Estimate half-life of thermoluminescence signals according to the different models by using Python

Nguyen Duy Sang
Department of Physics Education, School of Education, Can Tho University, Can Tho, Vietnam

ABSTRACT
In this study, the half-life is the time required for the thermoluminescence intensity to drop to half of its initial value. The half-life is a characteristic of the optical and thermal properties of the material. The half-life of the thermoluminescence signals under other models such as first order kinetics, second order kinetics, general order kinetics, mixed order kinetics and the one-trap one-recombination was calculated. The specific goals of this work are to give the half-life difference of the thermoluminescence signal of each model by using Python. The formulas allow to quickly determine the half-life of the simulated or empirical thermoluminescence curve, including one or more complex peak. Simulation results and calculations based on the figure of merit parameters allow to check the calculation of the half-life according to the most suitable model.

ARTICLE HISTORY
Received 17 July 2021
Revised 27 August 2021
Accepted 16 October 2021

KEYWORDS
Half-life; thermoluminescence; material; order kinetics; python; figure of merit

1. Introduction
The phenomenon of thermoluminescence (TL) describes a process in which light is emitted by an irradiated material when it is heated. Luminescence signals from natural and synthetic materials are widely used in dating and dosimetric applications. The most commonly used models for analyzing such signals are the first order kinetics (FOK), second order kinetics (SOK), the general order kinetics (GOK), mixed order kinetics (MOK) and the one trap one recombination center (OTOR) model. While there are many simulation studies of TL phenomena within these models, there has not been many studies the determination of half-life of TL traps by means of comparative models (GOK, MOK, OTOR). In practical situations, researchers are much interested in the type of half-life of TL signals, which is the time required for the TL intensity to decreased to half of its initial value. This type of half-life will be denoted by $t_{1/2}$ in the rest of this paper. The purpose of this paper is to present new analytical expressions for the half-life parameters $t_{1/2}$. The expressions are applicable for experiments carried out under either constant optical excitation, or under constant thermal excitation conditions. The new analytical expressions contain the model parameters characterizing both the experimental conditions, and the physical properties of the materials.

It was simulated the TL curve according to the initial parameters. The TL curve was modelled with a single peak following the different models. All simulated and empirical TL curves were analyzed and calculated the $t_{1/2}$ values according to the different models by Python software.

The specific goals of this work are:

1) To give $t_{1/2}$ difference of TL signals according to the different models.

2) To quickly determine $t_{1/2}$ of the simulated or empirical TL curve, including one or more complex peak by Python software.

3) To check the calculation of $t_{1/2}$ according to which model is the most suitable.

2. Material and methods
2.1. Evaluation and analysis Python software
For the analysis presented in this paper, multiple custom-made software packages are written in Python using several open-source packages. Most algorithms and calculations in the temperature reconstruction and glow curve deconvolution, including the fitting procedures are implemented by using functions from the SciPy library [1]. The results are saved in DataFrames of the pandas library [2], which can be exported to many different types of output files.

2.2. Glow curve modelling and simulation of the TL curves
A TL glow curve typically consists of several glow peaks. Equations simulate glow peaks of various orders. The
FOK, SOK, the GOK glow peak can be simulated using the following three ordinary equations, respectively [3]:

\[
\frac{dn}{dt} = \frac{-ns \exp \left( -\frac{E}{kT} \right)}{\beta} \quad (1)
\]

\[
\frac{dn}{dt} = \frac{-n^2 s \exp \left( -\frac{E}{kT} \right)}{N \beta} \quad (2)
\]

\[
\frac{dn}{dt} = \frac{-n^b s \exp \left( -\frac{E}{kT} \right)}{N \beta} \quad (3)
\]

where \( n \) is the concentration of trapped electrons, \( \frac{dn}{dt} \) is the rate of change of the concentration of trapped electrons, \( s \) is the frequency factor, \( E \) is the activation energy, \( T \) is the absolute temperature, \( k \) is the Boltzmann constant, \( N \) is the total concentration of the traps in the crystal, \( b \) is kinetic order, and is \( \beta \) the linear heating rate.

The approximate equation of the OTOR model derived using the quasi-equilibrium approximation can be described by [3]:

\[
\frac{dn}{dt} = \frac{-A_n n^2 s \exp \left( -\frac{E}{kT} \right)}{[nA_h + (N - n)A_h] \beta} \quad (4)
\]

where \( \frac{dn}{dt} \) is the rate of change of the concentration of trapped electrons, \( A_n \) is the probability coefficient of electron recombinating with holes in the recombination centre, \( A_h \) is the probability coefficient of electron retrapping in the traps.

The approximate equation of the MOK model derived using the quasi-equilibrium approximation can be described by Kitis [4]:

\[
\frac{dn}{dt} = \frac{-s n (n + c) \exp \left( -\frac{E}{kT} \right)}{(N + c) \beta} \quad (5)
\]

With \( c = \frac{n(1-a)}{a} \) and put in Equation (5) to get the Equation (6):

\[
\frac{dn}{dt} = \frac{-n^2 s \exp \left( -\frac{E}{kT} \right)}{[N + n \left( \frac{1-a}{a} \right)] \beta \alpha} \quad (6)
\]

where \( \alpha \) is an extra parameter.

To simulate a glow peak, the user needs to supply parameters of the initial concentration of trapped electrons. The user must supply temperature and TL signal values stored in a two-column data frame (or matrix). The data set can be loaded into Python software. Additional arguments that need to be specified for glow curve fitting include the number of glow peaks to be deconvoluted, the allowed maximum number of random trials, the allowed maximum total half-width of glow peaks, the allowed minimum distance between peak temperatures, etc. A plot showing deconvoluted glow peaks can be automatically produced once the calculation is terminated. The user can also specify a file to save the fit data for further usage.

First-order glow peaks appear if the recombination probability \( (A_n) \) is greater than that of retrapping \( (A_h) \) during excitation. The three parameters describing a glow peak are: the maximum intensity \( (I_m) \), the activation energy \( (E) \), and the maximum temperature \( (T_m) \). The empirical expression describing first-order glow peaks is available in function [5]:

\[
I(T) = I_n \exp \left[ \frac{1}{kT} - \frac{T_m}{kT} - \frac{T^2_m}{kT} \left( 1 - \frac{2kT}{E} \right) \right]
\]

(7)

Second-order glow peaks appear if the re-trapping probability is comparable with or greater than that of recombination during excitation. The three parameters describing a glow peak are the same as those of first-orders. The empirical expression describing second-order glow peaks is available in function [5]:

\[
I(T) = 4I_m \exp \left[ \frac{1}{kT} - \frac{T_m}{kT} - \frac{T^2_m}{kT} \left( 1 - \frac{2kT}{E} \right) \right]
\]

(8)

General-order glow peaks are produced in intermediate cases (neither of first-order, nor of second-order). The four parameters describing a glow peak are: \( I_m, E, T_m, \) and \( b \). The empirical expression describing general-order glow peaks is available in function [5]:

\[
I(T) = I_m b^\omega \exp \left[ \frac{1}{kT} - \frac{T_m}{kT} \right] \left( b - 1 \right) \left( 1 - \frac{2kT}{E} \right)
\]

(9)

OTO model based semi-analytical expressions have also been applied to fit glow peaks, by using either the Lambert W function [6–8] or the Wright Omega function [9–11]. The four parameters describing a glow peak are: \( I_m, E, T_m, \) and \( b \). The empirical expression describing OTO order glow peaks is available in function [5]:

\[
I(T) = \frac{1}{T_m} \exp \left[ \frac{-E}{kT} \right] \frac{\omega(Z_m) + [\omega(Z_m)]^2}{\omega(Z) + [\omega(Z)]^2}
\]

(10)

where

\[
Z_m = \frac{R}{1 - R} - \log \left( \frac{1 - R}{R} \right)
\]

\[
\frac{E}{kT_m} \log \left( \frac{1 - R}{R} \right)
\]

(11)
and
\[ Z = \frac{R}{1 - R} - \log \left( \frac{1 - R}{R} \right) + \frac{\exp \left( \frac{E}{kT_m} \right)}{kT_m (1 - 1.05R^{1.26})} F(T, E) \] (12)

Mixed-order kinetic models introduce an extra parameter \( \alpha = \frac{n_0}{R_m+M} \) where \( n_0 \) is the initial filled concentration of the active traps and \( M \) is the trap concentration of the thermally disconnected deep traps [12]. The four parameters describing a glow peak are: \( I_m, E, T_m, \) and \( \alpha \). The empirical expression describing mixed-order glow peaks is available in function [4]:
\[
I(T) = l(T) = I_m \exp \left( \frac{1}{R_m} - \frac{2kT_m}{E} \right) \left[ \exp \left( \frac{2kT_m}{E} \right) - \alpha \right] \exp \left( \frac{E}{kT} - \frac{T_m}{T_m} \right)
\]
\[
\exp \left( \frac{1}{R_m} - \frac{2kT_m}{E} \right) \left[ \exp \left( \frac{2kT_m}{E} \right) - \alpha \right] \exp \left( \frac{E}{kT} - \frac{T_m}{T_m} \right)
\]
\[
\exp \left( \frac{1}{R_m} - \frac{2kT_m}{E} \right) \left[ \exp \left( \frac{2kT_m}{E} \right) - \alpha \right] \exp \left( \frac{E}{kT} - \frac{T_m}{T_m} \right)
\]
\[
\exp \left( \frac{1}{R_m} - \frac{2kT_m}{E} \right) \left[ \exp \left( \frac{2kT_m}{E} \right) - \alpha \right] \exp \left( \frac{E}{kT} - \frac{T_m}{T_m} \right)
\]
(13)

where \( R_m = \frac{A_m+\alpha}{A_m} \) and \( A_m = \exp \left( \frac{A_{m-\alpha}}{A_m+\alpha} \left( 1 - \frac{2kT_m}{E} \right) \right) \)

2.3. The TL curves obtained from experiments

The experimental curves are the complex TL curves characterized by the overlap of many single peaks. The data are referenced from the GLOCANIN project [13,14]. This project result has now been widely used among the TL studies [15–17]. However, the determination of half-life for these curves of the GLOCANIN project has not been mentioned yet. Especially, the TL curves with the overlap of many single peaks have still been unknown for half-life. In this paper, the TL curves of Rg1, Rg2, Rg9 were used to calculate the individual half-life for each peak.

2.4. Calculation of half-life

In this experimental studies, the intensity \( I(t) \) of the TL signal is measured at time \( t \) after the beginning of the experiment. This TL intensity \( I(t) \) is proportional to the derivative \( -dn/dt \), depending on the measurement conditions. In empirical research, experimentalists are much interested in half-life of TL signals, which is the time required for the TL intensity \( I(t) \) to drop to half of its initial value [4].

Function glow curve deconvolution is used for deconvolving thermoluminescence glow curves according to various kinetic models.

For isothermal luminescence experiments \( I(t) \) the thermal excitation rate is \( \lambda \) :
\[
\lambda = \exp \left( \frac{E}{kT_m} \right)
\] (14)

2.4.1. First order kinetics (FOK)

Kitis et al. (5) [5] obtained the following analytical equation for the frequency factor:
\[
s = \frac{\beta E}{kT_m} \exp \left( \frac{E}{kT_m} \right)
\] (15)

The half-life are presented in the following equations [8,18,19] :
\[
t_{1/2} = \frac{\ln 2}{\lambda}
\] (16)

Taking into account Equations (1), (2) and (3), the half-life can be evaluated from the equation:
\[
t_{1/2} = \frac{\ln 2 kT_m^2}{\beta E}
\] (17)

2.4.2. s order kinetics (SOK)

Kitis et al. (5) [5] obtained the following analytical equation for the frequency factor:
\[
s = \frac{\beta E}{kT_m^2} \exp \left( \frac{E}{kT_m} \right)
\] (18)

The half-life can be evaluated from the following equation [8,18,19] :
\[
t_{1/2} = (N/n_0) \left( \sqrt{2} - 1 \right) / \lambda
\] (19)

Taking into account Equations (1), (4) and (5), the half-life is presented in the following equation:
\[
t_{1/2} = \frac{kT_m^2 (N/n_0) \left( \sqrt{2} - 1 \right) (1 + 2kT_m/E)}{\beta E}
\] (20)

2.4.3. General order kinetics (GOK)

Kitis et al. (5) [5] obtained the following analytical equation for the frequency factor:
\[
s = \left( \frac{\beta E}{kT_m^2} \right) \exp \left( \frac{E}{kT_m} \right) \left[ 1 + (b - 1) \frac{2kT_m}{E} \right]^{-1}
\] (21)

with \( b \) is the kinetic order.

The half-life (GOK) can be evaluated from the following equation [8,18,19] :
\[
t_{1/2} = \frac{(N/n_0)^{b-1}}{\lambda(b - 1)} \left( \frac{2^{b-1}}{b - 1} - 1 \right)
\] (22)

Taking into account Equations. (1), (8) and (9), the half-life is presented in the following equation:
\[
t_{1/2} = \frac{kT_m^2 [1 + 2(b - 1)kT_m/E] \left( \frac{2^{b-1}}{b - 1} \right) (N/n_0)^{b-1}}{\beta E(b - 1)}
\] (23)
2.4.4. Mixed order kinetics (MOK)

The frequency factor is computed [4]:

\[ s = \left( \frac{\beta E}{kT_m^2} \right) \exp \left( \frac{E}{kT_m} \right) \frac{\alpha R_m}{(1 - \alpha)} \]  

(24)

The final form of the term \( R_m \) is computed [4] by the equation:

\[ R_m = \frac{2.6 - 0.9203\alpha + 0.324\alpha^{3.338}}{2.6 - 2.9203\alpha + 0.324\alpha^{3.338}} \]

\( \alpha \) is the kinetic parameter describing the glow peak.

The half-life (MOK) can be evaluated from the following equations [18]:

\[ t_{1/2} = \frac{\left( 1 + \frac{n_0}{n_0(1-\alpha)} \right) \ln \left[ 1 - \alpha + \alpha^2 + (1 - \alpha)\sqrt{1 + \alpha^2} / \lambda \right]}{\beta E \alpha R_m} \]  

(25)

\[ t_{1/2} = \frac{\ln \left[ 1 - \alpha + \alpha^2 + (1 - \alpha)\sqrt{1 + \alpha^2} / \lambda \right]}{\beta E \alpha R_m} \]  

(26)

2.4.5. One trap one recombination center (OTOR)

The frequency factor is computed [16,20] by the equation:

\[ s = \left( \frac{\beta E}{kT_m^2} \right) \exp \left( \frac{E}{kT_m} \right) \left[ (1 + W[\exp(Zm)]^2 / 1 + 2W[\exp(Zm)]) \right] (1 - R) \]  

(27)

The half-life (OTOR) can be evaluated from the following equation [8,18]:

\[ t_{1/2} = \frac{-1 - 2R/y + R + A}{-2 \ln \left( \frac{A^{R+1}}{4(1+R/y-R)} - 2R \ln \frac{A^{R-1}}{2N/y^2} \right)} \]  

(28)

with

\[ A = \sqrt{(R-1)^2 - 8R(R-1)/y + 8R^2/y^2} \]

\( y = n_0/N \)

\( t_{1/2} = \frac{-1 - 2R/y + R + A}{-2 \ln \left( \frac{A^{R+1}}{4(1+R/y-R)} - 2R \ln \frac{A^{R-1}}{2N/y^2} \right)} \]  

(29)

The fitting the glow curves of TL depended on the figure of merit (FOM) given by:

\[ \text{FOM} = \frac{\sum_{p} |y_{\text{exp}} - y_{\text{fit}}|}{\sum_{p} y_{\text{fit}}} \]  

(30)

where \( y_{\text{exp}} \) and \( y_{\text{fit}} \) are the experimental data and the values of the fitting function, respectively.

3. Results and discussion

3.1. Simulate TL curves based on parameters in TL traps

The curves of the single peak TL are simulated according to trap parameters based on FOK, SOK and GOK models. They are simulated from given initial trapping parameters: \( n_0 = 10^8 \), \( N = 10^{10} \), \( E = 1.1 \) (eV), \( \beta = 1 \) (K/s), \( s = 8.10^{14} \) (s\(^{-1}\)) and kinetic parameters: \( b = 1.61, R = 0.008 \) or \( \alpha = 0.99 \). Then, the peak TL curve is estimated as the maximum peak temperature: \( T_m = 473 \) (K). In Figure 1, TL curves are simulated according to trap parameters based on FOK, SOK and GOK models.

In Figure 2, TL curves are simulated according to trap parameters based on GOK, MOK and OTOR. In Figure 3, TL curves from given trap parameters according to different models (FOK, SOK, GOK, MOK and OTOR) are simulated.

The evaluation of simulation results is based on the FOM coefficient. Simulation results show curves following different models with similar results. Then, the FOM of the simulation curves is very small. The simulation results also show that the temperature at the top of the TL curve is almost equal, the maximum intensity of the TL curve is different. Thus, in different models, the simulation results obtained on peak TL of TL curve are similar. Realizing that, in research models, GOK is the simplest model and the most suitable model compared to other models.

3.2. Simulate the TL curve based on peak parameters

From the parameters of the top of the curve TL were given as \( I_m = 8000, E = 0.95 \) (eV), \( T_m = 473 \) (K) and kinetic parameters: \( b = 1.61, R = 0.2 \) or \( \alpha = 0.0001 \), the frequency factor of peak TL is estimated: \( s = 8.10^{14} \) (s\(^{-1}\)). In Figure 4, TL curves are simulated according to trap parameters based on FOK, GOK and GOK models. In Figure 5, TL curves are simulated according to trap parameters based on GOK, MOK and OTOR models. Unlike the simulation method based on trap parameters, this method used a given spectral peak parameter, then estimates the frequency factor of the spectrum peak and evaluates the estimate based on the FOM coefficient. According to different models, the calculated FOM coefficient is also quite small and shows that the fit is suitable. The calculation results show that the obtained frequency factor is similar. Therefore, with given initial spectral peak parameters, the frequency factor can be estimated according to different models.

Consider the specific case for simulated TL curve with GOK models according to given TL peak parameters including \( I_m = 10968, E = 1.18 \) (eV), \( T_m = 490 \) (K) and kinetic order \( b = 1.0001 \). The frequency factor and half-life parameter of peak TL were estimated...
Figure 1. Simulate a TL curve from trapping parameters according to FOK, SOK and GOK models.

Figure 2. Simulate a TL curve from trapping parameters according to GOK, MOK and OTOR models.
to be: \( s = 8.1 \times 10^{10} \, (s^{-1}) \) and 12.150 (s). The results show
that the small FOM coefficient proves that the simula-
tion is suitable.

In general, with TL curve simulation according to dif-
ferent models and different ways, TL curve is evaluated
and analyzed clearly and accurately based on Python
software. The FOM coefficients are small, the escape
frequency and the half-life according to the models
are nearly equal, indicating that the simulation is suit-
able. Therefore, this simulation method can be used
in the simulation of the TL curve to estimate trapping
parameters.

Figure 3. The TL curves from giving trap parameters according to different models such as FOK, SOK, GOK, MOK and OTOR.

Figure 4. Simulate a TL curve with peak TL parameters according to FOK, SOK and GOK models.
3.3. Results of the calculation of the half-life of the experimental TL curve

Experimental TL curves showed peak TL parameters and peak intensity. Based on these parameters, we could estimate the frequency factor. Half-life is calculated by the frequency factor and initial parameters. The results show that the computing half-life values of the TL traps of simulated and empirical samples consist single or multiple overlapping peaks. The heating rate selected for all simulation and experiment curve is 1 K/s. The results of the TL curves are shown in Table 1.

The experimental curves in this study were referenced from the GLOCANIN project [13,14]. The results of the data set were commonly used in the TL curves study. This project was done seriously and quite meticulously in modern and famous laboratories in the world.

First, the TL curve is considered to be Rg1 from the GLOCANIN project [13,14]. Rg1 is a single peak so Rg1 is matched and computed with a peak. The TL curve of Rg1 is a single peak with one peak located the TL intensity at 10968 and temperatures at 490 (K). Results show that the half-life values of Rg1 are determined as 12.152 (GOK), 12.154 (OTOR) and 12.145 (s) (MOK). The FOM values of Rg1 were 1e-2 (GOK and OTOR) and 3e-2 (MOK). Therefore, the glow curve of Rg1 are consistent with GOK or OTOR model. The computation of the glow curve of Rg1 consists of the single peak given by Figure 6.

Calculation results with the Rg1 curve show that the FOMs of all models are very small. Therefore, the curve Rg1 has been matched very well and close to the experiment. The half-life results of the calculated models are similar. The half-life values according to the models are obtained equal, proving that the calculation method according to the models is suitable. The kinetic equations of the GOK model are simpler than the other models, so in the models, the GOK model gives the fastest calculation results (Table 2).

Next, the TL curve was considered to be Rg2 from the GLOCANIN project [13,14]. Towards the glow curve fitting Rg2, they consist of four main peaks and are given by Figure 7. The experimental curve Rg2 has four main peaks at peak intensity and temperature, respectively $I_m = 398$, 543, 835 and 1623; $T_m = 417$, 456, 484, 511(K). Results show that the half-life values of Rg2 of the four peaks are determined as 7.640, 8.457, 8.880, 7.824 (GOK), 7.782, 7.587, 8.869, 8.247 (s) (OTOR) and 1349.65, 408.269, 7.310, 40.193 (s) (MOK). The half-life

### Table 1. The results determine the half-life of the TL curves from the GLOCANIN project [13,14] according to GOK, MOK and OTOR models.

| TL  | Peaks | GOK t$_{1/2}$ (s) | OTOR t$_{1/2}$ (s) | MOK t$_{1/2}$ (s) | FOM |
|-----|-------|------------------|-------------------|------------------|-----|
| Rg1 | P1    | 12.152           | 12.154            | 12.145           | 7.1e-4 |
|     | P2    | 7.640            | 7.782             | 1349.65          | 2.6e-3 |
|     | P3    | 8.880            | 7.587             | 408.269          | 2.6e-3 |
|     | P4    | 7.824            | 8.869             | 7.310            | 40.193 |

3.3. Results of the calculation of the half-life of the experimental TL curve

Experimental TL curves showed peak TL parameters and peak intensity. Based on these parameters, we could estimate the frequency factor. Half-life is calculated by the frequency factor and initial parameters. The results show that the computing half-life values of the TL traps of simulated and empirical samples consist single or multiple overlapping peaks. The heating rate selected for all simulation and experiment curve is 1 K/s. The results of the TL curves are shown in Table 1.

The experimental curves in this study were referenced from the GLOCANIN project [13,14]. The results of the data set were commonly used in the TL curves study. This project was done seriously and quite meticulously in modern and famous laboratories in the world.

First, the TL curve is considered to be Rg1 from the GLOCANIN project [13,14]. Rg1 is a single peak so Rg1 is matched and computed with a peak. The TL curve of Rg1 is a single peak with one peak located the TL intensity at 10968 and temperatures at 490 (K). Results show that the half-life values of Rg1 are determined as 12.152 (GOK), 12.154 (OTOR) and 12.145 (s) (MOK). The FOM values of Rg1 were 1e-2 (GOK and OTOR) and 3e-2 (MOK). Therefore, the glow curve of Rg1 are consistent with GOK or OTOR model. The computation of the glow curve of Rg1 consists of the single peak given by Figure 6.

Calculation results with the Rg1 curve show that the FOMs of all models are very small. Therefore, the curve Rg1 has been matched very well and close to the experiment. The half-life results of the calculated models are similar. The half-life values according to the models are obtained equal, proving that the calculation method according to the models is suitable. The kinetic equations of the GOK model are simpler than the other models, so in the models, the GOK model gives the fastest calculation results (Table 2).

Next, the TL curve was considered to be Rg2 from the GLOCANIN project [13,14]. Towards the glow curve fitting Rg2, they consist of four main peaks and are given by Figure 7. The experimental curve Rg2 has four main peaks at peak intensity and temperature, respectively $I_m = 398$, 543, 835 and 1623; $T_m = 417$, 456, 484, 511(K). Results show that the half-life values of Rg2 of the four peaks are determined as 7.640, 8.457, 8.880, 7.824 (GOK), 7.782, 7.587, 8.869, 8.247 (s) (OTOR) and 1349.65, 408.269, 7.310, 40.193 (s) (MOK). The half-life
values of Rg2 in the GOK, OTOR, MOK model are not much different. The FOM values of Rg2 were very low and nearly equal each other (8e-3 and 9e-3). Therefore, Rg2 are consistent with GOK, OTOR or MOK model.

Calculation results show that FOM is very small, showing that the TL curve is well matched. The half-life values of the Rg2 curve are equal, proving that the model to calculate the Rg2 curve is suitable. Compare each other models, the GOK model gives the best results, the fastest execution time. Toward the MOK model, the programme takes a long time to calculate and give results. This is because the kinetic equations of the MOK model are relatively complex, requiring many iterations compared to the other two models.

In the case of the Rg9 curve from the GLOCANIN project [13,14], it is a complex curve with many peaks TL. The calculation results show that Rg9 curve is most suitable when fitting with nine peaks and according to GOK model. Fitting and half-life computation is shown in the Figure 8.

In general, for the experimental single-peak TL curve, the simulation and calculation of the half-life according to the models are quickly and accurately simulated. For the experimental TL curve, the complex includes the superposition of many peaks according to the existing dynamic models which are still simulated and calculated reasonably. However, when comparing GOK, OTOR and MOK models, the GOK model gives simple, fast calculation and is more suitable than the other models. The lower the FOM value, the TL curve is considered to be closer to the experiment. The model for the lowest FOM would be selected as a result of the half-life value. The determination of the half-life values of the TL traps of the simulated and experimental samples basing on the TL curves is investigated. The calculated results depend on the FOM values of GOK, OTOR and MOK model. The half-life values for the TL curves by others models are different each other. The reason of this difference comes from individual errors that lead to total errors during the calculation and fitting of models. Therefore, in the calculation process, if the errors of matching are too big, we cannot apply this method to determine the half-life values. In this study, the simulated and calculated TL of FOM values of GOK, OTOR and MOK model are very low. It is, therefore, possible to apply the half-life calculation method of the TL traps of the samples from the TL curves.
Figure 7. Calculate the half-life by fitting the TL Rg2 curve based on the GOK model.

Figure 8. Calculate the half-life by fitting the TL Rg9 curve based on the GOK model.
4. Conclusions

The results of the calculation are consistent with the model of simulation and experiment. The method of determining the half-life of the samples by comparing the kinetics parameters by the models of GOK, OTOR or MOK is investigated and applied. The method gets more suitable if the FOM values are low. The results show that, the half-life values of the Rg1, Rg2 have been approximately equal. Accurately determining the half-life values of the TL traps will be of great significance in determining the existence of the TL peaks over time that is a basis for studying applications related to dose measurement, the TL material preparation, detection and identification of irradiated food.

The article presents the method of calculating half-life of simulated and experimental samples including the peaks of glow curves of TL. The simulation and computation are performed based on Python. The simulation, computation and splitting peak TL curve of Python software to calculate the half-life was researched and applied for the first time. The potential for application of Python software in TL curve simulations and analysis is huge. Python applications in data science in general and in simulation and TL curve processing, in particular, will continue to grow significantly in the coming time.

Disclosure statement

No potential conflict of interest was reported by the author(s).

ORCID

Nguyen Duy Sang  http://orcid.org/0000-0001-5017-383X

References

[1] Jones E, Oliphant T, Peterson P. “SciPy: Open source scientific tools for Python”, 2001.
[2] McKinney W. “Data Structures for Statistical Computing in Python”, Proceedings of the 9th Python in Science Conference, pp. 51-56, 2010.
[3] Pagonis V, Kitis G, Furetta C. Numerical and Practical Exercises in Thermoluminescence. United States of America: Springer; 2006.
[4] Kitis G, Gomez-Ros JM. Thermoluminescence glow-curve deconvolution functions for mixed order of kinetics and continuous trap distribution. Nucl Instrum Methods Phys Res Sect A. 2000;440(1):224–231.
[5] Kitis G, Gomez-Ros JM, Tuyn JWN. Thermoluminescence glow-curve deconvolution functions for first, second and general orders of kinetics. J Phys D: Appl Phys. 1998;31(19):2636–2641.
[6] Kitis G, Vlachos ND. General semi-analytical expressions for TL, OSL and other luminescence stimulation modes derived from the OTOR model using the Lambert W-function. Radiat Meas. 2013;48:47–54.
[7] Sadek AM, Eissa HM, Basha AM, et al. The deconvolution of thermoluminescence glow-curves using general expressions derived from the one trap-one recombination (OTOR) level model. Appl Radiat Isot. 2015;95:214–221.
[8] Kitis G, Pagonis V. New expressions for half life, peak maximum temperature, activation energy and kinetic order of a thermoluminescence glow peak based on the Lambert W function. Radiat Meas. 2017;97:28–34.
[9] Singh LL, Gartia RK. Theoretical derivation of a simplified form of the OTOR/GOT differential equation. Radiat Meas. 2013;59:160–164.
[10] Singh LL, Gartia RK. Derivation of an expression for lifetime (\(\tau\)) in OTOR model. Nucl Instrum Methods Phys Res Sect B. 2013;308:21–23.
[11] Singh LL, Gartia RK. Derivation of a simplified OSL OTOR equation using Wright Omega function and its application. Nucl Instrum Methods Phys Res Sect B. 2015;346:45–52.
[12] Sunta CM, Ayta WEF, Chubaci JFD, et al. General order and mixed order fits of thermoluminescence glow curves—a comparison. Radiat Meas. 2002;35(1):47–57.
[13] Bos AJJ, Pitera TM, Ros JMG, et al. An intercomparison of glow curve analysis computer programs: I. Synthetic Glow Curves. Radiat Prot Dosim. 1993;47(1):473–477.
[14] Bos AJJ, Pitera TM, Ros JMG, et al. An intercomparison of glow curve analysis computer programs: II. Measured Glow Curves. Radiat Prot Dosim. 1994;51(1):257–264.
[15] Puchalska M, Bilski P. GlowFit - a new tool for thermoluminescence glow-curve deconvolution. Radiat Meas. 2006;41(6):659–664.
[16] Sadek AM, Eissa HM, Basha AM, et al. The deconvolution of thermoluminescence glow-curves using general expressions derived from the one trap-one recombination (OTOR) level model. Appl Radiat Isot. 2015;95:214–221.
[17] Peng J, Dong Z, Han F. tgcd: An R package for analyzing thermoluminescence glow curves. SoftwareX. 2016;5:112–120.
[18] Pagonis V, Kitis G, Polymeris GS. On the half-life of luminescence signals in dosimetric applications: A unified presentation. Physica B: Condensed Matter. 2018;539:35–43.
[19] Furetta C. Some remarks on the pre-exponential factor and the half-life in second and general order of kinetics. Journal of Materials Science Letters. 2003;22(20):1395–1397.
[20] Kitis G, Vlachos ND. General semi-analytical expressions for TL, OSL and other luminescence stimulation modes derived from the OTOR model using the Lambert W-function. Radiat Meas. 2013;48:47–54.