sum\{e^{-D/D_{0i}}\}_{i=(1\text{-}n)})$

In (12) and (14), I_S is independent of recombination probability and dI_S/dD ($D = 0$) is independent of the trapping probability. However, the relative trapping probability (at $D = 0$) is reflected in the mean dose of trap filling (D_0), which is equal to the standardised signal at saturation (I_{SMax}): an initially high rate of trapping at sites from which the charge will eventually yield luminescence, relative to sites where this will not occur, will produce low D_0 and I_{SMax} values, and vice versa. Where D_0 and I_{SMax} or I_{NMax} vary by the same proportion between different materials, samples, aliquots or individual grains (*e.g.* Olley *et al.*, 2004; Timar-Gabor *et al.*, 2011; Lamothe and Auclair, 1999; Forman and Pierson, 2002), this indicates differences in trapping probability. This behaviour is a consequence of the saturating exponential form of the dose response characteristic and the effect of normalisation using an accurate monitor of sensitivity. It does not relate to any particular material or signal, so variations in I_{SMax} or I_{NMax} and D_0 indicate different relative trapping probabilities for different samples, and variations about $I_{SMax}/D_0 = 1$ indicate deviations from the case where I_T accurately monitors sensitivity with respect to I. However, in practise a finite test dose response will also be subject to

saturation effects, which produce dependence of I_{SMax}/D_0 on test dose size (Burbidge *et al.*, 2006).

4. Standardised and normalised dose response characteristics for any fixed test response

Where the approximation of a small test dose is relinquished, the standardised signal is a function of the dose response characteristics of both the "signal" (I) in response to the "dose" (D) and the "test signal" (I_T) in response to the "test dose" (D_T). For single saturating exponential signal responses:

$$(15) \qquad I_S = D_T \, {I}/{I_T} = f(D, D_T) = D_T \, \frac{I_{Max}}{I_{TMax}} \frac{\left(1 - e^{-D/D_0}\right)}{\left(1 - e^{-D_T/D_{T0}}\right)}$$

$$(16) \qquad \frac{\delta I_S}{\delta D} = \frac{D_T}{D_0} \frac{I_{Max}}{I_{TMax}} \frac{e^{-D/D_0}}{\left(1 - e^{-D_T/D_{T0}}\right)}$$

$$(17) \qquad \frac{\delta I_S}{\delta D_T} = \left(\left(1 - e^{-D_T/D_{T0}}\right) - \frac{D_T}{D_{T0}} e^{-D_T/D_{T0}} \right) \frac{I_{Max}}{I_{TMax}} \frac{\left(1 - e^{-D/D_0}\right)}{\left(1 - e^{-D_T/D_{T0}}\right)^2}$$

Where a fixed test dose D_T is applied, and D_{T0} and I_{Max}/I_{TMax} are invariant with dose D, then the standardised dose response characteristic (15) takes the form of a single saturating exponential:

$$(18) \qquad I_S = I_{SMax}\left(1 - e^{-D/D_0}\right)$$

such that at $D = 0$, $\delta I_S/\delta D = I_{SMax}/D_0$, where:

$$(19) \qquad I_{SMax} = D_T \, \frac{I_{Max}}{I_{TMax}} \frac{1}{\left(1 - e^{-D_T/D_{T0}}\right)}$$

Thus, I_{SMax} varies as a function of test dose, but D_0 does not, so I_{SMax} (19) is no longer constrained to approximately equal D_0, and the gradient of the standardised dose response characteristic (16) at $D = 0$ is no longer constrained to approximate unity (*c.f.* section 3). For large test doses the exponential of $-D_T/D_{T0}$ approximates zero, so the gradient of I_{SMax} with respect to D_T is found to be I_{Max}/I_{TMax} and:

$$(20) \qquad D_T/D_{T0} \rightarrow \infty: I_{SMax} \rightarrow D_T \, I_{Max}/I_{TMax};$$

, for small test doses the exponential of $-D_T/D_{T0}$ approximates $(1 - D_T/D_{T0})$, and the gradient with respect to D_T is found to be $\frac{1}{2} \, I_{Max}/I_{TMax}$, so:

$$(21) \qquad D_T/D_{T0} \rightarrow 0, I_{SMax} \rightarrow (D_{T0} + D_T/2) \, I_{Max}/I_{TMax}$$

Examples are shown in Fig. 2. and Table 2. However, D_{T0} and I_{TMax} are not evaluated separately in a fit of the form of (18). The situation is simplified where the signal and test signal in (15) may be assumed to relate to the same dose response characteristic: in this case (10) is verified

for small test doses and the meaning of the assumption that "I_T accurately monitors sensitivity with respect to I" in this context is clarified, *i.e.* $I_{Max} = I_{TMax}$ and $D_0 = D_{T0}$.

Where the standardised dose response characteristic is composed of more than one saturating exponential component, due to the contributions of different trap types, then:

(22) $\delta I_S/\delta D\ (D = 0) = \sum\{I_{Ti}\ I_{SMaxi}/D_{0i}\}_{i=(1\text{-}n)} / \sum\{I_{Ti}\}_{i=(1\text{-}n)}$

and:

(23) $I_S\ (D = \infty) = I_{SMax} = \sum\{I_{Ti}\ I_{SMaxi}\}_{i=(1\text{-}n)} / \sum\{I_{Ti}\}_{i=(1\text{-}n)}$

However, unlike the case for non-normalised signals (4) or normalised signals using the small test dose assumption (14), D_0 cannot be well predicted from (22) unless the relative contribution of each signal component to I_T is known.

5. Dose response characteristics where the test response is affected by changes in recombination and / or trapping probability

In sections 3 and 4 calculations have been presented for a fixed test dose, assuming that this will provide a fixed test dose response. As mentioned in the introduction this is a simplification: in reality changes in recombination probability occur between the beginnings of the measurements I and I_T, and changes in trapping probability occur between the beginnings of the irradiations D and D_T. Let factor k represent relative recombination probability and factor l represent relative trapping probability. Thus k only affects I_{Max}, while l affects I_{Max} and D_0 equally:

(24) $I_{TMax} = kl\ I_{Max}$

(25) $D_{T0} = l\ D_0$

, and so:

(26) $$I_T = I_{TMax}\left(1 - e^{-D_T/D_{T0}}\right) = klI_{Max}\left(1 - e^{-D_T/lD_0}\right)$$

Where change in the relative recombination and trapping probability (k and l) between I and I_T is assumed to be a function of dose, D, then each is expected to respond as a function of filling of the electron and hole traps participating in the production of the signal. Assuming that each follows a single saturating exponential, but that this change is induced relative to a baseline level defined by non-dose responsive factors (k_0, l_0), then:

(27) $$k = f(D) = k_0 + k_{Max}\left(1 - e^{-D/D_{k0}}\right)$$

(28) $$l = f(D) = l_0 + l_{Max}\left(1 - e^{-D/D_{l0}}\right)$$

I_{TMax} and D_{T0} are now dose dependent variables, so the standardised dose response characteristic (15) no longer takes the form of a single saturating exponential (18). Substituting (26), (27) and (28) into (15) gives:

(29) $$I_{S(kl)} = \frac{D_T\left(1-e^{-D/D_0}\right)}{\left(k_0+k_{Max}\left(1-e^{-D/D_{k0}}\right)\right)\left(l_0+l_{Max}\left(1-e^{-D/D_{l0}}\right)\right)\left(1-e^{-D_T/D_0\left(l_0+l_{Max}\left(1-e^{-D/D_{l0}}\right)\right)}\right)}$$

, and hence:

(30) $$\frac{\delta_{I_{S(kl)}}}{\delta_D} = \frac{\frac{D_T}{D_0}e^{-D/D_0}}{kl\left(1-e^{-D_T/lD_0}\right)} - \frac{D_T\left(1-e^{-D/D_0}\right)\left(\frac{k}{l}\frac{l_{Max}}{D_{l0}}\frac{D_0}{D_T}e^{-D_T/lD_0}e^{-D/D_{l0}}+\left(1-e^{-D_T/lD_0}\right)\left(k\frac{l_{Max}}{D_{l0}}e^{-D/D_{l0}}+l\frac{k_{Max}}{D_{k0}}e^{-D/D_{k0}}\right)\right)}{\left(kl\left(1-e^{-D_T/lD_0}\right)\right)^2}$$

Equation (29) may be simplified as follows:
- If it is assumed that I and I_T are measured from the same dose response characteristic, differences in trapping and recombination probability induced by different treatments associated with the measurements notwithstanding, then $k_0 = l_0 = 1$.
- Where no changes in relative trapping or recombination probability are considered, then $k_{Max} = l_{Max} = 0$. If also $k_0 = l_0 = 1$, then (15) is obtained for the special case in which $D_{T0} = D_0$ and $I_{TMax} = I_{Max}$.
- Where only changes in relative recombination probability between the measurements I and I_T are considered, then $l_{Max} = 0$.
- Where only changes in relative trapping probability between the beginnings of irradiations D and D_T are considered, then $k_{Max} = 0$.

Examples of the form of the dose response characteristic obtained when considering changes in relative recombination and trapping probability separately are shown in Fig. 3, Fig. 4, and Fig. 5. These illustrate that the effect of the functions k and/or l is to transfer the dose response characteristic based on (15) from one saturating exponential trajectory to another; *i.e.* I_S at a given dose D is shifted at a rate controlled by k_{Max} and D_{k0} and/or l_{Max} and D_{l0} (see (2)), and by a magnitude controlled by k_{Max}, k_0, and/or l_{Max} and l_0. Where the normalisation or test dose response I_T is measured subsequent to the dose response I, the shift is worked on I_S through change in I_T as a function of dose D, (Fig. 3, Fig. 4, and Fig. 5 insets). Just as the test dose response I_T is constrained to be positive, statistical variations in real data notwithstanding, in the application of (29) k and l function as multipliers of I_T and so are also constrained to be positive. Where k_{Max}/k_0 or l_{Max}/l_0 is less than -1 then I_S vs. D is discontinuous and enters physically meaningless regions of negative values, but (29) can be used to calculate continuous dose responses in negative space if necessary, by making k_0 or l_0 negative. At $D = 0$ and $D = \infty$, $\delta(29)/\delta D =$ (16), but at intermediate doses it is altered by k and l. $\delta I_S/\delta D = 0$ if the two parts of (30), either side of the subtraction, are equal. This occurs at $D = \infty$, but when k_{Max} or l_{Max} is positive and D_{k0} is greater than D_0 it also occurs for a finite value of D. $\delta I_S/\delta D_T$ is not affected by k or l. At doses approaching zero the characteristic is always linear. Above zero dose the transfer produces the following cases:

1/ Superlinearity followed by ‘two phase saturation’.
2/ An inflection followed by ‘accelerated saturation’.
3/ Early onset sublinearity followed by ‘subdued saturation’.
4/ A peak followed by ‘negative saturation’.

Which case is evident depends on at what dose, at what rate, and to what magnitude the transfer takes place (k_{Max}, l_{Max}, D_{k0}, D_{l0}), in relation to the dose, rate and magnitude of the basic saturating exponential form of the dose response (I_{Max}, D_0). Thus, when multiple components with different D_0 values are present in the dose response characteristic of I, then for a given dose the effect of a given transfer function differs between the components. In addition to cases 1/ to 4/ this can produce:

5/ A peak, *i.e.* increase and decline in signal level, followed by a further increase to saturation (Fig. 7, curve a.).

6. Discussion

6.1. Superlinearity

The algebraic-geometric descriptions studied in the present work are just that, but their behavioural implications relate to the superlinearity (supra- in the case of extrapolation, see Chen and McKeever, 1994) predicted from simple physical models for un-normalised dose response characteristics (McKeever, 1985. Ch 3.4). Where a dose response subject to a given (proportional) effect is normalised to a test signal subject to the same effect, then the effect is cancelled. Thus, the “positive” or “negative” superlinearity observed in the present study (section 5) represents the *relative* levels of superlinearity in the dose response and the test dose response; hence the complete lack of superlinearity in the standardised/normalised dose response where no differences in trapping or recombination probability are considered (sections 3 and 4). Conversely, if the test dose (or reference point, whatever) were before the dose, then the change in trapping or recombination probability (k or l) would apply to I, not I_T. If the normalisation were then removed but the samples were considered uniform prior to irradiation and measurement, then any changes would apply to an initial uniform baseline (but unmonitored) state. As such the changes would be manifest in the un-normalised dose response: this is the superlinearity reported for un-normalised dose responses and predicted from rate equations in the literature (Charitidis *et al*., 2000; Chen and McKeever, 1994; Lawless *et al*., 2005; Mische and McKeever, 1989). Also, in the case of the dose normalised dose response characteristic, the test dose response appears to operate as a proxy for the availability or saturation of delocalised bands during irradiation: the gradient in I_{NMax} vs. D_T at low test doses is $(I_{Max}/I_{TMax})/2$, while at high test doses it is (I_{Max}/I_{TMax}) (Fig. 2). The factor of two difference between models calculated assuming non-equilibrium or quasi-equilibrium thermodynamics: ‘empty bands’ or ‘nearly-full bands’ is analogous to that discussed by McKeever (1985, Ch 3.4), in the context of superlinearity in dose response.

6.2. Standardisation and the effect of test dose size

In section 3 it was shown that where a standardised dose response characteristic is based on saturating exponential dose and test dose responses, each drawn from the same dose response characteristic and evaluated using a small fixed test dose with fixed test dose response, then $I_{SMax} \approx D_0$ and dI_S/dD ($D = 0$) = 1. Satisfaction of the constraints required to obtain this simple case appears relatively demanding, but studies examining the utility of common dose response characteristics for different aliquots, samples, sites or regions indicate that it is often approximated (*e.g.* Burbidge *et al*., 2006; Roberts and Duller 2004; Hong and Choi, 2008; Lai, 2006; Shen and Mauz, 2011; Telfer *et al*., 2008; and references in Wintle, 1997, section 5.1.5). The order-of-magnitude reduction in the effect of test dose size on signal level following standardisation (Fig. 2, Table 1, Table 2) illustrates that standardisation is a helpful first step in

facilitating comparisons between measurements made using different test doses. The effect of the magnitude of the normalisation or test dose on the standardised signal level can itself be described and accounted for (section 4).

Standardised dose response characteristics were previously analysed for the effect of test dose size by Burbidge *et al*. (2006), who used quadratic approximations ($I_S = aD^2 + bD + c$) to (1)., for limited ranges of D in order to separate gradient as an orthogonal component of the fits. A suite of samples were examined using test doses between 1 and 7 Gy, and change in b was found to be well approximated by a linear expression in this range (Burbidge *et al*., 2006, Eqn. 4). Burbidge (2003) analysed the same data for the saturating exponential case and found change in I_{SMax}/D_0 with D_T to be identical to change in b for the quadratic case, within uncertainties. Thus, for a fixed value of D_0, I_{SMax} was observed to be 10% higher for D_T = 7 Gy than for D_T = 1 Gy. Shen and Mauz (2011, Fig. 5) have measured an approximately linear increase in standardised luminescence response to a dose of 7.2 Gy with test doses between 1.8 and 35 Gy. They used this to establish correction factors for measurements made on fine grains prepared from loess using a variety of test doses. The increase they observed between D_T = 1.8 and 23 Gy was approximately 40%, but unlike in Fig. 2 their uppermost data point indicated a slight tendency for sublinearity. The results of the present study show that these linear relationships are approximations and that a more complete and accurate descriptor is provided by (29) and (30), in these cases simplifiable into the forms of (16) and (19), and illustrated in Fig. 2. The apparent sublinearity observed by Shen and Mauz (2011) may be the result of other factors and merits further investigation.

The simplified case (section 4) where the signal and test signal in (15) may be assumed to relate to the same dose response characteristic is likely to apply where the same type of signal is measured for the dose response and test response, following preheats of similar magnitude or at least of similar effect on trapping probability, *e.g.* in single aliquot regenerative optically stimulated luminescence (SAR OSL) measurement of quartz, or in infrared stimulated luminescence (IRSL) measurement of feldspars using matching preheats for dose and test dose responses. The general case for (19) applies where different signals are used to measure the dose response characteristic and the test response, *e.g.* in thermally transferred OSL (TTOSL) using an OSL test response or in OSL using the 110 °C thermally stimulated luminescence (TSL) test response, or where different preheats are applied to measure the dose response characteristic and the test response from a continuous trap distribution (a possibility for *e.g.* IRSL measurement of feldspars) (Table 2).

6.3. Dose dependent changes in recombination and trapping probability

In sections 3 and 4 calculations were made for a fixed test dose assuming that this would provide a fixed test dose response. Everyday experience with protocols such as SAR and studies such as Chen (1979), Stokes (1994) and Bailey (2000) show that test response relative to dose response varies as a function of dose, predose, and non-dose dependent factors. In particular, heating following irradiation tends to produce large increases in luminescence sensitivity in quartz, by increasing the relative availability of luminescent recombination sites. (OSL) measurement tends to reduce this, and hence to reverse any such increases, by recombination at such sites. The relative magnitude of each of these phenomena is different in different materials. For quartz, Stokes (1994, Fig 3) shows positive and negative changes of up to 2.5 times through the sequence. These appear to vary as a function of the saturating dose response, but their cumulative effects between I and I_T were much smaller. Murray and Wintle (2000, Fig. 3) report similar changes but focus only on this cumulative effect: decreases of 8 % and 17 % were observed. In both papers the changes occur at rates, with respect to increasing dose, D, which are apparently consistent with saturation based on a D_0 value *c.* 30-50 Gy and so relate to the level of the dominant OSL signal in the quartz samples in this dose range.

In section 5, k and l were introduced to describe changes in recombination and trapping probability between I and I_T ((24), (25)). Their effects were explored for the case that they follow saturating exponential functions of dose, D ((27), (28)). When considering the effects of k and l as described in the present study, some care is required with terminology for the comparison of certain results between other studies. It is the case that "D", the "dose" referred to in the present study and in the above discussion of Stokes (1994) and Murray and Wintle (2000), would be considered to be the "predose" in other contexts (*e.g.* Chen, 1979). In the present work, "predose" would refer to all irradiations prior to "D", but the focus of the present study is on dose (D) dependent effects and ignores the others. This is because the effects of D are generally predominant following a given irradiation, whether through simple dose response or through activated predose response, and it appears possible to explain many forms of standardised dose response characteristic (29) by assuming that transforms for recombination and trapping probability (k and l) are functions of D, without recourse to other effects (Fig. 3-Fig. 7, Table 3, Table 4).

In Fig. 3 and Fig. 5, k_{Max} and l_{Max} were chosen to be -0.99 and 100 to illustrate the extreme forms or end members of the effects of dose dependent change in k and l. k_{Max} was observed to have a far greater influence than l_{Max}, on the magnitude of changes produced in I_T relative to I, and hence in the form of the dose response characteristic, I_S (Fig. 4). For k_{Max} = -0.99 and 100, I_T decreased and increased respectively by 100 times, while for l_{Max} = -0.99 I_T decreased by 2.5 times and for l_{Max} = 100 I_T increased by only 1%. The lower sensitivity to l relates to the counterbalancing effects of its presence as a multiplier of both I_{Max} and D_0 ((24), (25)). Thus, a given change in trapping probability has much less effect on the form of the dose response characteristic than a change in recombination probability of similar magnitude. Where recombination or trapping probability was made to reduce with dose in (29) (Fig. 3a, Fig. 5a), results for case 1/ are similar to the shape commonly reported for superlinear un-normalised TSL dose response characteristics of TLDs (*e.g.* McKeever 1985, Fig 3.27). Case 2/ exhibits an inflection as do some dose response characteristics obtained using electron paramagnetic resonance (EPR) (*e.g.* Schellmann *et al*., 2008), but on a linear axis these curves tend towards an exponential plus linear appearance, which is commonly reported for (normalised) SAR OSL dose response characteristics (*e.g.* Murray and Wintle, 2000; Shen and Mauz, 2011). For increases in recombination or trapping probability with dose (Fig. 3b, Fig. 5b), case 3/ is similar to the shape commonly reported for superlinear un-normalised thermally stimulated luminescence dose response characteristics of heated quartz (*e.g.* McKeever 1985, Fig 4.1). Case 4/ is similar to dose normalised dose response characteristics reported for quartz by Burbidge *et al*. (2011), for OSL measurements subject to additional heating (thermal activation) between measurement of I and I_T .

In Fig. 6 are presented curves where l_{Max} is set to 0 and k_{Max} was chosen to produce differences in curve shape of magnitudes relevant to datasets obtained from real samples in luminescence analyses. The data in Fig. 6 a. and b. are calculated based on a *c*. ±20% change in the relationship between the sensitivity of the sample at the beginning of measurement I, relative to that of I_T, as a function of dose. The level of variability is similar to that observed between samples in single aliquot data, *e.g.* the differences between standardised growth curves observed by Hong and Choi (2008) and Telfer *et al*. (2008). Stronger variations in the form of the normalised dose response have been reported for individual grains than for multi-grain single-aliquot or multiple aliquot measurements (*e.g.* Duller *et al.*, 2000; Yoshida *et al.*, 2000). Such variability has been simulated in Fig. 6 c. and d. by assuming multiplicative or divisive changes of *c*. 5 times between I and I_T. In most cases the data are well approximated by a single saturating exponential within the fitted range of dose values (0-166), but exponential plus linear or even simpler linear fits appear more appropriate in some cases (Fig. 6, Table 3). However, the parameters of these fits do not relate directly to the fundamental dose response characteristics of the samples. If the curves in Fig. 6 a. and b. were reconstructed from a limited number of real data using dose values below 200 (say five or six dose points as in many of the studies in the bibliography of the present study), then they would simply appear to be single

saturating exponential curves with different characteristics. In the cases of Fig. 6 c. and d. it would be possible to identify some differences from the single saturating exponential form, but only if the data were precise and numerous at both high and low doses. When the (approximately) saturating exponential plus linear data in Fig. 6 are fitted with curves of this form, the 'plus linear' component reflects the average rate of the change in test response in the upper part of the dose range fitted but D_0 tends to be underestimated. This is similar to the behaviour of fits applied to signals composed of multiple saturating components (Fig. 1). Observations of variations in the contribution of 'plus linear' components (*e.g.* Shen and Mauz, 2011, section 3.2), which do not conform to a conventional view of proportional increases in I_{Max} and D_0 (as a function of trapping probability) may therefore be looked at as either a difference in the contribution of a signal component with a high D_0 value, or a greater degree of change in recombination probability between I and I_T.

6.4. Non-monotonicity

Burbidge *et al*. (2011) reported OSL measurements made within a TTOSL protocol, where a significant dose dependent increase in recombination probability is expected to have occurred between I and I_T, as a result of the additional heating prior to TTOSL measurement (see Stokes, 1994, Fig. 3). In Burbidge *et al*. (2011) the samples were also heated to 500 °C between measurement cycles to reset residual signals. As such the dose D, plus a test dose of 10.5 Gy, was thermally activated in each case and sensitivity increased between measurement cycles. Sensitisation was strongest for $D = 0$, and reduced by 30% to 90% as D was increased to 20 kGy. In the application of (29) this would indicate $k_{Max} \approx$ -0.3 to -0.9, while the rate of change with dose appeared consistent with D_{k0} values around 3 kGy. Dose response characteristics exhibiting superlinear (case 1) and non-monotonic behaviour were observed (cases 4/ and 5/). Fig. 7, curve c. is obtained straightforwardly using (29). It indicates a single component saturating exponential dose response characteristic affected by a strong dose dependent increase in recombination probability between I and I_T. In such cases the peak is located at the D value for which the two parts of (30) are equal, it moves to lower doses if values of $l_0<1$ are included, but $l_0>1$ has little effect. Curve a. in Fig. 7 is similar to c., but includes an additional saturating exponential signal component to account for renewed increases in signal level at doses above the peak (Table 4). However, it was not possible to describe accurately using (26), (27), and (29) the dose at which the peak maximum occurred, or the magnitude of the "trough" at slightly higher doses, using the value of k_{Max} that was required in order to bring I_S down to the observed levels. This also necessitated the use of a smaller D_0 value for component 1 when compared with curve c., which was very similar to curve a. but did not require component 2 (Table 4, and see end of previous paragraph). To be dose dependent, the down curve of the peak in curve a. would require descriptors other than (26) and (27). Curve b. in Fig. 7 was well approximated using (26), (27), and (29), but this required the employment of all the parameters in (29), often in ways that do not appear to square with the rationale developed in the present study, *viz.* the arbitrary use of l in addition to k, the use of k_0 and l_0 values other than unity, and the summing of a negatively saturating signal component.

The employment of more parameters than data points to fit a given set of data, in the case of curve b. in Fig. 7, illustrates that although there are many parameters in the construction of (29), they are non-orthogonal, *i.e.* they are interrelated just as in (1) (*c.f.* use of polynomials by Burbidge *et al.*, 2006). For this reason, the assumption that I and I_T are related through k and l as described in (24) to (30) is actually quite restrictive on the form of the curve that can be obtained. The restriction becomes increasingly evident the more I_S at $D = \infty$ deviates from $I_{SMax} \approx D_0$, *i.e.* the more extreme the value of k or l. Comparison with the extreme set of real data in Fig. 7, where Max. I is at least an order of magnitude lower than the D_0 value of the most rapidly saturating component (Table 4 and *c.f.* Table 3), indicates that while the use of (29) with the assumption that k and l follow saturating exponential functions of dose D can well describe many aspects of dose normalised dose response characteristics, it cannot describe them all. More complex numerical models (*e.g.* Bailey, 2001, for luminescence of quartz) may be better

able to describe these in detail (McKeever, 1985, Ch 3.4), but outputs from complex models themselves need to be analysed to understand which components are important or indeed relevant to the system under examination (Sivia, 2006). The analysis elaborated in the present study may be used to distinguish which forms are produced by dose dependent sensitivity change between I_S and I_T, and which may be due to other factors. Lawless *et al*. (2005) review and model non-monotonic luminescence dose responses: they demonstrate that the effect can be explained in relation to superlinearity and that traditional interpretations based on radiation damage effects are unnecessary. They obtained curves similar to Fig. 7, curve c, in cases dominated by competition (for holes) between two different recombination centres during excitation (irradiation in the terminology of the present study). Curves similar to Fig. 7, curve b were obtained for cases dominated by competition during heating (readout). However, additional components of signal increase were not considered, nor was the absolute position of the peak in the non-monotonic response, or variability in this.

6.5. Beyond dose dependent effects

Dose dependent effects produce differences in the form of the dose response characteristic but do not in themselves affect the evaluation of absorbed doses, *i.e.* the use of controlled irradiations of samples to calibrate, *a posteriori*, an unknown absorbed dose. Factors that do influence this include dose rate, cumulative "pre"-dose, and non-dosimetric chemical changes. In discussion of the results of Burbidge *et al.* (2011), when presented at UKLED2010, it was evident that similar forms of dose response characteristic had been observed by G.A.T. Duller, S.J. Armitage and R.M. Bailey; who indicated that they could be modelled using thermally unstable "R centres". These centres may correspond to a delocalised band discussed above in respect of superlinearity, but charge losses due to thermal instability imply dose-rate effects. Differences in trapping probability as a function of dose rate can only be evident where the rate of charge build-up (dose rate) differs significantly in relation to, but remains greater than, the rate of charge loss (de-trapping rate), and that the difference is integrated over a dose sufficiently large that a significant degree of saturation of the delocalised band is achieved (Groom *et al*., 1978). The dose dependence of dose rate effects, or vice versa, indicates that they could be described in (29) by adjusting the form of (27). To quantitatively reproduce some features of dose response characteristics at higher doses (*e.g.* Fig. 7), such an adjustment would need to augment the effect of relative trapping probability (l) on the form of (29), which presently appears weak when compared to relative recombination probability (k, section 5). The reader is reminded that since the signal is normalised, any proportional changes or differences that apply to both I and I_T cancel, so that it is the relationship between the two that is important. In the context of (26), (27), and (29), the predose and non-dose dependent changes require that k_0 and/or l_0 are not fixed, so that the basis value for each I, I_T pair is different, whether D is varied or not. Assuming consistent thermal pre-treatments and measurement conditions, this only applies where repeated I, I_T pairs are measured consecutively on the same sample (*e.g.* in protocols such as SAR or multiple activation predose. Bailey, 2000; Chen, 1979). The responses to cumulative predose and measurement cycle (non-dose dependent) could be based on the saturating exponential form, just as for dose and relative trapping and recombination probability in the present study, and related to dose as discrete functions when necessary.

7. Conclusions

The present study elaborates an approach to describing dose normalised dose response characteristics which, being based on the consequences of simple and established physical descriptions of dose response, can help to indicate what type of physical mechanism is involved in producing a particular form of dose response characteristic. The analysis was based solely on the consideration of dose response, normalisation/test dose response, and changes in trapping and recombination probability between dose and normalisation/test dose (irradiations and measurements), which were each assumed to follow saturating exponential functions of dose or normalisation/test dose. A combination of these functions was developed, described, and its

geometry explored, using basic algebraic manipulation and calculus, and illustrated with plots and tables of calculated examples and approximations to published datasets. It is able to quantitatively reproduce most observed features of dose-normalised dose response characteristics, and provides an analytical framework for the exploration of the effects of other factors on dose response and absorbed dose evaluation. The relevance of the algebraic-geometric analyses in the present study is further indicated by emergent relationships between aspects of the results and features of the basic physical models underlying their calculation. The present study did not investigate the particular chemical changes or solid state reactions that ultimately produce the effects described.

Signal levels at saturation in normalised dose response characteristics (I_{NMax}) depend strongly on test or normalisation dose size and this does not affect the mean-dose of trap filling (D_0). Standardisation of the dose response characteristic to the test or normalisation dose reduces this dependence, particularly for low test/normalisation doses. If generally adopted this manner of presentation would greatly facilitate inter-comparison between published works.

The assumption of a fixed linear test dose response was shown to result in a standardised saturating exponential dose response characteristic for which, by definition, the signal at saturation (I_{SMax}) is approximately equal to mean-dose of trap filling (D_0), and the gradient ($\delta I_S/\delta D$) at zero dose is approximately unity. This assumption is implicit in most published comments on dose normalised dose response characteristics in the literature: standardised dose response characteristics published to date indicate that it is commonly approximated. Deviations from this case can be used to identify samples exhibiting more complex behaviour.

Changes in recombination probability, as a function of dose, between the beginning of the measurement of the dose response and the measurement of the test/normalisation dose response, produce a dose response characteristic that does not follow the saturating exponential form, and which can exhibit non-monotonic behaviour (peaks and troughs) as the result of changes in recombination probability. Changes in trapping probability produce effects of a similar form but of much reduced amplitude.

A degree of variability in the parameter values obtained from saturating exponential fits may result simply from the presence of additional poorly resolved saturating components. However, even moderate changes in recombination probability between dose and test dose measurements produce fits with widely varying parameter values, even though the data are well approximated by the saturating exponential or saturating exponential plus linear forms, for limited ranges of doses. Complex non-exponential forms of dose normalised dose response are obtained where severe heating is applied between measurement of the dose response and the normalisation response, as a result of additional thermal activation. These differences from the saturating exponential form make fits of this type (or summed saturating exponential curves, or saturating exponential + linear curves) unreliable for parameter evaluation and extrapolation.

Most variations in the form of the dose normalised dose response characteristic can be described as functions of dose, D. In this case absorbed dose evaluation is not made inaccurate by the variations in the shape of the dose response characteristic, except through complicating data reduction. Variations in the form of the dose normalised dose response characteristic caused by dose rate, predose and non-dose dependent effects, will affect the accuracy of absorbed dose evaluations. The present study also provides an analytical framework through which these may be explored. It has focussed on radiation dosimetry using luminescence measurements, with a particular emphasis on the behaviour of OSL signals from quartz, but the approach and findings are expected to be relevant to other dosimetric methods where dose normalised signals are employed.

8. References

Aitken, M.J. 1985. Thermoluminescence dating. Academic Press, London.
Bailey, R.M. 2000. Circumventing possible inaccuracies of the single aliquot regeneration method for the optical dating of quartz. Radiation Measurements 32, 833-840.
Bailey, R.M., 2001. Towards a general kinetic model for optically and thermally stimulated luminescence of quartz. Radiation Measurements 33, 17-45.
Bird, J.O., 1988. Newnes mathematics pocket book for engineers. Butterworth-Heinmann Ltd., Oxford.
Burbidge, C.I. 2003. Luminescence investigations and dating of anthropogenic palaeosols from South Mainland Shetland. University of Wales, Aberystwyth. 396 p, Unpublished PhD Thesis.
Burbidge, C.I., Cabo Verde, S.I., Fernandes, A.C., Prudêncio, M.I., Botelho, M.L., Dias, M.I., Cardoso, G.O. 2011. Dosimetry in the multi kilo-Gray range using optically-stimulated luminescence (OSL) and thermally-transferred OSL from quartz. Radiation Measurements 46, 860-865.
Burbidge, C.I., Duller, G.A.T., Roberts, H.M. 2006. De determination for young samples using the standardised OSL response of coarse grain quartz. Radiation Measurements 41, 278-288.
Charitidis, C., Kitis, G., Furetta, C., Charalambous, S., 2000. Superlinearity of synthetic quartz: dependence on the firing temperature. Nuclear Instruments & Methods in Physics Research Section B- Beam Interactions with Materials and Atoms 168, 404-410.
Chen, R. 1979. Saturation of sensitization of the 110 °C peak in quartz and its potential application in the pre-dose technique. Specialist Seminar on TL Dating, Oxford, 1978. Council of Europe PACT Journal 3, 325-335.
Chen, R., McKeever, S.W.S., 1994. Characterization of nonlinearities in the dose dependence of thermoluminescence. Radiation Measurements 23, 667-673.
Duller, G.A.T., Bøtter-Jensen, L., Murray, A.S. 2000. Optical dating of single sand-sized grains of quartz: sources of variability. Radiation Measurements 32, 453-457.
Forman, L.S., Pierson, J. 2002. Late Pleistocene luminescence chronology of loess deposition in the Missouri and Mississippi river valleys, United States. Palaeogeography, Palaeoclimatology, Palaeoecology 186: 25-46.
Groom, P.J., Durrani, S.A., Khazal, K.A.R., McKeever, S.W.S., 1978. The dose-rate dependence of thermoluminescence response and sensitivity in quartz. Council of Europe PACT Journal 2, 200-210.
Grün, R., 1996. Errors in dose assessment introduced by the use of the «linear part» of a saturating dose response curve. Radiation Measurements 26, 297-302.
Hampshire, S. 1956. The age of reason, the 17th century philosophers. Mentor, New York.
Hong, D.G., Choi, J.H. 2008. Investigations on standardized growth curve (SGC) procedure for optical dating of heated quartz. Journal of Radioanalytical and Nuclear Chemistry 275, 613-617.
Lai, Z-P. 2006. Testing the use of an OSL standardised growth curve (SGC) for De determination on quartz from the Chinese Loess Plateau. Radiation Measurements 41, 9-16.
Lamothe, M., Auclair, M. 1999. A solution to anomalous fading and age shortfalls in optical dating of feldspar minerals. Earth and Planetary Science Letters 171(3): 319-323.
Lawless, J.L., Chen, R., Lo, D., Pagonis, V., 2005. A model for non-monotonic dose dependence of thermoluminescence (TL). Journal of Physics: Condensed Matter 17, 737-753.
McKeever, S.W.S. 1985. Thermoluminescence of Solids. Cambridge University Press.
Mische, E.F., McKeever, S.W.S., 1989. Mechanisms of supralinearity in lithium flouride thermoluminescence dosemeters. Radiation Protection Dosimetry 29, 159-175.
Murray, A.S., Wintle, A.G. 2000. Luminescence dating of quartz using an improved single-aliquot regenerative-dose protocol. Radiation Measurements 32, 57-73.
Olley, J.M., De Deckker, P., Roberts, R.G., Fifield, L.K., Yoshida, H., Hancock, G. 2004. Optical dating of deep-sea sediments using single grains of quartz: a comparison with radiocarbon. Sedimentary Geology 169, 175-189.

Roberts, H.M., Duller, G.A.. 2004. Standardised growth curves for optical dating of sediment using multiple grain aliquots. Radiation Measurements 38, 241-252.

Schellmann, G., Beerten, K., Radtke, U. 2008. Electron spin resonance (ESR) dating of Quaternary materials. Eiszeitalter und Gegenwart Quaternary Science Journal 57, 150-178.

Shen, Z., Mauz, B. 2011. Estimating the equivalent dose of late Pleistocene fine silt quartz from the lower Mississippi Valley using a standardized OSL growth curve. Radiation Measurements 46, 649-654.

Sivia, D.S., 2006. Data analysis: a Bayesian tutorial, 2nd Edn. Oxford University Press.

Stokes, S. 1994. The timing of OSL sensitivity changes in a natural quartz. Radiation Measurements 23, 601-605.

Telfer, M.W., Bateman, M.D., Carr, A.S., Chase, B.M., 2008. Testing the applicability of a standardized growth curve (SGC) for quartz OSL dating: Kalahari dunes, South African coastal dunes and Florida dune cordons. Quaternary Geochronology 3, 137-142.

Timar-Gabor, A., Vandenberghe, D.A.G., Vasiliniuc, S., Panaiotu, C.G., Dimofte, D., Cosma, C., 2011. Optical dating of Romanian loess: a comparison between silt-sized and sand-sized quartz. Quaternary International 240, 62-70.

Wintle, A.G., 1997. Luminescence dating: laboratory procedures and protocols. Radiation Measurements 27, 769-817.

Captions

Fig. 1. Un-normalised (I, a. - c.) and normalised or standardised (I_N, I_S, d. - e.) dose response characteristics calculated using (1) and (18). The D_T value used to calculate I_S was 1, so $I_N = I_S$. Two saturating exponential components were summed ($\sum \boldsymbol{I}$): a dominant component ($\boldsymbol{I_1}$), for which $I_{Max} = I_{TMax} = 4$, and $D_0 = D_{T0} = 50$, and a minor component ($\boldsymbol{I_2}$), for which $I_{Max} = I_{TMax} = 1$, and $D_0 = D_{T0} = 100$ (in a. and d.), 500 (in b. and e.) or 5000 (in c. and f.). $\sum I$ was approximated (**Predicted** $\sum \boldsymbol{I}$) by calculating dI/dD at $D = 0$ and I_{Max} (using (5), (6), (22), and (23)), and then assuming values of D_0 predicted from these equations, as if the curve were a simple saturating exponential and not a sum of saturating exponentials. $\sum I$ was then fitted using an equation of the form (1) in the range $D = 0$-166 (**Fit** $\sum \boldsymbol{I}$**, D = 0-166**), to illustrate the dose response characteristic that would be obtained from a dataset for a limited range of doses when single saturating exponential dose response was assumed. Input values and results of the calculations and fits are listed in Table 1.

Fig. 2. I_{SMax} and $\delta I_S/\delta D$ at $D = 0$ calculated for a range of test doses (D_T) using (16) and (19), assuming $I_{Max} = I_{TMax} = 1$ and $D_0 = D_{T0} = 38$ Gy: the D_0 value observed when low test doses were used by Burbidge *et al*. (2006). Inset a plot of the same data with axis extended, into the physically meaningless region of negative D_T, to illustrate the form of the curve. Limits for low and high D_T values ((20), (21)) are indicated by dashed lines. A linear fit to the calculated values of $\delta I_S/\delta D$ at $D = 0$ for D_T values between 1 and 7 Gy gives $y = 0.014\,x + 0.999$, *i.e.* the parameters are within errors of those in (**Error! Reference source not found.**). Examples of normalised and standardised dose response characteristics for D_T values between 1 and 7 Gy are presented in Burbidge *et al*. (2006), Fig. 1. An equivalent plot for I_{NMax} and $\delta I_S/\delta D$ at $D = 0$ is included to illustrate the much stronger variation of this signal with D_T; note logged axes.

Fig. 3. Standardised dose response characteristics calculated using (29), to illustrate how the form changes as D_{k0} is varied, relative to a D_0 value of 50, for different values of k_{Max}: *i.e.* for different rates and magnitudes of dose (D) dependent change in recombination probability, between the measurement of dose response I (D) and the measurement of the response to the normalisation or test dose (D_T), I_T. In a., $k_{Max} = -0.99$, in b., $k_{Max} = 100$. In each plot are shown curves for $D_{k0} = 0.5$, 5, 50, 500 and 5000. In all cases $D_T = 1$, $I_{Max} = 1$, $D_0 = 50$, $k_0 = 1$, $l_0 = 1$, $l_{Max} = 0$, and $D_{l0} = 1$. Since the D_T value used to calculate I_S was 1, $I_S = I_N$. The dotted line indicates the dose response characteristic for $k_{Max} = 0$, *i.e.* no change in recombination probability. Inset is the dose dependent change in a subsequently measured normalisation or test dose response, I_T relative to I, which produces the dose dependent change in the dose response characteristics.

Fig. 4. Standardised dose response characteristics calculated using (29), to illustrate how the form changes as k_{Max} is varied, for different values of D_{k0} (relative to a D_0 value of 50): *i.e.* for different magnitudes and rates of dose (D) dependent change in recombination probability, between the measurement of dose response I (D) and the measurement of the response to the normalisation or test dose (D_T), I_T. In a., $D_{k0} = 5000$ (*i.e.* $> D_0$), in b., $D_{k0} = 0.5$ (*i.e.* $< D_0$). In each plot are shown curves for $k_{Max} = -0.99$, -0.9, 0, 10, and 100. In all cases $D_T = 1$, $I_{Max} = 1$, $D_0 = 50$, $k_0 = 1$, $l_0 = 1$, $l_{Max} = 0$, and $D_{l0} = 1$. Since the D_T value used to calculate I_S was 1, $I_S = I_N$. Inset is the dose dependent change in a subsequently measured normalisation or test dose response, I_T relative to I, which produces the dose dependent change in the dose response characteristics.

Fig. 5. Standardised dose response characteristics calculated using (29), to illustrate how the form changes as D_{l0} is varied, relative to a D_0 value of 50, for different values of l_{Max}: *i.e.* for different rates and magnitudes of dose (D) dependent change in trapping probability, between the start of irradiation with the dose, D, and the start of irradiation with the normalisation or test dose, D_T. In a., $l_{Max} = -0.99$, and curves are shown for $D_{l0} = 0.5$, 5, 50, 500 and 5000. In b., $l_{Max} = 100$ and curves are shown for $D_{l0} = 50$, 500, 5000, 50000 and 500000. In all cases $D_T = 1$, $I_{Max} =$

1, D_0 = 50, l_0 = 1, k_0 = 1, k_{Max} = 0, and D_{k0} = 1. Since the D_T value used to calculate I_S was 1, I_S = I_N. The dotted line indicates the dose response characteristic for l_{Max} = 0, *i.e.* no change in trapping probability. Inset is the dose dependent change in a subsequently measured normalisation or test dose response, I_T relative to I, which produces the dose dependent change in the dose response characteristics.

Fig. 6. Standardised dose response characteristics calculated using (29), using different values of k_{Max} and D_{k0}, to illustrate variations in shape that are similar in form and magnitude to those observed in single aliquot (a. and b.) and single grain (c. and d.) data. In a., k_{Max} = 0.2, in b. -0.2, in c. 4, and in d. -0.8. In each plot are shown curves for D_{k0} = 5, 50, 500 and 5000. In all cases D_T = 1, I_{Max} = 1, D_0 = 50, k_0 = 1, l_0 = 1, l_{Max} = 0, D_{l0} = 1. Since the D_T value used to calculate I_S was 1, I_S = I_N. Each set of calculated data was fitted using an equation of the form (1) in the range D = 0-166, indicated by dotted lines, to illustrate the dose response characteristic that would be obtained from a dataset for a limited range of doses when single saturating exponential dose response was assumed. Selected characteristics of each curve and fit are listed in Table 3.

Fig. 7. Examples of quartz OSL multi-kGy dose response characteristics, where the dose D was subject to additional thermal activation, *i.e.* increase in recombination probability, in between the measurement of I and I_T (Stokes, 1994; Chen, 1979). The data are selected from Burbidge *et al*. (2011, Fig. 5), standardised, and approximated by curves calculated using (29) with the parameters in Table 4. The data are of dose normalised OSL, but measured within a TTOSL protocol: following irradiation with D, the samples were preheated and the OSL signal measured (I), then they were preheated again to a higher temperature before measurement of the TTOSL signal, following which the test/normalisation dose (D_T) was administered and the samples preheated to a lower temperature, then finally measured by OSL (I_T).

Table 1. Input values and results of the calculations and fits for the curves presented in Fig. 1. Also included are two examples designed to permit comparison of normalised and standardised dose response characteristics where $D_T >> 1$.

Table 2. Example calculations of I_{SMax} for different test doses, for D_0 values relevant to quartz OSL, feldspar IRSL and TTOSL (values are in arbitrary units, but D_0, D_{T0}, D_T, and I_{SMax} may be considered as if they were presented in Gy). Also included are equivalent values of I_{NMax}, to illustrate differences in the patterns of change with test dose size between standardised and normalised signals. In each case the gradient at D = 0 can be obtained by dividing the values by D_0.

Table 3. Maximum signal levels, gradients at D = 0 and saturation rates for the curves plotted in Fig. 6, and the single saturating exponential fits to these data in the range D = 0-166. An example where k_{Max} is set to 0 is included for comparison. Max. I_S was used for the data instead of I_{SMax}, so that where $k_{Max} > 1$, the signal level at the peak would be recorded. In all cases k_0, l_0, D_T and D_{k0} were set to 1, and l_{Max} to 0.

Table 4. Parameter values used to calculate the curves plotted in Fig. 7.

Tables

Table 1, double column table

			$\sum I$ No D_T		$(\sum I)_N = (\sum I)_S$ $D_T = 1$			$(\sum I)_N$ $D_T = 100$	$(\sum I)_S$
	Fig. 1.	a	b	c	d	e	f		
***I*nputs**									
$\boldsymbol{I_1}$	I_{Max}, I_{TMax}	4	4	4	4	4	4	4	4
	D_0, D_{T0}	50	50	50	50	50	50	50	50
$\boldsymbol{I_2}$	I_{Max}, I_{TMax}	1	1	1	1	1	1	1	1
	D_0, D_{T0}	100	500	5000	100	500	5000	5000	5000
Results									
$\boldsymbol{I_1}$	I_{Max}	-	-	-	50.5	50.5	50.5	1.16	116
	dI/dD at D=0	-	-	-	1.01	1.01	1.01	0.0231	2.31
	D_0[1]	-	-	-	50.0	50.0	50.0	50.0	50.0
$\boldsymbol{I_2}$	I_{Max}	-	-	-	101	501	5001	50.5	5050
	dI/dD at D=0	-	-	-	1.01	1.00	1.00	0.0101	1.01
	D_0[1]	-	-	-	100	500	5000	5000	5000
$\sum \boldsymbol{I}$	I_{Max}	5.00	5.00	5.00	56.1	61.6	63.0	1.44	144
	dI/dD at D=0	0.0900	0.0820	0.0802	1.01	1.01	1.01	0.0231	2.31
	D_0[12]	*55.6*	*61.0*	*62.3*	*55.6*	*61.0*	*62.3*	*62.3*	*62.3*
Fit ($\sum I$)	I_{Max}	4.89	4.31	4.03	54.8	53.0	50.8	1.2	116.0
(D = 0-166)	D_0	54.8	53.1	50.4	54.8	53.1	50.4	50.4	50.4
	I_{Max} /D_0[3]	0.0892	0.0811	0.0801	1.00	1.00	1.01	0.0230	2.30

[1] D_0 calculated as $I_{Max}/(dI/dD$ at $D = 0)$, [2] Not appropriate for $\sum I$, but used to calculate "predicted" curve in Fig. 1. for the purposes of illustration. [3] I_{Max}/D_0, = dI/dD at D = 0.

Table 2, single column table

	Example							
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
I_{Max}	1	1	1	1	0,5	1	1	1
D_0	50	50	50	50	50	25	1000	1000
I_{TMax}	1	0,5	0,5	1	1	1	1	1
D_{T0}	50	25	50	25	50	50	1000	50
D_T	$I_{NMax} = (I_{Max} / I_{TMax})/(1-e^{-D_T / D_0})$							
0,1	501	501	1001	251	250	501	10001	501
1	50,5	51,0	101	25,5	25,3	50,5	1001	50,5
10	5,52	6,07	11,0	3,03	2,76	5,52	101	5,52
100	1,16	2,04	2,31	1,02	0,58	1,16	10,5	1,16
1000	1,00	2,00	2,00	1,00	0,50	1,00	1,58	1,00
D_T	$I_{SMax} = D_T (I_{Max} / I_{TMax})/(1-e^{-D_T / D_0})$							
0,1	50	50	100	25	25	50	1000	50
1	51	51	101	26	25	51	1001	51
10	55	61	110	30	28	55	1005	55
100	116	204	231	102	58	116	1051	116
1000	1000	2000	2000	1000	500	1000	1582	1000

Table 3, double column table

Inputs		**Data**			**Fit**		
k_{Max}	D_{k0}	Max. I_S	dI_S/dD at D = 0	Predicted D_0	I_{SMax}	D_0	Predicted dI_S/dD at D = 0
0	**-**	*50.5*	*1.01*	*50.0*	*50.5*	*50.0*	*1.01*
0.2	**5**	42.1	1.01	41.7	41.9	49.4	0.85
($I_T(D=\infty)/I_T(D=0)$) = 1.2	**50**	42.1	1.01	41.7	41.3	42.6	0.97
	500	46.6	1.01	46.1	47.6	46.8	1.02
	5000	49.8	1.01	49.3	50.2	49.6	1.01
-0.2	**5**	63.1	1.01	62.5	63.4	50.8	1.25
($I_T(D=\infty)/I_T(D=0)$) = 0.8	**50**	63.1	1.01	62.5	65.3	61.5	1.06
	500	63.1	1.01	62.5	53.8	53.8	1.00
	5000	63.1	1.01	62.5	50.9	50.4	1.01
4	**5**	10.1	1.01	10.0	8.21	45.8	0.18
($I_T(D=\infty)/I_T(D=0)$) = 5	**50**	10.1	1.01	10.0	7.90	10.5	0.75
	500	25.3	1.01	25.1	22.6	20.5	1.10
	5000	43.1	1.01	42.6	43.3	41.7	1.04
-0.8	**5**	252.5	1.01	250	264	57.9	4.56
($I_T(D=\infty)/I_T(D=0)$) = 0.2	**50**	252.5	1.01	250	4512	3322	1.36
	500	252.5	1.01	250	68.5	71.0	0.97
	5000	252.5	1.01	250	52.0	51.7	1.00

Table 4, single column table

	Curve		
Parameter	**a**	**b**	**c**
D_T	10.5	10.5	10.5
I_{Max1}	1	1	1
D_{01}	1100	3750	1500
I_{Max2}	4.26	-1.6	0
D_{02}	15714	100000	1
k_0	1	100	1
k_{Max}	46	-70	24.5
D_{k0}	4000	1000	2500
l_0	1	0.0000017	1
l_{Max}	0	0.1	0
D_{l0}	1	3000	1

Figures

Fig. 1, double column figure

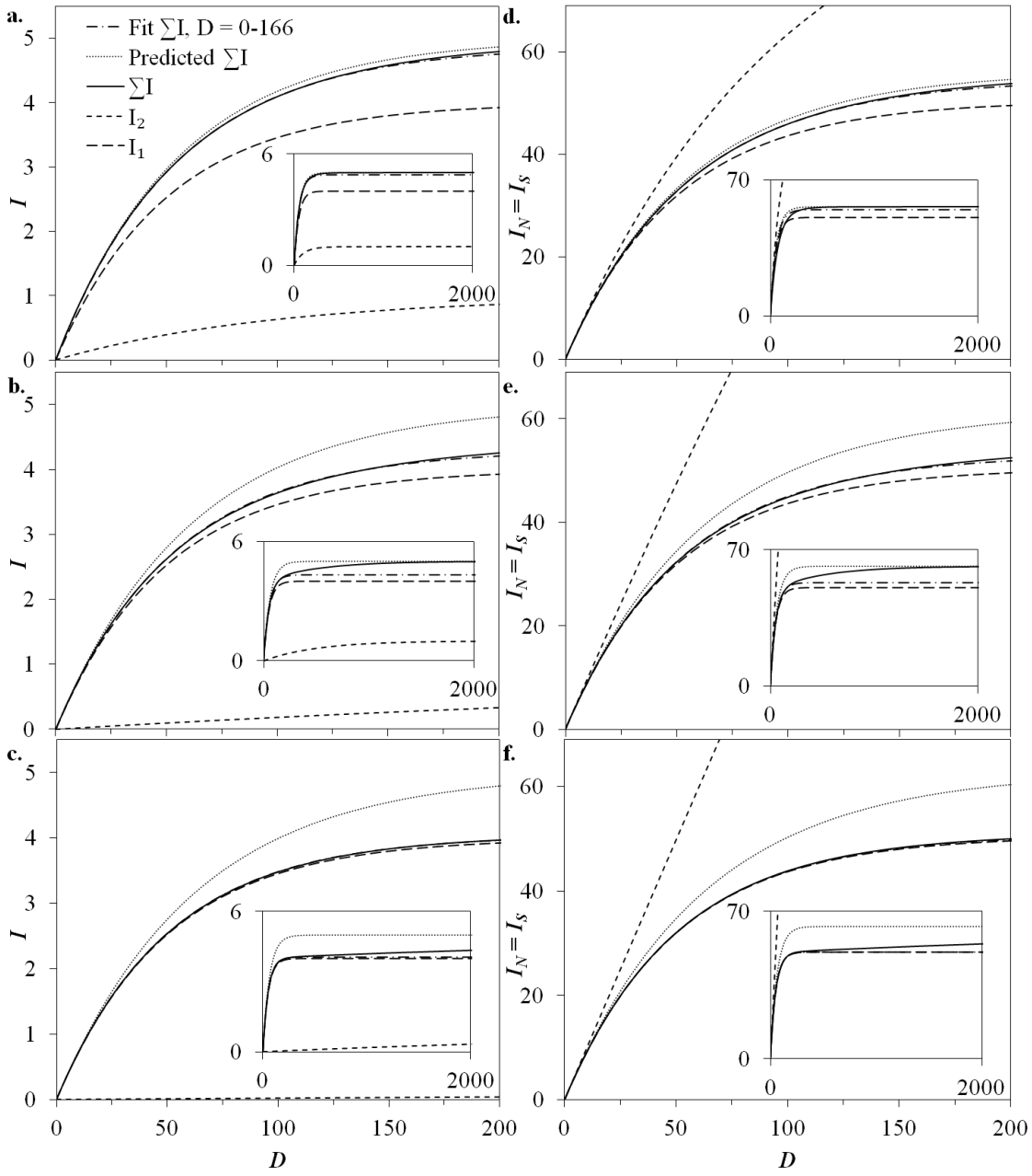

Fig. 2, single column figure

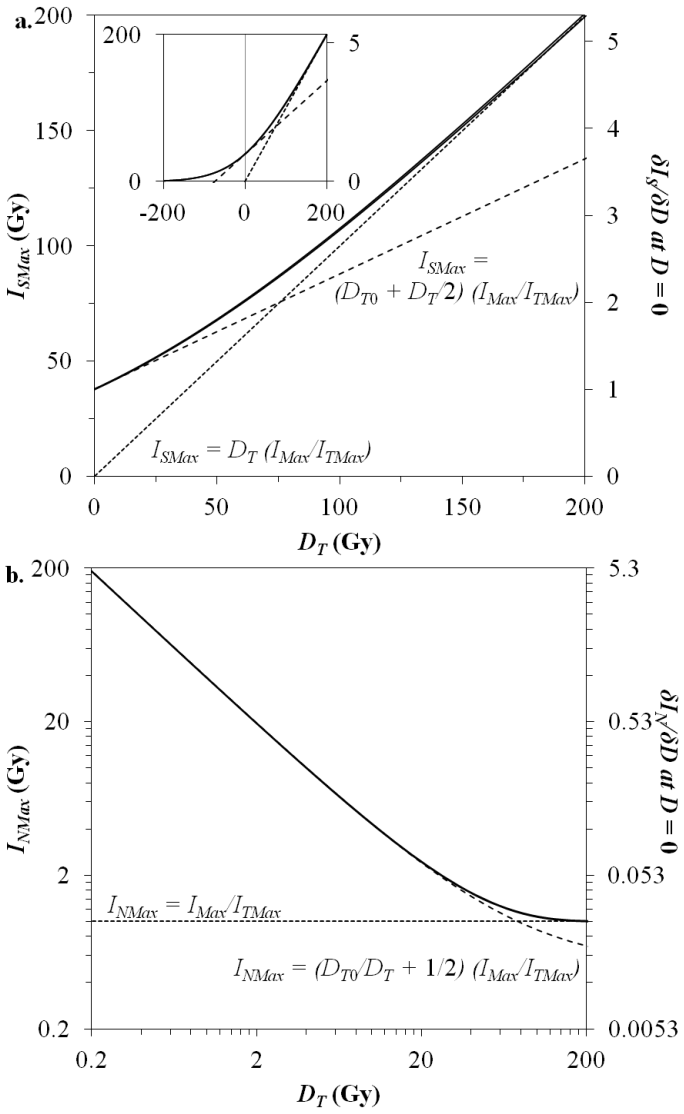

Fig. 3, single column figure

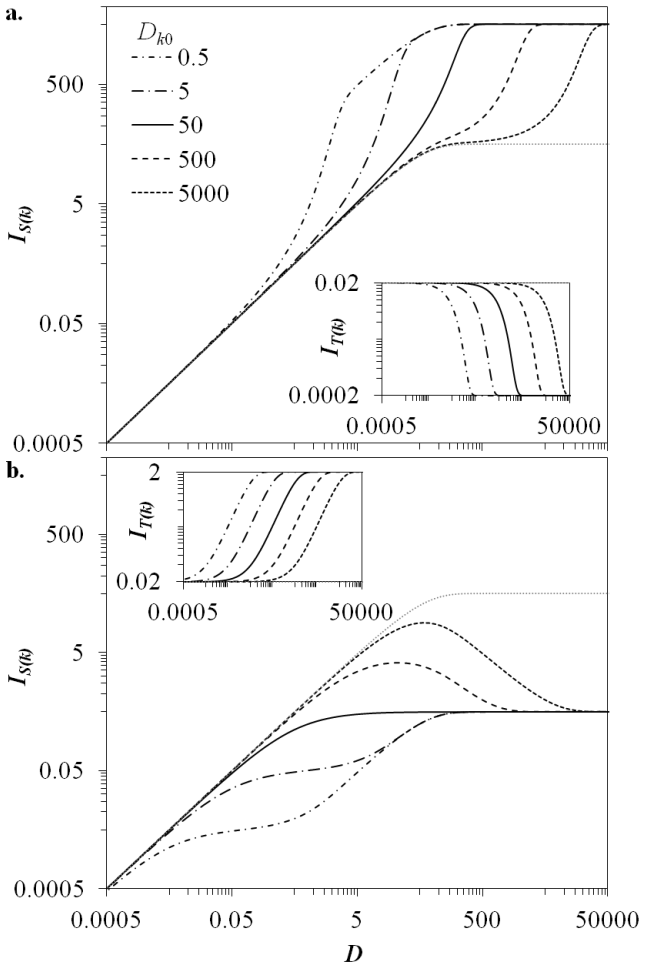

Fig. 4, single column figure

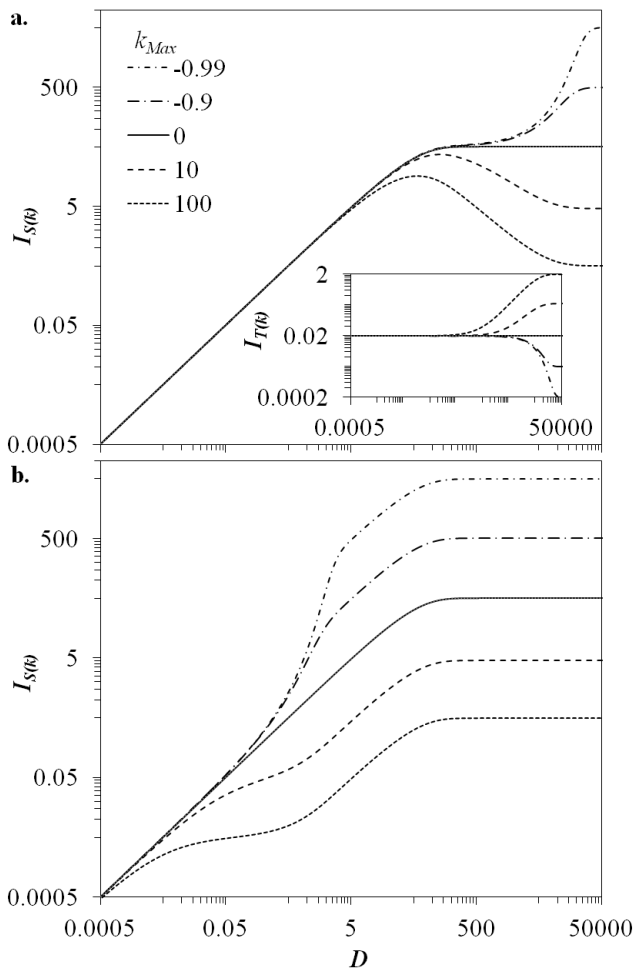

Fig. 5, single column figure

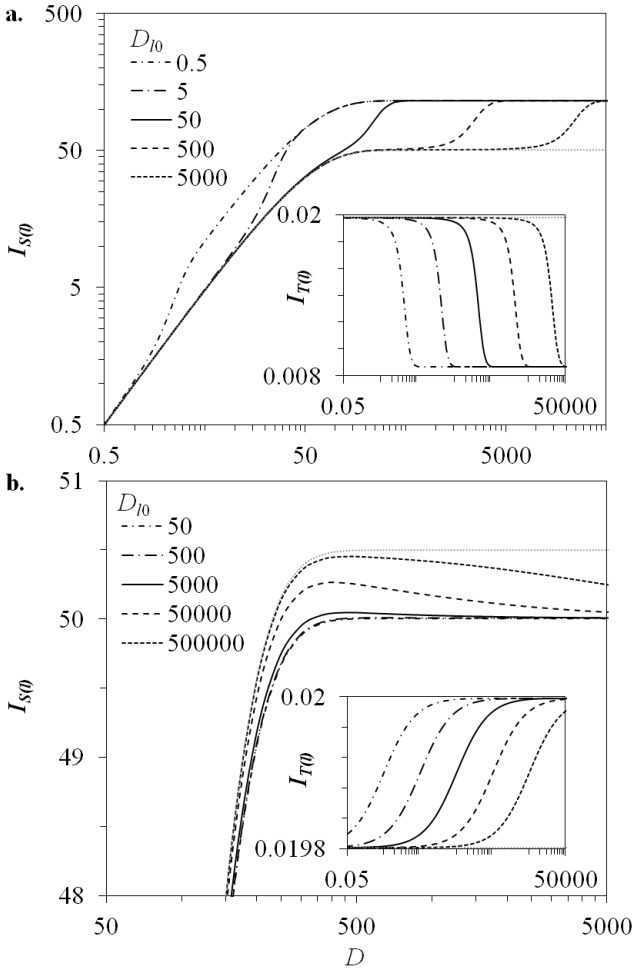

Fig. 6, double column figure

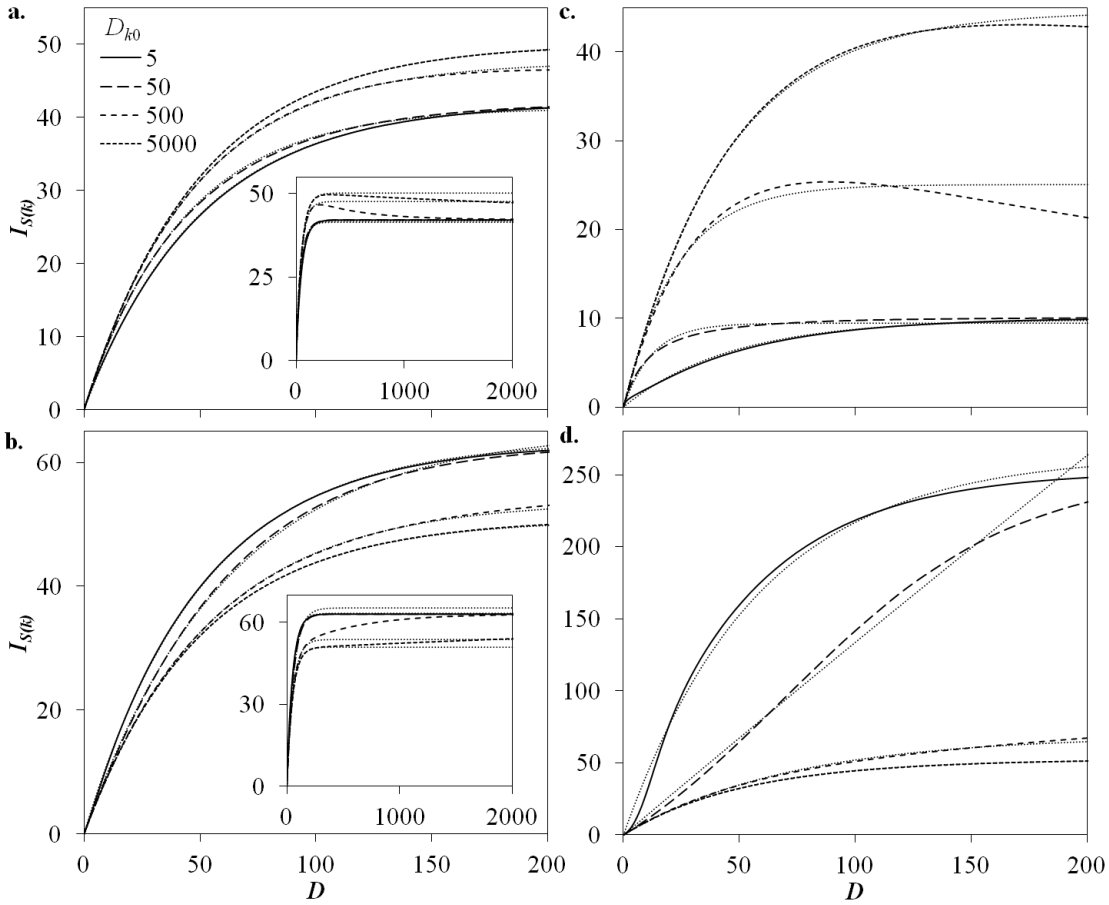

Fig. 7, single column figure

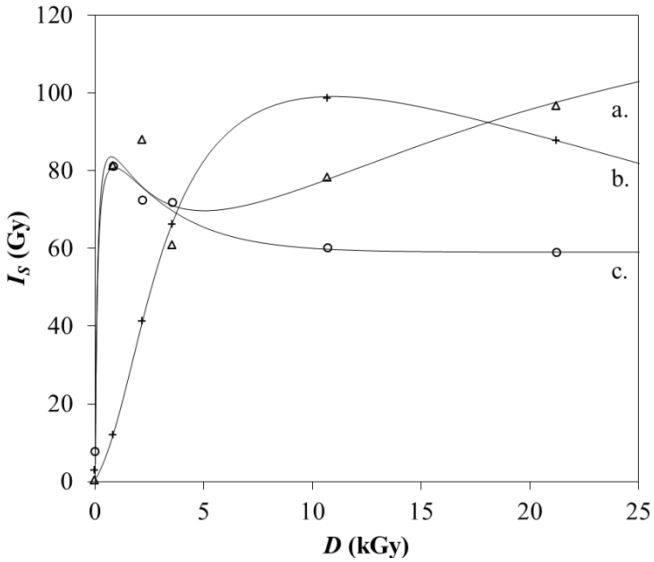

Figure 1

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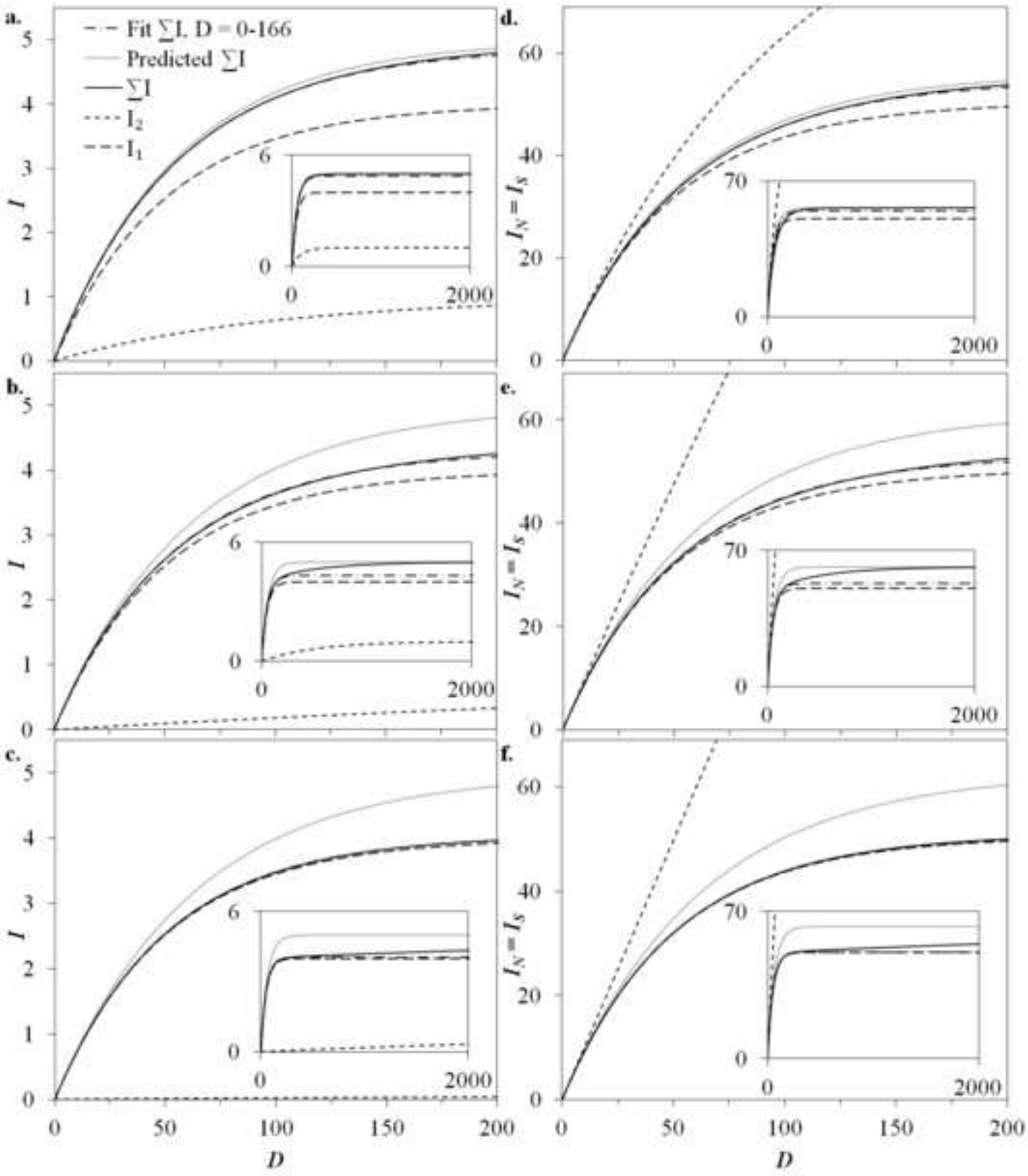

Figure 2

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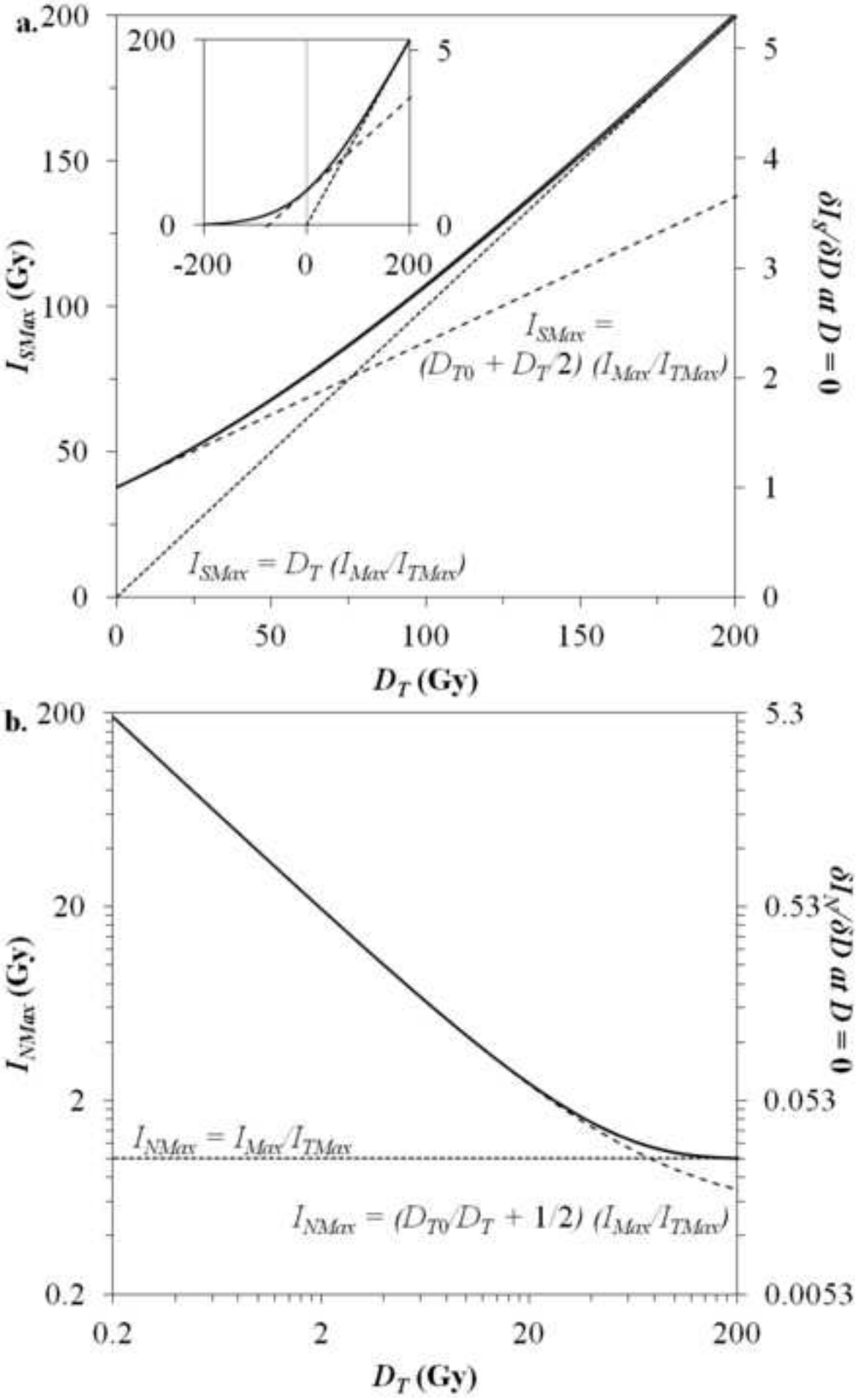

Figure 3

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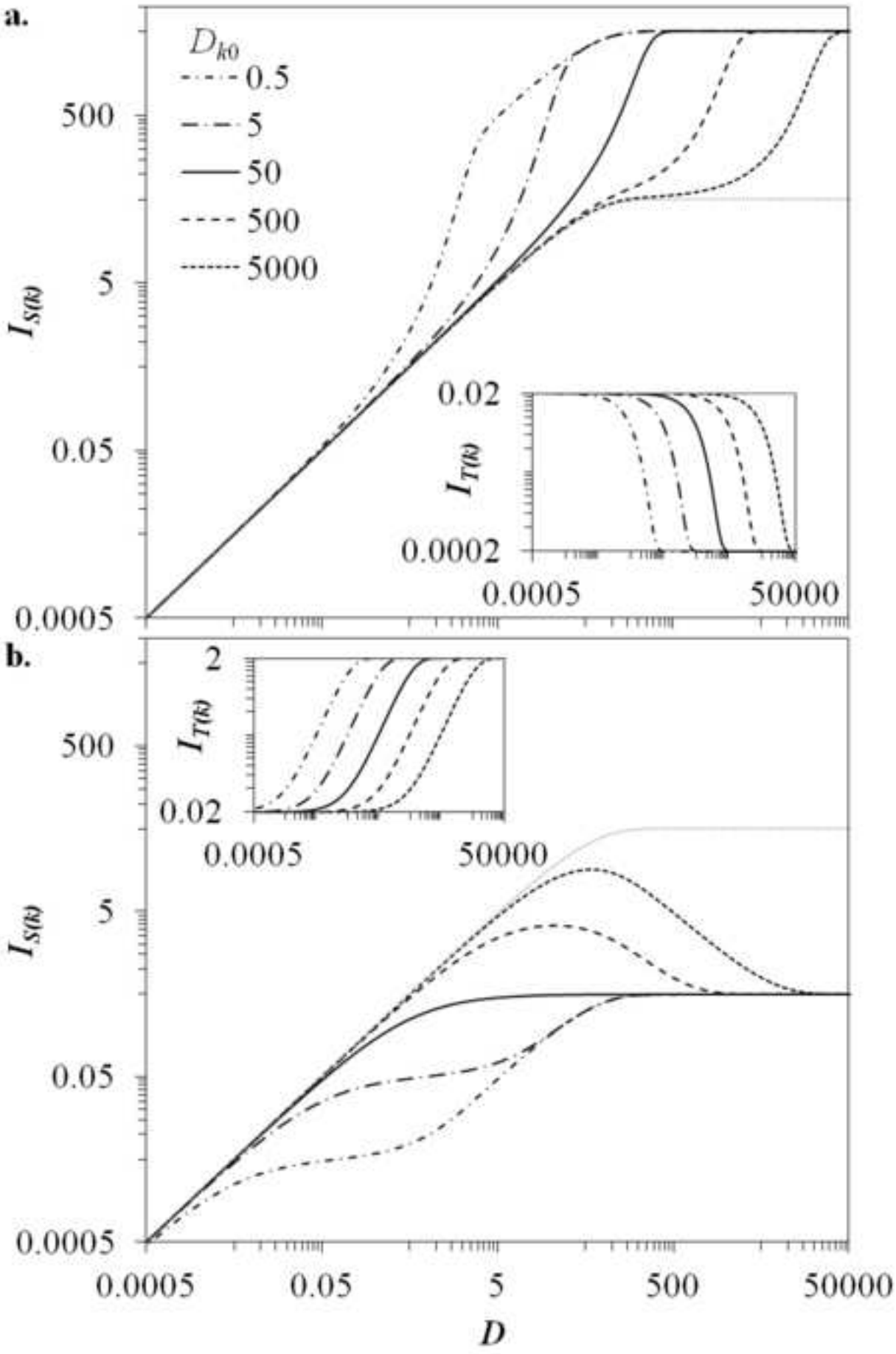

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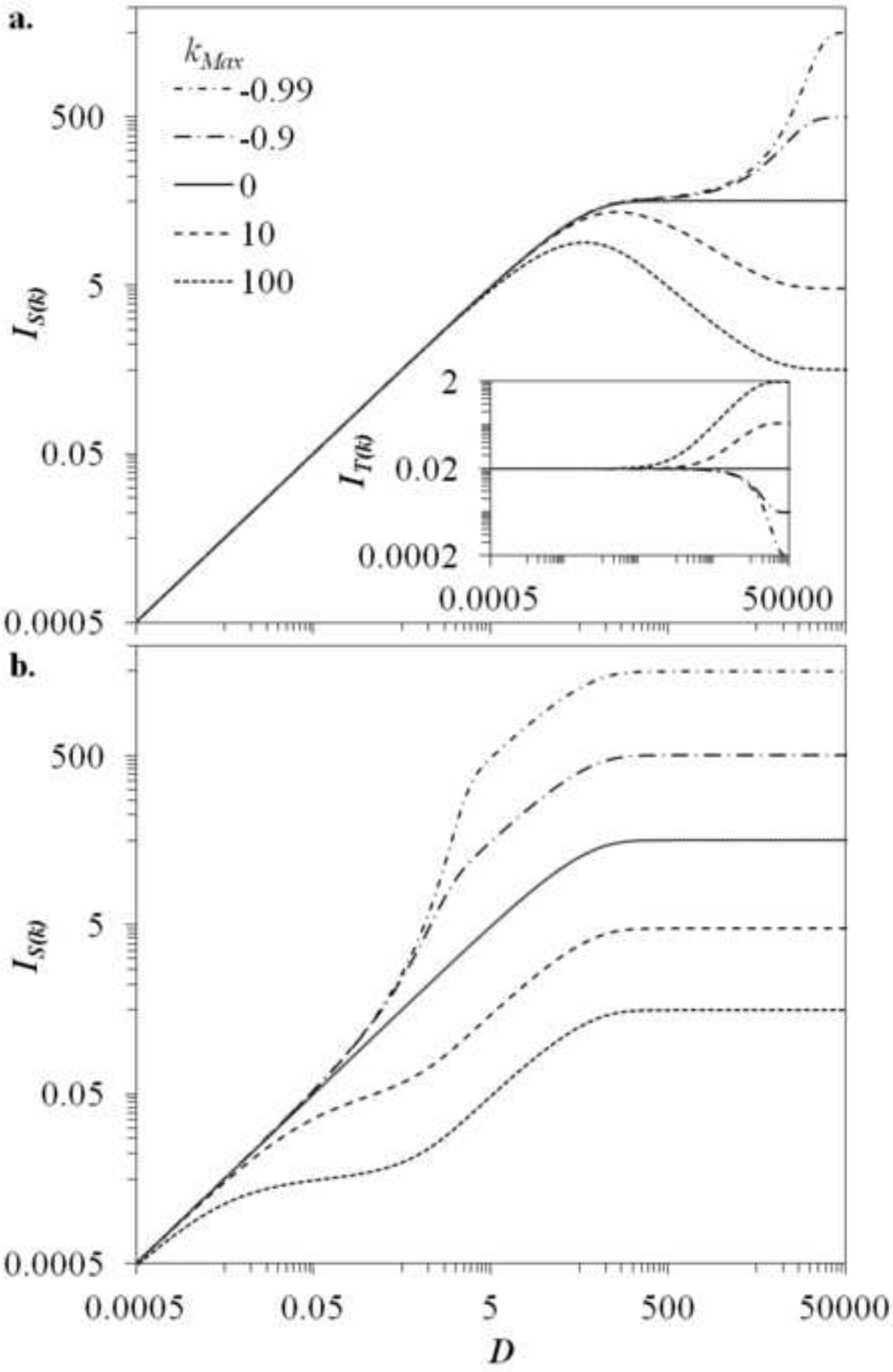

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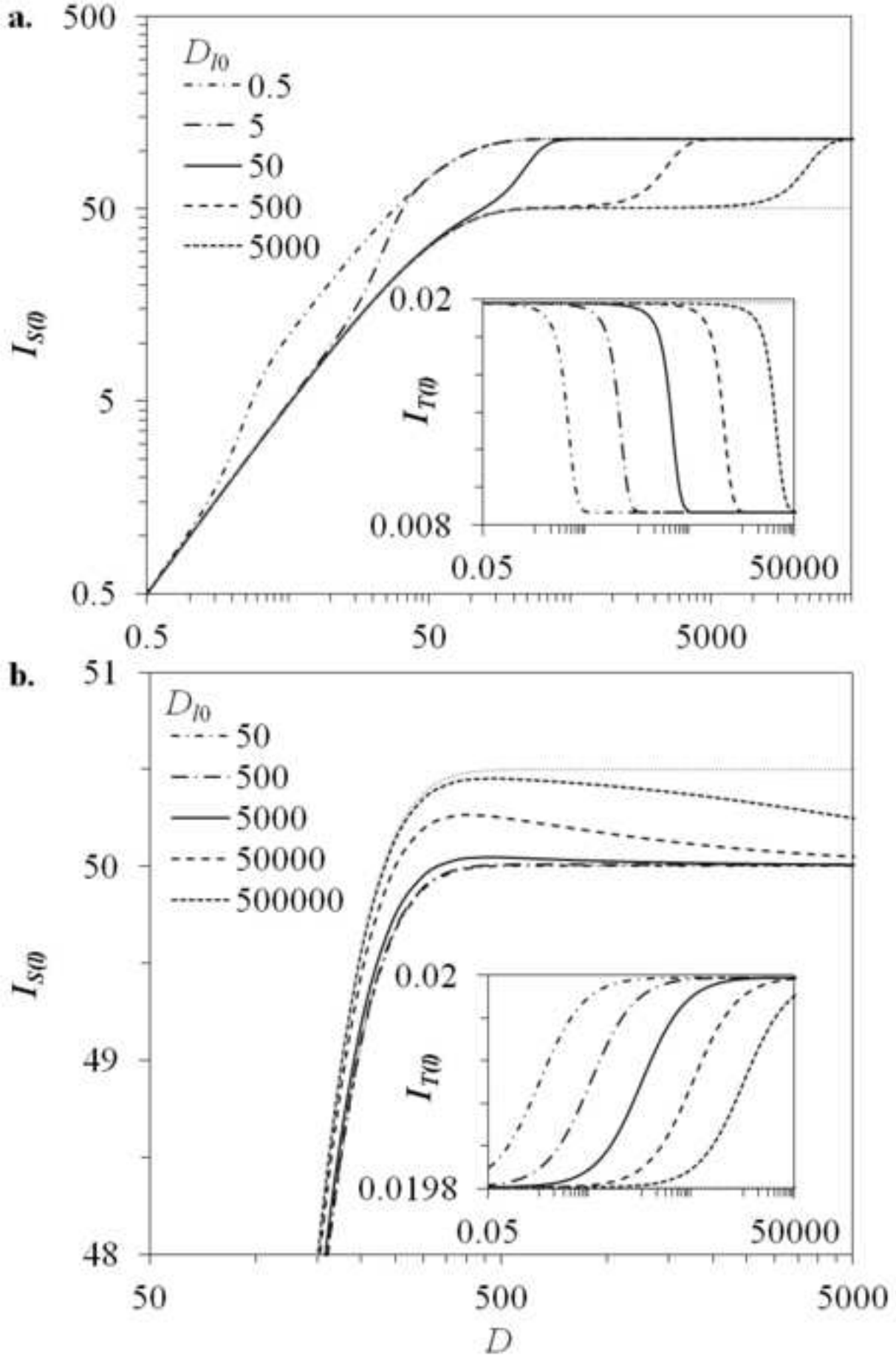

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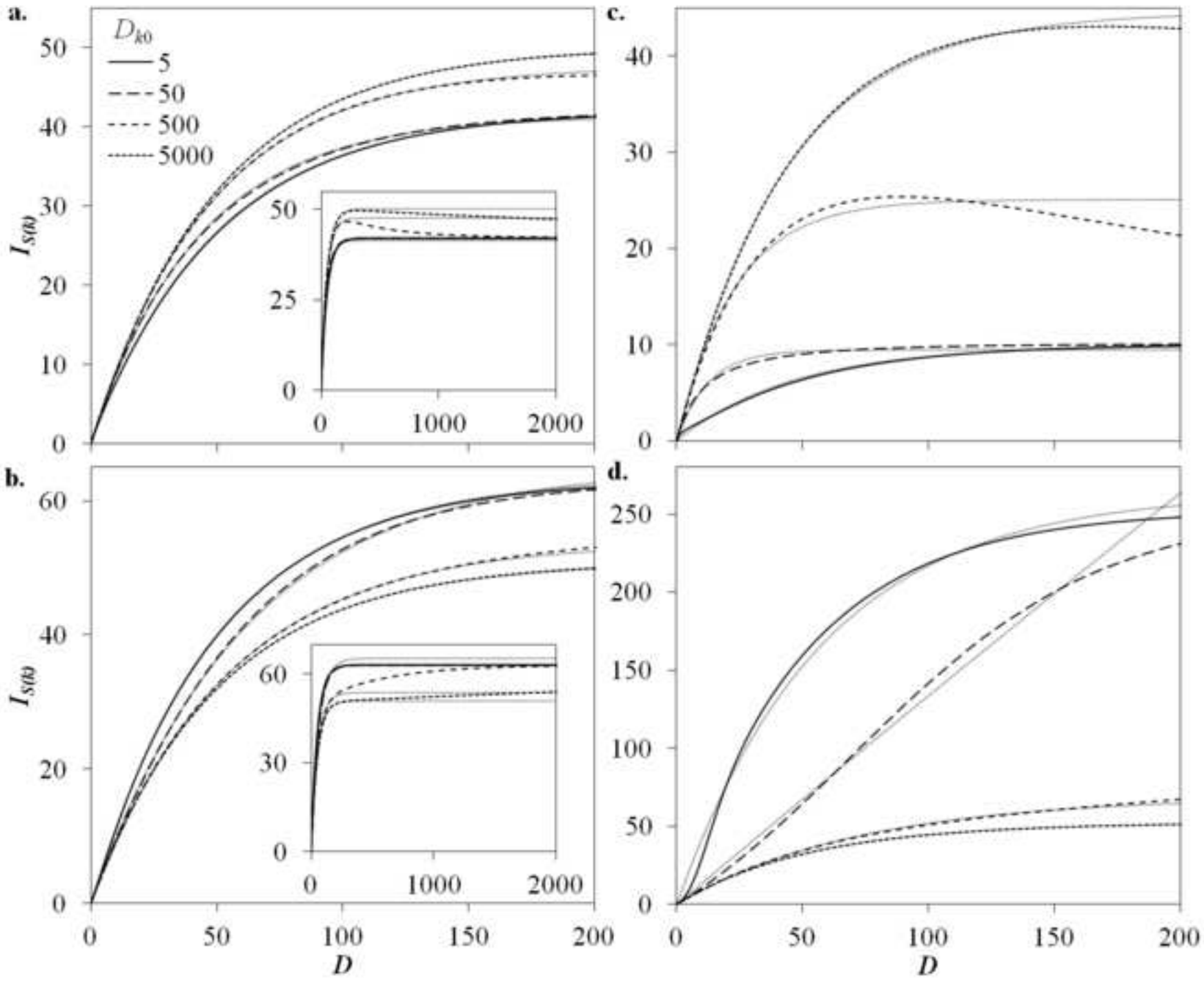

Figure 7

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