- MagSuite V2.5 : Help -

I-   Installation

I.A-   MagSuite_ForPC : Installation instructions

This installation should work on Windows XP, 7, 8 and 10.

(Remove previous versions if no needed).

- Unzip archive if needed.
- Execute the automatic installer "setup.exe".

    Note that "LabVIEW 2014 SP1 Runtime Engine" is needed.

    The installer will install it first, if needed.
- Follow instructions of the installer (it is recommended to keep default settings).
- To launch the application use the corresponding shortcuts of the Windows program menu.

To run properly,

- several config files ("*.cfg") are needed in a folder located in "c:\MagSuite_ConfigFile".
- "useLocaleDecimalPt=False" option has to be set in "*.ini" files

    located in "c:\Programfilex86\MagSuite".

I.B-   MagSuite_ForMAC : Installation instructions

This installation should work only 32 bit Mac system.

(Remove previous versions if no needed)

- Download and Install LabVIEW Runtime Engine version 2014 SP1 for Mac

    from NI.com ("LabVIEW2014SP1RuntimeEngine.dmg").
- Unzip archive.
- To launch the application, execute the corresponding "*.app" file.

To run properly,

- several config files ("*.cfg") are needed in a subfolder "_ConfigFile".
- "useLocaleDecimalPt=False" option has to be set in "*.preferences" files.

II-   Introduction

MagSuite is a collection of software applications programmed with Labview 2014.

- MagViewer

>   to sort and treat magnetic data.

- MagExplorer

>   to quickly visualize plots exported with MagViewer.

- MagFitterCC

>   to extract relaxation time values (*To*) from AC magnetic measurements.

- MagFitter

>   to perform single curve fitting.

- MagCalculator

>   to calculate molar weight or specific formulae.

III-   MagViewer

III.A-   Principle of the application

This application is to sort and treat magnetic data.

1- Raw data file that can be imported with format configurations, will be transformed in a normalized table. The normalized columns are:

t0	time (s)
t	temperature (K)
h	DC magnetic field amplitude (Oe)
m	DC magnetic moment (emu)
m1	AC magnetic moment in phase (emu)
m2	AC magnetic moment out of phase (emu)
h1	AC magnetic field amplitude (Oe)
f1	AC magnetic field frequency (Hz)

2- From this normalized table, series of data can be sorted (typically for static studies, field and temperature dependencies, and for dynamic studies, frequency and temperature dependencies).

3- For each series, data can be treated (correction with formula configurations, normalization with type normalization presets, and 1st derivative calculation).

4- Series can be previewed in a plot.

5- Series can be exported in standard ASCII file with export configurations.
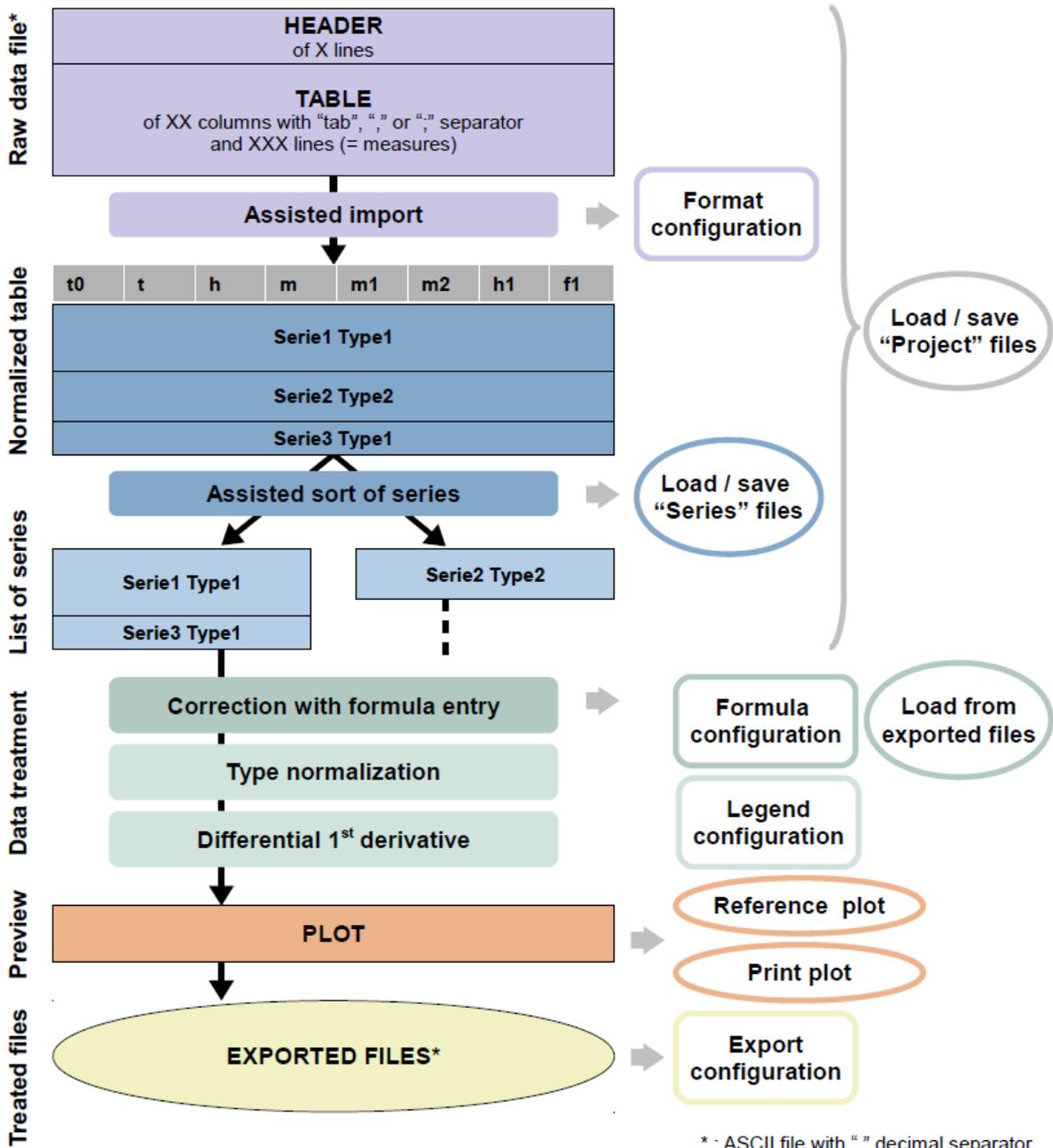
III.B-   Getting started

III.B.1-   Main window

In the menu bar, at the top of the window, you can find:

- **"Import datafile"** button to open the import window.

- **"Load / Save project"** buttons to save current information of the raw data file, the format configuration and the list of series.

The project will be saved automatically in the same folder as the raw data file with an extension ".prj". It is important to keep raw data file and project file in the same folder.

- **"Configuration"** button to open the configuration window.

- **"X"** button to close the application.

In the main part of the window, you can find from left to right:

- The normalized table and some controls to add series

Data of this table are set from the import window.

Columns are defined in *Principle of the application* chapter.

"**Values format**" is adjusting the format of the values (the syntax is similar to legend configurations, as described in *Configuration window* chapter).

To add series:

- select corresponding lines in the table (use "Shift" or "Ctrl" key if needed).
- set series parameters

A series is defined with 3 variables as: **Y=f(X) @ Z**. Select the column for X, Y and Z.

For example, you can set Y=m=f(X=h) @ Z=t.

"**DeltaZ**" is the maximum deviation of Z for a series (before creating a new series).

For example, you can select all lines for m=f(h) @ t=2K, m=f(h) @ t=3K, m=f(h) @ t=5K and m=f(h) @ t=8K with DeltaZ = 0,5, to add 4 series Z=t= 2 , 3, 5 and 8 K

"**Sort by X, Z**" option sort the lines by X values then Z values.

Typically this option is used for temperature dependencies AC measurements @ several frequencies (that have been recorded for several frequencies at each step of temperature).

- click on "**Add series**" button

- The list of series

You can select several series from the list for plotting and exporting (use "Shift" or "Ctrl" key if needed).

"**Up**", "**Down**", "**Clear**", and "**Del**" buttons allow the rearrangement of the list.

"Select lines from series" update the lines in the normalized table from the selected series.

"Load" and **"Save"** buttons save the list of series. The list will be saved automatically in the same folder as the raw data file with an extension ".ser". It is important to keep raw data file and series file in the same folder.

TIPS: To merge data from several series, you can select the corresponding series from the list, click on "Select lines from series" to select all the corresponding data, and click on "Add series" to create the right series. Then used "Del" button to delete old series.

- The data treatment section

(Treatment is described in *Data treatment* chapter)

You can set the **formula configuration**.

You can modify the formula and the parameters.

"**Save config.**" button load current formula and parameters in the configuration window to save it as new formula configuration.

"**Load from file**" button load the formula from an exported file (with the default export configuration).

When "**Keep parameters**" option is active, the parameter values will not be affected by a modification of the formula configuration.

When "**Auto update plot**" option is active, the plot will be automatically updated during parameter modification. This option has to be used wit care.

You can choose the **type normalization** preset.

You can enable/disable the **1st derivative differential**.

You can choose the **legend configuration**.

- The plot section

"**Plot series**" button calculates for the selected series the corrected and normalized data and plot the result. "X" button aborts the process.

"**Print plot**" button copy the image of the plot. You can paste it directly in a ".doc" file for example.

"**X=**" and "**Y=**" indicators show values of the cursor.

"**LogX**" and "**LogY**" enable/disable the log scales.

You can plot a reference for comparison. The reference is a file exported with MagViewer (with the default export configuration).

    - Set the file with the "**...**" browse button and select the X and Y values.

    - Activate the "**Plot reference**" option.

- Calculate the plot with the "**Plot series**" button.

The plot window provides tools for zooming, cursor manipulation, plot selection, etc... that are specific to LabView... see LabView reference if needed.

- The export section

The "**Export series**" button will save the data of the current plot in a ".txt" file with export configurations.

It is recommended to use the "**Default**" configuration for compatibility with the other applications (*MagExplorer, MagFitter, MagFitterCC..).*

The "**Default**" configuration sets a 6 lines header (with useful information as version, type and formula), and independent "X,Y" columns without any interpolation, to save as much as possible information from measurements.

Other configurations can be used for special needs:

"**Phi single plot**" and "**Phi multi plot**" configurations are set for the use of *Phi* software (Nicholas Chilton). In that case, you have to convert field values in tesla in accordance with the convention of *Phi (i.e. replace "x=x0" with "x=x0/10000" at the beginning of the formula)*.

You can set manually the path and the filename of the exported file.

By default, they are automatically set with the path and the name of the raw file, with an extension based on the series definition and the type normalization.

Files can't be overwritten.

III.B.2- Import window

- Set the raw data file with the "**...**" browse button.

> The left table will display the raw data file.

> The right table will display the normalized table with the current format parameters.

- Set the **format configuration**.

> You can modify manually the parameters.

> You can upload the current format parameters in the configuration window with the "Save config." button.

- You can edit a value of the table.

> Click on a cell, type the new value and validate with Enter key.

- Click on "**Import for sorting**" button, to load the normalized table in the main window.

III.B.3- <u>Configuration window</u>

- The **default file path** can be set. It is recommended to reboot the application after modification.

When a raw file is loaded the application use its path by default.

(This information is saved in "_ConfigFile/Param.cfg".)

- With the four tables, you can manage different configurations for "**Format**", "**Formula**", "**Legend**" and "**Export**".

Double click on a line of a table, to load the corresponding values in the form.

The corresponding information is saved in "Format.cfg", "Formula.cfg", "Legend.cfg" and "Export.cfg" of the directory "_ConfigFile".

III.C- **Data treatment**

III.C.1- Main schematic
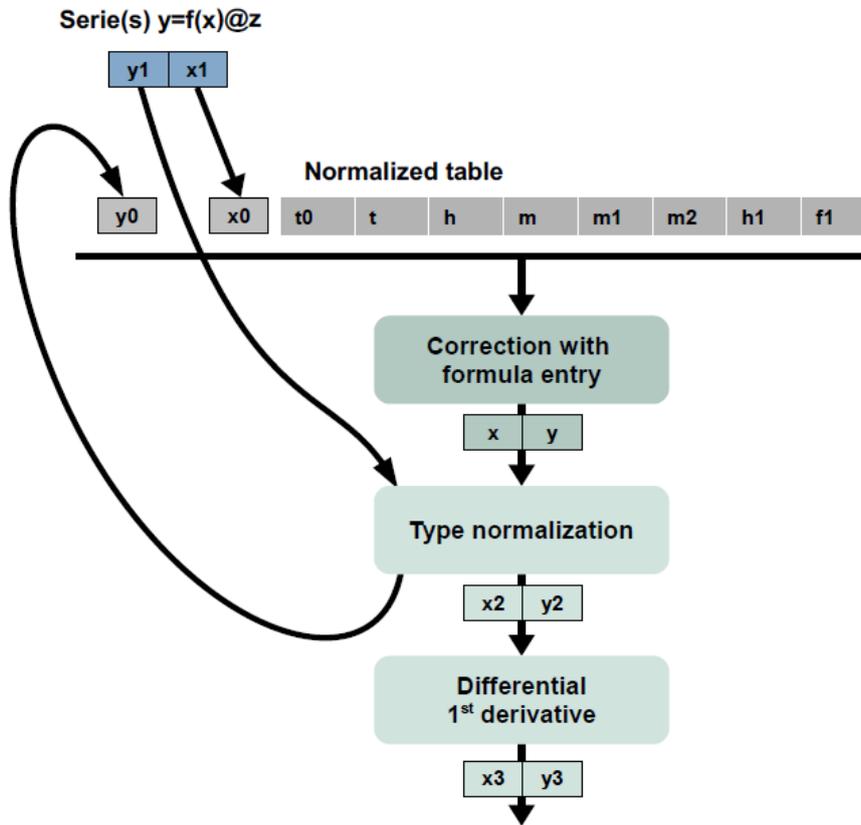
III.C.2- Type normalization

---	y0 = y1		y2 = y	x2 = x
M				
M(Bohr)			y2 = y / 5585.02	x2 = x / t
M(BohrT)	y0 = m			
Khi		x0 = x1	y2 = y / h	x2 = x
1/Khi			y2 = h / y	
KhiT			y2 = y * t / h	
M'	y0 = m1		y2 = y	
M"	y0 = m2			
Khi'	y0 = m1		y2 = y / h1	
Khi"	y0 = m2			

The type normalization affects data treatment before and after the **correction formula**.

From the "X;Y" variables as defined from the series ("x1;y1" as described in *Main schematic* chapter), the type normalization preset calculates "x0;y0" and "x2;y2" values.

This behavior aims to display different common normalizations (susceptibility, Bohr magneton normalized magnetization, etc...) with a unique correction formula based on magnetization values only.

Type normalization presets can't be modified.

III.C.3- Differential 1st derivative

"**---** ":

$$y3 = y2 \qquad\qquad x3 = x2$$

"**1st derivative**" :

$$y3 = \frac{y2_{i+1} - y2_i}{x2_{i+1} - x2_i} \qquad x3 = \frac{x2_{i+1} + x2_i}{2}$$

Differential presets can't be modified.

III.C.4- Correction formula

Syntax

Thanks to the formula entry you can perform custom calculations.

You can do "x;y" calculations from the "X;Y" variables as defined from the series and **type normalizations** ("x0;y0" as described in *Main schematic* chapter) and from all the variables from the normalized table (t0, t, h, m, m1, m2, h1 and f1 as described in *Principle of the application* chapter).

For example, you can check the stability in temperature for a series (independently to the definition of "X;Y"), by setting "x=t0;y=t" with a type normalization "---".

Syntax is based on the LabView formula node syntax.

You can refer to:

https://zone.ni.com/reference/en-XX/help/371361R-01/lvhowto/formula_node_syntax/

Formula definition can be saved with **formula configurations**.

"DC mol-1 with Bag+DiaMol+KhiD" formula

$$M_{Measured} = M_{SamplePara} + M_{SampleDia} + M_{SampleTIP} + M_{Bag}$$

or

$$M_{SamplePara} = M_{Measured} - M_{SampleDia} - M_{SampleTIP} - M_{Bag}$$

with:

$$M_{SamplePara} = M_{SamplePara(mol^{-1})} \cdot \left(\frac{Mass_{Sample}}{MolarMass_{Sample}} \right)$$

$$M_{SampleDia} = \chi_{SampleDia} \cdot H = -0,5 \, x10^{-6} \cdot MolarMass_{Sample} \cdot H \cdot \left(\frac{Mass_{Sample}}{MolarMass_{Sample}} \right)$$

$$M_{SampleTIP} = \chi_{SampleTIP(mol^{-1})} \cdot MolarMass_{Sample} \cdot H \cdot \left(\frac{Mass_{Sample}}{MolarMass_{Sample}} \right)$$

$$M_{Bag} = \chi_{Bag} \cdot H = \left[-7.62x10^{-7} + \left(\frac{6.541x10^{-7}}{T+2.91} \right) \right] \cdot Mass_{Bag} \cdot H$$

and with:

$$p1 = MolarMass_{Sample}$$

$$p2 = Mass_{Sample}$$

$$p3 = Mass_{Bag}$$

$$p4 = \chi_{SampleTIP(mol^{-1})}$$

$$M_{SamplePara(mol^{-1})} = \left(\frac{p1}{p2} \right) \cdot \left([M_{Measured}] - [(-0,5+p4)\,x10^{-6} \cdot p2 \cdot H] - [(-7.62x10^{-7} + (\frac{6.541x10^{-7}}{T+2.91})) \cdot p3.H] \right)$$

$$\chi_{SamplePara(mol^{-1})} = \frac{M_{SamplePara(mol^{-1})}}{H}$$

IV- Mag Explorer

IV.A- Getting started

In the menu bar, at the top of the window, you can find:

- **"..."** button to open a folder.
- **"X"** button to close the application.

In the main part of the window, you can find from top left to bottom right:

- The "Explorer" section

The table on the left lists all files ("*.txt") of the folder. You can select one or several files (use "Shift" or "Ctrl" key if needed).

The text box above displays the header of the selected file.

The table on the right lists all the series of the selected files. You can select one or several files.

When the "**Preview**" checkbox is activated, all selected series from the table will be plotted. When it's deactivated, only selected series from "**Data to plot**" section are plotted.

The "**Add series**" button adds selected series in the table of the "**Data to plot**" section.

- The "Data to plot" section

From the table you can select the series to plot.

"**Down**", "**Up**", "**Clear**", and "**Delete**" buttons allow the rearrangement of the list.

TIPS: You can plot series from different files and from different folder.

- The plot section

"**Print plot**" button copy the image of the plot. You can paste it directly in a ".doc" file for example.

"**X=**" and "**Y=**" indicators show values of the cursor.

"**LogX**" and "**LogY**" enable/disable the log scales.

- The export section

The "**Export series**" button will save the data of the current plot in a ".txt" file with export configurations.

It is recommended to use the "**Default**" configuration for compatibility with the other applications (*MagViewer, MagFitter, MagFitterCC..*).

The "**Default**" configuration sets a 6 lines header (with useful information as version, type and formula), and independent "X,Y" columns without any interpolation, to save as much as possible information from measurements.

Other configurations can be used for special needs.

Export configurations can be managed with *MagViewer*.

You can set manually the path and the filename of the exported file.

V- MagFitterCC

V.A- Principle of the application

This application is to extract relaxation time values (*To*) from AC magnetic measurements.

1. Raw data has to be exported with *MagViewer* with the default export configuration. Two exported files are necessary: in phase *Khi'* and out of phase *Khi"* frequency dependencies with same series of data.

2. Some data points of a series can be disabled.

3. Series can be plotted and fitted with a generalized Debye model.

   Fits are based on the average of fits on *Khi'* and *Khi"* frequency dependencies.

4. According to the series, evolution of fit results can be previewed in a plot.

5. Fit data points and fit results can be exported in standard ASCII file.

Conventions used for variables are described in "*Data treatment*" chapter.
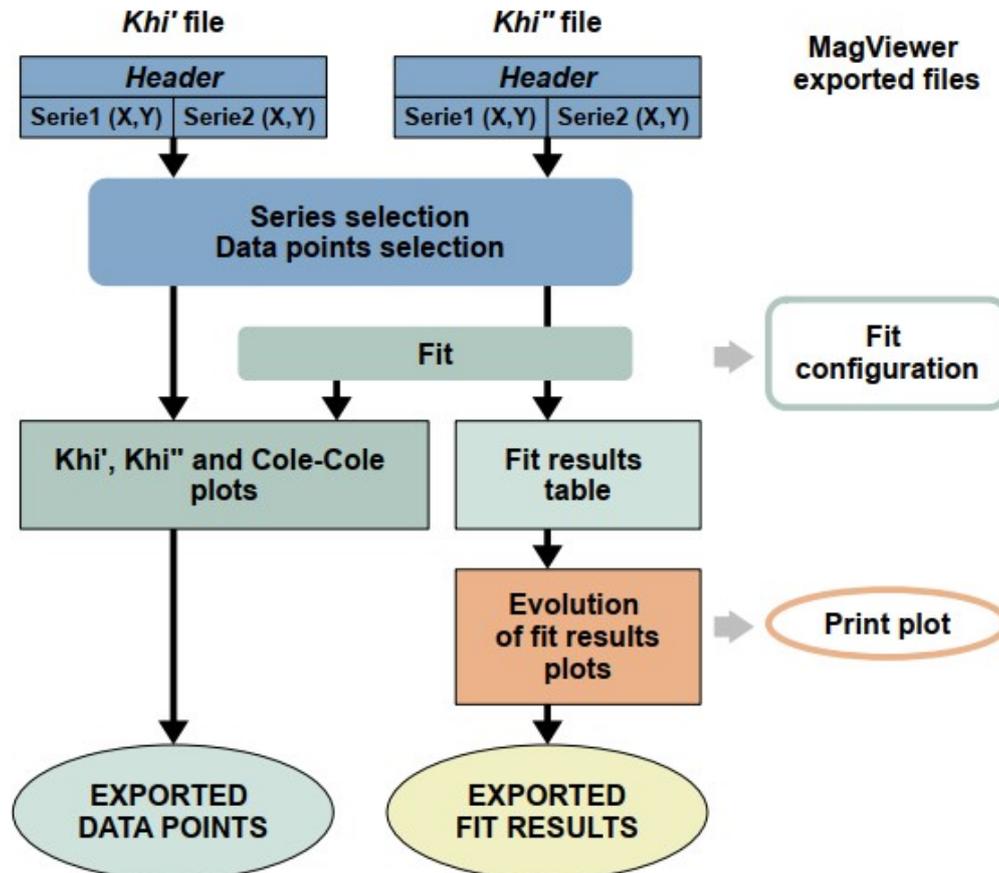
V.B-   Getting started
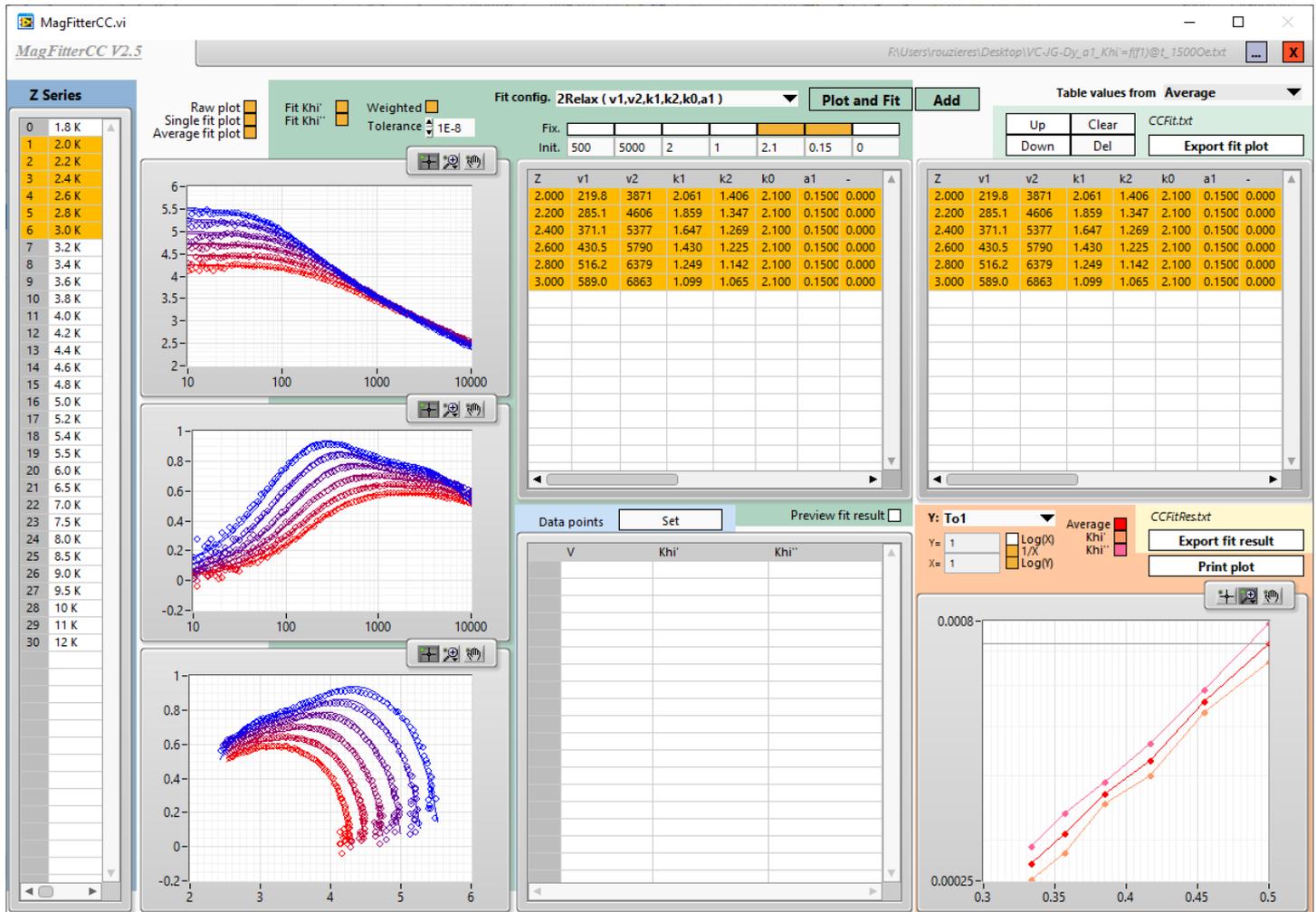
In the menu bar, at the top of the window, you can find:

- **"..."** button to open consecutively *Khi'* and *Khi''* files.

- **"X"** button to close the application.

In the main part of the window, you can find from top left to bottom right:

- The list of "Z series"

You can select several series from this list for plotting and fitting (use "Shift" or "Ctrl" key if needed).

To display data point values in the "**Data points**" table, double-click on a series.

To disable some data points, unselect the corresponding lines in the "**Data points**" table and click on "**Set**" button.

- The plot and fit section

You can set the **fit configuration**.

You can modify the fit parameters:

>   Select the plots to fit with "**Fit khi'**" and "**Fit khi''**" checkboxes.

>   Set the tolerance.

>   Use weighted values with values with "**Weighted**" checkbox.

>   Set initial values with the "**Init.**" table.

>   Fix initial values with the "**Fix.**" checkboxes.

Click on "**Plot and fit**" button to calculate the fit and to plot the selected series.

You can mange plots to display with "**Raw plot'**", "**Single fit plot''**" and "**Average fit plot**" checkboxes.

Temporary fit results are displayed in the table just below the "**Init.**" table.

To plot these results in the **final fit results plot**, enable the "**Preview fit result**" checkbox.

Use "**Add**" button to add to the final fit results table on the right, values from the selected series.

You can use the "**Table values from**" list, to switch between "**Average**", "**Khi'**" and "**Khi''**" fit results (for these two tables).

"**Up**", "**Down**", "**Clear**", and "**Del**" buttons allow the rearrangement of the final table.

The "**Export fit plot**" button export raw data and average fit values in a ASCII file.

- The final fit results plot (evolution of fit results)

The plot is automatically updated from the final fit results table.

The "**Y:**" list select the result to display:

>   You can select all variables from the fit, and *To* ("**ToX**"), *-ln(To)* ("**-lnToX**") and error bars on *To* ("**E-ToX**", "**E-ToX**").

"**X=**" and "**Y=**" indicators show values of the cursor.

"**LogX**", "**1/X**" and "**LogY**" enable/disable the specific scales.

"**Average**", "**Khi'**" and "**Khi''**" checkboxes select the corresponding plots.

The "**Print plot**" button copy the image of the plot. You can paste it directly in a ".doc" file for example.

The "**Export fit result**" button export final fit results in a ASCII file.

V.C- Recommended strategy

Do not try to plot and fit too many series, to avoid big time of calculations.

Start with a fully described relaxation mode, with default fit parameters..

Set the initials values of the fit as close as possible to real values.

    vX, **kX** and **k0** values can be graphically deduced from plots.

Fix fit variables to make **raw data**, **single fit** and **average fit** converge to single curve for **Khi'**, **Khi"** and **CC** plots.

V.D- Data treatment

V.D.1- Conventions and variables

Khi'	χ'	In phase AC susceptibility
		/ frequency dependence of the in phase AC susceptibility
Khi"	χ''	Out of phase AC susceptibility
		/ frequency dependence of the out of phase AC susceptibility
CC		Cole-Cole plot *Khi"=f(Khi')*

X	a digit from 1 to 9

vX	v_0	characteristic frequency
kX	$\Delta\chi = \chi_0 - \chi_\infty$	difference of isothermal and adiabatic limits of susceptibility
k0	χ_∞	adiabatic limit of susceptibility
aX	α	width of the distribution in relaxation times

V.D.2- Generalized Debye model

M' and M'' are defined as in phase and out of phase magnetization in response to an oscillating field excitation $H(t) = H_{AC} \cos(2\pi\nu.t)$:

$$M(t) = M'\cos(2\pi\nu.t) + M''\sin(2\pi\nu.t)$$

with t the time and ν the frequency

$$\chi' = \frac{M'}{H_{AC}} \qquad \chi'' = \frac{M''}{H_{AC}}$$

For a single mode, generalized Debye function describes the frequency dependency of both χ' and χ'', taking into account a distribution of relaxation times:

- ν_0 :   characteristic frequency (at the maximum of χ'') directly related to the relaxation time

$$\nu_0 = \frac{1}{2\pi\tau}$$

- α :   width of the distribution in relaxation times
- χ_∞ :   adiabatic limit of susceptibility (χ' when ν tends to infinity)
- χ_0 :   isothermal limit of susceptibility (χ' when ν tends to 0)
- $\Delta\chi = \chi_0 - \chi_\infty$

$$\chi'(\nu) = \chi_\infty + \Delta\chi \cdot \frac{1 + \left(\frac{\nu}{\nu_0}\right)^{1-\alpha}.\sin\left(\frac{\alpha\pi}{2}\right)}{1 + 2\left(\frac{\nu}{\nu_0}\right)^{1-\alpha}.\sin\left(\frac{\alpha\pi}{2}\right) + \left(\frac{\nu}{\nu_0}\right)^{2-2\alpha}} \qquad \chi''(\nu) = \Delta\chi \cdot \frac{\left(\frac{\nu}{\nu_0}\right)^{1-\alpha}.\cos\left(\frac{\alpha\pi}{2}\right)}{1 + 2\left(\frac{\nu}{\nu_0}\right)^{1-\alpha}.\sin\left(\frac{\alpha\pi}{2}\right) + \left(\frac{\nu}{\nu_0}\right)^{2-2\alpha}}$$

And for the Cole-Cole plot:

$$\chi''(\chi') = \sqrt{\left(\frac{\Delta\chi.\tan\left(\frac{\alpha\pi}{2}\right)}{2}\right)^2 + \Delta\chi(\chi' - \chi_\infty) - (\chi' - \chi_\infty)^2} - \left(\frac{\Delta\chi}{2}.\tan\left(\frac{\alpha\pi}{2}\right)\right)$$

"1Relax (v1,k1,k0,a1)" fit configuration

For two relaxation modes, can be described with the sum of two generalized Debye model. In that case we will use:

- a unique adiabatic limit of susceptibility

$$\chi_{\infty total} = \chi_{\infty 1} + \chi_{\infty 2}$$
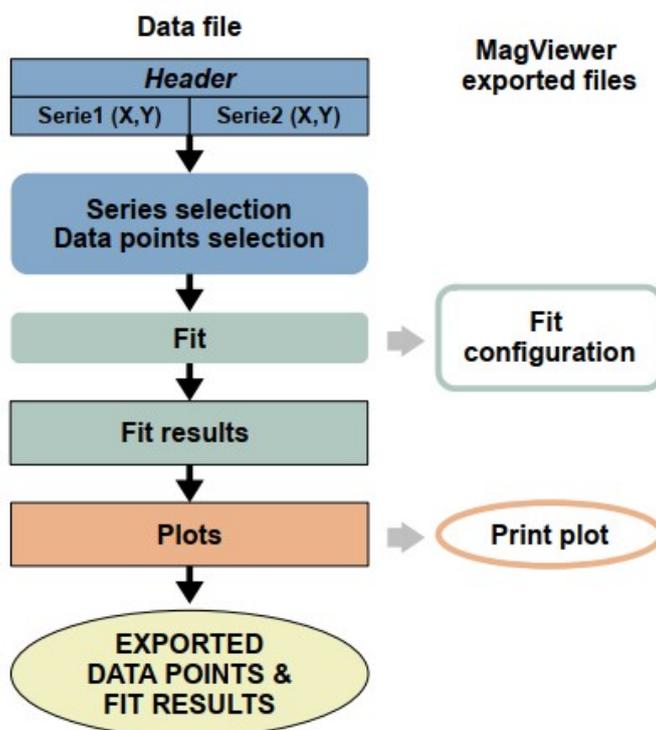
- an average width of the distribution in relaxation times

$$\alpha_{average} = \alpha_1 = \alpha_2$$

"2Relax (v1,v2,k1,k2,k0,a1)" fit configuration

VI- MagFitter

VI.A- Principle of the application

MagFitter is a simpler version of MagFitterCC, to fit a single curve.

VI.B- Getting started

In the menu bar, at the top of the window, you can find:

- "**...**" button to open the data file.

- "**Configuration**" button to manage fit configurations.

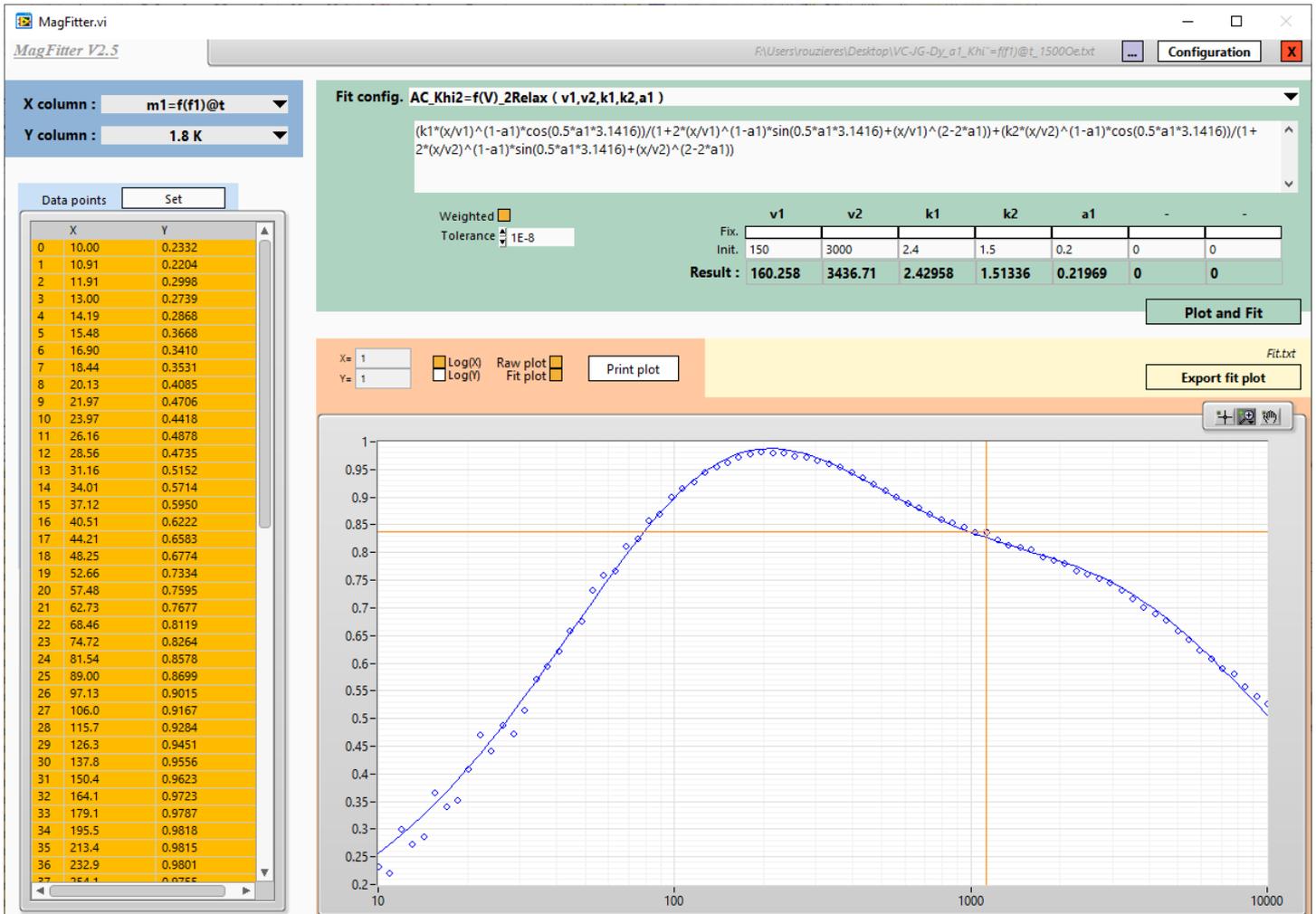- "**X**" button to close the application.

In the main part of the window, you can find from top left to bottom right:

- "X column" and "Y column" selector

You can select the series to plot.

Data point values in the "**Data points**" table, will be updated.

To disable some data points, unselect the corresponding lines in the "**Data points**" table and click on "**Set**" button.

- The plot and fit section

You can set the **fit configuration**. You can modify the fit parameters:

   Modify the formula if needed.

   Set the tolerance.

   Use wheighted values with values with "**Weighted**" checkbox.

   Set initial values with the "**Init.**" table.

   Fix initial values with the "**Fix.**" checkboxes.

Click on "**Plot and fit**" button to calculate the fit and plot the result.

Fit results are displayed in the table just below the "**Init.**" table.

You can mange plots to display with "**Raw plot'**" and "**Fit plot**" checkboxes.

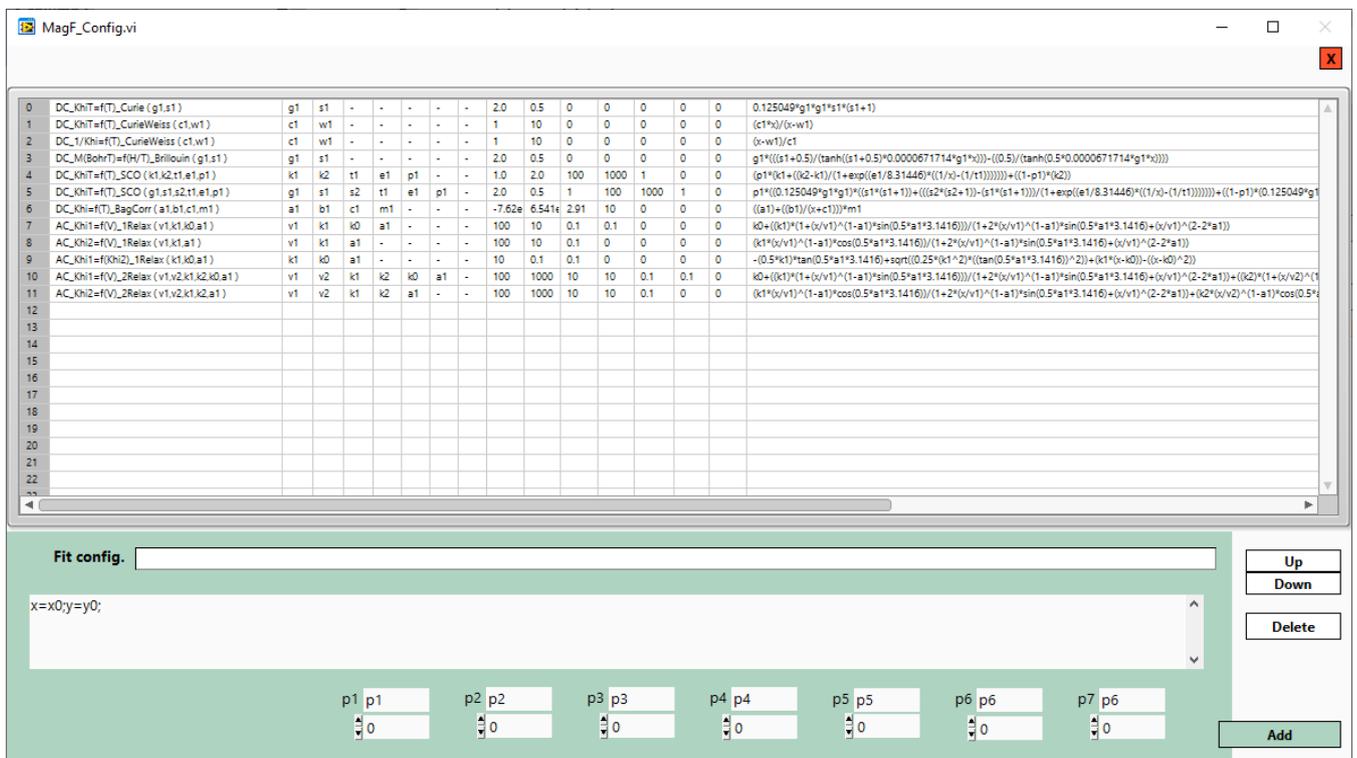"**X=**" and "**Y=**" indicators show values of the cursor.

"**LogX**" and "**LogY**" enable/disable the specific scales.

The "**Print plot**" button copy the image of the plot. You can paste it directly in a ".doc" file for example.

The "**Export fit plot**" button export plot with fit results in a ASCII file.

VI.C-   Configurations

You can edit / add / delete fit formulae from the configuration window.

Conventions used for variables are described in the chapter "MagFitterCC / *Data treatment / Fit variables*".

Syntax is based on the LabView formula node syntax.
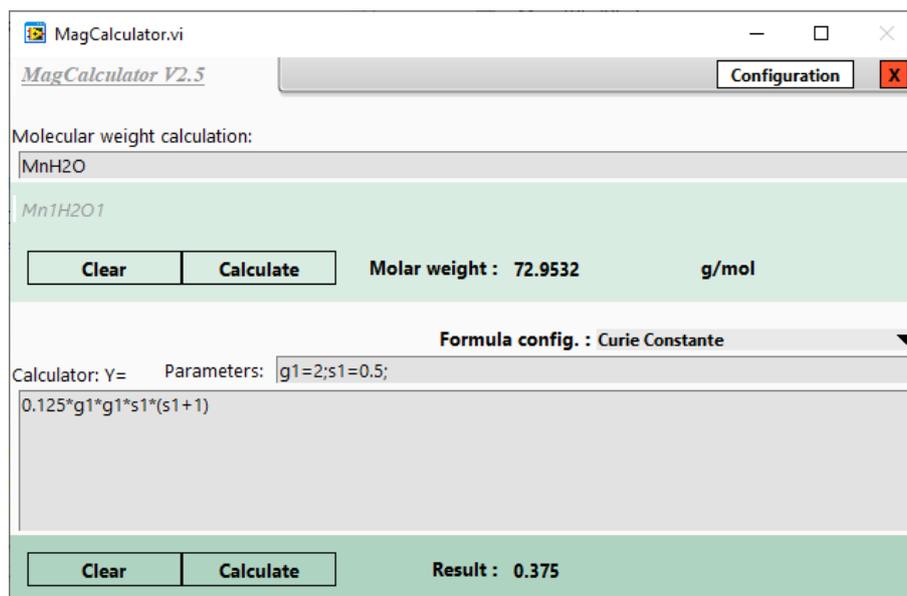
You can refer to:

https://zone.ni.com/reference/en-XX/help/371361R-01/lvhowto/formula_node_syntax/

VII- MagCalculator

This application is a calculator with specific tools useful when you treat magnetic data.

The top part is dedicated to molar weight calculations, and the lower part to formula calculations.

VII.A- Getting started

In the menu bar, at the top of the window, you can find:

- **"X"** button to close the application.

- **"Configuration"** button to manage calculator configurations.

In the "**Molecular weight calculation**" section:

You can copy-paste in the input text box the text of the formula you want to calculate.

- For element specifiers only the first letter has to be a capital character.

- Number of elements has to be set after the element specifier.

When you click on "**Calculate**" button, the formula taken into account is indicated (that should be the same as the input formula if everything is fine).
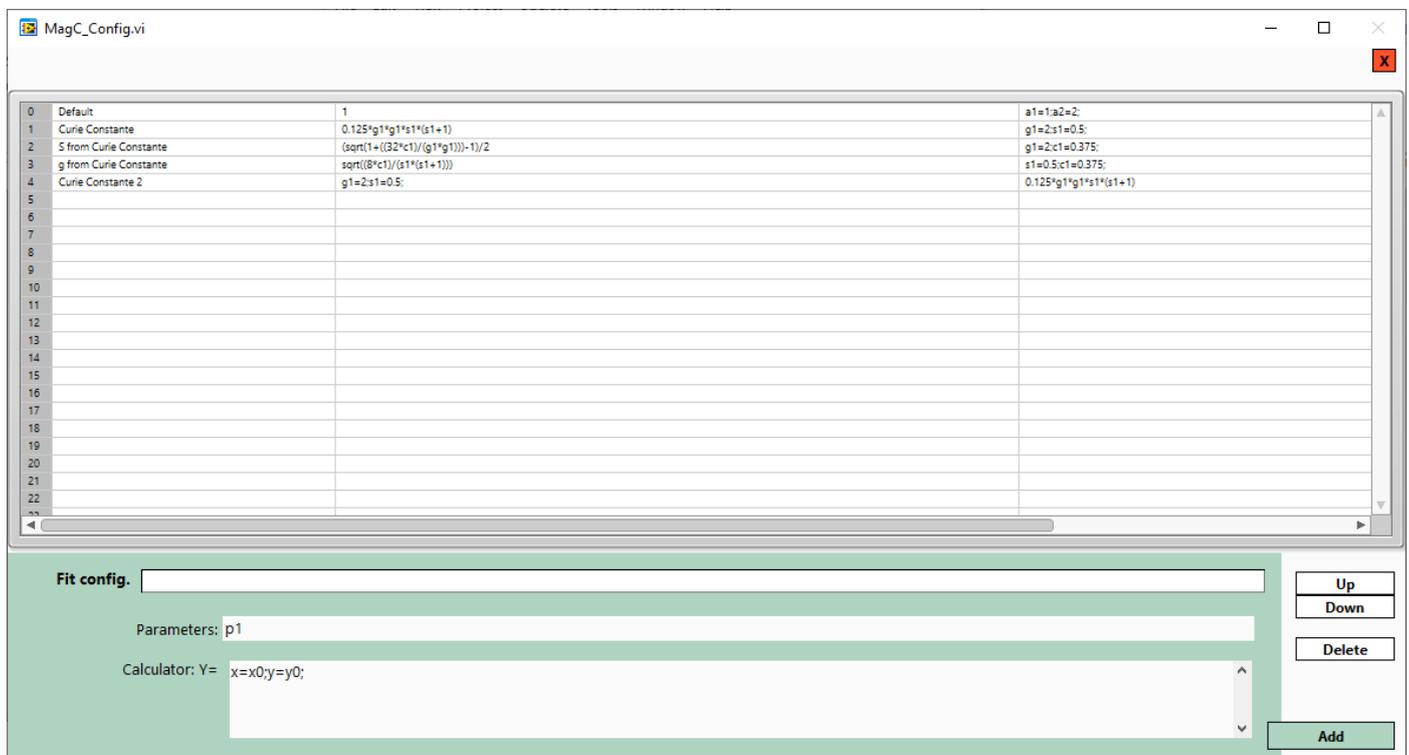
In the "**Calculator: Y=**" section:

You can select existing formula configurations to set specific formula and parameters with the "**Formula config.**" list.

You can manually modify the formula ("**Calculator:Y=**" text box) and the parameters ("**Parameters:**" text box).

VII.B- Configurations

You can edit / add / delete calculator formulae from the configuration window.

Syntax is based on the LabView formula node syntax.

You can refer to:

https://zone.ni.com/reference/en-XX/help/371361R-01/lvhowto/formula_node_syntax/