

User Guide for the PATISSIER Program



PATISSIER

Quanterra
rue de la Grise 28, 1007 Lausanne,
Switzerland
www.quanterra.org
Mail: support.quanterra.org

Institut de Minéralogie et Géochimie
Université de Lausanne
BFSH2, CH-1015 Lausanne Switzerland
Tel: ++ 41 21 692.43.00
Fax: ++ 41 21 692.43.05

Written by M. Jaboyedoff

By M. Jaboyedoff



Quanterra

Ch. Tour-Grise 28, 1007 Lausanne, Switzerland
www.quanterra.org E-Mail: support.quanterra.org

And

Institut de Minéralogie et Géochimie
Université de Lausanne, BFSH2
CH-1015 Lausanne, Switzerland
Tel: ++ 41 21 692.43.00 Fax: ++ 41 21 692.43.05"

1. INTRODUCTION	3
2. GENERAL SETTINGS.....	3
2.1 INSTRUMENTAL EFFECT REMOVAL.....	3
2.2 PLOTTING A POINT	4
3. OPTIONS.....	5
3.1 GRID LINES.....	5
3.1.1. <i>Export Constant line</i>	5
3.2 REICHWEITE	5
4. THE FILE MENU	6
4.1 TREAT FILE	6
4.2 PRINT.....	6
5. EDIT MENU (FIG. 6).....	6
5.1 COPY TO CLIPBOARD.....	7
5.2 CLEAR ALL.....	7
5.3 CLEAR POINTS	7
6. DRAW.....	7

Installing

The program was compiled under Windows 98 with VB 6.0 SP5. Unzip the file in a directory and click on setup.

Questions may be addressed to support.quanterra.org. Remarks for the program improvement are welcome.

1. Introduction

This software is designed for the "illite crystallinity" interpretation. Detailed description of the theory can be found in:

JABOYEDOFF, M. and THÉLIN, P. (2002): PATISSIER: software to estimate the smectite content and number of consecutive illite layers in mixed-layer illite-smectite using illite crystallinity data Schweiz. Mineral. Petrogr. Mitt., 82

JABOYEDOFF, M., BUSSY F., KÜBLER, B. and THÉLIN, P. (2001a): Illite crystallinity revisited. Clays and Clay Minerals 49,156-167.

MOORE, D. M. and REYNOLDS, R. C. (1997): X-ray diffraction and the identification and analysis of clay minerals. Oxford University Press, Oxford, 378 pp.

REYNOLDS, R.C.J. (1985): NEWMOD a computer program for the calculation of one-dimensional X-Ray diffraction patterns of mixed-layered clays. Reynolds, R.C.Jr., 8 Brook Dr., Hanover, New Hampshire.

REYNOLDS, R.C.Jr. and REYNOLDS, R.C.Jr. III. (1996): NEWMOD© a computer program for the calculation of one-dimensional diffraction patterns of mixed-layered Clays, 8 Brook Dr., Hanover, New Hampshire, Reynolds, R.C.Jr..

This program allows the estimation of the coherent scattering domain of diffraction (CSD) characteristics. Mean thickness (N) of illite-smectite (I/S) with low %S content (=illite s.l.) can be estimated, as well as %S, and the number of consecutive illite in the CSD equal to N_{fp} . This is realized by measuring both full width at half maximum (FWHM) of 10 Å diffraction peak on both air dried (AD) and glycolated (Gly) diffractograms.

When FWHM is not corrected for instrumental, it is named illite crystallinity (IC) and when instrumental broadening is removed the FWHM is called illite width (IW).

The estimation is used using a diagram IWAD versus IW_{Gly}, which means that N, %S and N_{fp} are estimated on the basis of the position of a point in a graph IWAD - IW_{Gly}

The program has been designed using the Newmod© program (Reynolds (1985) using $^{\circ}\Delta 2\theta\text{CuK}\alpha$ units.

2. General settings

2.1 Instrumental effect removal

The first step to use this software is to choose the type of removal effect (Fig.1). In the upper right file of the window the full width at half maximum of the instrumental broadening must be inputted to $^{\circ}\Delta 2\theta\text{CuK}\alpha$ units. The method to remove the instrumental broadening is set at the left of the windows. Four choices are possible: **Gaussian**, **Lorentzian**, **Mixture**. Mixture corresponds to the geometric mean of the two previous methods. Another possibility is to use a file (with extension *.cor) containing a table of correspondence between the FWHM of the experimental profiles (IC) and the profile after instrumental effect removal (IW). This file must contain a comment in its first line, in the second line the starting FWHM of the corrected data (equivalent to IW). In the third line the step between IW corrected, and then the list of value corresponding to uncorrected data equivalent to IC (Table 1).

Couple of data are given by (V1, start), (V2, start + step), (V3, start + 2*step), ... For example 0.074 $^{\circ}\Delta 2\theta\text{CuK}\alpha$ correspond to 0.01 $^{\circ}\Delta 2\theta\text{CuK}\alpha$ corrected IW.

Theory	Example
Nom	Profile rigaku pearson IIV m=2 powder convolution
Start ($^{\circ}\Delta 2\theta\text{CuK}\alpha$)	0.005
Step	0.005
V1	0.066
V2	0.074
V3	0.08
....	0.087
	...

Tables 1: Structure of the instrumental correction file, a file example is P7m2pow.cor was designed for a Rigaku diffractometer.

2.2 Plotting a point

With a click on **Draw** button, the value in the field **Air-dried IC** and **Ethylene-Glycol IC** are corrected for instrumental broadening, with the current settings, and plotted on the graph IW-2w IW-2gly. IW-2W IW-2gly, displaying the value of N, %S, N_{fp} and k which link %S to N by $\%S/100 = k/N$. The k values are primarily plotted in the graph.

Clicking in the graph, but under the 1/1 diagonal can directly plot a point and over the higher k value line plotted (Fig. 1). The position of the mouse is displayed in $^{\circ}\Delta 2\theta\text{CuK}\alpha$ in the white field.

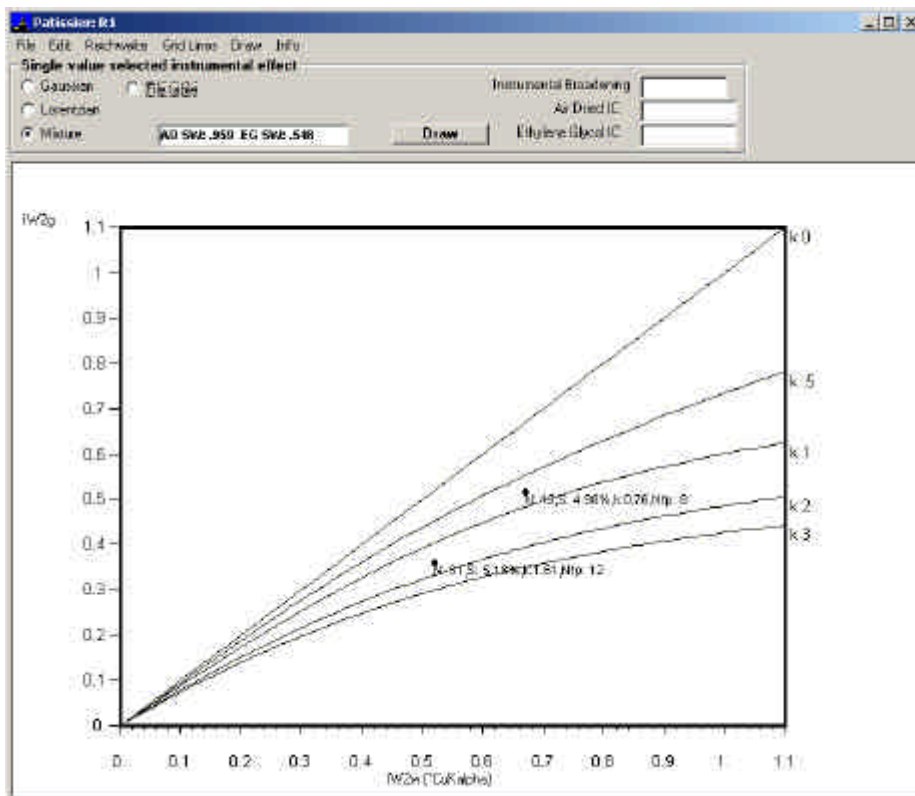


Figure 1: View of the window of the program, with the graph and the settings above. K-lines are displayed.

3. Options

The displayed graph can be changed using a series of options, which allow modifying to display lines or to change the Reichweite of the I/S (Fig. 3).

3.1 Grid lines

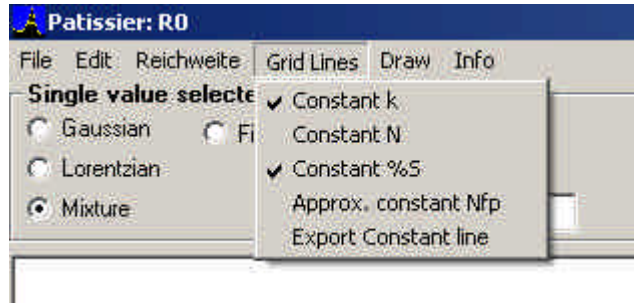


Figure 3: Menu Grid Lines

In the graph some of the characteristics of the graph may be plotted. Lines with **Constant** values of **k**, **N**, **%S**, **approximate N_{fp}** can be plotted, either all together or separately, by checking menu.

3.1.1. Export Constant line

In order to import the raw data of the constant lines to another program, it is possible to export all the "constant lines" raw data that are currently checked in a file (*.IWL), except k-lines, which are not exported.

Constants proportion lines

Reichweite: R0				R1				R2				R3			
N	%S	Gly	...	N	%S	Gly	...	N	%S	Gly	...	N	%S	Gly	...
0.722	0.712	0.15	0.442	...	0.18	0.127	0.31	0.227	...	0.08	0.06	0.11	0.061
0.75	0.704	0.275	0.388	...	0.188	0.155	0.395	0.256	...	0.08	0.064	0.11	0.067

Table 2: format of the exported lines file. N, %S and N_{fp} values are indicated, and the corresponding IW-SA and IW-Gly are listed below.

3.2 Reichweite

The ordering of the I/S stacking may be chosen with the same definition used in Newmod. **R0** (no order), **R1** and **R3** are possible (Fig. 4).



Figure 4: Reichweite menu.

4. The File menu



Figure 5: Menu File.

4.1 Treat File

A file (with extension *.IW) containing couple of IC AD - IC Gly data is read and plotted on the graph as points using current settings of the instrumental broadening removal (Figs. 1 and 5). The result are exported in a file with *.IWO extension. You can find one example in *FREY_DIGIT.IW*. During the treatment, if data are outside the zone of validity of the method, an error is generated.

The first line of the file is a comment, the second the number of data couple and the third is the instrumental broadening (Table 3). In the fourth line, the data are in two columns, the first being the IC AD and the second the corresponding IC Gly. Tabulators separate data.

```
FREY AND KISCH DATA
210
.168
0.81  0.75
0.83  0.73
0.78  0.74
0.73  0.69
0.66  0.66
0.74  0.66
0.74  0.66
0.76  0.68
0.78  0.67
...
```

Table 3: (corresponding file is FREY_DIGIT.IW)

4.2 Print

Simply print the graph windows (Figs. 1 or 7)

5. Edit Menu (fig. 6)

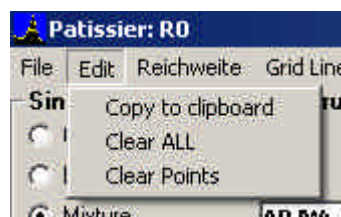


Figure 6: Menu edit

5.1 Copy to clipboard

A bitmap copy of the current graph is copied in the clipboard (Fig. 7).

5.2 Clear all

Remove all points and lines from the graph except the k-lines.

5.3 Clear points

Remove only the points displayed on the graph.

6. Draw

This menu permits to draw for each point displayed on the graph, the lines which have the **Identical** values **k**, **N**, **%S** or **N_{fp}** to the points displayed (Figs. 7 and 8). The corresponding lines are displayed if the sub-menus are checked

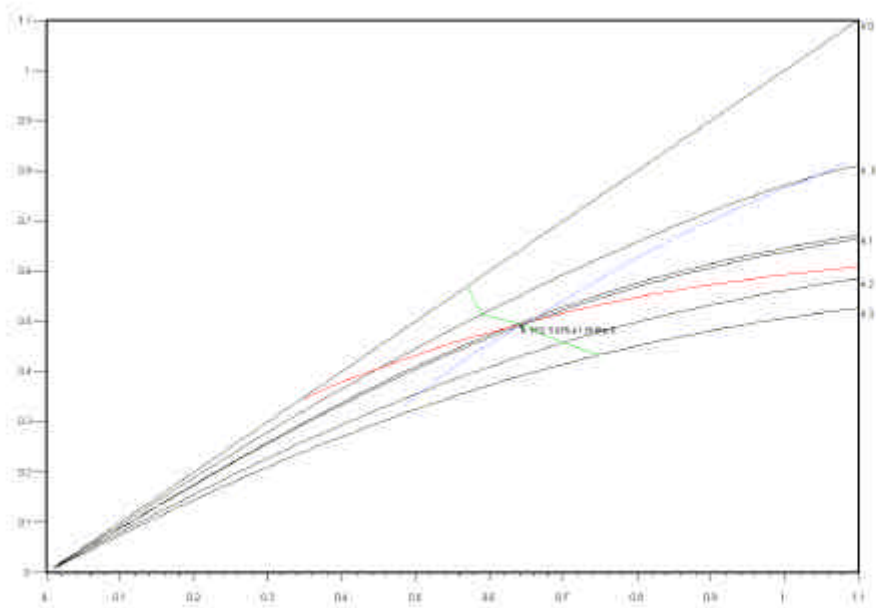


Figure 7: Bitmap of the window containing only one point with identical K, N, %S and N_{fp} lines.

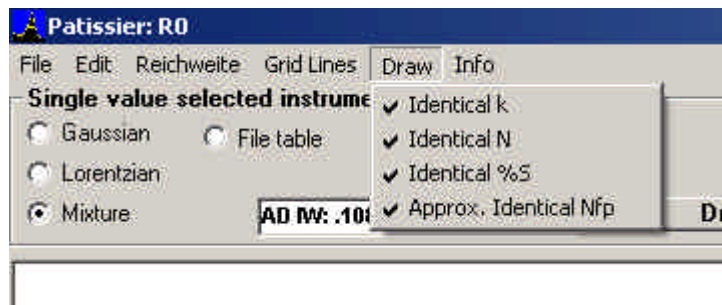


Figure 8: Draw menu indicating that all lines are drawn.

Michel Jaboyedoff
Quanterra
Lausanne, 10th July, 2002