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Influence of scatter data and temperature lag on the analysis of thermoluminescence glow peak: A Monte Carlo simulation study

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ABSTRACT

The effects of the scattering data that might appear at the low radiation doses and the temperature lag that might occur between the heater pan and the detector on the thermoluminescence (TL) glow-curve have been addressed. The scattering data were mathematically induced in the TL glow curve using the Monte Carlo (MC) algorithm. While the phenomenon of the temperature lag has been simulated, assuming an exponential function. The deconvolution analysis has been carried out by TL expressions based on a presumed kinetics order value in comparison with the general-order kinetics equation. It has been found that even though the glow peak is known to obey the first- or second-order kinetics model, using the general-order kinetics equation in the deconvolution analysis is better than using the corresponding model equation.

1. Introduction

The analysis of the thermoluminescence (TL) glow-curve is mainly based on the TL kinetics model. The first-order kinetics model was introduced by Randall and Wilkins (Randall and Wilkins, 1945), assuming negligible retrapping during the heating stage. Garlick and Gibson (Garlick and Gibson, 1948) considered that the retrapping dominates, and established the second-order kinetics model. Later, the general-order kinetics (GOK) model was empirically developed (May and Partridge, 1964) with the adjustable order of kinetics parameter ranging from $b = 1$ to $b = 2$ as the glow-peak goes from the first-to second-order kinetics model. Chen (1969) studied the characteristics of the TL glow peak arising from each model and found that the first-order glow-peak is characterized by a symmetry factor of $\mu_g = 0.42$, while the second-order glow peak is characterized by a symmetry factor of $\mu_g = 0.52$.

Kitis et al. (Kitis et al., 1998) developed transformed expressions for the original first-, second- and general-order kinetics equations so that they can be conveniently used in the deconvolution analysis of the TL glow-curve. Nonetheless, due to the fact that the GOK equation is strictly empirical, whenever the glow-peaks are known to obey the first- or second-order kinetics model, the corresponding model equation is used in place of the GOK equation (Horowitz et al., 1986; Horowitz and Moscovitch, 1986; Horowitz and Yossian, 1995; Bos, 2001). However, applying the first- or the second-order kinetics model requires the experimental glow-curve to have precisely the same characteristics of the applicable model. Besides, using an inappropriate model that does not fit the shape of the TL glow-peak would lead to an unreal *extra* residual. This residual is usually decreased by increasing the number of deconvolved peaks (Horowitz and Yossian, 1995). In this case, additional *fake* glow-peaks will be included in the deconvolution analysis process, and thus unrealistic kinetics parameter values will be obtained (Sadek et al., 2018).

Under certain circumstances, external factors may influence the TL glow peak and change its characteristics. One of these factors is the scattering data that appear, especially in low doses. Typically, the scattered data is produced by induced noise signal that does not belong to the actual measured property. Such scattered data will lead to an error in the evaluation and the interpretation of data because of the possibility of considering a high scatter data point instead of the corrected one (Fruhwirth et al., 2000). In TL glow-curve, the scattered data appear as sharply discontinuous points on the glow peak and may arise not only from statistically improbable events but also from apparatus malfunction (Horowitz et al., 1986). Besides, these scattered data influence not only the shape of the glow-peak, but also the accuracy of the evaluated kinetics parameters (Matignon, 2007).

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The non-ideal heat transfer between the heating strips and the TL sample may also result in unrealistic evaluated kinetics parameters (Piters and Boss, 1999; Stadtmann et al., 2002). Indeed, during the TL readout, there is always a difference between the temperature of the heating element and the surface of the sample (Betts et al., 1993). This phenomenon is called the *temperature lag* (Kitis and Tuyn, 1999; Delice, 2018) and was observed for various TL samples. Gotlib et al. (Gotlib et al., 1984) reported a temperature lag of 7 K for LiF samples of thickness 3 mm with a linear heating rate of 4.3 K s^{-1}. While, a temperature lag of 14 K was reported for the same sample type but with thickness 9 mm and a linear heating rate of 6 K/s (Piters and Boss, 1999). The temperature lag between the heater pan and the sample is dependent on the heating rate and thickness of the sample. However, other factors, such as the temperature gradient in the heating element, the non-ideal thermal contact between the heater element and sample, the temperature gradient across the sample, and effects of the inert exchange gas in the chamber, should be considered (Sunta, 2015). On the other hand, the effect of the temperature gradient across the sample was found to be relatively small compared to the other factors (Piters and Boss, 1999). Indeed, Kitis and Tuyn (Kitis & Tuyn, 1998, 1999) reported that the thermal gradient across 1 mm thick samples of LiF : Mg, Ti and Al_2O_3 : C is practically zero.

The current work aims to investigate the effect of the scattering data and temperature lag phenomenon on fitting the first- or second-order glow peaks by their respective model equation compared to the GOK equation. Consequently, the suggestion of fitting the first- or second-order peaks by the GOK equation, under certain circumstances, will be addressed.

2. Simulation and peak fitting TL models

In the present study, the general-order kinetics TL equation of May and Partridge (1964) has been used to simulate the TL glow-peaks.

$$I(T) = n_o s \exp\left(-\frac{E}{kT}\right)\left[\frac{(b-1)s}{\beta}\times\int_{T_0}^{T}\exp\left(-\frac{E}{kT}\right)dT + 1\right]^{-\frac{b}{b-1}} \quad (1)$$

where n_0 (cm^{-3}) is the initial concentration of the trapped electrons in, s (s^{-1}) is the frequency factor, E (eV) is the activation energy, β (s^{-1}) is the linear heating rate, b is the order of kinetics. The first-order glow peaks have been simulated by setting $b \approx 1$ while the second-order peals have been simulated with $b = 2$.

In the fitting process, the first- and second-order peaks have been fitted with the TL expressions given, respectively, as (Kitis et al., 1998):

$$I(T) = I_m \exp\left[1 + \frac{E}{kT}\frac{T-T_m}{T_m} - \frac{T^2}{T_m^2}\times\exp\left(\frac{E}{kT} - \frac{T-T_m}{T_m}(1-\Delta) - \Delta_m\right)\right] \quad (2)$$

$$I(T) = 4I_m \exp\left(\frac{E}{kT}\frac{T-T_m}{T_m}\right)\times\left[\frac{T^2}{T_m^2}(1-\Delta)\exp\left(\frac{E}{kT}\frac{T-T_m}{T_m}\right) + 1 + \Delta_m\right]^{-2} \quad (3)$$

where I_m and T_m are the maximum peak intensity and maximum peak position, respectively, $\Delta = 2kT/E$ and $\Delta_m = 2kT_m/E$.

The equations provided by Eq.[2] and Eq.[3] are transformed versions of the original first- and second-order kinetics models, respectively. These equations are more convenient to be used in the deconvolution analysis because the starting values of the fitting parameters I_m and T_m can be obtained from the experimental glow-curve. The deconvolution analysis results obtained using these expressions have been compared with the analysis results using the GOK equation.

The GOK equation was widely used in the deconvolution analysis of TL glow-curves (Ortega et al., 2017). The accuracy of the GOK equation in fitting the one trap – one recombination (OTOR) glow-peak was revised by Sadek et al. (Sadek et al., 2014a; Sadek et al., 2014b; Sadek et al., 2015). It was concluded that the GOK equation could reliably describe the first- and second-order kinetics glow-peaks with an error of less than 1% in the activation energy value. While, for the intermediate cases ($1.0 < b \leq 2.0$), the error in the activation energy value was less than 5%. Therefore, it is not anticipated that there will be a significant difference in the analysis results of the TL expressions based on presumed kinetics order, and the results of the GOK expression. The transformed expression of the GOK equation as a function of $I = I(T_m, I_m, E, b)$ is given by (Kitis et al., 1998);

$$I(T) = I_m b^{\frac{b}{b-1}}\exp\left(\frac{E}{kT}\frac{T-T_m}{T_m}\right)\times\left[(b-1)(1-\Delta)\frac{T^2}{T_m^2}\exp\left(\frac{E}{kT}\frac{T-T_m}{T_m}\right) + Z_m\right]^{-\frac{b}{b-1}} \quad (4)$$

$$Z_m = Z_m = 1 + (b-1)\Delta_m,\ \Delta_m = \frac{2kT_m}{E} \quad (5)$$

In the transformed equation, the TL integral appearing in Eq.[1] was solved using the first term of the series provided by Eq.[6] (Kitis et al., 1998);

$$F(T,E) = \int_{T_0}^{T}\exp\left(-\frac{E}{kT}\right)dT = T\exp\left(-\frac{E}{kT}\right)\sum_{n=1}^{\infty}\left(\frac{kT}{E}\right)(-1)^n\, n! \quad (6)$$

In addition, the solution of this integral was also proposed via the exponential integral function E_i (Horowitz and Yossian, 1995; McKeever and Chen, 1997) as;

$$F(T,E) = T\exp\left(-\frac{E}{kT}\right) + \left(\frac{E}{k}\right)E_i\left(-\frac{E}{kT}\right) \quad (7)$$

Nevertheless, it was reported that the two solutions are almost equivalent (Gomez-Ros and Kitis, 2002).

The quality of the fitting has been assessed using the figure of merit (FOM) (Balian and Eddy, 1977);

$$FOM(\%) = \sum_{j_i}^{j_f}\frac{|y_i - y(x_i)|}{A}\times 100 \quad (8)$$

where *FOM* is the figure of merit, j_i is the first channel in the region of interest, j_f is the last channel in the region of interest, y_i is the information content of channel j, $y(x_i)$ is the value of the fitting function in channel j, and A is the integral of the fitted glow-peak in the region of interest.

The quality of the fitting reflects the capability of the applied model to fit the data. However, it is crucially dependent on the starting values provided for the fitting parameters. Therefore, poor-fitting could be obtained due to incorrect starting values. Thus, in the present study, the starting value of the activation energy parameter has been set to the true (input simulation) value. In this way, the comparison between the FOM values of the different TL models reflects the capability of each model to fit the data, if the correct starting values were provided.

3. Simulation of induced scatter data and heater-sample temperature lag

3.1. Modeling the scatter data in TL glow-peak

The random error ε is defined as the deviation of the measured property from its expectation value and characterized by a Gaussian distribution (Gallagher, 2006). Unfortunately, it is not possible to correct for the random error (ISO 3534-2, 2006); however, it can be controlled by increasing the replicate number. Thus, for a true value x, the scattering data is defined as;

$$\xi = x + u(x)z:\ \varepsilon = \xi - x \quad (9)$$

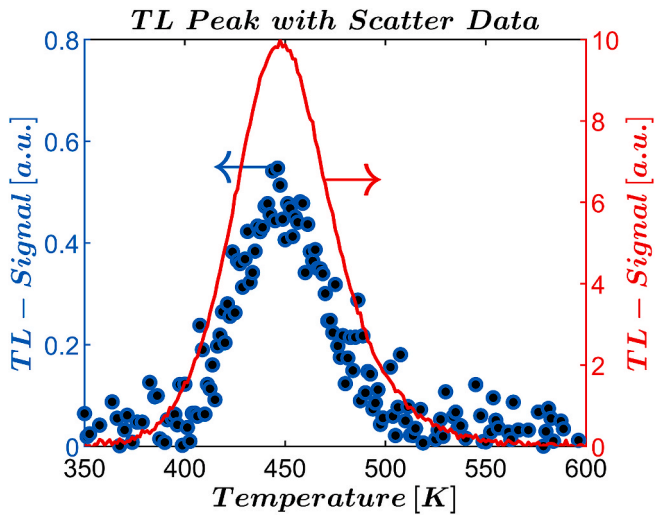

Fig. 1. An example of TL glow-peak simulated under the influence of the scatter data generated using the Monte Carlo method in cases of low and high doses (i.e., TL Signal).

where $u(x)$ is the adjustable standard error and z is the standard Gaussian distribution of mean 0 and standard error 1. Thereby, the degree of the dispersion (i.e., the scattering data) in the simulated data can be simulated via varying the standard error $u(x)$. In the present study, the scattering data have been induced empirically in the TL glow curve using Eq.[9]. The variation of each point in the TL glow curve has been modeled using the following procedure;

i. The TL glow-peak has been generated using the general-order kinetics eq.[1] equation for different concentrations of the trapped electrons n_0 *i.e.,* different doses.
ii. For each x_i data point in the glow-peak, a random variable with a Gaussian distribution has been generated using Eq.[9] for certain iteration number M, where $u(x_i)$ was arbitrarily set to control the dispersion level of the scattering data.
iii. To have high scatter data at the two tails of the TL spectrum, and low scatter data at the maximum of the TL spectrum, the standard error $u(x)$ was fixed to a constant value for all the generated TL peaks.
iv. The glow-peak has been analyzed, and the kinetic parameters have been obtained.
v. Steps (i-iv) have been repeated for a sufficient iteration number so that all the calculated parameters have a reliable standard error.

An example of TL glow-peaks simulated at relatively low and high doses (i.e., n_0 values) are presented in Fig. 1.

3.2. Modeling the temperature lag phenomenon

Another disturbance that may change the shape of the TL glow-peak is the temperature lag between the heater-pan and the TL sample. The temperature lag causes a shift in the temperature of the TL glow peak. A similar shift can also be induced due to changing the heating rate (Bos and Piters, 1993). However, in this case, all the data points in the glow peak will be shifted by a constant factor $\Delta T = const$. While, in the case of the temperature lag phenomenon, the shift in the temperature of the TL peak is a function of the temperature $\Delta T = \Delta T(T)$ in such that it increases with increasing the temperature (Kitis et al., 2015). In the current study, the temperature lag phenomenon has been simulated using an exponential function given by;

$$T_{lag}(t) = T(t)\, e^{\alpha t} \tag{10}$$

T_{lag} is the apparent temperature reading, $T(t)$ is the actual temperature of the heater, $\alpha(s^{-1})$ is a constant describing the degree of the temperature lag, and t is the readout time. The effect of the temperature lag can be observed on the TL glow peak as a shift in the maximum peak position, as shown in Fig. 2.

It is evident that the shift in the temperature $\Delta(T)$ increases as the temperature rises. Several studies were carried to estimate a correction for this temperature shift (Kitis & Tuyn, 1998, 1999). However, it seems it would be difficult to estimate a correction for each temperature value T_i. Therefore, these studies attempted to estimate a correction for the shift in the peak position and apply it to the entire temperature range. In the present study, the temperature lag between the heater element and the TL sample can be expressed in terms of the shift in the maximum peak position.

4. Geometrical and integral symmetry factor

The shape of a TL glow-peak can be characterized by the symmetry factor given by (Chen, 1969)

$$\mu_g = \frac{\delta}{\omega},\ \delta = T_2 - T_m,\ \omega = T_2 - T_1 \tag{11}$$

where T_1 and T_2 are the temperatures at the peak half-maximum at the lower and higher temperature sides, respectively. On the other hand, the integral symmetry factor μ_g' was also introduced to characterize the shape of the TL glow peak. It is defined as the ratio of the high-temperature half-integral of a glow-peak over its total integral (Halperin and Braner, 1960):

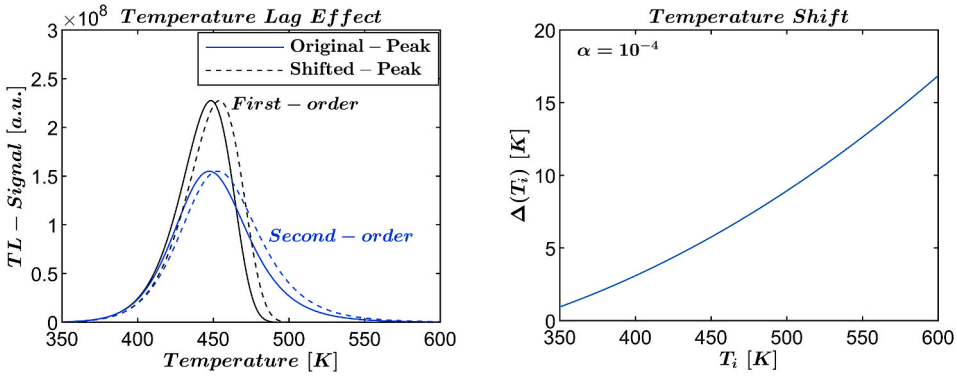

Fig. 2. The shift in the peak temperature due to the temperature lag effect. The original peak is represented by a solid line, while the dashed line represents the shifted peak. The shift $\Delta(T_i)$ for each temperature T_i is also represented.

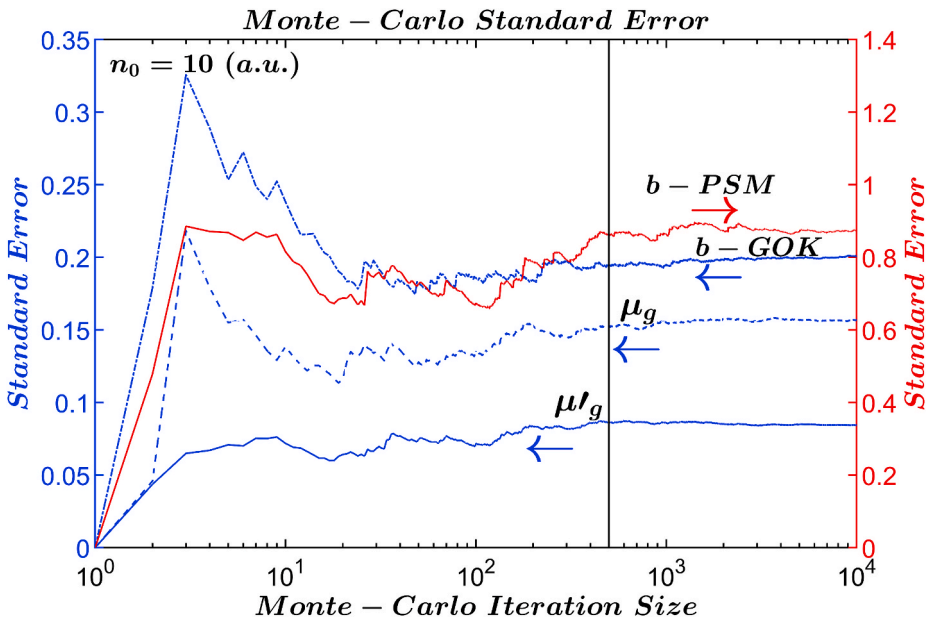

Fig. 3. The standard error of some of the parameters calculated from simulated glow-peaks under the influence of the scatter data induced using Monte Carlo (MC) method.

$$\mu_g^{'} = \frac{n_m}{n_0} \tag{12}$$

where $n_m = \int_{T_m}^{\infty} I\,dT$ is the high-temperature half integral of the glow-peak.

It is to be noted that in the previous work of Halpern and Braner (Halperin and Braner, 1960), the parameter n_m/n_0 was defined as the geometrical symmetry factor. Following the work of Kitis and Pagonis (Kitis and Pagonis, 2007), in the current work, this parameter has been denoted as the integral symmetry factor, and δ/ω is the geometrical symmetry factor.

5. Results and discussion

5.1. Monte Carlo standard error: selection of iteration number

Although many problems of simulating stochastic processes can be performed using Monte Carlo (MC) algorithm, the results are never exact because of the randomness behavior of the MC algorithm (JCGM-101, 2008). The MC algorithm should, therefore, be performed for a sufficient number of iterations to have reliable and reproducible results. In the present study, the MC iteration number has been selected so that the standard errors of the evaluated parameters remain constant. In such a case, increasing the iteration number does not affect the results. Fig. 3 presents the standard error over the iteration number for most of the calculated parameters in the current study.

The standard error of the calculated parameters becomes stable approximately at 500 iterations. Further increasing the iterations number does not improve the standard error of the estimated parameters implying that the true uncertainties have been approached. It is worthwhile to mention that the simulation presented in Fig. 3 was performed at the lowest dose, *i.e.*, $n_0 = 10$ $(a.u.)$ at which the scattering data is maximum. Therefore, it would be practical to use the same iteration number for the higher doses.

5.2. Influence of scattering data on the evaluation of the peak symmetry factor

It has been shown in the previous sections that the shape of the TL glow peak is characterized by either the geometrical or integral symmetry factor. In the current section, the influence of the scattered data on the peak symmetry factors has been investigated. Sets of first and

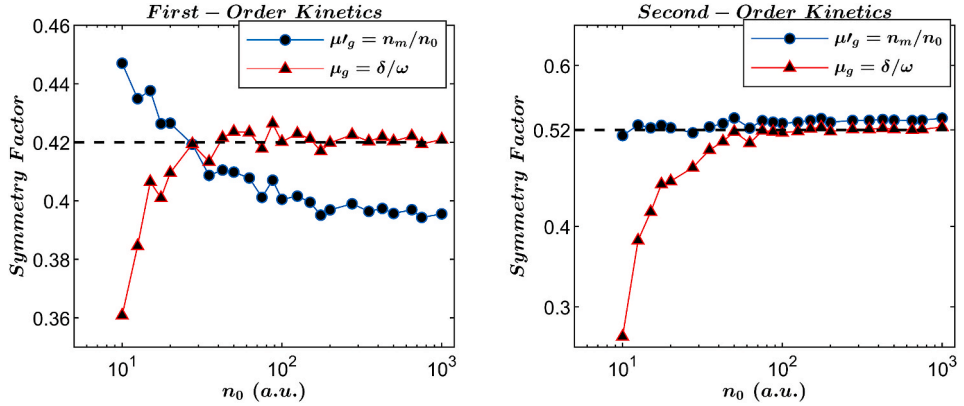

Fig. 4. Geometrical and integral symmetry factor parameters evaluated for first- and second-order peaks generated using the general-order kinetics equation with different doses (i.e. n_0) under the influence of scattering data. Each value is represented by the average of 10 samples and its standard deviation.

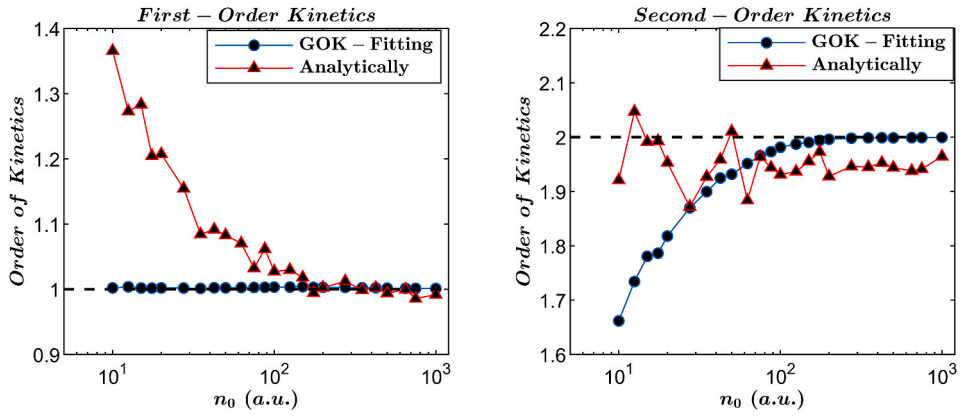

Fig. 5. Order of kinetics evaluated computationally through the GOK-fitting and analytically using Eq.[14].

second-order glow-peaks have been simulated over different absorbed doses using the GOK equation Eq.[1]. For both cases, the constant parameters were $E = 1$ eV and $s = 10^{10}$ s^{-1}. The order of kinetics values b have been set to ~1 and 2 for the first- and the second-order kinetics cases, respectively. The geometrical and integral symmetry factor parameters have been evaluated for each glow-peak. Fig. 4 shows a comparison between the geometrical and integral symmetry factors evaluated for the first- and second-order glow peaks simulated over a wide range of doses.

In case of the second-order kinetics, the integral symmetry factor μ_g' was found to be more reliable than the geometrical symmetry factor μ_g at the low doses. This is because μ_g is calculated from a few points on the glow-peak, and therefore, it is more susceptible to the effects of the scattering. While μ_g' is calculated from the integration of the glow-peak over the temperature range. It is also noticeable that for the first-order peaks, $\mu_g' < \mu_g$, while for the second-order peaks, $\mu_g' > \mu_g$. This observation could be interpreted using the mathematical relationship deduced by Chen (1969) as;

$$\mu_g' = \eta\, \mu_g \tag{13}$$

where η was found to be dependent on the order of kinetics in such that $\eta \approx 0.94$ and $\eta \approx 1.025$ for the first- and second-order peaks, respectively.

The key conclusion in this section is that the kinetics parameters of a TL glow peak that is suffering from high scattering data cannot be accurately evaluated using the geometrical symmetry factor μ_g. In this case, the integral symmetry factor is preferable over the geometrical symmetry factor. Therefore, Kitis and Pagonis (Kitis and Pagonis, 2007) derived an analytical relationship which allows the calculation of the order of kinetics using the integral symmetry factor μ_g'.

$$\mu_g' = \left(\frac{b}{1+(b-1)\Delta_m}\right)^{-\frac{1}{b-1}},\ \Delta_m = \frac{2kT_m}{E} \tag{14}$$

Nevertheless, the order of kinetics b can also be computationally evaluated through the fitting of the glow peak by the GOK expression. Fig. 5 illustrates the effect of the scattered data on the evaluation of the order of kinetics b computationally by the fitting procedure and analytically via the solution of Eq.[14].

For the first-order peaks, the order of kinetics values evaluated analytically using the solution of Eq.[14] were overestimated at low doses due to the effect of the scattered data. At the same time, the GOK-fitting procedure could provide reliable values over the entire dose range. Nevertheless, for the second-order glow peaks, the fitting method failed to provide accurate b values, while the solution of Eq.[14] could. In fact, the scattered data influence the shape of the TL glow peak in such a way the order of kinetics evaluated by the fitting process is always underestimated. However, this underestimation can be observed only in the case of the second-order peaks where b can have values $b < 2$. While in the case of the first-order peaks, the b values could not be underestimated because the GOK equation is not solvable in this range. Therefore, for the first-order peaks, the GOK fitting process approached the lowest possible values for the order of kinetics, i.e., $b \approx 1$. On the other hand, the deviations in the kinetics order values obtained from the analytical expression Eq.[14] was anticipated due to the effect of the scattered data on the evaluation of μ_g'.

The general conclusion that can be drawn in this section is that it is the scattered data influence the shape of the TL glow peak. Therefore it

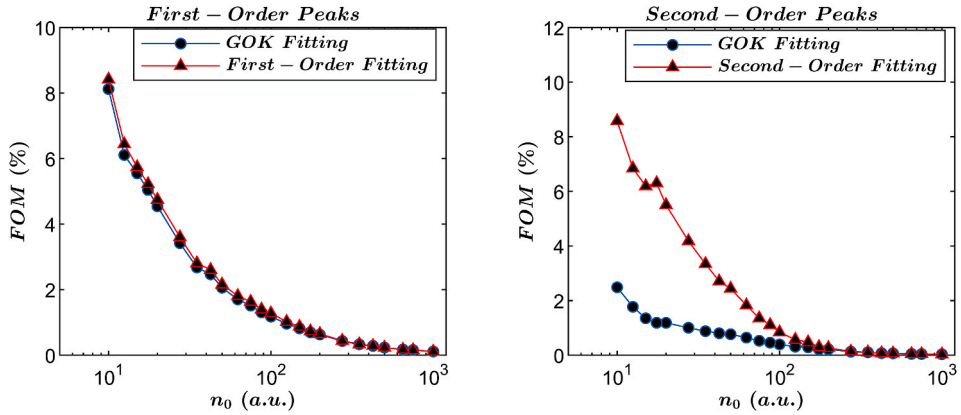

Fig. 6. The quality of fitting values evaluated over different doses for the first- and second-order glow peaks using the corresponding model in comparison with the GOK model.

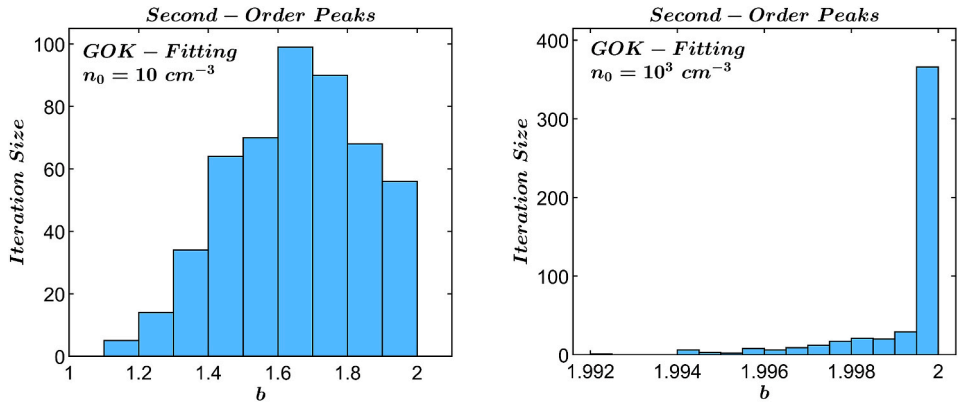

Fig. 7. Distribution of the kinetics order values obtained from fitting the second-order glow peaks using the GOK at the low and high doses.

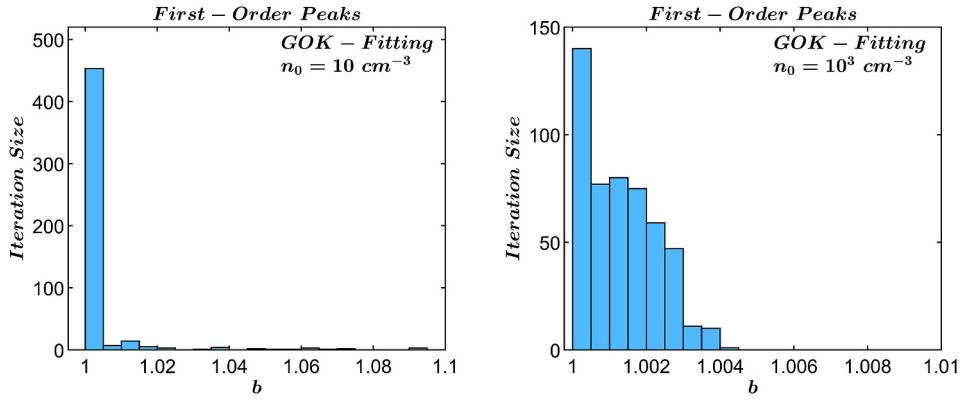

Fig. 8. Distribution of the kinetics order values of the first-order glow peak over the MC iteration in cases of low and high doses.

will not be possible to have an accurate estimation for the trapping parameters neither by the peak fitting nor the peak shape methods. Hence, the estimation of the kinetics parameters should be avoided at low doses.

5.3. Influence of the scatter data on the quality of fitting

The deconvolution analysis may also be used for purposes other than estimating the kinetics parameters of the TL glow peak. Indeed, advantages were also found from applying the deconvolution analysis in the low TL dose dosimetry applications (Horowitz and Yossian, 1995). In this case, the fitting quality will be the focus of concern. Of course, as the number of the fitting parameters increases, the fitting quality is expected to increase. However, this was not a sufficient reason to prefer the GOK equation, with the additional order of kinetics parameter, to the first- or the second-order kinetics equation. The fact that the GOK equation is purely empirical limited its use in the deconvolution analysis. Therefore, in the current section, the fitting quality using the GOK equation has been compared with the fitting quality using the first- and second-order TL expressions. Sets of first and second-order glow-peaks have been simulated for differentn_0, and each glow peak was fitted by its corresponding model equation in comparison with the GOK equation. The quality of the fitting values evaluated by Eq.[8] over the dose range are shown in Fig. 6.

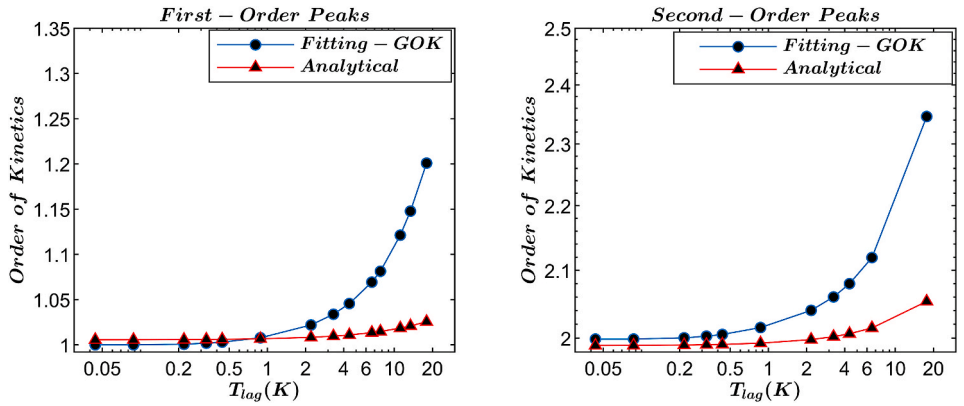

Fig. 9. *The order of kinetics obtained from the GOK fitting and the solution of eq.[14] as a function of the shift of the maximum peak position.* The values of α have been randomly selected from the range $\alpha = [10^{-6} : 4 \times 10^{-4}]$.

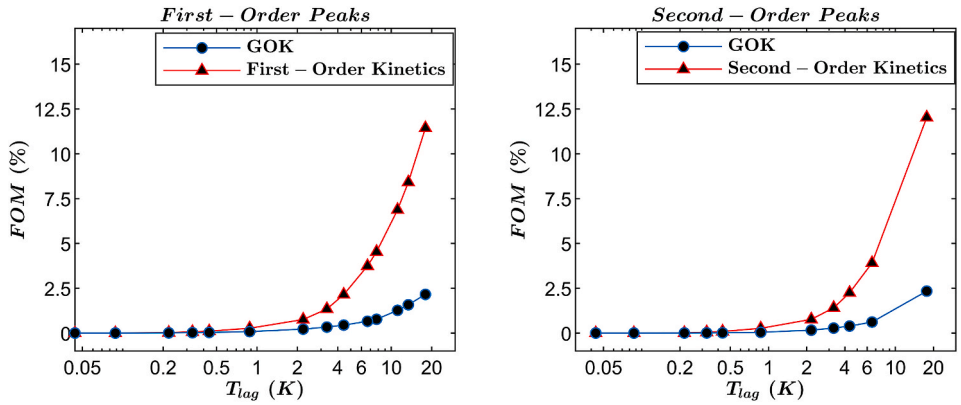

Fig. 10. The FOM values of fitting first and second-order TL glow-peaks simulated under the influence of scattering data over different temperature lag parameter values. The values of α have been randomly selected from the range $\alpha = [10^{-6} : 4 \times 10^{-4}]$.

At low doses, a significant improvement in the fitting quality has been achieved when the GOK equation was used instead of the second-order kinetics equation. The change in the kinetics order of the glow peaks as a result of the scattered data could be handled with the GOK equation, with the adjustable b parameter. Hence, at low doses, a wide range of b values has been adopted by the fitting process to approach the optimum FOM value, as shown in Fig. 7. While, when the dose increased ($n_0 = 10^3$), and thus, the effect of the scattering data decreased, all of the b values determined by the fitting process were almost $b \approx 2$. On the other hand, the presumption of $b = 2$ set in the TL expression of the second-order kinetics model has led to high FOM values.

For the first-order peaks, the underestimation in the order of kinetics values could not be handled by the GOK equation since it has no solution for $b < 1$. At low doses, the optimum order of kinetics values that could be approached by the GOK fitting were $b \approx 1$ (Fig. 8), which is already presumed in the TL expression of the first-order kinetics model. In addition, when the dose increased ($n_0 = 10^3\ cm^{-3}$), the order of kinetics values obtained by the GOK fitting approached the typical, expected values ($b \approx 1$). Therefore, the fitting quality using the TL expression of the first-order kinetics model is similar to the fitting quality using the GOK expression over the entire dose range.

5.4. Influence of the temperature lag on the quality of fitting

The temperature lag between the heating element and the TL detector is another factor that may influence the shape of the TL glow peak. However, unlike the scattered data, this effect cannot be observed in the experimental glow curve. Therefore, in the present study, this effect has been simulated for different temperature lags between the heating element and the TL detector. The temperature lag interval has been adjusted through the parameter α in Eq.[10]. The effect of this temperature lag on the TL glow peak has been measured as the shift in the maximum peak position. Thus, the values of α have been selected so that $T_{Lag} \leq 20\ K$. The first- and second-order glow-peaks have been fitted with the corresponding models' equations in comparison with the GOK equation. The order of kinetics values obtained computationally from GOK-fitting compared with the analytical Eq.[14] are presented in Fig. 9.

An overestimation has been observed in the order of kinetics values evaluated either computationally by the GOK fitting or analytically by the solution of Eq.[14]. This overestimation was found in the fitting carried out by the first- and the second-order kinetics glow peaks. Therefore, fitting these glow peaks with the expressions of presumed kinetics order value has led to high FOM values. On the other hand, again, the GOK equation with the adjustable order of kinetics value could recover this high FOM with the advantage of the adjustable b parameter, as depicted in Fig. 10.

6. Conclusions

- Both of the scattered data and the temperature lag influence the shape of the TL glow peak resulting in either overestimation or underestimation of the order of kinetics value. If this underestimation/overestimation in the order of kinetics value has not been corrected, fitting the TL glow peak with presumed order of kinetics value will result in high FOM value.
- The GOK equation could recover this high FOM value with the advantage of the adjustable order of kinetics parameter.
- It is recommended to use the GOK equation in fitting the experimental glow peaks even though the glow peaks are known to follow the first- or second-order kinetics models, especially in low doses, and the presence of temperature lags between the heater and the sample.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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