PeakCounter 2.1.5: a user-friendly Windows programme for high resolution analysis of multi-parameter data from the ItraxTM core scanner

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Abstract

This paper describes new software *PeakCounter 2.1.5* that was specifically developed for using multi-parameter data from the Itrax[™] core scanner for varve counting, but it is also an extremely useful tool for all fine-scale analysis of such data. The X-radiograph and the optical images can be viewed adjacently. An active window selector plots up to six different parameters (e.g. greyscale from X-radiograph, chemical elements and/or ratio between them, as well as any other parameter measured by the scanner). The active area of the optical image can also be viewed in a separate window (magnified). A cursor line moves simultaneously in all active windows, allowing the user to check correlation between different curves. Recognised varve/laminae limits can be marked with the numbers denoting the varve clarity to the human counter, allowing a measure of varve quality to be incorporated into the count. Weighted/unweighted moving averaging can be used to overcome noisy element profiles that can result when scanning at very high resolution. Distinct sedimentary structures that are often used to correlate cores (e.g. turbidites, tephras, etc.) can be marked and described. These new data appear as four additional columns in the output file: greyscale from X-radiograph, varve limit, marker layer number and notes.

1.0 Introduction

X-ray fluorescence (XRF) core scanning of split sediment cores was developed in the late 1990s (Jansen *et al.*, 1998) and is a powerful analytical technique. It is relatively rapid, requires no sample preparation, is non-destructive, and can detect most chemical elements of the periodic table down to limits of a few parts per million, depending on acquisition dwell time and sample conditions. A new generation of XRF core scanners allowing extremely high resolution analysis, with improved count rates and detection limits (even with reduced count time), have become widely available. The ItraxTM core scanner takes high resolution radiographic and optical images at the same time as XRF measurements. Rather than using a single spot X-ray beam, which most alternative scanners use, the ItraxTM scanner is equipped with a unique flat X-ray beam that means that grain-to-grain variance is averaged across the horizontal core axis, ensuring predominance of the environmental signal through depth without compromising resolution along the depth axis. This is a particular advantage when measuring laminated sediments at very high resolution and is one of the main reasons why researchers in this field are beginning to choose this type of XRF core scanner

over alternatives. The X-radiographic images are also extremely useful in allowing grey scale profiles to be produced of sediment density variations as well as in the detection of hidden clacks and sedimentary structures that are not visible from the sediment surface.

A growing number of studies utilise digital analysis of core images as an objective method of analysing sediment features, including varves, both manually and automated (Ripepe et al., 1991; Cooper, 1997; Petterson et al., 1999; Saarinen and Petterson, 2001; Ojala and Francus, 2002; Haltia-Hovi et al., 2007). Automated peak counting software has been developed for use in characterising laminated sediments and varve counting; using profiles derived from images but also geochemical data, and allow the option of spectral analysis on output datasets (Weber et al., 2010). However, for such approaches to be viable the laminations must be extremely well preserved, clearly and consistently distinguishable (optically or geochemically) and continuous for the entire period of interest. In most laminated and varved sediment encountered sequences this is not the case. These methods detract from actually studying and characterising sediment composition and understanding the process of deposition, for which there is no substitution. However, using a multi-parameter approach allows complicated sedimentary sequences to be robustly characterised through their optical, density, and geochemical properties, and therefore provides a greater insight that is necessary for accurate lamina recognition and varve counting.

PeakCounter 2.1.5 is a new programme that was developed by Takeshi Nakagawa using Visual Basic 6 and thoroughly tested by Michael Marshall for varve counting using multi-parameter data from the ItraxTM core scanner for the Lake Suigetsu 2006

Varved Sediment Core (SG06) Project (Nakagawa *et al.* in press), but it is also an extremely useful tool for all fine-scale analysis of such data. Although the software was originally developed for internal use of the SG06 project, the performance and the user-friendly interface attracted attention from outside of the project and therefore the demand for a comprehensive description for the user became high. This paper is aimed at helping a general audience to fully benefit from this new software and should be considered complementary to its specific application for varve counting for the SG06 project described in detail in Marshall *et al.* (in prep) and also very briefly by Francus *et al.* (2009).

2.0 Scanner configuration

PeakCounter 2.1.5 requires that the number of pixels along the depth axis of the Xradiograph is the same as the number of XRF measurements. In other words the resolution (stepping interval) needs to be identical for both X-ray radiography and XRF scanning. This is the only requirement for the scanner settings. Optical core images can be taken in different resolution and using different devices such as digital cameras. Users can include as many elements as they want for detection. The scanning resolution (defined by the user) must be constant within each scanned segment. PeakCounter 2.1.5 displays one XRF measurement in one pixel on the monitor. Therefore the use of a coarse step size results in images that are too small. Therefore, PeakCounter may not be the best analytical tool for materials that do not require high-resolution scanning.

3.0 Installation of PeakCounter 2.1.5

PeakCounter 2.1.5 runs on Windows XP Service Pack 3 (SP3) or later. It has been reported by several users that it does not run on Windows XP (SP2) or earlier. Currently there is no plan to develop PeakCounter for Macintosh or Linux. An installer package of PeakCounter 2.1.5 can be downloaded from the web page <<u>http://dendro.naruto-u.ac.jp/~nakagawa/</u>>. The download has no limitation and is free of charge. Extract the downloaded zip file and double-click SetUp.exe file. Next, simply follow the ordinary procedures of installing Windows software. If successfully installed you will find a shortcut to the PeakCounter software in your Start menu (Start> Program Files > PeakCounter > PeakCounter 2.1.5). You do not need to restart your computer to activate the software. If you have already installed an older version of PeakCounter and are trying to update it, it is usually possible to simply download the "compressed" version and replace the old .exe file (which is normally in C/Program Files/PeakCounter/) unless otherwise stated on the web site. The PeakCounter.exe file needs to be in the same directory as the "References" folder. A folder containing sample images and XRF data is also included in the installer package to allow users to test or familiarise themselves with the software prior to acquiring their own data from ItraxTM core scans. A malfunction of PeakCounter 2.0.0 was reported by a French Windows user. The more recent version 2.1.5 seems to be free from this problem. If the problem persists, an easy solution is to use PeakCounter version 1.6.2 (also available at http://dendro.naruto-u.ac.jp/~nakagawa/) which has less capacity to customise the user interface but does essentially the same thing as the latest version.

4.0 Formatting data and image files

PeakCounter 2.1.5 requires the data file containing the XRF data to be in comma separated value (.csv) format and the X-radiograph and optical images to both be in either bitmap (.bmp) or Jpeg (.jpg) format. The XRF data file ("result.txt") can be imported/opened in Excel and saved as a .csv file using any name. Apart from this format conversion, users do not need to modify original data table generated by ItraxTM (as of 06 Dec. 2010). The optical image ("optical.tif") can be saved as a .bmp/.jpg file using standard graphics software (e.g. Adobe Photoshop, GIMP etc), as can the X-radiograph image ("radiograph.tif"), although this must first be converted to an 8 Bits/Channel image (from 16 Bits/Channel) before it can be saved as a .bmp/.jpg file. Standard image enhancements (e.g. brightness, contrast) may need to be made prior to the conversion, in order to avoid loss of signal resolution (using wider range from light to dark grey is important in case of 8 bit grey scale, because it can resolve only 256 levels, whereas 16 bit grey scale divides the range from white to black into >65,000 levels and can resolve subtle difference between very similar tones). However, all core sections from the same master sequence should be edited using identical settings to allow consistent master grey scale profiles to be constructed from the X-radiograph images.

Any available optical image of the core section may be used, whether that recorded by the ItraxTM scanner or taken in the field or laboratory by any devices such as ordinary digital camera or microscope. XRF data, radiograph and optical image files in required format are included as sample fines in the installer package.

5.0 Importing files and user interface manipulation

5.1 X-radiographic image

The user navigates to the location of PeakCounter 2.1.5 and opens the programme. The user then selects the "Import radiograph" button in the PeakCounter 2.1.5 control panel (or uses "File", "Import radiograph"), navigates to the required radiograph .bmp/.jpg file, selects it (or the "Radiograph.bmp/.jpg" file from the sample data folder), and clicks "Open" (or double-clicks the file). This opens the full radiograph image in the X-radiograph "Preview" window at the top of the screen with the core top to the right, including the file location path (Fig. 1). The red rectangle is the "active window selector" (Fig. 1) and denotes the smaller core section of Xradiograph image that is plotted in the first of the active windows that is also opened (Fig. 1, "1: Grey scale"). Details on the "Active years" window that is also opened are provided below. The position of the active window can be changed by clicking inside the active window selector and dragging to the required position down/up core, and can be resized by clicking and dragging either side of the selector. The green line is the greyscale profile (Fig. 1) calculated from the area between the two dashed white lines on the X-radiograph image, the position and width of which can be changed by clicking and dragging within, or on the lines (in either the active window, where the width in pixels is also shown, or in the full X-radiograph preview window, see Fig. 1). The Y-axis scale can be edited by changing the limits of greyscale value at the top and bottom right hand corners. The position of the greyscale selector determines the values that are saved in the additional column; labelled "greyscale" created in the output file - one column to the right of "coh" (coherent scatter), see Fig. 4. The brightness and contrast of the X-radiograph can be changed by using the corresponding scroll bars in the PeakCounter 2.1.5 control panel, which will not change the values saved in the additional column in the output file; *i.e.* the function is only to enhance visibility on the monitor without altering signal quality.

5.2 XRF data

The user selects the "Import XRF data" button in the PeakCounter 2.1.5 control panel (or uses "File", "Import XRF data"), to navigate to the required XRF data .csv file (or uses the "XRF data.csv" file from the sample data folder), selects it and clicks "Open" (or double-clicks the file). This opens five other active windows, which contain element profiles plotted in green on a background of the X-radiograph image. Two scale bars are also opened; one showing the full core section length above the Xradiograph preview window (Fig. 1) defined by the core scan length, and the other showing the length of the active windows (Fig. 1) defined by the active window selector. The scale bars automatically reflect the analytical resolution (stepping interval) recorded in the XRF data file. The position of the windows can be changed by clicking and dragging them. They can be arranged and aligned by right-clicking on the upper-most window and clicking "Align forms" (Fig. 2), or going to "Tool", "Align forms" in the control panel menu. A single active window can be viewed by right-clicking the window of interest and clicking on "Hide others" (Fig. 2). Users can also right-click and click "Show 1-3" to just show the first three active windows, or alternatively "Show 4-6" (Fig. 2). To display all six windows the user right-clicks and selects "Show all" (Fig. 2) or selects "Tool", "Show all" in the control panel menu.

5.3 Core photograph (optional)

The user selects the "Import core photo" button in the PeakCounter 2.1.5 control panel (or uses "File", "Import core photo"), to navigate to the required core photo .bmp/.jpg file (or uses the "Core photo.bmp/.jpg" file from the sample data folder), selects it and clicks "Open" (or double-clicks the file). Once open, the

window displaying the optical image can be aligned to the X-radiograph image. The window can be resized both horizontally (i.e. along the long axis of the core) and vertically by clicking and dragging at its edge. If it is resized horizontally, then the optical image stretches or shrinks to the width of the window. This function is particularly useful when aligning the core image, independently taken by a digital camera, to the X-radiograph image. Vertical resizing only trims the core image, which is useful to save space on the monitor. The position of the image within the window can be moved vertically (i.e. the short axis of the core) by clicking and dragging the image. If the overlap between images encompasses the active window selector on the X-radiograph (red rectangle), an active window selector will also appear on the optical image (Fig. 1). This moves horizontally when the user changes the position of the active window selector on the X-radiograph image. It can be moved vertically by clicking and dragging within it in the core photo window. If the user changes the position or size of the core photo then it is necessary to click on the active window selector in the core photo to re-align it to that within the X-radiograph image preview window.

5.3.1 Magnifying the core image (optional)

The user right-clicks on the core photo and selects "Crop" to open a magnified image of the core section defined by the active window selector in a separate window. This can be moved and resized both vertically and horizontally. The brightness and contrast can be changed by using the corresponding scroll bars in the PeakCounter 2.1.5 control panel. Once in the required position (i.e. aligned with the active windows), the user right-clicks the magnified image and selects "Align scale", to align the active window scale below the cropped core photo, and to align the active cursor line (orange line with cross-hair) between this and the other active windows. The method used for aligning the active cursor is defined by either the absolute position of the core photo compared to the X-radiograph image, or by the relative scale between the two. The user right-clicks on the cropped optical image and selects "Pointer link", then either "Position" or "Scale". The "Scale" mode is more useful when the optical core image was taken by the ItraxTM, when it usually has the exact same scale as the X-radiograph image. The "Position" mode can better solve the problem of imperfect alignment between core images taken independently by a digital camera and the X-radiograph. In "Position" mode, the orange cursor lines (with crosshair) in the magnified image and the active windows can be finely aligned by changing the width of the magnified core image window and the position of the scale to which the cursor line is linked. Initially three green profile lines appear on the magnified image corresponding to L^* , a^* , and b^* colour components which are derived from the area between the dashed white lines, the colour profile selector. As with the X-radiograph active window, this area can be moved and resized by clicking and dragging between or on the dashed white lines. The user can right-click on the cropped optical image and select "Colour profile", then either "RGB", to change the plotted profiles to red, green, blue additive colour components, or "grey scale", to plot the greyscale of the image, equivalent to the surface reflectance (Fig. 1). The Y-axis can be re-scaled/stretched by clicking and dragging vertically on the image anywhere outside the dashed white lines.

5.4 Screen resolution

One pixel in each active window precisely corresponds to one measurement by the ItraxTM core scanner. Users are advised to reduce their screen resolution to improve

the visibility of extremely fine-scale changes in parameter profiles. A trial and error approach is advocated so that the user can view the programme at a reduced resolution while maximising use of screen space. In Windows Vista users must rightclick on the desktop, select "Personalize", then click "Display settings".

6.0 Using PeakCounter 2.1.5

6.1 Further active window manipulation

All the components displaying the multi-parameters derived from the ItraxTM core scanner should now be arranged so they are all visible and fill the screen (Figs. 1, 3 and 4).

The drop-down menu at the top left corner of each of the six active windows can be used to select from the list which of the parameters is plotted in the window. As well as all of the chemical elements of interest selected by the ItraxTM user to measure, this list includes greyscale, kilo-counts per second (kcps), and mean square error of prediction (MSE). In active windows 4-6 it is also possible to plot element and/or parameter ratios by ticking the "ratio" box and selecting the desired element/parameter(s) from the two drop-down menus. The parameter profiles may be stretched by changing the upper and lower Y-axis values at the right of each active window. The Y-axis may also be reversed by right-clicking on the active window and selecting "Flip vertical" (Fig. 2). Weighted moving averages (equally- or centrallybiased, 3- or 5-point) can be plotted by right-clicking on the desired active window and selecting "Moving average" (Fig. 2) and then one of the possibly weightings ("0:33:33:33:0", "0:25:50:25:0", "20:20:20:20:20", or "10:20:40:20:10"). To bring both the active window scale bar and the X-radiograph scale bar to the front of all the windows at any time to the user selects "Tool", "Show scale" from the PeakCounter 2.1.5 control panel menu.

6.2 Varve counting

The active cursor line (orange line with cross-hair) moves simultaneously in all active windows allowing the user to examine correlation between elements, parameters and their ratios at extremely high resolution. This allows varve (or other laminae/sediment structure) limits to be precisely marked in the active windows (and the output file to scan increment resolution). The cursor line can be deactivated/activated by either right-clicking on any of them and unticking/ticking the "Activate" command (Fig. 2), or by using "Ctrl-A". The user is able to mark different levels of varve signal clarity resulting due to differing degrees of correlation between indicator parameters and signal strength, but also denoting the counter's judgement that it represents a true varve. By left-clicking at the desired position in any of the active windows (not including the magnified core photo) the user can mark a "Level 1" line (red) in all active windows which is also registered in the "Active years" counter window (Fig. 3) that counts all marked years within the current active window view. The user rightclicks at the desired position in any of the active windows to select any level of certainty from 1 to 5 (and to 9 by selecting "(more)"), which will be shown as different colour lines and registered in the corresponding "Active years" counter window (Fig. 3, click "more" in the counter window to see levels 6-9). The user can also move the mouse to the desired position and use the number keys (1-9) on the computer keyboard to mark varve limits with differing certainty. The user is able to change the corresponding line (and count) colour by going to "Setting" in the control panel menu, "Colour setting", selecting the level colour they wish to change, clicking

on the desired colour and clicking "OK". Default settings can be set by going to "Setting", "Colour setting", and selecting "Default".

The user can "Undo" their last marked level lines by right-clicking on any of the active windows and selecting the appropriate command (Fig. 2), or by using "Ctrl-Z". The undo function can be repeated for up to 50 times. Marked lines may be deleted by hovering the active cursor line over the particular marked line, right-clicking and selecting "Delete" [this cannot be undone]. An additional column is created in the output file labelled "year" where the marked level number is recorded in the spreadsheet row corresponding to the precise "Position (mm)" from the top of the ItraxTM core scan (Fig. 4) (one row in the spreadsheet corresponds to one pixel in the active windows).

If the varve clarity and/or signal are poor in places, then more clearly varved sections can be used to estimate the spacing/position of varves in the poorly varved section (i.e. sedimentation rate). The user either clicks the "Show tools" button in the PeakCounter 2.1.5 control panel (Fig. 3, which will also bring the "Active year" window to the front), or uses "Tool", "Show elastic scale", to open/show the "Elastic scale" bar aligned with the active windows. The user clicks and drags horizontally inside the bar to reveal markers and circles in the bar and active windows, respectively. The user can drag them to the desired spacing (noted in the elastic scale bar in mm) as indicated by the position of the marked varves in the clearly varved section (Fig. 3). The bar can be placed anywhere and the circles will move accordingly. It is emphasised that this tool should only ever be used as an approximate guide, and any varve limits marked using the tool should be marked at an accordingly low degree of certainty (i.e. a high level number, see Fig. 3). An objective method for varve interpolation that is statistically robust and does not rely on using sedimentation rates fro neighbouring sections can be found in Schloaut *et al.* (in prep).

6.3 Labelling laminae and describing sediment characteristics

To precisely mark a particular sedimentary structure the user right-clicks in an active window at the desired position and selects "Labelled lamina" (Fig. 2). This opens a separate window where the user can label the lamina in the first box and describe it in the second (Fig. 2). Clicking "OK" closes the window. A blue line will appear in the marked position in all active windows. The lamina label and note (in brackets) text appear when the user hovers the active cursor line over the blue line in any of the active windows. The labelled lamina may be deleted by hovering the active cursor line over the particular marked line, right-clicking and selecting "Delete" [this cannot be undone]. A blue line also appears in the X-radiograph preview window of the full core section which makes it easier for the user to align and re-scale (if required, i.e. when not using the core photo from the ItraxTM scan) the core photo to the Xradiograph image using the position of distinct sedimentary structures (e.g. turbidites, tephra) as marker layers (Fig. 1, 3 and 4). Two additional columns are created in the output file labelled "lamina" and "note" where these are recorded (Fig. 4). This therefore makes it easy for the user to find the marker layers in the output file which are particularly useful when used to correlate overlapping core sections, either when taken as parallel "Double-L" channel (a.k.a. "LL-channel" or "Nakagawa channel") sub-samples (see: Nakagawa (2007); Nakagawa et al. (in press)) (advocated here when core scanning at extremely high resolution for varve counting) from the same master core section, or from overlapping bore holes.

In the same way, the user can precisely mark notes at any required position by rightclicking in any of the active windows and selecting "Note" (Fig. 2). This opens a new window where the note can be made, either manually, or by selecting a note from the drop-down library list, and then clicking "OK" (Fig. 2). A short white line will appear in the active windows. This note will be shown as text when the user hovers the active cursor line over the white line in any of the active windows. Unlike "Labelled lamina", the line does not appear in the X-radiograph preview window. The note may be deleted by hovering the active cursor line over the particular marked white line, rightclicking and selecting "Delete" (this cannot be undone). The note will be recorded in the "note" column in the output file (Fig. 4).

6.4 Saving

When saving the output file for the first time, the user clicks the "Save as" button in the PeakCounter 2.1.5 control panel. This opens a window where the user can navigate to the desired folder location for saving. Alternatively, the user may click "File", "Save as", select the output file (or change its name), and click "Save". For saving after the first time, the user either clicks on the "Save" button in the PeakCounter 2.1.5 control panel, or clicks "File", "Save", in the control panel.

By clicking "File", "Save summary" a separate .csv file is created in which the sum of each level number (1-9) between each "Labelled lamina" is recorded (Fig. 5). This is extremely useful when comparing varve counts between marker layers in parallel core sections.

6.5 Closing PeakCounter 2.1.5

The user either clicks on the "Quit" button on the control panel, or uses "File", "Quit". If the user has made and changes to the file since the last save, then they are able to choose whether they want to save those changes prior to quitting.

7.0 Questions and bug reports

Queries and bug reports should be sent directly to the author of the software (E-mail: takeshi.nakagawa@newcastle.ac.uk).

8.0 Summary

PeakCounter 2.1.5 is a user-friendly Windows based programme for high resolution analysis of multi-parameter data from the ItraxTM core scanner. Although it was specifically designed to enable an objective approach to manual varve counting it is also an extremely useful and powerful tool for all high resolution analysis of sedimentary core sequences measured on the ItraxTM core scanner. As the programme uses a configuration of one pixel per measurement increment the user is able to mark lamina and define other sedimentary structures extremely precisely (only restricted by scan resolution). PeakCounter is continually updated, and the authors are receptive to the suggestions of other researchers. The features described in this paper are found in the current version of the programme, Version 2.1.5. Peakcounter 2.1.5 is free of charge to all interested scientific researchers.

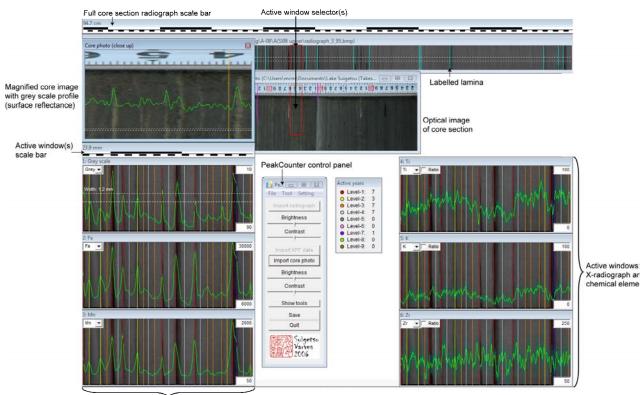
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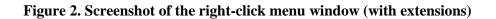
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Figure 1. Screenshot of PeakCounter 2.1.5, with all windows displayed



Marked varves (level/colour denotes class)



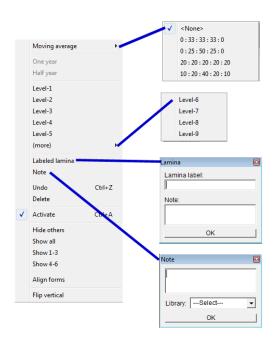


Figure 3. Screenshot of PeakCounter 2.1.5. The profile in active window 4 (Ti) has been smoothed using the weighted average tool. The profile in active window 5 shows the use of the ratio tool (Fe/Ti), and has been smoothed using the weighted average tool. Varve limits have been marked using different levels of certainty. The elastic scale tool is also shown (above active window 1).

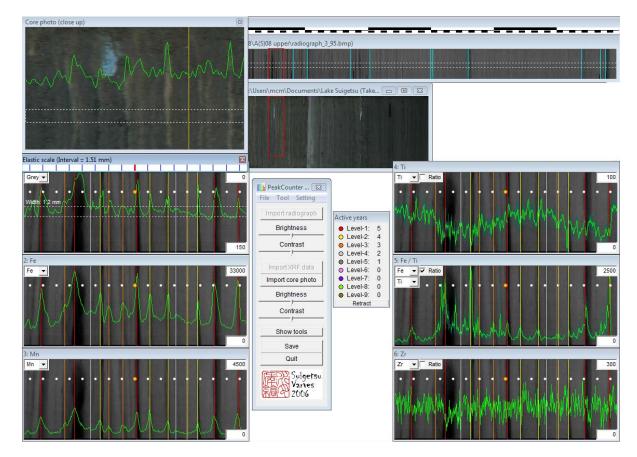


Figure 4. Screenshot of the output file opened in Excel showing additional columns created by PeakCounter 2.1.5.

AM	AN	AO	AP	AQ	AR	
inc	coh	greyscale	year	lamina	note	
1825	446	225				
2128	523	220				
2492	580	216				
2561	593	211				
2802	627	206				
2767	659	200				
2743	585	198				
2678	656	192				

	A	В	С	D	E	F	G	Н		J
1										
2										
3	Boundaries	Level-1	Level-2	Level-3	Level-4	Level-5	Level-6	Level-7	Level-8	Level-9
4	'Section top'									
5		3	6	37	30	0	0	0	0	0
6	'01a'									
7		0	0	4	1	0	0	0	0	0
8	'01b'									
9		0	0	6	6	0	0	0	0	0
10	'01c'									
11		18	28	129	118	0	0	0	0	0
12	'02'									
13		22	39	95	78	0	0	0	0	0
14	'03a'									
15		0	1	4	2	0	0	0	0	0
16	'03b'									
17		0	0	0	6	0	0	0	0	0
18	'03c'									
19		30	21	31	41	0	0	0	0	0
20	'04a'									
21		7	4	12	9	0	0	0	0	0
22	'04b'									
23		25	47	131	101	0	0	0	0	0
24	'Section bottom'									

Figure 5. Screenshot of the "Summary" output file opened in Excel showing the sum of each level of marked lamina/varves between each "Labelled lamina".