Duller, G., 2015. *The Analyst software package for luminescence data: overview and recent improvements.* Ancient TL 33(1): 35-42. https://doi.org/10.26034/la.atl.2015.489

Ancient TL

The Analyst software package for luminescence data: overview and recent improvements

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1. Introduction

Luminescence data collected for geochronology and dosimetry requires different types of manipulation and analysis in order to extract the information of interest. As automated systems for measurement of luminescence signals have developed (Bøtter-Jensen et al., 2010), the rate at which data can be acquired has increased. In addition, the development of equipment to obtain luminescence signals from individual mineral grains, whether using scanning systems (Duller et al., 1999) or imaging systems (Thomsen et al., in press), has further exacerbated this situation. It is not uncommon to make equivalent dose measurements of thousands of grains for each sample, involving tens of thousands of individual luminescence measurements.

In recent years a number of routines for analysis of luminescence data have been written in R (e.g., Kreutzer et al. 2012, Peng et al. 2013). These provide a range of tools for the manipulation and analysis of luminescence data and have the advantage that at least some of them (Kreutzer et al., 2012) are open source and thus it is explicit what numerical operations are undertaken. However, although these packages are capable of extremely complex analyses, they do require some understanding of the R environment, and there is currently no visual interface so interaction is primarily through command line statements (or scripts).

Analyst is a Windows based software package written in Delphi that has been developed over the last 15 years. It was originally written to analyse data collected in instruments built at Risø National Laboratory (e.g. Bøtter-Jensen et al. 2003), but can also be used for the analysis of data collected on other instruments provided that they generate compatible data files. Although the software has been used widely during the last 15 years, an overview of the capabilities of the software has never been given. Furthermore, a recent update to the software has included a number of significant enhancements. This paper seeks to summarise the overall capabilities of the software and to focus on recent improvements and additional capabilities.

2. Overview of software capability

The data format used by instruments built at Risø consists of a series of records, one for each luminescence measurement that is made. Each record contains a header (Table S1) which includes more than 60 parameters, some of which describe the conditions used to collect the data (e.g. the type of light source used for optical stimulation, the heating rate used for TL measurements, or the number of data points collected), and some of which are used to store information that can be used during data processing (e.g. whether the measurement is of a natural signal, or a regenerated signal). Following each header is a block of data collected during the measurement. The number of data points is specified in the header. The BINX file format consists of any number of headers and data blocks (i.e. header, data block, header, data block, header, data block...). The BIN file formats that were generated by previous versions of the Sequence Editor have the same overall structure as the BINX files, but the headers contain fewer parameters. Analyst is able to read all versions of BIN and BINX files.

Analyst provides a means for manipulating and viewing thermoluminescence (TL) and optically stimulated luminescence (OSL) data. The functionality can be split into three groups: (a) editing the header contents and selecting which data is appropriate for analysis, (b) visualisation of data, and (c) data analysis (e.g. construction of dose response curves, fading tests or component fitting).
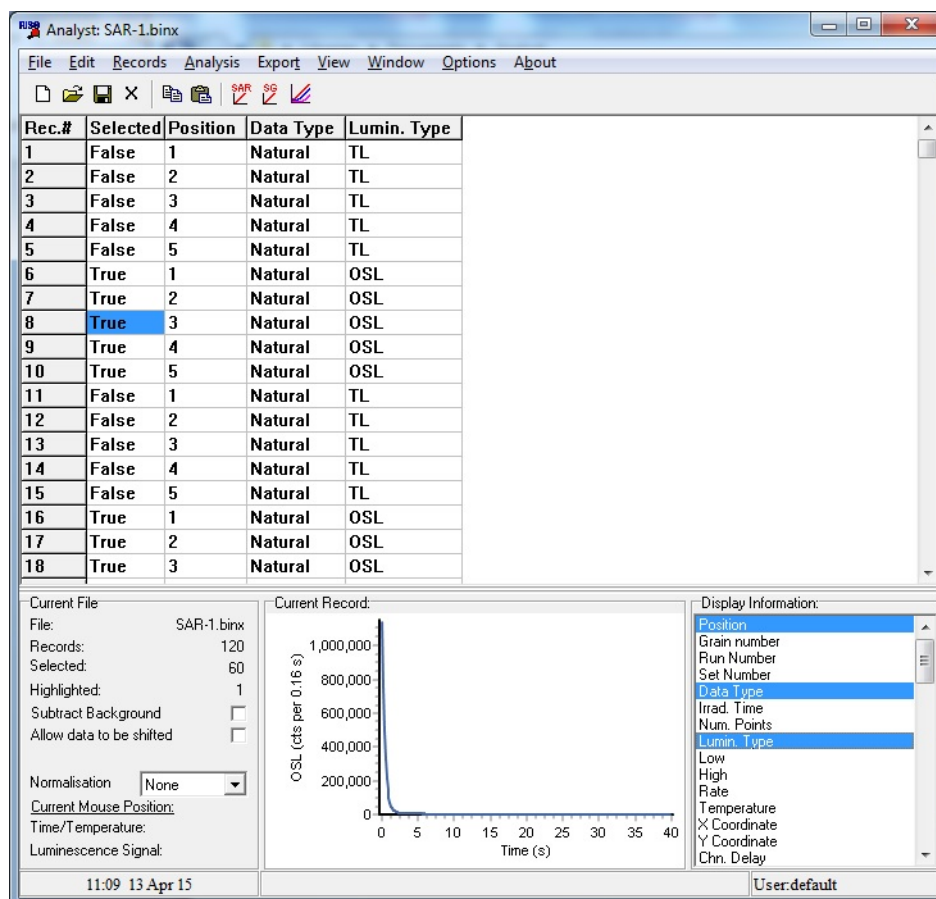
Figure 1: The front page of Analyst can be customised to show whichever parameters from the header are wanted - in this case the sample position on the carousel, the type of data and the type of luminescence measurement.

3. Editing header contents and selection of data

A large number of the parameters stored in the header for each luminescence measurement are set during data collection, for example the number of data points, the date and time of collection, the temperature at the time of collection, the heating rate that was used to reach this temperature, and if appropriate the type of optical stimulation that was used and the percentage stimulation power. Within the main screen of Analyst the user can select which of these parameters to display (Figure 1).

Some parameters are not set at run time, but can be edited in Analyst to give additional information that can be used in data analysis. For instance, when determining equivalent dose (D_e) using multiple aliquots it is important to specify which aliquots retain their natural luminescence signal, and which have had additive doses given, or regeneration doses given. Analyst allows any of the parameters in the header (except the number of data points) to be edited, either working on individual records at a time, or selecting a block of records and changing parameters for all of the records (using the 'Block Edit' function). The irradiation dose given to different aliquots is also important if equivalent dose is to be determined. The irradiation that each aliquot received prior to measurement may be edited in Analyst, though the irradiation time can also be automatically inserted into the BINX file by the Sequence Editor making it unnecessary to edit this parameter manually.
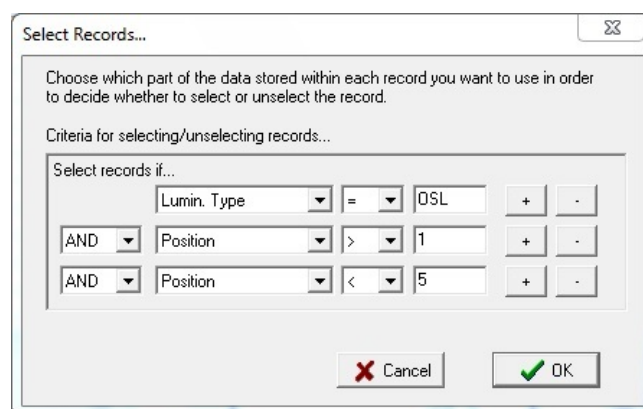

Figure 2: Selecting records from a BINX file for data collected for carousel positions 2, 3 and 4 and which are OSL measurements.
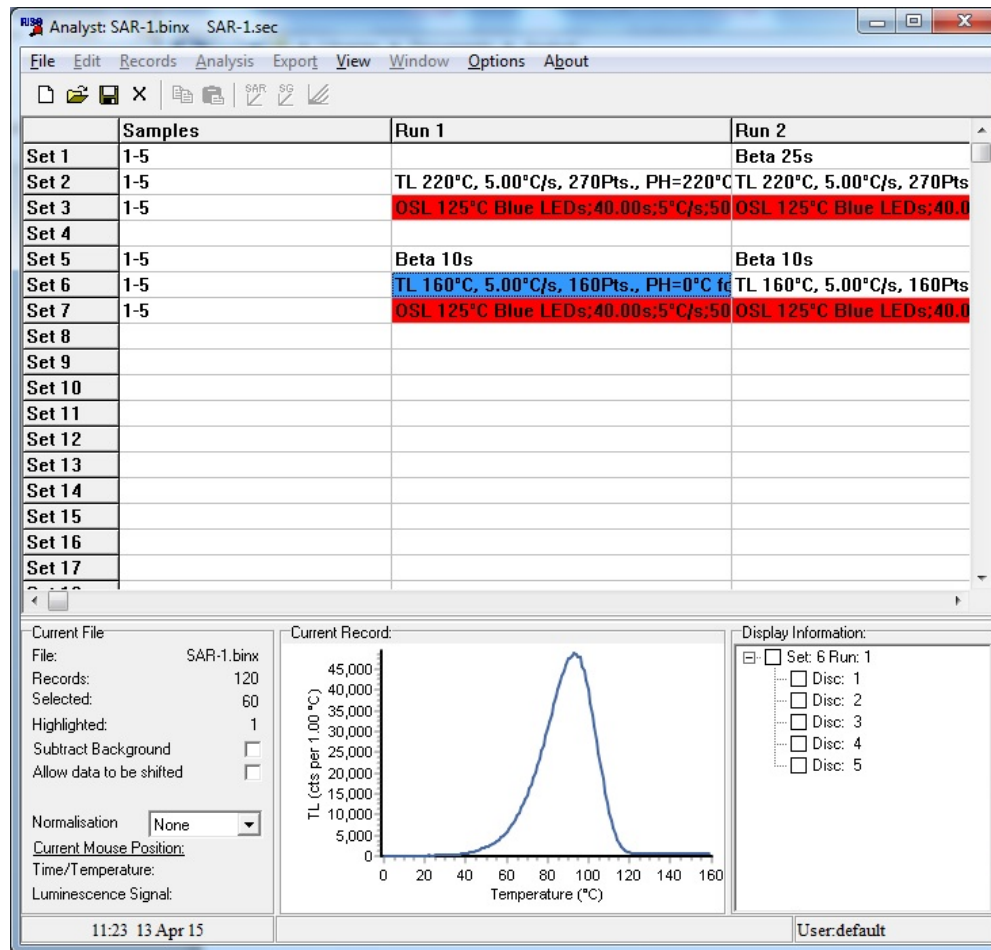
Figure 3: Visualising a BINX file using the sequence used to collect the data. In this example the cell shown in blue is highlighted. This part of the sequence collected TL data for aliquots in positions 1 to 5, and a list of these data is shown in the bottom right hand side of the screen. At present, none of this TL has been selected for analysis and so none of the tick boxes in the bottom right panel are selected, and the cell in the main panel is not coloured red.

Perhaps the most common activity under this heading is to select which of the records in a BINX file are to be used in subsequent data analysis. It is possible to delete records, but this deletion is permanent. A better approach is to mark which records are to be selected for subsequent analyses, and which are not. This is done by setting the 'Select' entry in the header of each record. Individual records can be selected or unselected individually using key strokes, but a more sophisticated approach is to filter which records are to be selected or unselected based upon some aspect of the header information (Figure 2). A common application of this approach would be in post-IR IRSL procedures (Thomsen et al., 2008) where IRSL has been measured at two or more temperatures (e.g. IR$_{50}$ and IR$_{225}$), but analysis is required using only one of these data sets. This can be achieved by selecting records where the temperature parameter in the header is equal to 225, or can be achieved by selecting specific set numbers or run numbers.

A recent addition to Analyst is the ability to display the data in a format that reflects the sequence used to collect the data (Figure 3). This option is available if the copy of the sequence file (.SEC) used to collect the data is stored in the same directory where Analyst accessed the BINX file. This option is useful for navigating through complex sequences, and can also be used to conveniently select all the records collected by a command in the Sequence file.

4. Visualisation of data

Visualisation is an essential part of exploring data and Analyst provides a range of opportunities to do this. In the main display the data for individual luminescence measurements is displayed at the bottom of the screen. A new facility within the package is to be able to compare up to 30 records simultaneously by plotting them on the same graph (Figure 4a). It is possible to select which records to display either by dragging and dropping them onto the graph page, or by using a filtering command similar to that used to select data (Figure 2). The drag and drop option makes it possible to compare records from different BINX files. As many
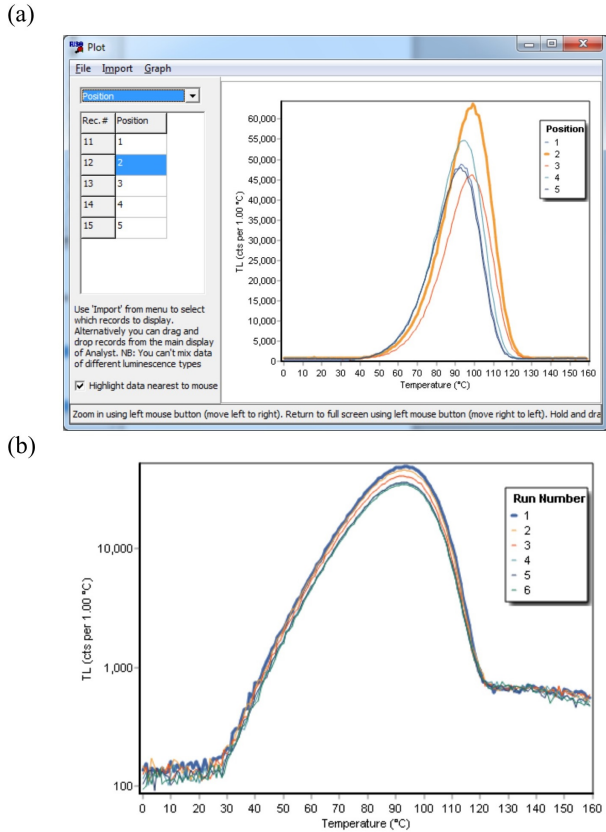
(a)

(b)

Figure 4: Selecting records from a BINX file for data collected for carousel positions 2, 3 and 4 and which are OSL measurements.

graphs as required can be displayed simultaneously. Furthermore, the characteristics of these graphs can be manipulated by the user, for instance whether to use logarithmic axes, what range of data to show on the axes, and the font size (e.g. Figure 4b).

5. Data analysis

Four major types of data analysis are supported in Analyst, (1) multiple aliquot determination of equivalent dose (D_e), (2) single aliquot (and single grain) determination of D_e, (3) calculation of fading rates and (4) component fitting of CW-OSL data.

5.1. Multiple aliquot D_e determination

Equivalent dose determination using multiple aliquots has been a feature of Analyst for many years, and both the additive dose and regenerative dose methods are supported. In each case it is possible both to calculate a D_e based upon integration of a region of interest (e.g. a specific temperature range for TL measurements, or a specific part of the OSL decay curve), and also to calculate a D_e plateau over a range of values (Figure 5). A variety of equations can be used to

fit the dose response curve and the most important ones are listed in Table 1.

5.2. Single aliquot and single grain D_e determination

The same range of equations (Table 1) are also available when fitting dose response curves generated from single aliquot or single grain data sets. It has long been possible in Analyst to apply a range of acceptance criteria (Jacobs et al., 2006) to individual aliquots in order to assess whether the D_e value should be accepted for subsequent analysis or not. One of the more recent additions is the ability to screen on the basis of recuperation. The recuperation is assessed by looking at the signal when no dose has been given to the aliquot in the SAR sequence. The magnitude of the recuperated signal can be expressed in one of three ways. The first and most commonly used in published work, is to express the recuperated signal as a percentage of the natural signal. However, where samples are very young and the natural signal is weak, this may yield misleading results. One alternative is to express the recuperation as a percentage of the largest regeneration dose, and the final possibility is to extrapolate the dose response curve to where it intersects the dose axis and to use this as the 'apparent recuperated dose'. This provides an absolute measure (expressed in seconds or Gy) of the magnitude of the recuperated signal.

The assessment of uncertainty of the calculated D_e is critical, and the approach used in Analyst has been described previously by Duller (2007). The uncertainty in the measurement of individual luminescence signals is calculated from the counting statistics using the method described in Galbraith (2002), and an additional uncertainty associated with instrumental uncertainty (e.g. Armitage et al. 2000, Thomsen et al. 2005) can be combined in quadrature. Two approaches are possible in Analyst for how to propagate these uncertainties in luminescence intensity into uncertainties in equivalent dose. The default approach is to use the uncertainty calculated for the natural signal and propagate this through the interpolation onto the dose response curve. In

Linear
$$y = a + bx$$

Saturating exponential
$$y = a\left(1 - e^{-\frac{x+c}{b}}\right)$$

Saturating exponential plus linear
$$y = a\left(1 - e^{-\frac{x+c}{b}}\right) + gx$$

Sum of saturating exponentials
$$y = a\left(1 - e^{-\frac{x}{b}}\right) + c\left(1 - e^{-\frac{x}{d}}\right) + g$$

Table 1: Some of the equations available within Analyst for fitting dose response curves generated from multiple aliquot, single aliquot or single grain data sets.
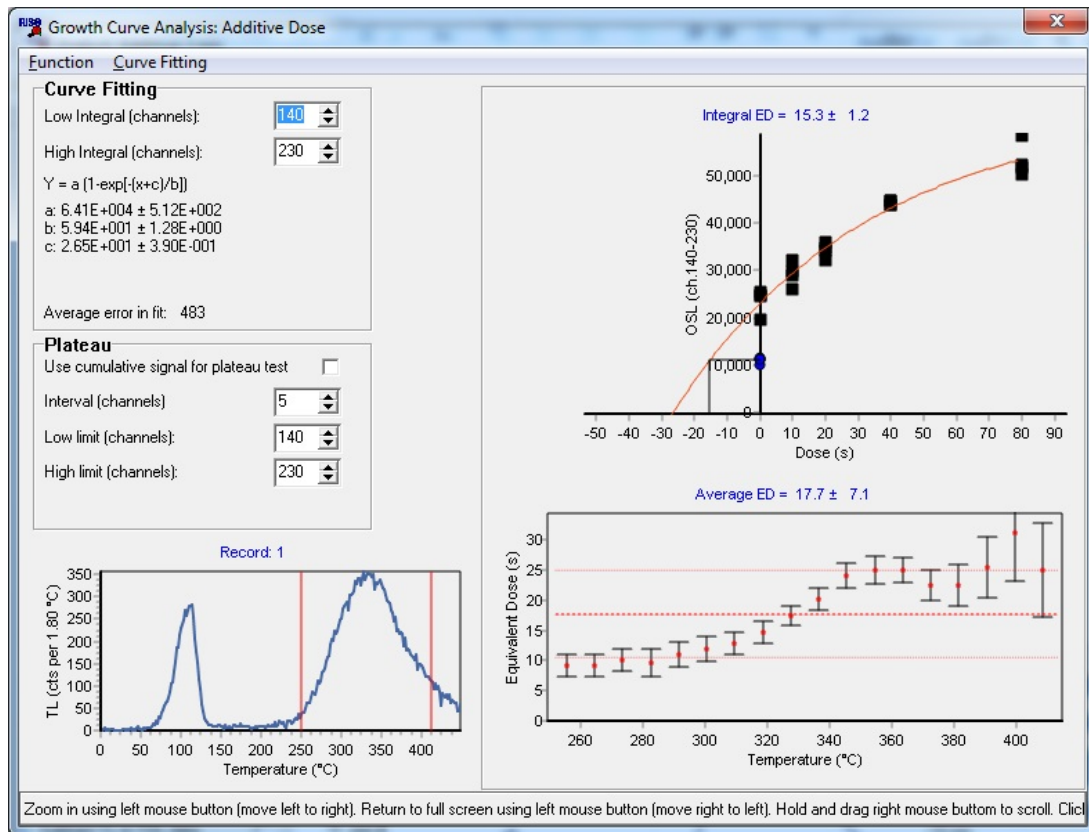
Figure 5: Example of analysis of a multiple aliquot additive dose data set, both showing the De calculated over a broad integral (upper right), and a plateau test (lower right) across a range of temperatures from 250 to 410°C

this approach, additional uncertainty in the fit of the data to the dose response curve is accounted for by including an additional uncertainty calculated from the average deviation of data points from the dose response curve (Eqn. 7 of Duller
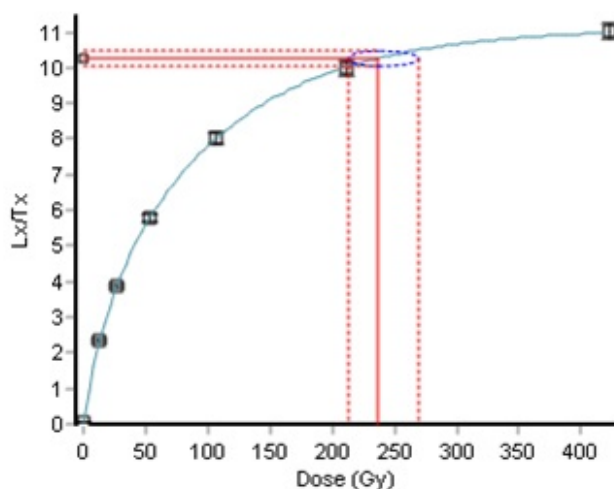

Figure 6: Dose response curve where the dose is expressed in Gray, generated by Analyst.

2007). A second approach is to use a Monte Carlo method to determine the impact of uncertainties in all the L_x/T_x ratios determined for an aliquot upon the D_e. Whilst the Monte Carlo method requires greater computational time, analysis using this method is still fast on most modern computers. These two approaches are still available in Analyst. At high doses where there is significant curvature of the dose response curve the uncertainties are likely to be asymmetric (Murray & Funder, 2003) and Analyst will now calculate estimates of the positive and negative uncertainties (e.g. 230^{+25}_{-14}).

Analysis of BINX files containing data for tens, hundreds or thousands of equivalent dose measurements would take a long period of time to step through individually. Analyst is able to automatically step through a BINX file and attempt to calculate a D_e value for every aliquot or grain. In such automated analysis the acceptance criteria (e.g. recycling, recuperation) are used to decide whether an individual D_e estimate is accepted or rejected. A further addition to Analyst is the display of a range of summary statistics for the suite of D_e values obtained from a BINX file (at present these are based only on symmetrical uncertainties). The range of summary statistics describing the distribution of D_e values includes the mean, weighted mean, common age model, central age model, overdispersion (Galbraith et al., 1999) and mean square of weighted deviates (MSWD).
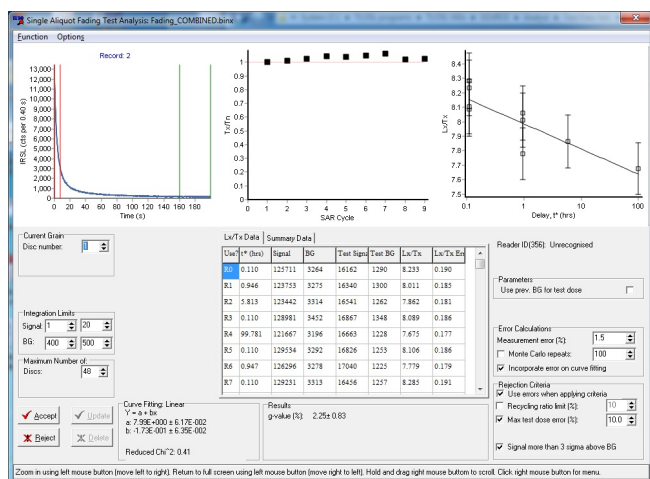
Figure 7: Fading data combining data measured for short storage periods (up to 6 hours) undertaken as part of a single sequence with data obtained after storage for 100 hours outside the instrument.

A final change in the most recent version of Analyst is the ability to calculate D_e values in Gray as well as seconds. The latest BINX format includes a parameter defining the dose rate of the source used for irradiation, so that irradiation times in seconds can be converted to Gy. This dose rate parameter may either be set automatically by the Sequence Editor when the data is collected, or changed in Analyst. Providing that a dose rate is set, the user can select whether to work in seconds or Gy when calculating D_e values. This makes it relatively simple to generate dose response curves of moderate quality for talks or publication which are expressed in Gy (e.g. Figure 6), and not seconds.

5.3. Calculating fading rates

The development of analytical protocols designed to isolate a signal from feldspar which has negligible anomalous fading (Thomsen et al., 2008) has reinvigorated study of this mineral group for geochronology. An important part of many studies is to explicitly test the rate of fading observed over laboratory timescales, and the methods outlined by Huntley & Lamothe (2001) and Auclair et al. (2003) are commonly used. These involve making prompt and delayed measurements, with a test dose correction applied. Critical to calculation of fading rates is knowledge of the time between irradiation and luminescence measurement so that t^* can be calculated (Auclair et al., 2003). The time since irradiation is one of the new parameters stored in BINX headers. If irradiation and subsequent measurement are undertaken within a single measurement sequence then this time since irradiation is set automatically when data are collected. If storage outside the automated reader is used to obtain data extending over longer periods of time, to improve the characterisation of the fading rate, then the time since irradiation needs to be input into the header by the user in Analyst. Once this time

since irradiation parameter has been set, Analyst is able to calculate t^*, plot the drop in luminescence as a function of time (t^*) and fit the data to obtain a g-value (normalised to 2 days; Figure 7).

5.4. Component fitting of CW-OSL data

An experimental part of Analyst that has been included in the most recent version can be used to fit a sum of exponential decays to continuous wave OSL (CW-OSL) data (Figure 8). The equation used for fitting is

$$ y = a + \left[n_1 . b_1 e^{-b_1 t} \right] + \left[n_2 . b_2 e^{-b_2 t} \right] + \left[n_3 . b_3 e^{-b_3 t} \right] $$

where the number of components can be changed from one to three (the equation above is for a three component fit). A Levenberg-Marquardt method is used for fitting. Initial estimates of the parameters are generated automatically, but the user can edit these initial estimates if desired. Additionally, the user can fix any parameter (for instance the parameter b_1 which is the rate of decay of the fastest component, e.g. Rowan et al. (2012). The challenges of this type of fitting have been described by Bailey et al. (2011). Initial experiments to incorporate routine curve fitting of this type into Analyst so that component resolved D_e values can be determined have been undertaken, but at present the system is not sufficiently robust to be reliable, and more complex approaches such as the differential evolution method described by Bluszcz & Adamiec (2006) may be required to ensuring that global best fits are always obtained rather than falling into localised minima.

6. Accessibility of data

Analyst provides a range of options for manipulating, interrogating and analysing luminescence data, but any package of this nature can never be a complete solution to all the requirements that users may have. Analyst has been designed to make it as easy as possible for data to be exported so that it can be analysed using other software and so that more complex graphs can be generated. The main display of Analyst provides the opportunity to export both information from the headers and the luminescence data via the Windows clipboard, making it simple to paste into other packages (e.g. Excel), and similar facilities are available to export the data generated during single aliquot D_e determination or fading analysis for individual aliquots, or for groups of aliquots. The new graph tool used throughout the package also makes it possible to export both the raw data used to generate the graph (e.g. the doses and L_x/T_x ratios used to generate a dose response curve), and any of the analytical data produced (e.g. the dose response curve that is fitted, or the results of the Monte Carlo replicates used to estimate the uncertainty on D_e values).
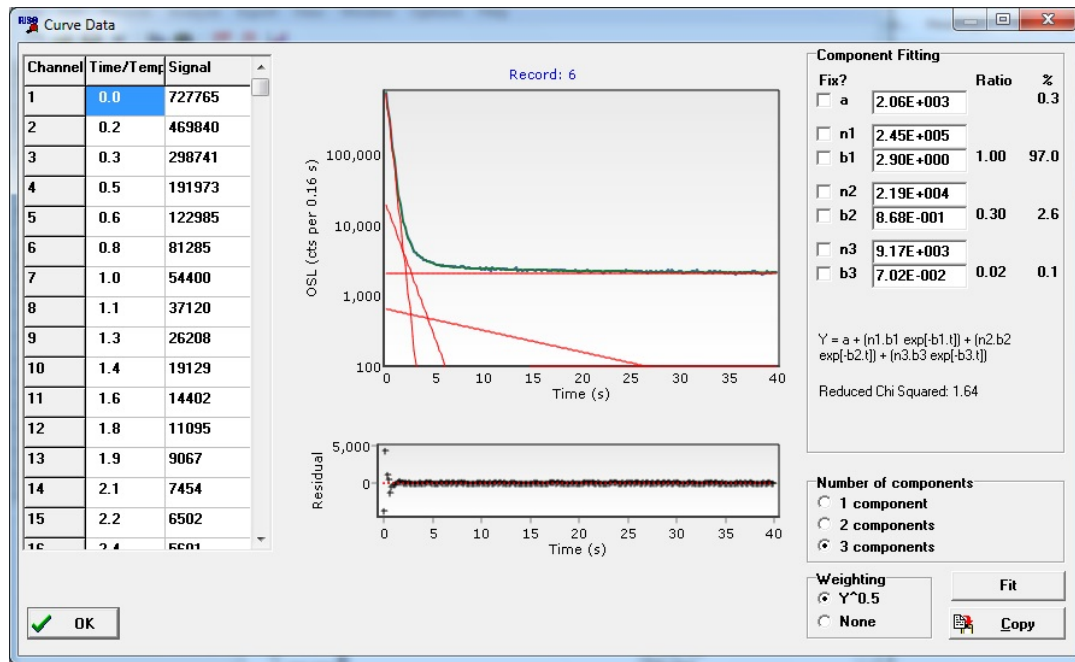
Figure 8: Example of component fitting a CW-OSL decay curve. The fitted parameters are given on the right hand side of the screen and can easily be copied to the clipboard for further processing.

7. Conclusion

The latest version of Analyst (v.4.31.7) is freely available either from the Aberystwyth Luminescence Research Laboratory website (http://www.aber.ac.uk/alrl) or from the DTU Nutech website (http://www.nutech.dtu.dk/english/Products-and-Services/Dosimetry/Radiation-Measurement-Instruments/TL_OSL_reader/Software). In addition to the new facilities described above, the package now contains an integrated context-sensitive help system (available by pressing F1 at any time) and a 77 page manual (Duller, 2015). It is hoped that this package will provide a user friendly, and highly visual, tool for analysing a range of luminescence data.

Supplementary Information

Table S1 is available as Supplementary Information at http://www.ecu.edu/cs-cas/physics/Ancient-Timeline/ancient-TOC33.cfm

Acknowledgments

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Reviewer

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