THE SFU PROGRAM SUITE

These programs are for analyzing luminescence data taken for optical
dating or for thermoluminescence dating.

The suite consists of four programs as follows: Programs 2, 3 and 4 require that the data be in a specified format. Data that are in some other formats can be rewritten in this required format using program 1.

1) **SFF-MAKE** is a program to read data from files in various formats, normalize the data, print it, view it and plot it. However, the main purpose of this program is to create a new file in a particular format; this file is given an .**SFF** extension. Programs 2, 3 and 4 require that the data be in this particular format

2) **REGEN** is a program to fit additive-dose data and regeneration data to a single function using the "Australian Slide".

3) **INTCPT** is a program to fit
   (a) additive-dose data only.
   (b) additive-dose with the thermal transfer correction (for optical dating).
   (c) additive-dose and partial bleach data (for TL dating).
   (d) additive dose extrapolated to a constant intensity.

4) **b-VALUE** is a program to jointly fit additive-dose data (beta or gamma) and additive alpha dose data to a single curve, the scaling factor for the two dose scales being the b-value.

Each program is described in some detail in the following sections. Some features that are common to the three main programs are described separately under the heading “common features”. A formal description of the **.SFF** file format is given at the end.

System Requirements and Options

Requirements: IBM compatible operating system operating under DOS or similar operating system. EGA, VGA or compatible monitor. If DOS is used from Windows, full-screen mode should be used.

Recommended equipment:

Any normal printer. A nicer printout of the fitting parameters is obtained if you have a Hewlett-Packard printer that uses PCL (Hewlett Packard’s printer control language). The Deskjet 670C and the Deskjet 500 with Prestige Elite cartridge (22706B) are known to work.

Any plotter that uses HPGL (Hewlett-Packard graphics language). Most plotters do. The plotter should be set at 9600 baud. Alternatively, the graphs may be obtained using a printer and methods for doing this are described.

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definitions

record means the information on a file that is obtained from a measurement on a single aliquot, for example one glow curve or one shine-down curve.

channel refers to a position in the record in which a number, which is usually the number of photon counts, is recorded.

column is used in the same sense as it is used in a spreadsheet.

point refers to a single datum, ie photon count.

SFF-MAKE

General description

The main purpose of this program is to read data from one or more existing files and then to write a new file with the data in the format that the other programs will read. This format is called **.SFF** format. The program also allows the user to view, plot and print the data. There are other options which are useful for making the outputs of the main programs more useful.

The program is designed to read data in files in:

- Daybreak binary format
- Daybreak .ASC format
- Risø sequential data file format (2 kinds)
- Adelaide Kym format
- Lian's TXT format
- **.SFF** format (files written by this program)

Details of these formats are provided at the end of this section.

The program

The program proceeds as follows:

(i) The user is asked for the disk drive that the data are on.

(ii) The user is asked for the file name; a path can be used if needed in which case one must type everything needed after the drive letter and colon. If a mistake is made and the file does not exist the program will terminate.

(iii) The data are then read from the files. If there is information on the files that is relevant other than the data, and it can be allocated to the appropriate variable in the program, then it is read into that variable. Examples of such information are the radiation doses and sample name.

(iv) The user is then given a menu in which several items of information are asked for. These are the sample name, grain size and type, excitation, filters used and so on. None of these are needed, but they make the resulting graphs and printouts more meaningful. This can have a long-term benefit by avoiding the necessity of looking at old notebooks. If normalization values are to be entered later, Y or y must be given in answer to the relevant question in this table.

(v) There follows a page in which information about each aliquot is asked for. These are:

- the code
- the dose
- the normalization value (if in the previous menu a Y or y is given in answer to the relevant question). If the doses are found on the original file they may be shown and not asked for. Information about each record may be displayed also if it is read from the files as this may help the user to enter the correct code and dose. The codes and doses are needed for the subsequent SFU software that requires a file in .SFF format. The choice of required codes is shown at the top of the screen, and will stay there until this

operation is finished. The codes are case-sensitive and must be entered exactly as given. If a mistake is made, an opportunity is presented at the end to make changes.

(vi) If normalization values are input then the user will be asked whether the data should be divided by them or multiplied by them. The default is divided-by. Data to be normalized may contain a component, such as a dark count, which should not be normalized. Provision is made for this; the user will be asked to provide a number for the constant component. Normalization is then done.

(vii) The user is then given the opportunity to add + or - to the codes (see the Common Features section for an explanation) if normalization values have been entered.

(viii) The next menu allows the user to:

- view the data and plot it
- to list it on a printer
- create a file of the data in **.SFF** format

In each case the user can select records to be included or excluded. For plotting, read the section in “Common Features” on plotting graphs.

(ix) When making a file in **.SFF** format:

the user chooses the starting and ending channels of the data, and how many channels that are to be summed at a time (eg. with 250 channels of data one may wish to sum channels 51 to 200, 10 at a time).

the heading of each column in the **.SFF** file is the first channel number of those channels that are summed.

if a mistake is made during this process it is necessary to complete it; the user is then returned to the menu at which point it is possible to repeat the process.

when the user is asked to provide a name for the **.SFF** file, the complete file specification must be given, including the drive letter, colon and path if needed (the default drive letter is not that of the original data).

the **.SFF** file can be edited with any text editor if one wants to add other information, change the sample name, or make other corrections.

This SFF-MAKE program is in the development stage, and is provided as such. If you find errors in the output or bugs in the operation, please let me know. If appropriate, please include a diskette with the data files on it.

If your data are in a format that this program will not read, please send a formal description of the data format and a diskette with some example data files on it and I will endeavour to make the program read them. The program will not currently (October, 1998) read Risø binary files; if anyone can provide the detailed information necessary to read them I would very much appreciate it; an interim measure for those using Windows software is to use the method described under “Lian’s text files” in the section on file formats.

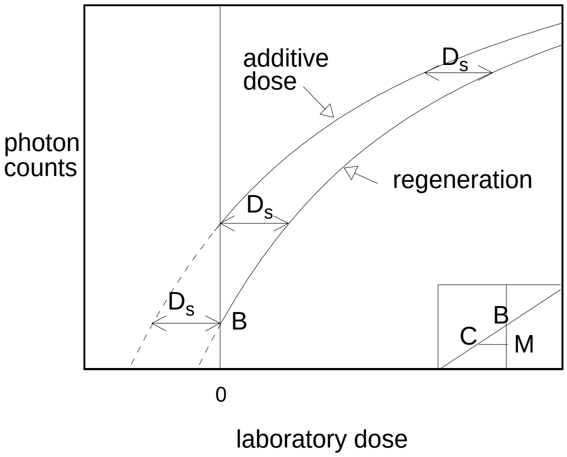
Thank you,
D.J.Huntley, Physics Dept, SFU, Burnaby, B.C., V5A 1S6, Canada
fax: 604-291-3592
e-mail: huntley@sfu.ca

REGENERATION PROGRAM

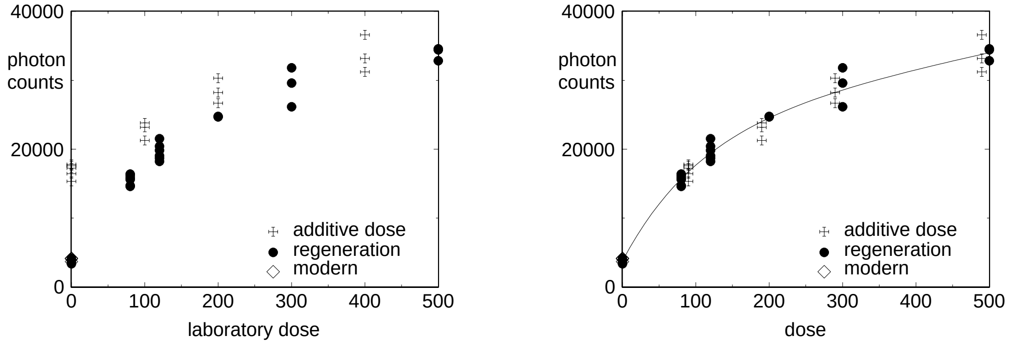
General description

The purpose of this program is to take two data sets and bring them into coincidence by a shift of one set along the x axis, and, optionally, a vertical scaling factor. This is just as described in the paper 'Estimation of equivalent dose in thermoluminescence dating - the *Australian slide* method' by J.R.Prescott, D.J.Huntley and J.T.Hutton; Ancient TL, vol.11, pp.1-5, 1993.

The ideal case is illustrated in the first figure below in which the ordinate is luminescence intensity and the abscissa is laboratory radiation dose. The two curves are labelled "additive dose" and "regeneration". They are identical except for a horizontal shift, D_s, which may be taken to be the past radiation dose. The user is expected to have two sets of data, one for each curve.



The additive-dose data must be coded **UN**, **UN+** or **UN-** and the regeneration data coded **Reg**, **Reg+** or **Reg-** These data must be in a file in **.SFF** format. This format is described in an appendix at the end of this manual. Note that the codes are case-sensitive and must be exactly as specified. Such a file can be created by the user in any way the user wishes, or by using the SFF-MAKE program. The left figure below shows an example of the two data sets, and the right figure shows the result of the fitting procedure in which the additive-dose data have been shifted to the right in order to obtain an optimum fit of both data sets to a single function, shown by the solid line.



Program

The user is first presented with an information screen and then proceeds as follows:

(i) The user is asked for the disk drive that the data are on.

(ii) The user is asked for the file name; a path can be used if needed in which case one must type everything needed after the drive letter and colon. If a mistake is made and the file does not exist the program will terminate.

(iii) The user is then shown how many records and how many "columns" of photon-count data there are in the file. The word "column" is used by default and if something is assigned to $Head in the file header, that term will be used instead.

(iv) The user is then asked for the first "column" to be analyzed; if the first "column" in the file is wanted, just pressing enter will get it.

(v) The user is then asked for the last "column" to be analyzed; if a non-existent "column" number is entered then the largest existing smaller one will be used.

(vi) A number of questions are now asked about the function to be fitted and the output desired. The program then reads the first set of data to be analyzed; the numbers are shown briefly on the screen and then displayed on a graph.

(vii) The user is now asked for initial guesses for the fitting parameters; defaults are provided and are usually adequate.

(viii) Next the program does a least-squares fit to the regeneration data in order to obtain better estimates of the fitting parameters. Then the program does a fit of the selected function to both data sets jointly; in this fit the shift of the additive-dose data along the dose axis is a parameter in the fit. If the optional intensity scaling factor is chosen to be a variable it is also a parameter in the fit.

(ix) If data for modern analogues are present in the .SFF file then a correction (M–C in the inset to the first figure above) is calculated and combined with the dose shift to give the equivalent dose (D_{eq}). For this the data for the modern analogue are simply averaged; no uncertainty is calculated.

(x) All the determined quantities may be printed on a printer or written to a file, and a fit shown on the screen can be plotted. Various ways of obtaining a plot are described under "Common Features".

Five functions are currently available to choose from:

- a straight line: $Y = k(D-D_i)$
- a quadratic: $Y = k_1(D-D_i) + k_2(D-D_i)^2$
- a cubic: $Y = k_1(D-D_i) + k_2(D-D_i)^2 + k_3(D-D_i)^3$
- a saturating exponential: $Y = Y_o\{1- \exp[-(D-D_i)/D_c]\}$
- a saturating exponential + linear: $Y = Y_o\{1- \exp[-(D-D_i)/D_c]\} + k(D-D_i)$

where Y is the luminescence intensity (ordinate variable), D is the dose (abscissa variable) and all other symbols are parameters. D_i is the dose at which the curve crosses the dose axis and will normally be negative; D_c is the characteristic dose of the saturating exponential and is the dose at which the intensity is (1 - 1/e) times the saturation value. The program is written in such a way that adding other functions is relatively straightforward and requests to do so will be entertained if accompanied by appropriate data and arguments.

Sometimes one is not sure whether to use a linear fit or a non-linear fit because the data look as though there might be a slight departure from linearity. In such cases one should first use the quadratic fit; if the quadratic coefficient (k_2) is not significantly different from zero one should then reprocess the data using a linear fit, otherwise one should reprocess the data using a saturating exponential fit.

Recommended running procedure

The recommended procedure is as follows. Run the program with the intensity scale fixed at unity. Then run the program again with the intensity scale as a variable parameter. Note those fits for which the intensity scale parameter is within 2 standard deviations of unity; for these one can accept the D_{eq} evaluated when the intensity scale was fixed at unity.

One should examine, and preferably plot, some of the fits in order to ensure they look reasonable. In most cases they will be, but it is possible to get data that are fitted by the program but for which the fit is clearly inappropriate.

As with any optimization routine there is no guarantee that the program will arrive at the global optimum, or at the optimum you wish (which could be different). With good data there need be no concern about this. With poor data the user should be alert and examine the fits to see if they make sense; if they do not, different initial parameters should be tried.

The data are assumed to have a scatter about the “true curve” that is described by a normal distribution with a standard deviation that is proportional to the intensity. Another way of putting this is that it has a constant fractional “error”. The value of the fraction is a parameter in the fit and is denoted by σ in the output. Actually there are two σ‘s, one for the additive-dose data set and one for the regeneration-data set. In the outputs these are quoted as percentages. If “short-shine” normalization is used in optical dating then the above model for the treatment of errors is inappropriate, and the scatter of the additive-dose data should be described differently, using two σ‘s for it. An option to do this is provided. It is described in detail in the “common features” section.

Test Data

A file named REG-TEST.SFF is provided as an example of correct formatting and for the user to test the program. A sample plot of a fit and a sample printout of the fitting parameters are also provided.

INTERCEPT PROGRAM

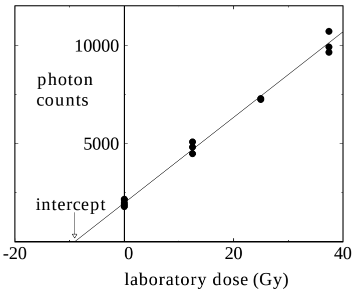
General description

The purpose of this program is to make fits to the following kinds of data and to find the appropriate intercept.

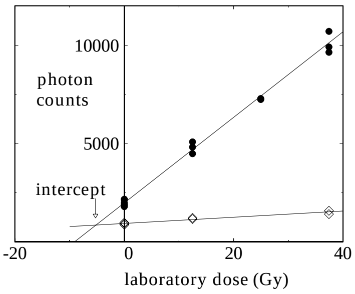
1. Additive-dose data
2. Additive-dose data with thermal-transfer-correction data for optical dating.
3. Additive-dose data with partial-bleach data for thermoluminescence dating.
4. Additive-dose data extrapolated to a constant intensity, as in the total-bleach method.

Examples are shown in the following three graphs. In the first one a line is fitted to a single set of data and the intercept with the axis is found. In the other cases there are two data sets and the intercept of the two fitted lines is found.

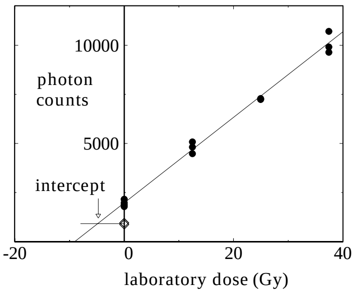
1



2 & 3



4



Types 2 and 3 are functionally equivalent and only differ in the way the data are coded. Type 4 is the same as one of the Type 2 or 3 options and again only differs in the way the data are coded.

The data must be in a file in **.SFF** format. This format is described in an appendix at the end. Such a file can be created by the user in any way the user wishes, or by using the **SFF-MAKE** program.

Program

The user is first presented with an information screen and then proceeds as follows:

(i) The user is asked for the disk drive that the data are on.

(ii) The user is asked for the file name; a path can be used if needed in which case one must type everything needed after the drive letter and colon. If a mistake is made and the file does not exist the program will terminate.

(iii) The user is then shown how many records and how many “columns” of data there are in the file. The word “column” is used by default and if something is assigned to $Head in the file header, that term will be used instead.

(iv) The user is then asked for the first “column” to be analyzed; if the first “column” in the file is wanted, just pressing enter will get it.

(v) The user is then asked for the last “column” to be analyzed; if a non-existent “column” number is entered then the largest existing smaller one will be used.

(vi) A number of questions are now asked about the function to be fitted and the output desired. The program then reads the first set of data to be analyzed; the numbers are shown briefly on the screen and then displayed on a graph.

(vii) The user is now asked for initial guesses for the fitting parameters; defaults are provided and are usually adequate.

(viii) Next the program proceeds with the fit.

(ix) All the determined quantities may be printed on a printer or written to a file, and a fit shown on the screen can be plotted. Various ways of obtaining a plot are described under “Common Features”.

(x) At the end, a plot of the intercept dose vs “column” number is shown on the screen and an option to plot it is presented if there is more than one intercept to plot.

The different types of fits will now be described.

Additive Dose - UN coded data

With this option only data coded **UN**, **UN+** or **UN-** are read from the file. There is a choice of functions for the fit as follows:

- a straight line: $Y = k(D-D_{int})$
- a quadratic: $Y = k_1(D-D_{int}) + k_2(D-D_{int})^2$
- a cubic: $Y = k_1(D-D_{int}) + k_2(D-D_{int})^2 + k_3(D-D_{int})^3$
- a saturating exponential: $Y = Y_o\{1- \exp[-(D-D_{int})/D_c]\}$
- a saturating exponential + linear: $Y = Y_o\{1- \exp[-(D-D_{int})/D_c]\} + k(D-D_{int})$

where Y is the luminescence intensity (ordinate variable), D is the dose (abscissa variable) and all other symbols are parameters.The main parameter of interest will be the intercept on the dose axis, denoted D_{int}.

A simple additive-dose fit should usually only be used for rough work or for information. It is never exactly the right thing to do to obtain an equivalent dose. The reason is that there is always a non-zero background from the photomultiplier tube; there may also be contributions to the background from scattered incident light or incandescence. Some people subtract the background and then do an additive dose fit to find the dose-axis intercept; if one does this one will not, and cannot, get the statistics of the fit correct; if the background correction is small, however, the error will be insignificant.

Caution should be used with any additive-dose fit because one simply does not know the correct form of the extrapolation.

Additive Dose with Thermal Transfer Correction - UN and TT coded data

With this option, data coded **UN**, **UN+**, or **UN-** are read from the file as additive-dose data and data coded **TT**, **TT+** or **TT-** are read for the thermal transfer correction. These are treated as measurements corresponding to two functions as follows:

$$Y_{TT} = Y_{int} + f(D-D_{int})$$
$$Y_{add} = Y_{TT} + g(D-D_{int}) = Y_{int} + f(D-D_{int}) + g(D-D_{int}).$$

Y_{int} and D_{int} are the intensity and dose at which the two functions intercept. The two functions *f*( ) and *g*( ) are are chosen by the user from menus. D is the dose read from the file. Note that with this model the additive-dose intensity is considered to be equal to the thermal-transfer intensity + an additional intensity.

The choice of functions for the fits is:

- a constant k
- a straight line: $k(D-D_{int})$
- a quadratic: $k_1(D-D_{int}) + k_2(D-D_{int})^2$
- a cubic: $k_1(D-D_{int}) + k_2(D-D_{int})^2 + k_3(D-D_{int})^3$
- a saturating exponential: $Y_o\{1- \exp[-(D-D_{int})/D_c]\}$
- a saturating exponential + linear: $Y_o\{1- \exp[-(D-D_{int})/D_c]\} + k(D-D_{int})$

First the user is asked which of these to pick for *f*( ) for the **TT** coded data. Then the user is asked which to pick for *g*( ), the addition. There is a restriction that *g*( ) cannot be less complicated than *f*( ). The quantities k, k_1, k_2, k_3, Y_o and D_c are parameters in the fits.

Additive Dose with Partial Bleach - UN and PB coded data

This is functionally the same as the additive dose with thermal transfer correction option and differs only in that data coded **PB** are read from the file instead of data coded **TT**.

Total Bleach - UN and TB coded data

This is functionally the same as the previous two options when *f*( ) is a constant. Thus the additive dose data are fitted to

$$Y = Y_{TB} + g(D-D_{int})$$

where Y_{TB} is a constant, determined by the maximum likelihood fit to the **TB** coded data, and *g*( ) is a function from the list above.

Other - UN and dc or ec or rh coded data

This is identical to the previous option except that **TB** is replaced with one of the following:

dc (for dark count)
ec (for empty chamber)
rh (for reheat)
a code entered from the keyboard (your choice)

One might want to use one of the first two when doing a simple additive-dose measurement. The third one would be useful for a TL measurement in which the incandescence was significant and measured by a reheat.

Test data

A file named INT-TEST.SFF is provided as an example of correct formatting and for the user to test the program. A sample plot of a fit and a sample printout of the fitting parameters are also provided.

b-VALUE PROGRAM

General Description

This program takes additive-alpha-dose data and additive-beta or gamma-dose data and jointly fits them to a single function. In doing so the alpha doses are scaled to yield the optimum fit. This scaling factor is a parameter in the fit and is what is defined as the b-value.

Program

The .SFF file must have the following two sets of data,

code	data
UN, **UN+** or **UN-**	additive β- or γ-dose data
αUN, **αUN+**, or **αUN-**	additive α-dose data

An example of a fit to obtain a b-value is shown in the following graph.

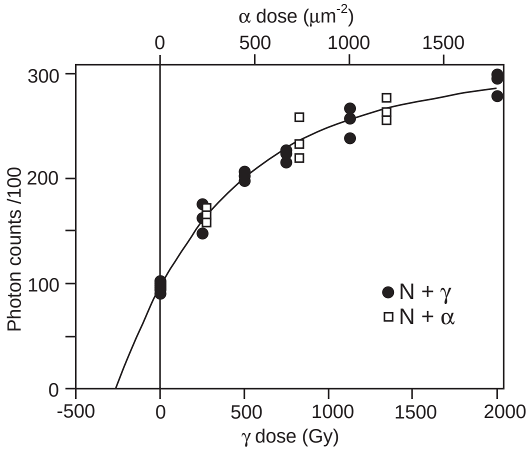


figure courtesy of O.B.Lian

Any units can be used for the two dose units according to the taste of the operator, but the header in the **.SFF** file is designed so that the units of the b-value are properly given if the "values" to the following are given in the header.

$DoseUnit, $DoseType, and $AlphaDoseUnit.

Thus for example if the header includes

$DoseUnit,Gy
$DoseType,β
$AlphaDoseUnit,μm^{-2}

the units of the b-value will be shown as Gy.μm^{2} on the screen, in the table or in the file.

If the information provided in the header is, for example, minutes for the alpha doses, minutes for beta doses, and β for the dose type, then the b-value will be given in minutes β per minute α and this can then later manually be converted to proper units. If no information is given in the header the b-value will be given without units. If the **.SFF** file is made using the SFF-MAKE program then the proper header will be written if the user has entered the appropriate information when asked for it.

The functions that can be used to fit the data are the same as those listed under additive-dose fits:

- linear
- quadratic
- saturating exponential
- saturating exponential + linear

All the parameters in the fits, and their uncertainities, are printed to a file if that option is chosen.

Because of the way a-values are defined, it is not possible to make a program that yields a-values without requiring the user to use specific units, thus if a-values are desired then the user should calculate b-values and later make the conversion as follows:

$$\text{a-value} \quad = \quad \frac{\mathrm{b-value}}{13\,\mathrm{Gy}\cdot\mu\mathrm{m}^2}$$

The a-value has no units.

COMMON FEATURES

Plotting the graphs

When a graph of a fit is shown on the screen you are asked if you want to plot it. If you do not want to plot it just press the enter key since the default is “no”. You can press the enter key in advance to prevent the program stopping at the graphs as many times as you want.

If you answer Y or y (for yes) then you will be asked whether the graph is to be output to COM1, COM2, or a file. Select COM1 if a plotter is connected to the COM1 serial port, or COM2 if a plotter is connect to the COM2 serial port. The plotter should use HPGL (Hewlett-Packard graphics language); almost all plotters do. The plotter should be set to 9600 baud. If you select the “File” option the program asks you for a file name and then writes the HPGL code to the file. You can then take the file to another computer with a plotter attached and just “copy” the file to the plotter. Alternatively you can import this file into a graphics program for further processing.

If no plotter is available but you have a printer, there are two further options. The first is to use the “Print Screen” key on the keyboard. In order for this to work the DOS GRAPHICS command must be executed before starting the program. Type and enter HELP GRAPHICS to obtain the details. Do not use the “Print Screen” key if you have chosen to print the fitting parameters to the printer as the two will interfere with each other.

The second option will give you a much nicer graph on your printer, but is more trouble. You must obtain a copy of the program PRINTGL. It is shareware and can be downloaded from the web page of Ravitz Software Inc. in Kentucky, U.S.A. at http://www.concentric.net/~ravitz/. The procedure is to obtain the HPGL file of the graph as described above, and use PRINTGL to print the graph on your printer. The resulting graph will probably be even nicer than one obtained using a plotter.

Writing the result to a file

If you choose this option you are asked for a file name. A header is first written to the file with information about the sample and the type of fits made to the data. The fitting parameters (and their uncertainties) for each column of the data are then written as they are calculated. The end result is a table, including the column headings for it. Strings are written in quotation marks and commas are used as delimiters. The file is designed to be imported into a spreadsheet and should be quite readable there.

Precision and fitting

All calculations are double precision.

Maximum likelihood calculations are used to obtain the fits. The uncertainties in the parameters are evaluated by inverting the Hessian, which is evaluated numerically.

Maximization is done using a simplex routine. While this is taking place the current values of the parameters are shown in groups on the screen. The top left number of each set is proportional to the negative of the likelihood, and will generally be decreasing with time. When it no longer changes within the precision set by the user, the parameters are deemed to be optimized; the simplex routine is then repeated using this new set of parameters as a starting point, again until the likelihood no longer changes. The purpose of the repeat is to attempt to find a better maximum. The other numbers displayed in each group are the parameters in the fit and ending with the σ's.

The simplex routine used for the optimization is slower than other strategies, but has several advantages. It can be used with any function that can be programmed (even non-analytic ones), it is easier to program, and it cannot crash. It is, however, possible for the program to crash during evaluation of the likelihood, although most possibilities have been eliminated. If a crash occurs it is probably due to a poor choice of the initial parameters, or poor data. Note that the calculated intensity at any of the data dose values is restricted to being positive; this will normally be expected anyway.

The desired precision in the maximum likelihood routine is set by the user. If the number is set very small, for example 10^{-15}, the program will take longer, and could end up in an endless loop and never terminate. If the number is set relatively large the program will take less time, but may not reach a proper maximum; if this happens the user will be notified. For safety the program should be run with successively smaller values until there is no change in the output. A value of 10^{-13} will probably suffice for most good data.

Printing the data

The option of printing the data is to allow the user to debug incorrectly formatted data.

Initial Parameter Estimates

The user is asked to provide initial estimates of the parameters. The data are shown on the screen to make this easy. Defaults are provided and should normally suffice.

If the program fails to produce a fit, run it again but choose the initial estimates of the parameters carefully. It is unlikely that this will be necessary, except occasionally with very scattered data.

Codes with + and - added (e.g. UN+, Reg-)

The extra + and - have no effect on the data processing, but the final graphs produced by the regeneration and intercept programs show on each point whether the normalization value was larger or smaller than 1. The + and - are added to the codes on the basis of whether the normalization reduces or increases the intensity, respectively. If the code for the point has a + sign the top half of the symbol will be shown filled in; if the code has a - sign the lower half of the symbol will be filled in. Thus for example:

UN+ points will be shown as **Reg+** points will be shown as

UN- points will be shown as **Reg-** points will be shown as

The intent is that the + or - signs are to be used to see whether or not there is a correlation between normalization value and position relative to the fit for the set of points. If there is a systematic effect of points above the line having low normalization values and points below the line having high normalization values, then one has cause for concern. This may be an indication that not all the grains were well exposed to sufficient sunlight at the time of deposition. This is discussed in D.J.Huntley and G.W.Berger, Scatter in Luminescence Data for Optical Dating - some Models. Ancient TL 13, pp.5-9, 1995.

Fixed or variable σ for the additive dose (N+dose) data

There is a choice of two ways to treat the scatter in the additive dose data.

(a) The scatter can be treated in the analysis as though it can be described by a normal distribution with, for each point:

mean value = calculated intensity

standard deviation = a fixed fraction of the calculated intensity. This fraction will be denoted by σ. The actual fraction is a parameter in the fit. It is likely to come out to be in the range σ = 0.01 to 0.10 (ie 1-10%). This number is shown on the screen, plotted graph, printed table and results file, depending on which of these the user asks for. This option will be appropriate if the scatter results from the aliquots having different masses, or different sensitivities to radiation for the different aliquots, in either case with a normal distribution.

(b) The scatter can be treated in the analysis as though there is one σ for the zero-dose (naturals) intensity, and a different σ for any additional intensity. The reason for introducing the two σ's is that in optical dating one usually does an initial "short shine" on all the aliquots, and uses these intensities to normalize the final data. This has the effect of greatly reducing the scatter in general, and can reduce the scatter for the zero-dose points to a very small value, possibly under 1%. The scatter in the points at added doses will not usually be as small. For example, σ for the zero-dose points may be 1% while the scatter at the largest applied dose may be 5%. In this case the model in option (a) is inappropriate, and this option (b) would be apropriate as the intensity can be considered as the sum of two components. When using this option both σ's are shown on the screen and graph. When the results are printed on a printer both σ's are printed on a separate line after all the other parameters. When the results are written to a file they are listed as

σ(Nat) ± eσ(Nat) and σ(add) ± eσ(add).

When you are using the two-σ option the optimizing routine is more likely to go astray and not find the proper fit. If this happens run the program using option (a) and make a note of the fitting parameters. Then run it again using option (b) using these fitting parameters instead of the default ones.

Final Note

For cases, admittedly very rare, in which Poisson statistics (i.e. counting statistics) make a significant contribution, these programs will not deal with the statistics correctly.

Bugs

The graphs and printouts of the fitting parameters are designed to accomodate reasonable values of them. If unusual numbers are used (for example a set of doses such as 0, 2 x 10^{-6}, 4 x 10^{-6}) then the formatting may produce something unreadable. The correct values will be written to a file if that option is chosen.

If DOS is run from Windows one should do so using the full screen mode; if it is run from a window it may crash.

Please report other bugs to D.J.Huntley, preferably accompanied by a diskette with the data file and a description of the bug.

The version number of your software is printed on the screen with the copyright notice at the end when you have finished running the program.

Specifications of the various data formats that can be read.

Risø Sequential Data Files

These should not be confused with Risø Sequence files; they have nothing to do with each other. There are two kinds of Risø Sequential Data Files; they are referred to here as old and new. The following are taken from Risø manuals.

(1) Old: (after Fig 27 of the Risø TL Dating System Model TL-DA-10 manual, - with added notes)

```
  Test file for Rainer a note
24                          number of glow curves
700                         max end point temp
200                         lower integration temp
400                         upper integration temp
1                           run no
1                           group no
1                           sample no
 0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 0.000E+00  0.000E+00
 0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 0.000E+00  0.000E+00
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 0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 0.000E+00  0.000E+00
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 0.000E+00  0.000E+00
1
1
2
 0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 0.000E+00  0.000E+00
 0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 0.000E+00  0.000E+00
.
        .                       etc
```

(2) New: (copied from the Risø Model TL/OSL-DA-12 manual)

```
Note  - file information
12     - number of samples
2      - sample type (1=TL, 2=infrared OSL, 6=green, 5=short shine)
600    - max temp/time (x 0.1 sec)
1.319 E + 0003 - integral
1      - run no.
1      - sample no.
158
174
179
164
168

.            (channel counts(250))
```

<u>Daybreak .ASC files</u>

Each row in these files is one record. Each record consists of the following sequence, each item having a defined position (field) in the record:

glowcurve run number
text description in quotes including a bleach code (B for before irradiation, A for after, plus bleach time in minutes (M suffix) or hours (H suffix)
0 or 1 (1 indicates the natural TL is included)
alpha dose in μm^{-2}
beta dose in Gy
gamma dose in Gy
0 -1 or 1 (0 for no bleach, -1 if bleach before irradiation, 1 if after)
bleach time in minutes
a set of numbers which are 10 °C averages from 250 to 450 °C .

Daybreak binary files

Each file consists of a continuous sequence of records, each being 990 bytes long. Each record is as follows. Double means double precision. Note that several bytes are not used and that counting starts at zero. This description is for TL, but the extension to optical excitation can be imagined.

bytes	type	variable
0-1	integer	actual number of entries in the glow curve
2-3	integer	# of degrees C between subsequent points in the glowcurve (set at 5)
4-5	integer	run # - this is a serial #, the 1st aliquot measured is 0, the 2nd is 1 etc.
6-7	integer	the position in the turntable
8-9	integer	identifies the record as a TL measurement if it is <2000
10	integer	# of points in the record. This is fixed at 99, for 100 points.
12	boolean	true for a 1st glow, false for 2nd glow
14	boolean	true for TL measurement, false for a background measurement
16	boolean	true if bleaching was before irradiation, false if bleaching was after
18-25	double	bleach time
26-33	double	ramp rate
34-41	double	dose rate for the gamma source
42-49	double	dose rate for the beta source
49-57	double	dose rate for the alpha source
58-61	double	gamma dose
66-73	double	beta dose
74-81	double	alpha dose
82-89	double	shift (?), 4 time bases and background count rate
91-97	string	units of gamma irradiation
99-105	string	units of beta irradiation
107-113	string	units of alpha irradiation
115-121	string	bfilter (?)
123-129	string	type of gamma source
131-137	string	type of beta source
139-145	string	type of alpha source
147-148	date	bits 1-7 are the year-1900, 8-12 are the day, and 13-16 are the month
149-189	string	remark about this aliquot measurement
190-989	double	the 100 points of the data

note: the 2-byte integers should be read in reverse order.

Lian's text files

The data are formatted as follows. Here each record is a column. s_1, s_2 etc are the column headings and are text. The n's are the photon counts.

s_1, s_2, s_3, s_4, s_5, s_6, s_7, ...
n_{11}, n_{21}, n_{31}, n_{41}, n_{51}, n_{61}, n_{71}, ...
n_{12}, n_{22}, n_{32}, n_{42}, n_{52}, n_{62}, n_{72}, ...
n_{13}, n_{23}, n_{33}, n_{43}, n_{53}, n_{63}, n_{73}, ...
n_{14}, n_{24}, n_{34}, n_{44}, n_{54}, n_{64}, n_{74}, ...
.
.
.

The SFF-MAKE program figures out how many records and channels there are by reading the file.

Such a file can be created in many ways. A simple way to do it from Risø windows software is to:

open the VIEW menu
load the binary files you want
select all the records in the file by dragging the mouse
use the special 'copy' command
(the records have automatically been converted to ASCII, and are now in the Windows clipboard)
open a windows spreadsheet
paste
(you now see all the data, but only the data)
transpose the data
manually add the header for each column
save this as a text file with commas as delimiters.

FILE FORMAT of .SFF FILES

Bold upright items must be as shown (but not in bold font).
Items in italics are parameters as described below, in which: s or t indicates a string
d, n or z indicates a number.

**$Name,**$s_1$
**$Info,**$s_2$
**$DoseUnit,**$s_3$
**$DoseType,**$s_4$
**$AlphaDoseUnit,**$s_5$
**$Head,**$s_6$
**$Points,**$n_p$
**$Columns,**$n_c$
$**$
Head,Dose,n_1,n_2,n_3, ...
t_1,d_1,z_{11},z_{12},z_{13}, ...
t_2,d_2,z_{21},z_{22},z_{23}, ...
t_3,d_3,z_{31},z_{32},z_{33}, ...
.
.
t_i,d_i,z_{i1},z_{i2},z_{i3}, ...

where:
s_1 = sample name
s_2 = other information you wish on the output
s_3 = units of the radiation doses (eg: Gy or minutes).
s_4 = type of radiation, either β or γ.
s_5 = units of the α doses.
s_6 = meaning of the column headings, ie what the *n*’s mean (eg channel, temperature etc)
t_i = the code for this row of data, specifically:
 t_i = **UN** for additive dose data (N + dose, unbleached aliquots)
 t_i = **αUN** for additive α dose data (N + α dose, unbleached aliquots)
 t_i = **Reg** for regeneration data (N + bleach + dose aliquots)
 t_i = **TT** for thermal-transfer correction aliquots (N + dose + bleach aliquots)
 t_i = **PB** for partial bleach aliquots (N + dose + partial bleach aliquots)
 t_i = **TB** for total bleach aliquots (N.+ total bleach aliquots)
 t_i = **Mod** for modern analogue aliquots
 t_i = **Nnp** for natural no preheat aliquots
 t_i = **Bnp** for natural + bleach but no preheat aliquots
 t_i = **dc** for dark count
 t_i = **ec** for empty chamber
 t_i = **rh** for reheat (for TL)
d_i = the dose associated with this row of data.
z_{ij} = are the photon counts; there are n_p rows and n_c columns. Each row contains the data for one record, i.e. shine-down curve or glow curve.

The column headings, n_i, are the channel numbers, temperatures, or whatever you wish, for that column, as indicated by s_6. They must be in increasing order.

The **UN**, **αUN**, **Reg**, **TT** and **PB** codes may have a + or - sign added to the code to indicate whether the normalization value for the aliquot was >1 or <1. Here normalization value is taken to mean the number by which the raw data were divided by during normalization. Additional valid codes are thus: **UN+**, **UN-**, **αUN+**, **αUN-**, **Reg+**, **Reg-** and so on.

The initial group of lines which start with $ signs have some flexibility. They can be in any sequence except that **$**$** must be the last one. Other lines can be inserted but they will be ignored. The **$Points**, **$Columns** and **$**$** are required; the others are optional, and are used to enhance the information on the output graphs, tables and files.