QCM Analyzer Version 0.3 User's Guide

August 2015, Lubos Brieda, https://www.particleincell.com

1. About

"QCM Analyzer" is an HTML/Javascript program for analyzing and postprocessing QCM log files. This version supports QCM Research and CrystalTek files. Key features include:

- Computation of frequency rates using central difference
- Automatic calculation of delta-deltas
- Ability to perform TGA and support for reference curves
- Removal of multiple headers and joining of appended datasets
- Shifting of comments from new lines to the last column
- Graphical user interface with dual X/Y axis and zooming

2. Requirements

The analyzer runs within a web-browser and has been tested in Mozilla Firefox, Google Chrome, and Internet Explorer. As Internet Explorer does not support resizable elements, it is recommended that you use either Firefox or Chrome to run it.

3. Tutorial

If the code was delivered as "qcm_analyzer.txt", start by renaming the file to "qcm_analyzer.html". Double click the file to open it. If IE is your default browser, right click and select Open With, Mozilla Firefox or Google Chrome. You should see a window similar to Figure 1.

Axis X1: range: Y1: range: X2: range:	0 2553.6 0	QCM Ana : 49.58 : 16660.24 : 1	dx: 5 , dx: 5 , dy: 140 , dx: 0.1	(v0.3)	T R		Drop blank	the i area	input a belo	file	e into	the
Y2: range: Channels	-12247	: 7106.45	, dy:190			< >				_		

Figure 1. Blank startup window

Next, drag and drop "M2000.log" into the empty white area. It will turn yellow during the drag.

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Figure 2. Drag and drop the QCM log file to load it

You should next see the view shown below in Figure 3. The analyzer loaded multiple channels from the log file, and frequency for the first channel is being shown. Each dataset contains several options controlling the graphing output. The first two check boxes control whether the line and/or markers are shown. The X1/X2 and Y1/Y2 radio buttons control which axis to use for plotting. The final colored button allows you to change the default color.

The axis properties are controlled using the top set of input boxes. The buttons at the end of each axes allow you to rescale the axis automatically based on range of all data sets plotted on that particular axes. You can also to use the "view undo" button to return to the previous view.



Figure 3.QCM analyzer showing frequency

Also note that a link to download "output.txt" appeared in the top right corner. Click the link, and you will get an option to save the postprocessed data. This file contains the loaded data, but with multiple appended datasets joined together, comments moved to a separate column, frequency rate set from central difference, and delta-delta computed as shown below. This file can be opened with Excel for additional analysis.

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🥁 output.txt	
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from: data:	
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95	4/4/2015 21:50	96	20	0	2418.67	0.48	59.04	2944.24							
96	4/4/2015 21:51	97	20.01	0	2418.83	0.45	67.83	2943.47							
97	4/4/2015 21:52	98	19.58	0	2424.36	10.63	78.36	2940.71							
<mark>98</mark>	4/4/2015 21:53	99	18.59	0	2425.36	0.06	89.82	2935.97							
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101	4/4/2015 21:56	102	15.56	0	2429.83	0.62	141.93	2909.78							
102	4/4/2015 21:57	103	14.55	0	2431.56	1.68	154.92	2897.08							
103	4/4/2015 21:58	104	13.55	0	2433.68	2.21	171.96	2882.38							
104	4/4/2015 21:59	105	12.55	0	2435.84	-2.26	205.72	2865.7							
105	4/4/2015 22:00	106	11.54	0	2439.04	5.86	248.75	2847.03							
106	4/4/2015 22:01	107	10.55	0	2442.84	4.41	300.86	2826.37							
107	4/4/2015 22:02	108	9.55	0	2447.44	4.88	363.64	2803.72	6370.2 0	hange shr	oud temp	to 60C, MG	SE to 20C,	TQCM to -20	0
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109	4/4/2015 22:04	110	7.54	0	2460	6.4	516.36	2752.45							
110	4/4/2015 22:05	111	6.54	0	2468.49	9.74	607.32	2723.83							
111	4/4/2015 22:06	112	5.54	0	2478.86	18.25	705.81	2693.22							
112	4/4/2015 22:07	113	4.56	0	2490.37	13.23	813.26	2660.62							
113	4/4/2015 22:08	114	3.57	0	2505.13	20.41	927.62	2626.04							
114	4/4/2015 22:09	115	2.56	0	2520.57	19.69	1049.46	2589.46							
115	4/4/2015 22:10	116	1.56	0	2539.02	21.18	1176.88	2550.9							
116	4/4/2015 22:11	117	0.57	0	2559.25	21.5	1306.59	2510.34							
447	4/4/2015 22:12	440	0.44	0	2502.02	22.41	1400 50	0467.0							

Figure 5. The post-processed data can be opened in Excel. Note that comments are moved to a new column

Next, we take a look at frequency rate. Click the check boxes for both "line" and "markers", and also select "Y2". Next, use the vertical rescale button next to Y2 axes to rescale the data. Since this will yield some very negative values, type in a more reasonable minimum range (like 0) into the "min" box. Also set the spacing to 500.

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Figure 6. Comparison of frequency and frequency rate

We next take a look at "delta delta". In the plot below, the delta-delta is plotted on Y2 and rate is now on Y1.



Figure 7. The analyzer automatically computes delta deltas

The figure below shows delta deltas for the four channels present in this data file, showing the rates saw by the four QCMs track each other really well.



Figure 8. Comparison of delta-deltas from four QCMs

4. <u>TGA</u>

The analyzer also allows you to compute TGA. Reload the analyzer by pressing F5. Next drag and drop "M2000-tga.log". Frequency and crystal temperature for this data file is shown below.



Figure 9. Frequency and temperature from "M2000-tga.log" file

Notice the TGA performed around hour 40. Use the mouse to highlight the region between 40 and 46. Double click in the highlighted yellow box to zoom in.



Figure 10. Use the mouse to highlight the region of interest. Then double click to zoom in.

The figure below shows the zoomed in view. You can always easily return to the default view by clicking the rescale button next to X1 axis or return to previous view using the "undo" button.

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Figure 11. Zoomed in view after double clicking.

Next, highlight the first TGA (the region corresponding to the linearly increasing temperature). Then click the "T" button.



Figure 12. Highlight the first TGA and click the "T" button

Clicking the "T" button will generate a TGA plot. The "X" axis is the temperature and the "Y" axis the derivative of frequency in respect to temperature. The "X" button can be used to close this plot.

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Figure 13. TGA plot

Also note that a new link to save "tga.txt" appeared in the top corner. You can use this to save the TGA data, and load into Excel. Also, note that the TGA is computed for the first channel with "frequency" plotted either as a line or markers.



Figure 14.tga.txt data loaded into Excel

The analyzer also supports reference TGA curves. Highlight the second bakeoff, and click the "R" button. The TGA plot is automatically updated by subtracting this reference curve. By comparing the plot below to Figure 16, you may notice some slight differences.

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Figure 15. Select the second TGA and press "R" button to subtract the reference curve

The TGA calculation and reference curves subtraction can also be performed using the keyboard alone. To do this, set the "X1" range to span the TGA. Then press the "T" button. Next, set the "X1" range to cover the reference curve. Press the "R" button to subtract the reference curve.



Figure 16. TGA curve with reference curve subtracted out

5. Delta Delta Calculation

This section briefly discusses how the code computes delta deltas. This section uses screen-shots from an earlier version of the analyzer. Since a typical QCM collection contains numerous crystal bake offs, it's first necessary to remove these. The code does this automatically by looking for times when the crystal temperature is increasing. The figure below shows the correlation between the frequency rate and the crystal temperature rate.



Figure 17. Comparison of frequency rates and crystal temperature. The correlation between the two is clearly visible.

The temperature rate is used to "binarize" the data, by marking time ranges when QCM was sampling (1) and when it was being baked off (0). This is shown in Figure 18.

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QCM Analyzer
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Figure 18. Automatic determination of times when QCM collection was active

Next, the code picks up frequency rates at 15 minute interval in the "sampling" blocks and fits a cubic spline to the points. The end points of each block are also collected. The fitted cubic is shown below in green.



Figure 19. Cubic spline fit to frequency rates at 15 minute intervals in the "sampling" regions

Since frequency rate is now approximated by a piece-wise analytical function, delta delta can now be obtained from the first derivative.



Figure 20. Derivative of the cubic spline gives the delta-delta

6. <u>Revision List</u>

version 0.3, added the following features, 8/19/2015

- fixed background text highlighting in chrome when dragging mouse to select zoom area
- performing TGA and TGA-R using the keyboard alone using "T" and "R" buttons

- changed elapsed time in output.txt from minutes to hours per user request
- fixed resize handle not showing up in Chrome. Learned that Chrome does not allow shrinking. Also changed the default size to 600x400 since IE does not support resizing
- TGA limits are "niced" to the nearest 10 and 1
- added time stamp for start of x data to the xy plot
- fixed TGA plot not reappearing after closing
- added view undo

version 0.2, adding support for CrystalTek QCM, 6/8/2015

version 0.1, initial release, 6/1/2015

- supports QCM research log files
- multiple headers are stripped and data appended
- comments are moved to a new column
- rate is recomputed using central difference
- delta-delta is computed by automatically fitting cubic to non-crystal bakeout data
- tga can be computed by user using user interface
- user interface supports multiple channels, two X and two Y axis
- view can be zoomed in by double clicking selection
- TGA can be computed by pressing T button
- TGA reference curve can be subtracted by pressing R button
- 7. Contact

Questions/Comments/Bug reports/Suggestions?

Email me: lubos.brieda@particleincell.com