Probe Analysis Package for Igor (PAPI) Manual

Vol. 2: SP2 Data

DOC-0251 Revision D-2, PAPI v0.30

DROPLET MEASUREMENT TECHNOLOGIES

2545 Central Avenue
Boulder, CO 80301 USA

2545 CENTRAL AVENUE
BOULDER, COLORADO, USA 80301
TEL: +1 (303) 440-5576
FAX: +1 (303) 440-1965
WWW.DROPLETMEASUREMENT.COM

Trademark Information

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1.0 Introduction

The Probe Analysis Package for Igor (PAPI) is freeware, developed and provided by DMT as a courtesy to customers. This document describes SP2-specific features in PAPI version 0.30. Information on later versions is given in Appendix D, *Release Notes*.

For an overview of PAPI, including how to use it with files generated by the Particle Analysis and Display System (PADS), see Vol. 1 of the PAPI Manual (DOC-0232).

On the most general level, PAPI is used to perform two tasks with SP2 data: calibration and analysis. Instructions for these steps appear in section 2.0 and section 4.0. Since both calibration and analysis involve many steps, users are advised to save their Igor experiment (.pxp file) frequently. This will ensure that new data files, waves, graphs and so on are easily accessible and do not need to be recreated.

When you open PAPI, you will see a Notebook file with information about fixes and version numbers. Minimize this window as shown below.

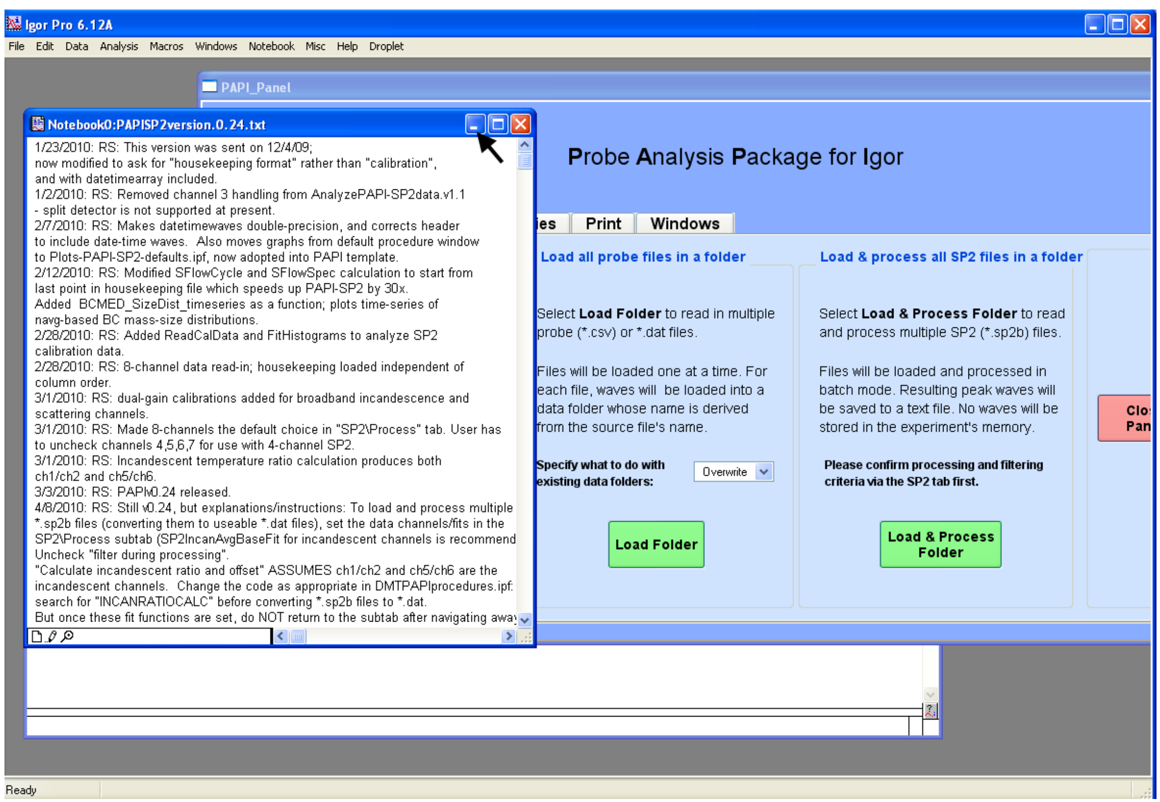


Figure 1: Minimizing the Notebook File

1.1 Requirements for using PAPI for SP2 Calibration and Data Analysis

1.1.1 Hardware Requirements

DMT recommends loading PAPI on a computer with an Intel® Core™ processor or better. If you choose to use an older computer, PAPI may not work.

1.1.2 Data Requirements

To use PAPI successfully, your SP2 data should be in the following format:

- Data files should be in a parent folder named in YYYYMMDD format
- .hk and .ini files should be included
- Raw data files should be in *.sp2b format, which is created with v2.9.5 or later versions of the SP2 data acquisition software, or should be converted from older *.sp2 formats to the newer *.sp2b format using the sp2-to-sp2b utility provided along with the data acquisition software.

For calibration data, you will also need to know the corresponding particle masses or sizes for each file.

1.2 Note on Terminology

While many aspects of working with SP2 data in PAPI are forms of data processing, in this document and in PAPI itself the term "processing" has a more specific meaning. In particular, "processing" refers to reducing the binary-format raw data (.sp2b files) into.dat files, which contain peak heights, peak positions and other useful information.

2.0 SP2 Calibration

2.1 Overview

Calibration should be performed once every six months and before and after every field campaign. There are five basic steps involved in calibrating SP2 data in PAPI (see Figure 2). These are as follows:

1. Preparation:
    a. PAPI processes .sp2b binary data into .dat files

   b. User creates Exptdetail.txt file (this associates each calibration file with a specific PSL/DMA size)
   c. User identifies minimum and maximum values for each channel, to eliminate noise peaks and saturated signals
2. Automated processing of calibration data via the **SP2 → Utilities** tab
3. Manual processing of calibration data (to verify the automated results)
4. Calibration Coefficients entered on the **SP2 → Calculate** tab

These steps are depicted in the flow chart below.

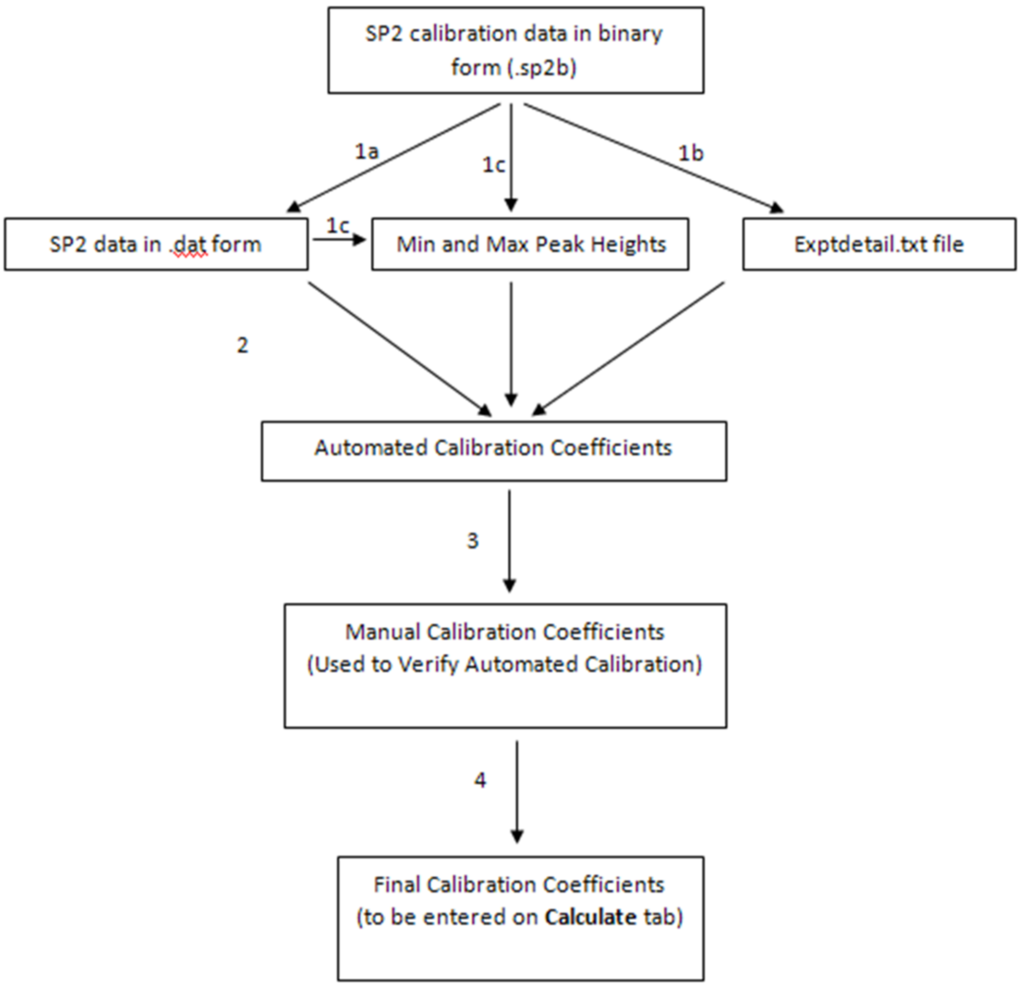


Figure 2: Processing SP2 calibration data

2.1.1 Manual vs. Automated Processing of Calibration Data

In cases where manual curve-fitting results differ from automated curve-fit results, manual results are usually preferred. The automated routine's "Fit Histograms" operation works well for normal distributions, but it is less successful for skewed distributions. In such cases manual curve-fitting allows the user to select only the "good" portion of the distribution and fit the Gaussian to this segment. This allows for more accurate coefficients.

Manual fits are also preferred near the minimum and maximum signal values, i.e. for the smallest and largest PSL/DMA sizes. It is thus particularly important for the user to verify automated curve-fit results in these cases. During the first few calibration sessions, however, it is recommended that SP2 users check the automated routine by manually fitting the histograms for *all* PSL/DMA sizes and comparing the two sets of results. Once the user has determined for which particular PSL/DMA sizes the automated and manual results typically differ, manual curve-fitting can be performed only on these sizes.

2.2 Step-by-Step Instructions

Step 1a: Creating .dat calibration files

This step creates .dat files from .sp2b calibration files. (.sp2b files are raw binary data, whereas .dat files are processed files containing peak-height information.) If you have already created .dat files from the .sp2b calibration files, make sure that all these files are in a folder named in YYYYMMDD format. Also make sure this folder contains .ini and .hk files. Then skip to *Step 1b: Creating Exptdetail.txt file*.

1.) If you do not yet have .dat files, go to the **SP2** → **Process** tab.

2.) In the white center box, check the channels according to your instrument type and the type of calibration being performed (see table below). Figure 3 shows how the screen would look when loading PSL calibration data on a typical eight-channel instrument.

	For PSL Calibration	*For Aquadag Calibration*
four-channel Instrument	Channel 0	Channel 1 Channel 2
eight-channel Instrument	Channel 0 Channel 4	Channel 1 Channel 2 Channel 5 Channel 6

Note: The table assumes a default configuration: Channels 0/4 are the scattering detectors, Channels 1/5 are the broadband incandescence, and Channels 2/6 are narrowband incandescence.

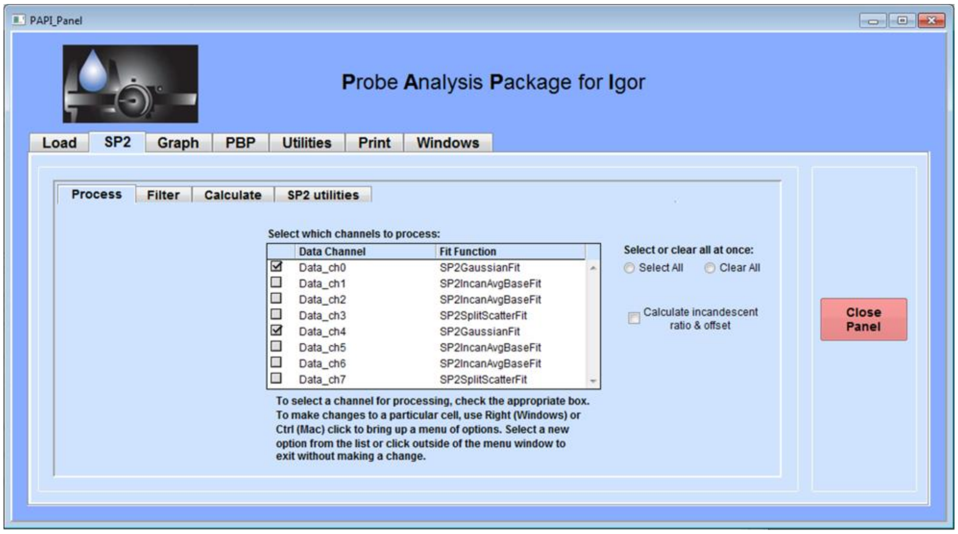
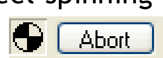


*Figure 3: **SP2→Process** Tab when Processing Calibration Data for a Typical Eight-Channel Instrument*

3.) For PSL calibrations, uncheck **Calculate incandescent ratio and offset.**

4.) Return to the **Load** tab. (Do not go back to the **SP2 → Process** tab, as the settings there will return to the defaults.)

5.) Click on **Load & Process Folder**. Navigate to the folder where your .sp2b calibration files are. Click on **OK** twice. PAPI will ask where you want the .txt file stored; put in the location where you want the processed .dat file. (The original data folder is usually a good choice.) While the files are being loaded and processed, you will see a black-and-white wheel spinning in the lower left corner of the program window that looks like this: 

Processing may take a while. After processing is finished, the program will have created .dat files with the data waves listed in Appendix A.

Step 1b: Creating Exptdetail.txt file

This step creates the Exptdetail.txt file, which PAPI uses during automated curve-fitting of calibration data (see *Step 2: Automated processing…*). The Exptdetail.txt file is simply a text file listing .dat calibration file names and the associated PSL/DMA values for these files. It must be in the format specified below for the automated routine to work properly.

1.) Create a text file named YYYYMMDDExptdetail.txt, where YYYYMMDD is the date of the parent folder (i.e., the date data acquisition occurred). *Note: you can create this file in Excel and save it as a tab-delimited .txt file. If you create it in a program like WordPad or NotePad, make sure that each column is separated by a single tab, not multiple tabs.*

2.) In this text file, make three tab-delimited columns. Label these columns as follows:

Diameter FileStart FileEnd

You can also include additional columns for other variables you want to track. However, the above columns are required, while other columns are ignored.

3.) On a separate row for each PSL/DMA setting, put the mobility (for DMA) or actual (for PSL) diameter in nm, the file start number, and the file end number. E.g., if you have nine calibration files named 20100525x001.dat through 20100525x009.dat, which measure PSL sizes 200-430 nm, your 20100525Exptdetail.txt file might look like this:

Diameter	FileStart	FileEnd
200	1	1
220	2	2
240	3	3
258	4	4
269	5	5
304	6	6
329	7	7
364	8	8
430	9	9

The .dat files and the newly created .txt file should be in a folder named 20100525.

Note that column headings and values may not visually match up if you are using a program like WordPad or NotePad.

Step 1c: Identifying Minimum and Maximum Channel Values

This step identifies minimum and maximum values for each channel, which are used to eliminate noise peaks and saturated signals. The process is identical to the one performed when analyzing ambient data, so it is described in section 3.0. Follow the steps in section 3.0, and then proceed to the steps below to complete the calibration process.

Step 2: Automated processing of calibration data

During automated curve-fitting, PAPI examines calibration .dat files associated with specific PSL/DMA values and calculates the SP2's peak height response in A/D counts for each PSL or DMA value. For the routine to work properly, PAPI must be supplied with an Exptdetail.txt file (created in step 1b) and .dat calibration files. The results of the routine are then used to derive calibration coefficients that are entered into the **SP2 → Calculate** tab.

1.) Navigate to the **SP2 → SP2 Utilities** tab.

2.) Click on **Load Calibration Data.**

3.) Navigate to the folder that contains the .dat files and the YYYYMMDDExptdetail.txt file.

4.) Click **OK** twice.

5.) After PAPI loads the relevant *.dat files, click on the **Fit Histograms** button.

6.) Enter the starting bin value (typically 0), the bin width (6 for eight-channel systems, 4 for four-channel systems), and the number of bins (11000 or 1100 respectively).

7.) Click on **Continue.**

8.) Enter the Minimum and Maximum Peak Heights determined in the previous step. The default value for the peak height fraction is fine. (Igor Pro's Gaussian curve-fitting routine uses this parameter to determine the range over which to fit the Gaussian.)

9.) Click on **Continue.**

10.) When the process is complete, the Igor experiment will have created HistGaussFit_ch#_Cum waves for all relevant channels. HistGaussFit_ch#_cum contains the SP2 response in peak height (A/D counts) corresponding to each PSL size or BC mass.

11.) *For PSL calibrations:* Calculate (or look up from a table, which DMT can supply) the scattering cross-section (Scatter, in cm^2) for each PSL diameter, and plot Scatter vs. SP2_PkHt_ch0. For an eight-channel instrument, also plot Scatter vs. SP2_PkHt_ch4.

For Incandescence calibrations: Convert the mobility diameters to mass, and plot BC mass vs. SP2_PkHt_ch1. For an eight-channel instrument, also plot BC mass vs. SP2_PkHt_ch5.

Step 3: Manual processing of calibration data

Manual processing is used to validate results from the automated processing (*Step* 2). It may not be necessary to manually determine the peak SP2 response at every PSL/DMA size; see section 2.1.1 for a discussion of when to do so.

Manual processing differs from automated processing in that the user selects the portion of the distribution over which to fit the Gaussian curve, after generating and visually inspecting the histogram for that particular PSL size/DMA set point.

A good first step is to copy and rename the wave containing the automated processing results. Then the original automated curve-fit results can be replaced in cases where the manual fit is preferable. The following instructions guide the user through this procedure.

1.) Duplicate the HistGaussFit_ch#_Cum wave and rename it “ManualFit_ch#” by doing the following:

    a. Navigating to **Data → Duplicate Waves** in the IgorPro menu bar
    b. Selecting HistGaussFit_ch#_Cum as the Template
    c. Selecting a data folder
    d. Typing “ManualFit_ch#” under names
    e. Clicking “Do it”

2.) In the Command window, type “Edit ManualFit_ch#” to bring up the newly created wave.

3.) Go to the **PBP→Bin Def** tab. Skip “Create PBP bins.”

4.) Set the bin boundaries by selecting “Calculate bins from parameters,” setting #bins to 1100 and Step size to 4 (for a four-channel instrument) or #bins to 11000 and Step size to 6 (for eight-channel instrument).

5.) Go to the **PBP → Data** tab, expand the data folder for the PSL size/DMA set under consideration, and select the PkHt_Ch# wave to bin[1].

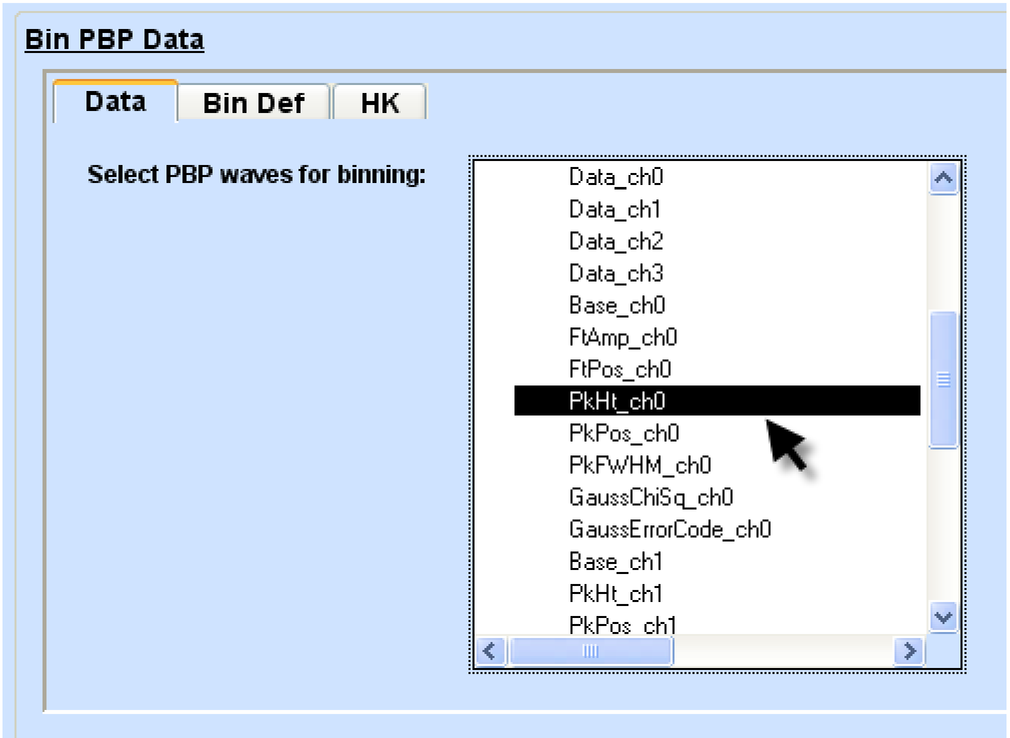


Figure 4: Selecting PkHt_ch# Wave to Bin

6.) Click on "Create 1 Histogram." You should see a graph somewhat similar to the one below.

[1] Typically, if you have PSL data, you will want to look at PkHt_Ch0 (four-channel instrument) or PkHt_Ch0 and PkHt_Ch4 (eight-channel instrument). If you have black carbon data, you will want to look at PkHt_Ch1 (four-channel instrument) or PkHt_Ch1 and PkHt_Ch5 (eight-channel instrument). You will need to create separate histograms and fits for different channels.

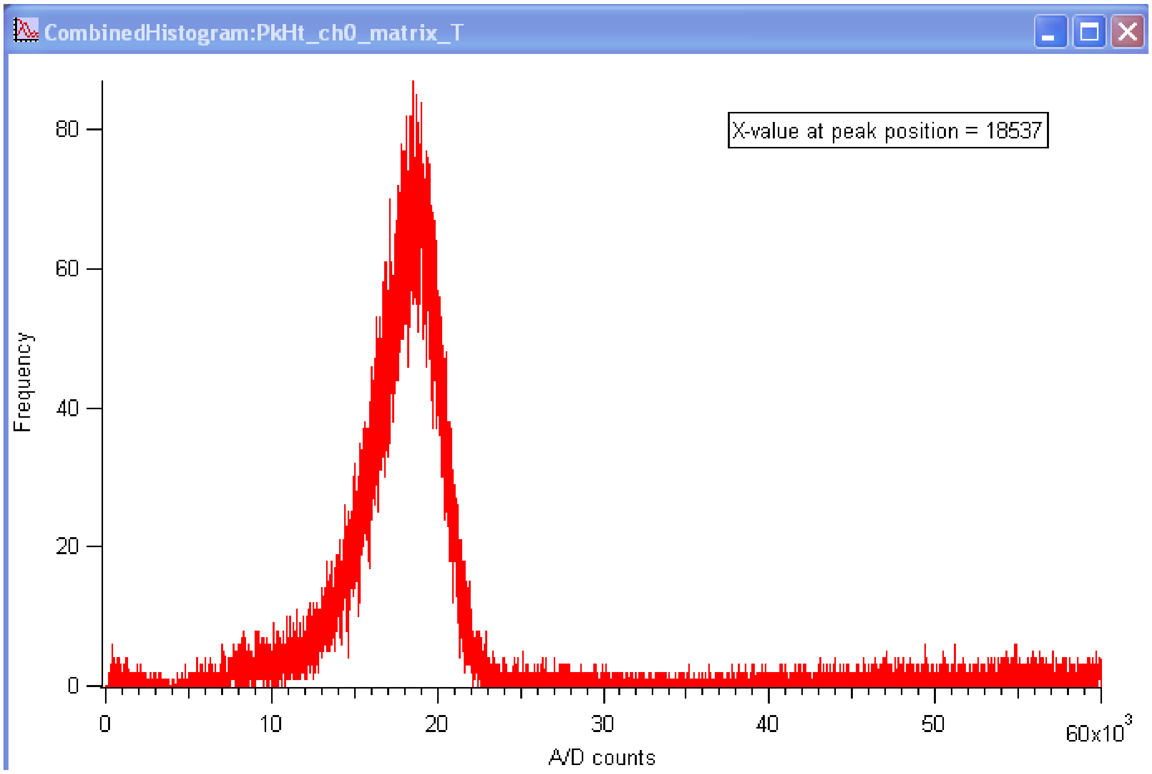


Figure 5: Results of "Create 1 Histogram"

7.) To fit a Gaussian curve to the distribution, do the following (see Figure 6):

a. Drag the A and B cursors at the bottom of the window to the fit points on the curve. Use the largest curve, as any smaller curves to the right are from doubly and triply charged particles (seen with DMA-sizing). In the event of a skewed distribution, use the cursors to select only the best portion of the curve. In Figure 6, for instance, the curve is slightly skewed with a tail to the left of the peak; the cursors omit this section.
b. Right click on the curve.
c. Click on “Quick fit.”
d. Make sure “Fit between cursors” is checked, and Textbox preferences are set to display the fit coefficients (“Display Quick Fit Info Textbox”, “Coefficient Report”, “Values” and “Errors” should all be checked).
e. Click “gauss.”

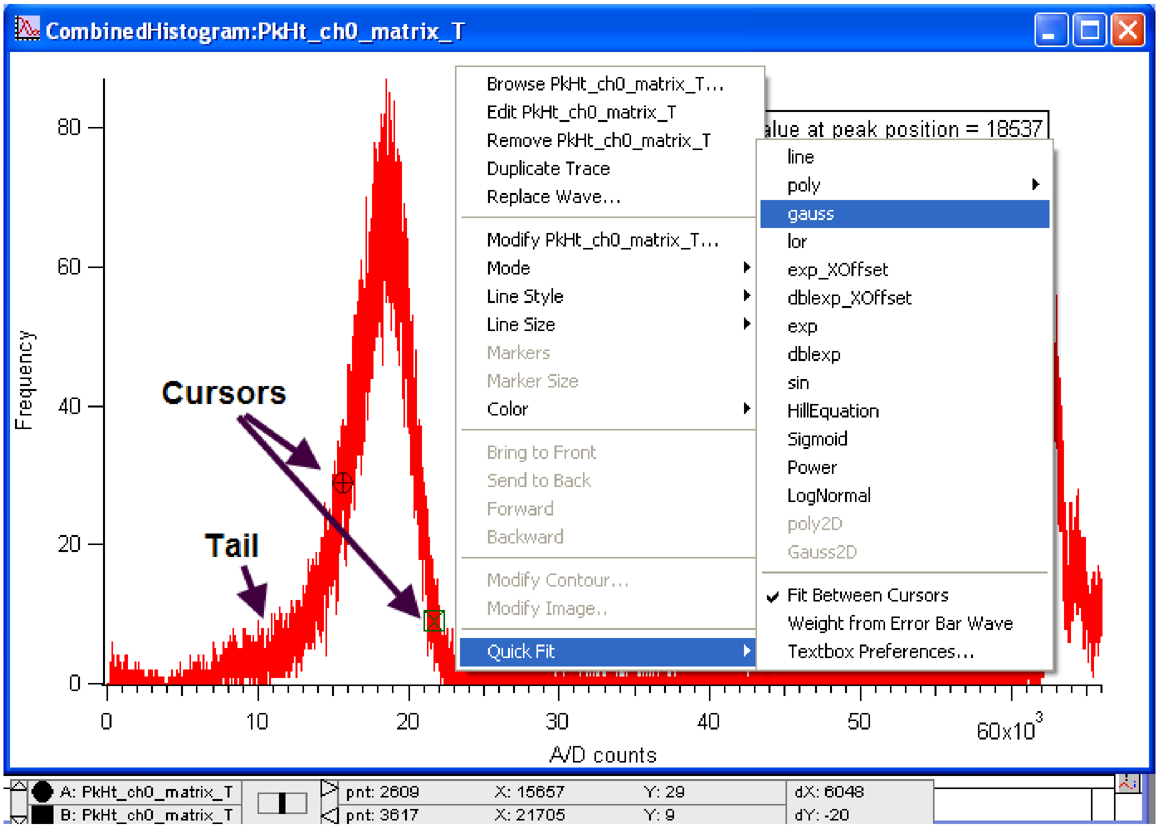


Figure 6: Fitting a Gaussian distribution to the Peak-Height Graph

A Gaussian fit curve will appear, along with the fit coefficients in a textbox on the graph.

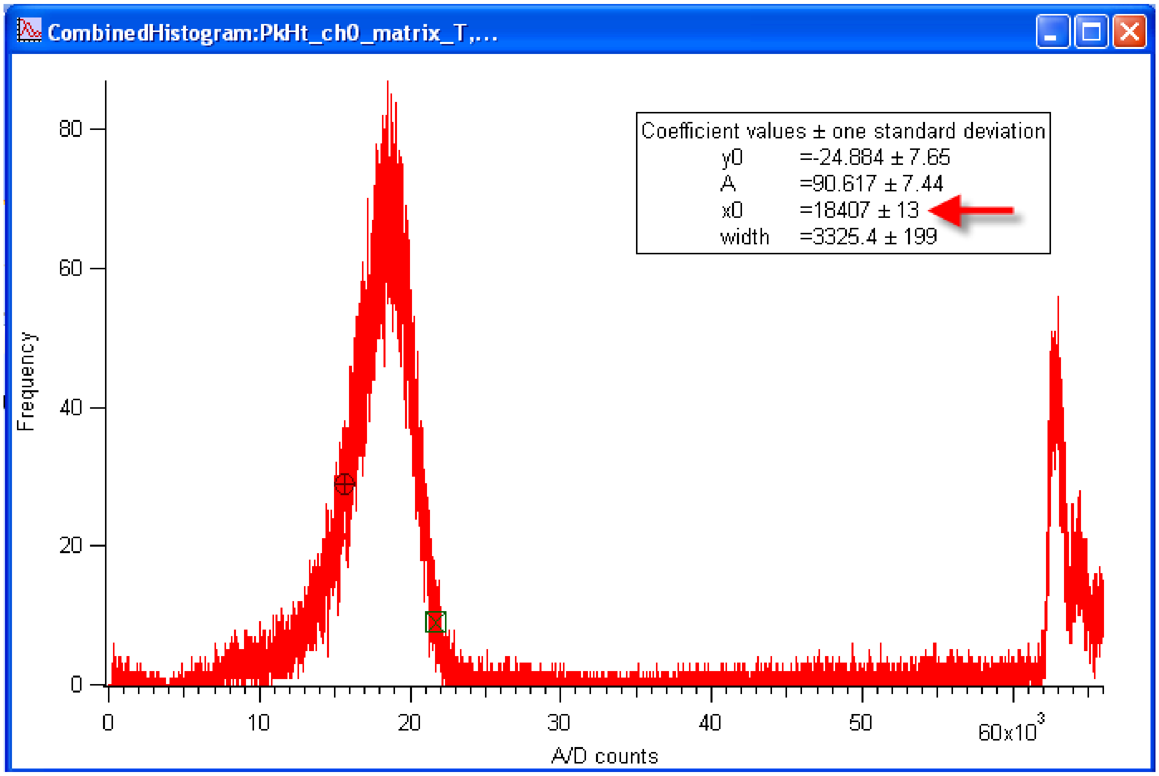


Figure 7: Gaussian Curve with Fit Coefficients

To exactly replicate the PAPI procedure, you may want to repeat this curve-fit while holding y0 = 0 (See Igor instructions on how to do this using the "Analysis\Curve fit" menu.) Alternately, you can copy the "Curvefit…" command from the Igor command window, replace "Curvefit/" with "k0=0;Curvefit/H="1000"/" and re-execute the command.

8.) Check the Gaussian mean (x0) value (see arrow in above figure) against the automated fit result for that particular PSL size or BC mass.

9.) Replace the automated fit results with the manual fit results if the latter are significantly different. (You can view and edit the ManualFit_ch# wave by typing "Edit ManualFit_ch#" in the Command window.) *Note:* The automated fit generally produces good results for values that are not too close to the noise or saturation values; manual fitting usually produces better results in these extreme cases.

10.) Repeat the above steps for as many different particle sizes or masses as you have. You will end up with a table of x0 values (Gaussian means) for each PSL diameter (or BC mass).

11.) Calculate (or look up from a table, which DMT can supply) the expected scattering cross-section (Scatter, in cm^2) for each PSL diameter, and plot Scatter vs. ManualFit_ch0 (or ch4). For calibration of the incandescence channel, this plot should be the BC mass (determined from the mobility diameter and a known or assumed mobility density) vs. ManualFit_ch1 (or PkHt_ch5).

12.) Fit the curves. The calibrations should normally have a zero-intercept, and the high-gain channels are expected to give a linear fit. The low-gain channels cover a wider range of scattering cross-section (or BC mass), and so a quadratic (2^{nd}-order) fit may be required.

Step 4: Inserting Calibration Coefficients

1.) Navigate to the **SP2 → Calculate** tab.

2.) Insert the new calibration coefficients, obtained from the curve-fits in *Step 3(12)* above.

Note: For four-channel systems, all coefficients should be inserted in the High-gain rows.

3.0 Identifying Minimum and Maximum Peak Height Values

Both SP2 calibration and data analysis require the user to identify minimum and maximum peak height values for SP2 channels. Signals below the minimum are assumed to be noise; signals above the maximum have saturated the detector, and hence are not reliable indicators of particle mass or size.

To identify minimum and maximum peak heights, follow the steps below. It is assumed that you already have processed .dat files at this point. If you do not, follow the instructions outlined in section 2.2 (step 1a).

1.) Load two or three .dat files using the **Load Folder** button on the **Load** tab. ***Note:*** If you have a lot of .dat files, you can move a small subset of them to a temporary folder so that you load only these selected files).

2.) Go to the **PBP → Bin Def** tab.

3.) Set bins by doing one of the following:

a. Use "Automatically Calculate Bins" and set number of bins, e.g. 1,000 for a four-channel instrument or 10,000 bins for an eight-channel instrument

b. Use "Calculate bins from parameters," setting #bins to 1100 and Step size to 4 (for a four-channel instrument) or #bins to 11,000 and Step size to 6 (for eight-channel instrument).

4.) Go back to **PBP → Data** tab and select PkHt_Ch0 (or PkHt_Ch1 for incandescence channel data). You may need to expand the folder to see the available waves. See the figures below.

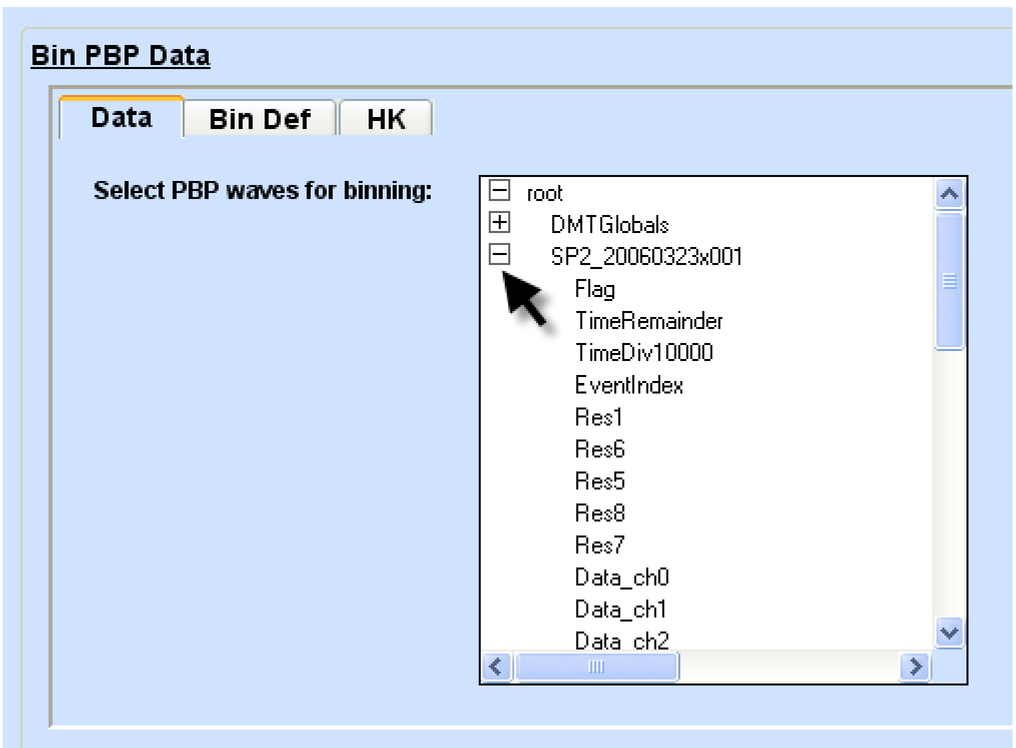


Figure 8: Expanding a Folder

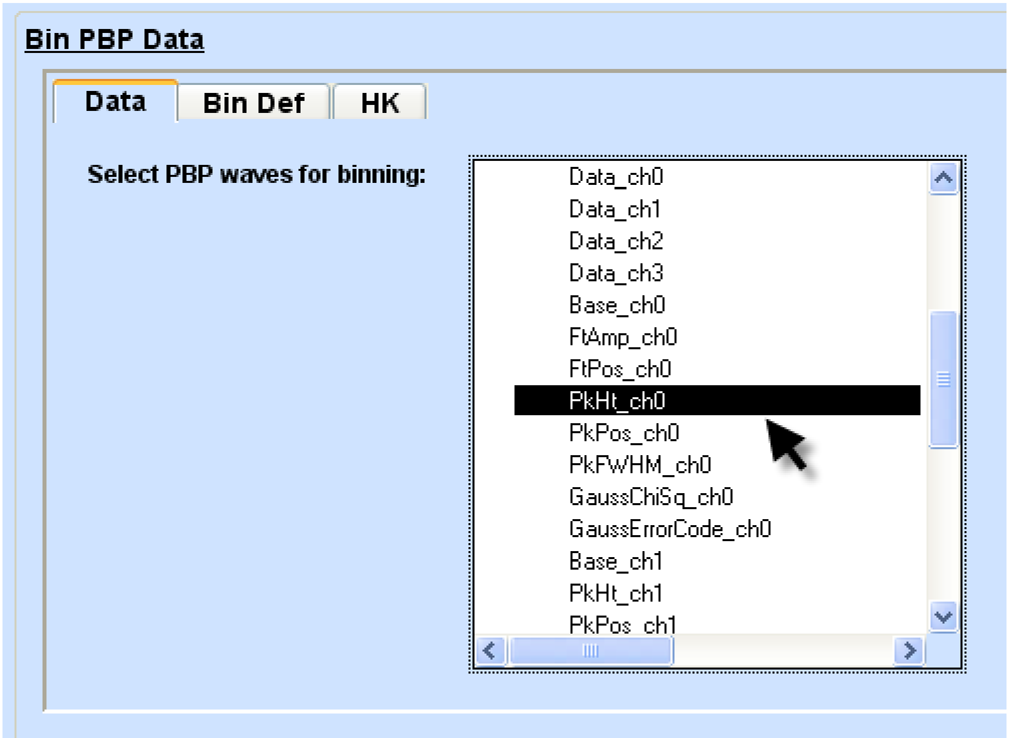


Figure 9: Selecting a Wave for Binning

Using Ctrl-click, select PkHt_Ch0 from all the files you have loaded. Keep the relevant folders expanded during this process, as collapsing them deselects all their waves.

5.) Click on “Create 1 Histogram.” You should see a graph.

6.) Zoom in on the area where the minimum peak value should fall. For instruments with a 0-4096 A/D range (usually four channels), zoom in on the 0-100 range. For instruments with a 0-65536 range (usually eight channels), zoom in on the 0-1000 A/D range. To zoom, draw a marquee around the area of interest, right-click, and select “Expand.”

7.) You should see a small signal peak in this section of the data. Set the minimum at the very end of this peak. E.g., for the figure below, an acceptable minimum would be around 4000.

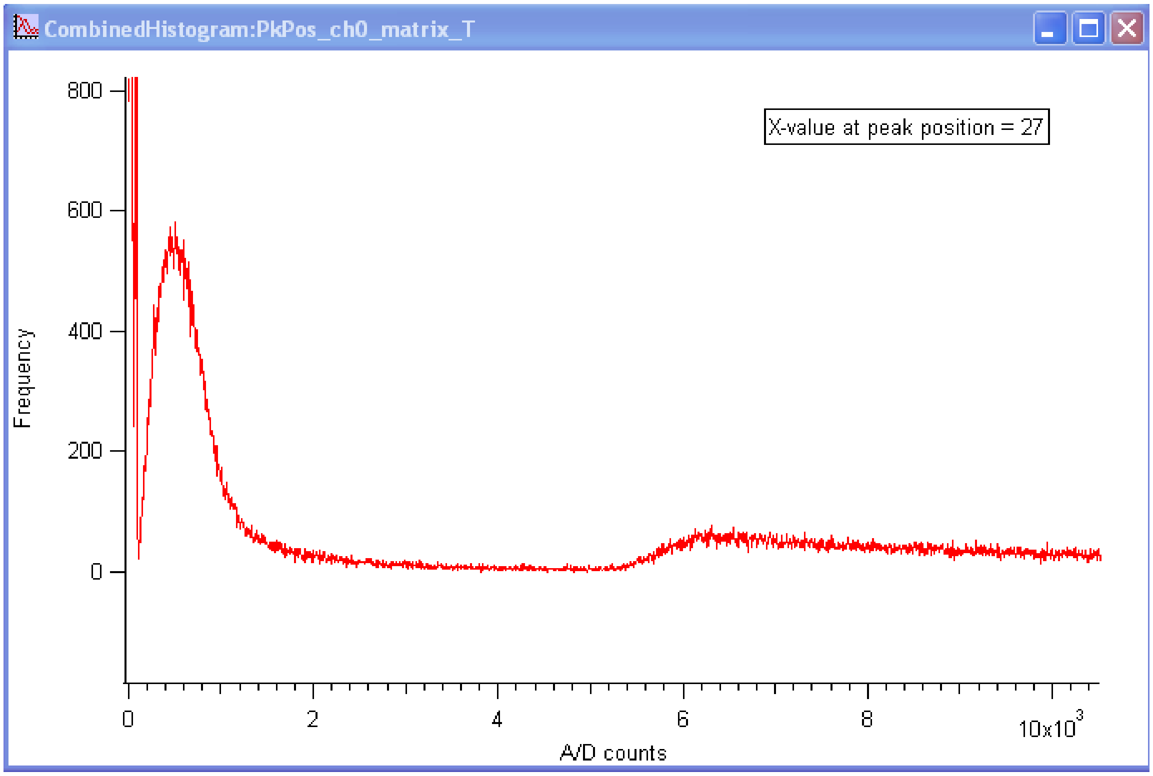


Figure 10: Identifying a Minimum Peak Height

8.) Bring up the full-scale graph again by right-clicking and selecting "Autoscale Axes."

9.) Zoom in on the area where the maximum peak value should fall. For instruments with a 0-4096 A/D range (usually four channels), zoom in on the 3500-4000 range. For instruments with a 0-65536 range (usually eight channels), zoom in on the 60,000-65,000 A/D range. To zoom, draw a marquee around the area of interest, right-click, and select "Expand."

10.) You should see a small signal peak in this section of the data. Set the minimum at the beginning of or just before this peak. E.g., in the figure below, a good minimum would be 62,000 A/D counts. If you do not see a peak, it may be that the saturation limit has not been reached, in which case a safe value of 60,000 can be used (4000 for four-channel SP2s). The particle-by-particle data can be examined to verify this (see steps below).

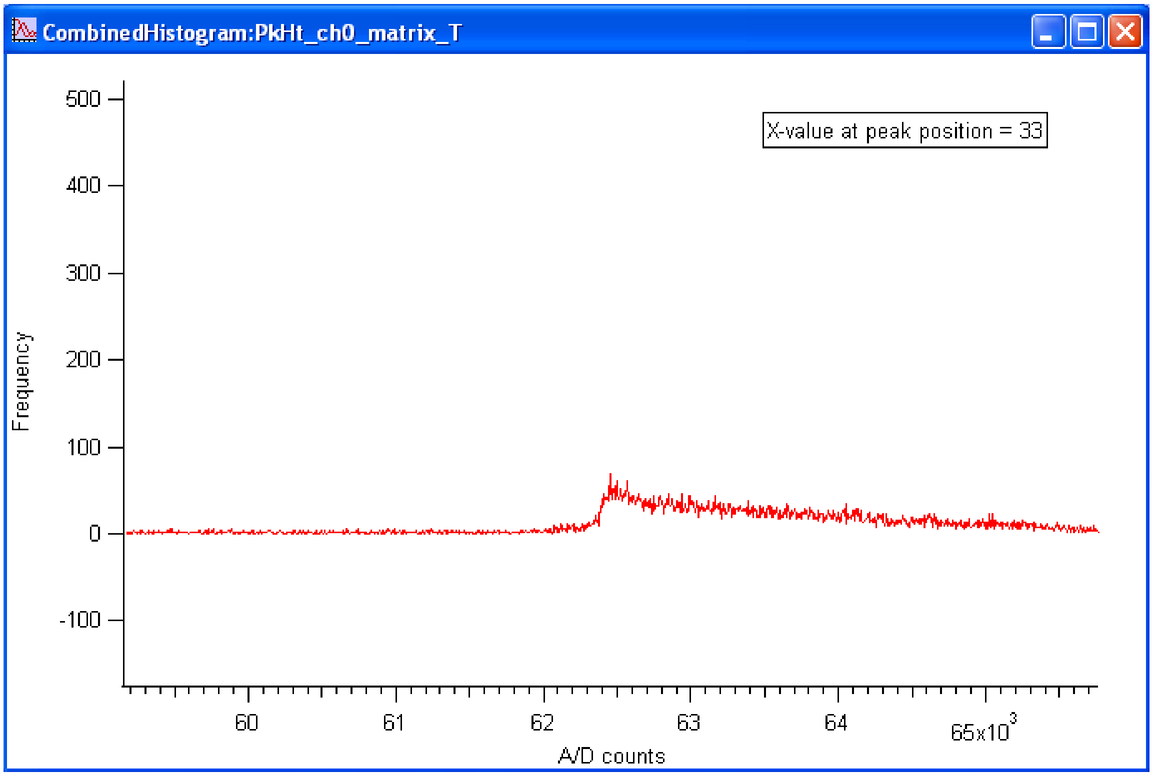


Figure 11: Identifying a Maximum Peak Height

11.) Repeat the process above for any remaining channels for which you want to identify filtering criteria.

12.) If you do not see clear choices for minimum and maximum peak heights, you should be able to identify a noise baseline (the minimum) and saturation level (the maximum) using the original .sp2b files and the SP2 Data Reader. (See *DOC-0092 SP2 Software Manual* for details on how to use the SP2 Data Reader.) Note that the scale of the A/D counts may shift between PAPI and the Data Reader, i.e., the Reader uses a scale from -32768 to 32768, while the peak heights in the *.dat files are baseline-corrected to a range of 0-65536 counts. Saturated particles have flat tops to their signal curves, and the **Saturation** box is checked. The figure below shows the Data Reader displaying information about a Saturated particle. This figure would suggest a scattering (Ch0) peak-height maximum of about 62,000. This value is obtained by zooming in to check the baseline and the value at saturation, and then subtracting the baseline from the saturation.

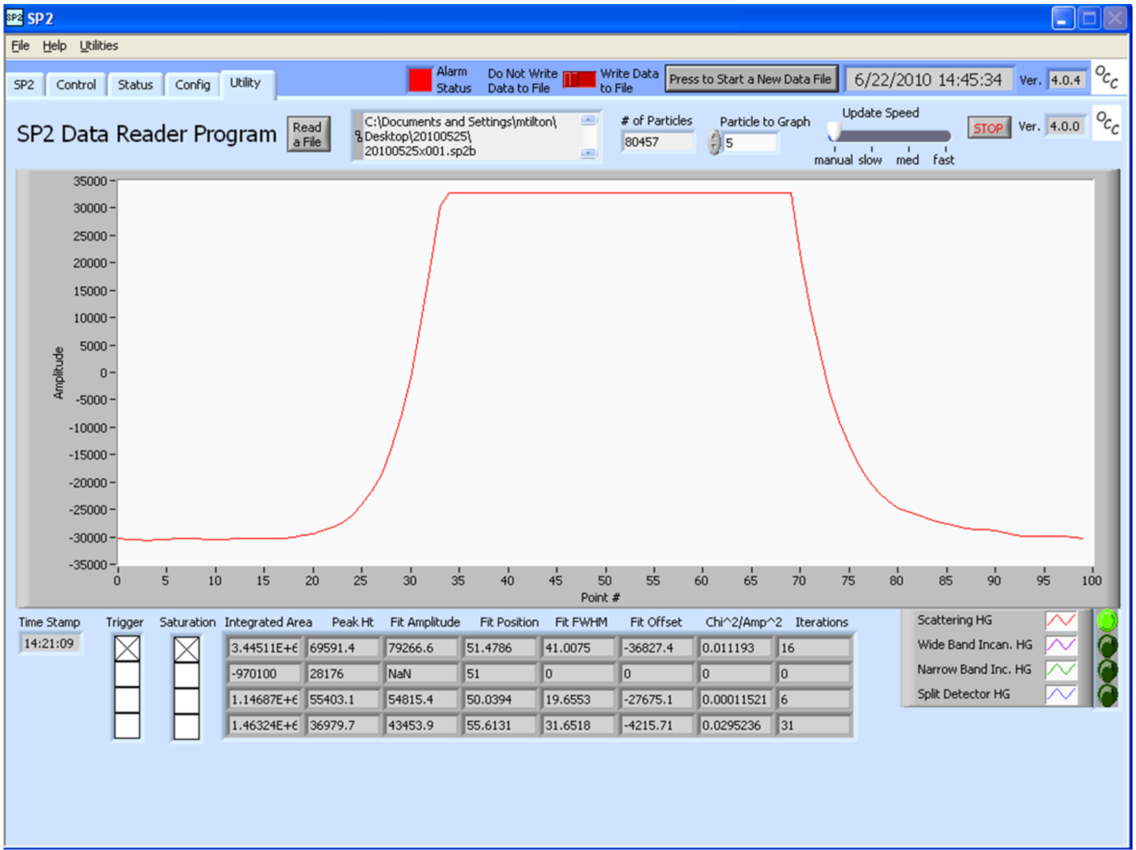


Figure 12: Using the SP2 Data Reader to Identify a Minimum and Maximum

13.) If minimum and maximum peak heights are still unclear, the system default values can be used for instruments with a 0 – 65536 A/D range (usually eight-channel systems). For systems with a 0 – 4096 A/D range (usually four-channel systems), the following defaults can be used:

	Min Peak Ht	Max Peak Ht
Ch0	20	4000
Ch1	10	4000
Ch2	10	4000

14.) The minimum and maximum peak heights can now be used in two ways:

- Entered into PAPI during automated processing of calibration data, as described in section 2.2
- Entered in on the **SP2 → Filter** tab for use during data analysis, as described in section 4.2.

4.0 Analyzing Ambient Data

4.1 Overview

There are four basic steps involved in processing and analyzing SP2 data in PAPI (see flow chart). These are as follows:

1.) Reducing the binary *.sp2b files to *.dat files
2.) Setting filters to remove noise and cases where the detector has been saturated
3.) Analyzing the data to determine BC mass and number concentrations, BC number fraction, and ensemble BC and scattering particle-size distributions
4.) Graphing the data

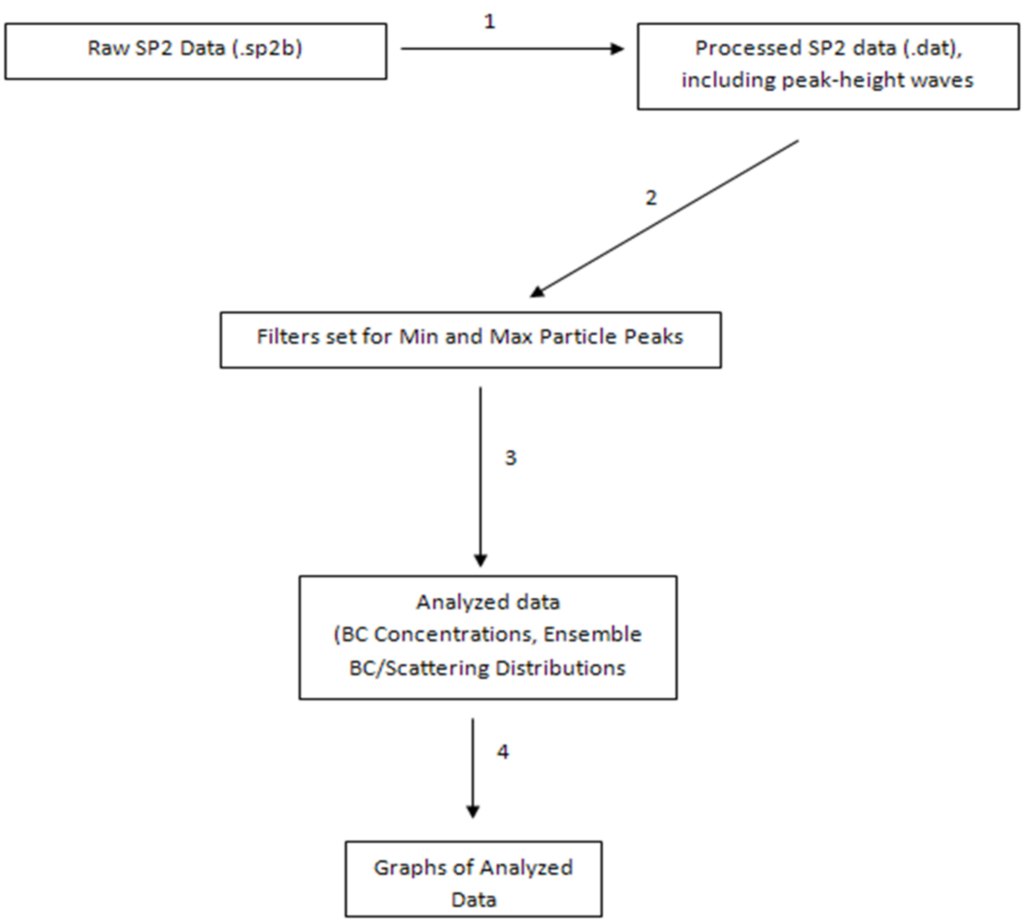


Figure 13: Analyzing Ambient SP2 Data in PAPI

4.2 Step-by-Step Instructions

Step 1: Loading and Processing .sp2b Files

This step creates .dat files from .sp2b calibration files. (.sp2b files are raw binary data, whereas .dat files are processed files containing peak-height information.) If you have already converted the .sp2b files to .dat files, load the .dat files using the **Load Folder** button and skip to *Step 2: Identifying Filters for Minimum and Maximum Peak Heights*. (Remember to include .hk files in the folder being loaded.) If you do not yet have .dat files, proceed with the steps below.

1.) Open PAPI and go to the **SP2 → Process** tab. If you have a four-channel Sp2, uncheck Data_ch4 through Data_ch7. See the figure below for an example with a standard eight-channel instrument. Make sure the "Calculate incandescent ratio & offset" box is checked.

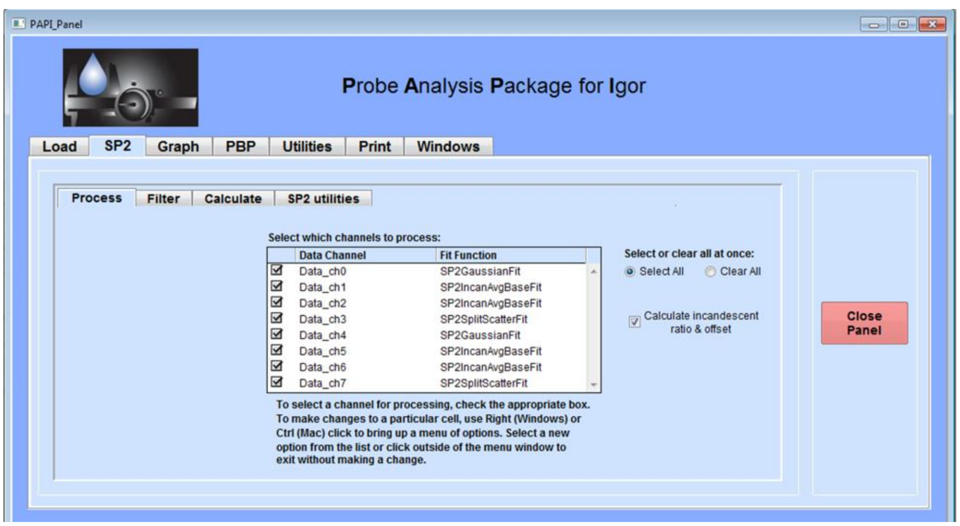
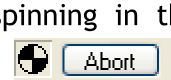


*Figure 14: **SP2→Process** Tab for a Typical Eight-Channel Instrument When Loading Ambient Data*

2.) Return to the **Load** tab.

3.) Click on **Load & Process Folder**. Navigate to the folder where your .sp2b files are. Click on **OK** twice. PAPI will ask where you want the .txt file stored; put in the location where you want the processed .dat file. (The original data folder is usually a good choice.) While the files are being loaded and processed, you will see a black-and-white wheel spinning in the lower left corner of the program window that looks like this: 

After processing is finished,

the program will have created .dat files with the data waves listed in Appendix A. Note that these files are not stored in PAPI memory, as they may be quite large.

Step 2: Identifying Filters for Minimum and Maximum Peak Heights

This step identifies minimum and maximum values for each channel, which are used to eliminate noise peaks and saturated signals. The process is identical to the one performed when calibrating the SP2, so it is described in section 3.0. Follow the steps in section 3.0, and then proceed with the instructions below.

1.) Go to the **SP2 → Filter** tab.

2.) Enter the minimum and maximum values for channels 0-2 in the **Min Peak Ht** and **Max Peak Ht** columns. (Typically, you will not set filters for Channel 3 or set filters other than those listed in these two columns.)

3.) Check the checkboxes next to Channels 0-2. Make sure the checkbox next to Channel 3 is unchecked, as is the checkbox for Channels 1 & 2 under "Specify filtering parameters (additional incandescent)." See the figure below.

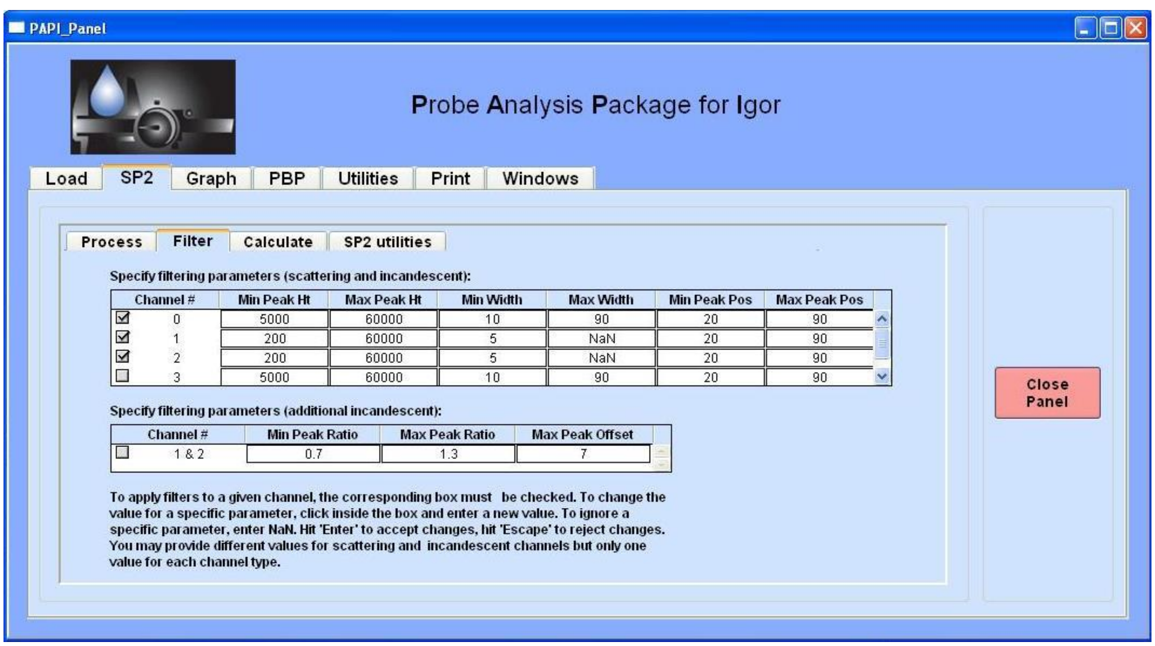


Figure 15: Setting Minimum and Maximum Filters

Step 3: Analyzing Data

This step analyzes the ambient data files to determine BC mass and number concentrations, BC number fraction, and ensemble BC and scattering particle-size distributions. The results are stored in two new .dat files, OutputWaves.dat and SizeDist.dat.

The Igor experiment contains more information than is written out in these two files, and can also be used to plot the output without reloading the data or repeating the experiment. Thus it is highly recommended that the Igor experiment be saved as a .pxp file.

1.) Go to the **SP2 → Calculate** sub-tab

2.) Click **Analyze Data.**

3.) The system will prompt you for an SP2 data folder (where the .dat files are). It will then ask you to enter the following information:

    a. The averaging interval in seconds for mass and number concentrations
    b. The averaging interval in seconds for spectra (i.e., time-resolved size distributions)
    c. The bin widths for spectra in micrometers

    The defaults should usually suffice.

4.) The history window will show the results of the data analysis. There will now be two new .dat files in the folder, YYYYMMDDOutputWaves.dat and YYYYMMDDSizeDist.dat. The waves in these files are listed in Appendix B. These waves are also stored in the Igor experiment, in addition to other output waves not stored to disk.

5.) To view the waves in the OutputWaves.dat and SizeDist.dat files in tabular form, you have several options:

    a. Open up the files in a spreadsheet program like Excel.
    b. Type “Edit [Wave Name]” in the PAPI Command Window.

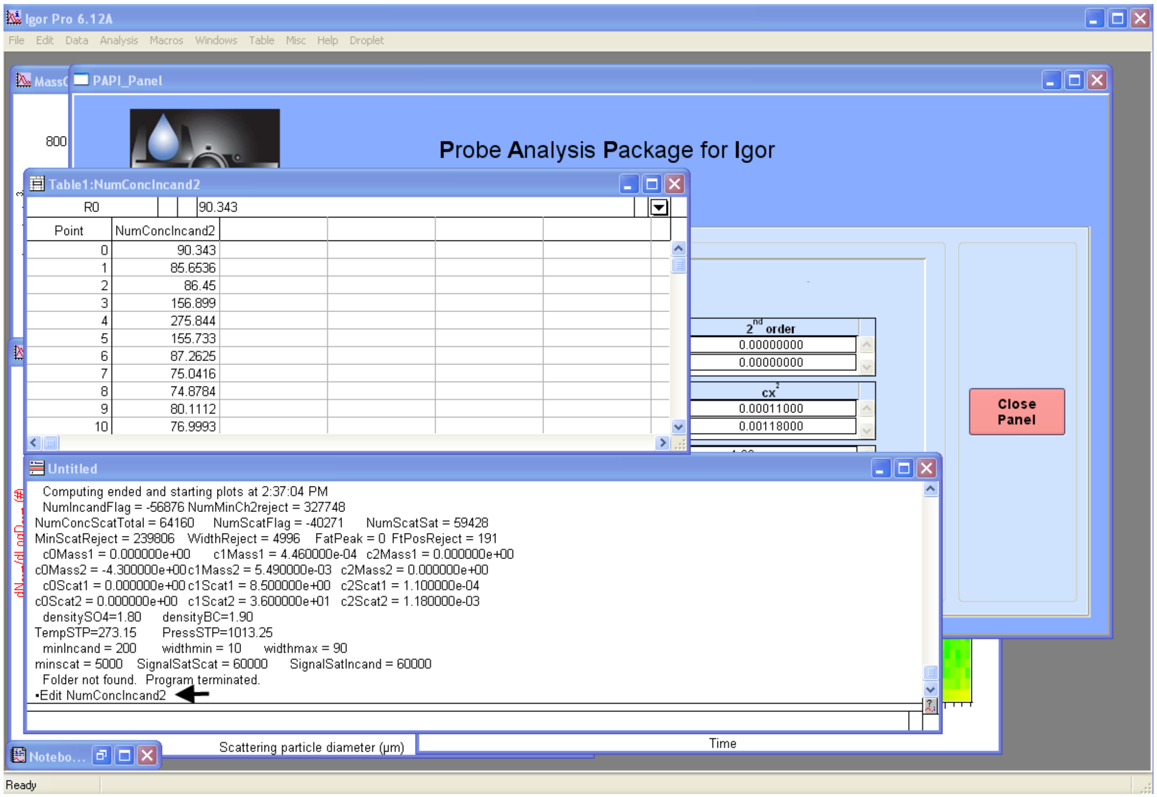


Figure 16: Viewing New Wave Data

Step 4: Graphing Analyzed Data

This step graphs the waves calculated in Step 3. To save these graphs, save your PAPI experiment as a .pxp file.

1.) Go to the **Graph** tab.
2.) Click on **Plot Analyzed Data**.

You will see graphs like those shown below. Note that you may have to minimize some windows to see all graphs.

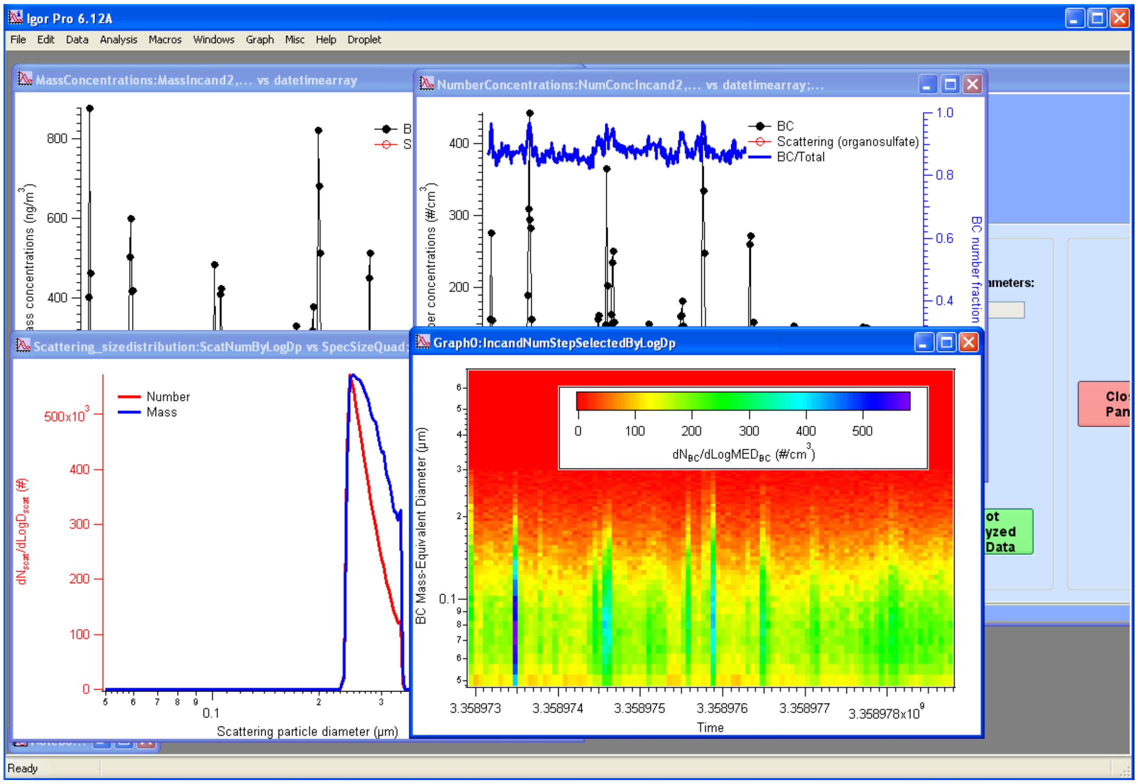


Figure 17: Plotting Analyzed Data

5.0 Loading Already-Processed *.dat Files

Already-processed files will be in *.dat form. These can be loaded using the **Load Folder** button on the **Load** tab. There are several common and easily surmountable errors that can occur during this process; see section 7.1.

6.0 Other Features of the SP2 Tab

6.1 Process Tab

6.1.1 Calculate Incandescent Ratio & Offset

If this checkbox is checked, PAPI will generate IncanPkOffsetch1ch2 and IncanRatioch1ch2 waves during processing. For eight-channel instruments, it will also calculate IncanPkOffsetch5ch6 and IncanRatioch5ch6. This step should be considered mandatory for ambient data and for incandescent channel calibrations, so this checkbox should always be checked in these cases.

6.1.2 Process Spectra Button (obsolete)

This button is rarely used. In the event that the user loads .sp2b files individually using the **Load File** button, clicking on **Process Spectra** will generate the same additional waves that are typically stored in .dat files. However, using **Load File** and **Process Spectra** does not store these waves except in PAPI memory, so a better choice is to use **Load & Process Folder** to process .sp2b files. This creates .dat files that can be quickly loaded for future analysis.
Note: This button has been removed as of PAPI-SP2 v0.30.

6.2 Filter Tab

6.2.1 Specify Filtering Parameters – Additional Incandescent

This feature can be used after preliminary filters have been identified and applied. Contact DMT for details.

6.2.2 Filter Data Button (on Filter Tab) (obsolete)

This button should not be used. Filters are applied automatically when the **Analyze Data** button is clicked.
Note: This button has been removed as of PAPI-SP2 v0.30.

7.0 Frequently Asked Questions

7.1 Loading Data

Why are there three load buttons?

They all serve different functions. **Load Folder** and **Load & Process Folder** are the options commonly used with the SP2. **Load & Process Folder** allows you to load and process a lot of .sp2b files automatically. This converts them to .dat files. **Load Folder** is useful for loading pre-processed *.dat files, since loading and processing .sp2b files takes a long time.

Load File is used mostly with other instruments and is not recommended for use with the SP2. Loading .sp2b files with this button requires you to process the files with the

Process Spectra button, and the resulting waves are stored only in PAPI memory, not in .dat files.

On **SP2 → Utilities** tab is yet another load button: **Load Calibration Data.** Clicking on this button allows the user to specify .dat calibration files and a YYYYMMDD.Exptdetail.txt file that can then be used to determine Gaussian fits for the calibration files. See step 2 in section 2.2 for details.

Why does the Load & Process Data command not keep .sp2b and .dat files in PAPI memory?

Since .sp2b files are very large, it is inefficient and often impossible to story many of them in RAM. Likewise, it does not make sense to store many processed .dat files in RAM unless there is a need to do so. PAPI can work faster by running operations ("Analyze Data," e.g.) by loading *.dat or *.sp2b files one at a time. Thus the **Load & Process** command does not store files in memory.

7.2 Processing and Filtering

What is the difference between processing and analyzing data?

"Processing" refers to converting raw .sp2b binary files to .dat files. "Analyzing" refers to determining variables like black carbon mass and number concentrations after filtering outlier particle events. (Outlier particle events include cases where noise triggered an event, or where a detector was saturated and its signal cannot be used to accurately assess particle characteristics.)

How do I change the fit function when I am processing data?

On the **SP2 → Process** tab, you can select what type of fit you would like for each channel to be processed by right-clicking on the Fit Function value. The default fits should suffice in most cases, however. A full description of fit functions appears in Appendix C.

I'm trying to find a peak-height maximum filter. What should I do if I suspect the saturation peak isn't appearing on my histogram?

Try expanding the x-axis range by increasing the step size by 1 or increasing the bin# by 20%. Both of these settings are on the **PBP → BinDef** tab.

Are there any default data filters I can use?

It is best to determine filters based on your particular data. However, if you want to use generic defaults, you might be able to do so. See section 3.0 for more information, and contact DMT with specific questions

What are the different ways to apply filters?

Filters are applied in several ways. During automated processing of calibration data, PAPI will prompt you to enter minimum and maximum peak-height filters. During analysis, when you click on **Analyze Data** (on the **SP2 → Calculate** tab), filters will be applied during the data analysis based on the parameters entered on the **SP2 → Filter** tab. In both of these cases, filters are applied to pre-existing .dat files. In addition, during the initial conversion of raw *.sp2b files to *.dat files, the filters on the **SP2 → Filter** tab are applied to the data, and two "key" waves, "ScatRejectKey" and "IncanRejectKey" are generated. At present, however, these key waves are not used in post-processing of the *.dat files, and so are not considered further in this manual.

7.3 Common Error Messages and What to Do About Them

Errors during Loading .dat Files

1.) "DateTimeWave could not be created for housekeeping data because date information was missing"

This message frequently appears when you load calibration .dat files, and in such cases does not affect the loading process. If you are comfortable programming in Igor and want to remove the error message, go to **Windows** (in the Igor Pro Menu Bar) → Procedure Windows → DMTPAPIProcedures.ipf. Search on "DateTimeWave could not be created." You will see a line that says

```
printf "DateTimeWave could not be created for housekeeping data because date information was missing for %s\r", LoadFileName
```

Commentize this line (by inserting "//" in front of it), click "compile," and resume data loading.

2.) "Configuration data was not loaded for [Filename]! No corresponding configuration data files were found."

Click OK. This message frequently appears when you load calibration .dat files, and in such cases does not affect the loading process. The system will generate the error message again each time a .dat file is encountered without a corresponding .ini file, and you will need to click OK in each case.

3.) "Identify instrument for YYYYMMDDOutputWaves.dat" (or "for YYYYMMDDSizeDist.dat") along with a drop-down list of instruments that does not include the SP2.

This prompt commonly occurs when you try to load a folder of .dat files after you have performed an "Analyze Data" operation. In theory this sequence should not happen; the only time you need to load .dat files is to identify filters, which presumably have been set by the time the Analyze Data button is clicked. However, there are easy ways around the problem: simply move YYYYMMDDOutputWaves.dat and YYYYMMDDSizeDist.dat to a temporary folder.

Errors during Analyze Data (SP2→ Calculate Tab)

There are reasons why the **Analyze Data** command may not work. If the system did not load .hk files along with the *.dat or *.sp2b files, it will not be able to calculate flow and hence will not be able to perform concentration calculations. To fix this issue, reload files from a folder with .hk files included. Another possible issue is that you are using data generated with an older version of the SP2 software, which isn't compatible with PAPI. Make sure your files were generated with SP2 data acquisition software version 4 or later. (Processing of files generated with v2.9.5 and earlier need some modifications to PAPI-SP2; contact DMT for details).

Appendix A: Waves Created During Processing (when .sp2b files become .dat files)

If date information was successfully obtained from the .sp2b file, PAPI generates two additional time waves, **DateTimeWaveUTC and DateTimeWave**, that include date information in addition to time in seconds. Additionally, corresponding SP2 configuration (.ini) files are automatically loaded as a text wave with the name **ConfigTextW**. If more than one configuration file is found for a given SP2 file, the contents of each .ini file are concatenated into a single text wave. Finally, corresponding housekeeping (.hk) data files are automatically loaded into a subfolder of the SP2 data folder with the name **HK**. Names for housekeeping waves are taken from column names. If duplicate wave names are encountered, PAPI automatically generates new names by adding a unique numerical suffix to subsequent occurrences of the name. If more than one .hk file is found for a given SP2 file, the data from subsequent files is appended to the appropriate existing waves.

When PAPI loads SP2 data from a LabView binary file (.sp2b), a 2D wave of individual particle spectra is generated for each data channel.

When PAPI converts *.sp2b files to *.dat (reduced) form, the following columns are produced:

TimeWave	The time-stamp in seconds past midnight
DateTimeWaveUTC	UTC date and time in seconds past midnight on January 1, 1904
DateTimeWave	Local* date and time in seconds past midnight on January 1, 1904
Base_ch1	Baseline of the particle spectrum
PkHt_ch1	Peak height of the spectrum, after correcting for the baseline
PkPos_ch1	Location of the actual peak height (in 0.2 μs divisions)
PkStart_ch1	Start of the spectrum (signal rises above the baseline), in 0.2 μs divisions
PkEnd_ch1	End of the spectrum (signal falls below the baseline), in 0.2 μs divisions
PkHalfRise_ch1	Position of the half-peak, on the rising side
PkHalfDecay_ch1	Position of the half-peak, on the falling side
IncanRatioch5ch6	Incandescent temperature ratio**, Channel 5/Channel 6 (low-gain)
IncanPkOffsetch5ch6	PkPos_ch5 - PkPos_ch6
IncanRatioch1ch2	For Ch1/Ch2***
IncanPkOffsetch1ch2	For Ch1/Ch2
Base_ch0	The baseline (y0) calculated by fitting a Gaussian curve to the data.
FtAmp_ch0	The baseline-corrected peak amplitude of the Gaussian curve fitted to Gaussian signals
FtPos_ch0	The position of the Gaussian fit amplitude
PkHt_ch0	The actual baseline-corrected peak height of the event spectrum.

PkPos_ch0	Location of the actual peak height
PkFWHM_ch0	The Gaussian FWHM
GaussChiSq_ch0	Gaussian fit parameter
GaussErrorCode_ch0	Gaussian fit parameter

***** Caution: The DateTimeWave values can sometimes be wrong, especially when the "Restart files at midnight" option is not used during data acquisition.

** The incandescent temperature ratio is calculated by (1) calculating the ratio of Channel 5/Channel 6 at each 0.2 µs location starting at PkPos_ch5, all the way to PkHalfDecay_ch5; and (2) averaging these ratios.

*** For Ch1Ch2, the same method applies as for Ch5Ch6.

Appendix B: Waves Created During "Analyze Data" Operation

In YYYYMMDDOutputWaves.dat:

Start time: The start time in seconds.
End time: The end time in seconds.
Start DateTime: The start time (UTC) in seconds since midnight of January 1, 1904.
End DateTime: The end time (UTC) in seconds since midnight of January 1, 1904.
Scattering conc (#/cm3-STP): Scattering number concentration at standard temperature and pressure.
Incandescent Conc (#/cm3-STP): Incandescent number concentration at standard temperature and pressure.
Scattering mass conc (ng/m3-STP): Scattering mass concentration at standard temperature and pressure.
Total scattering mass conc (ng/m3-STP): The total* scattering mass concentration at standard temperature and pressure.
Incandescent mass conc (ng/m3-STP): Incandescent mass concentration at standard temperature and pressure.
Total incandescent mass conc (ng/m3-STP): The total* incandescent mass concentration at standard temperature and pressure.

"Total" concentrations include saturated particles, with the mass assumed as the value corresponding to the saturation peak height. By definition, this would be an underestimate of the true particle mass.

In YYYYMMDDSizeDist.dat:

SpecSizeQuad: The mid-point of the size bin in microns.
IncandNumByLogDp: The ensemble incandescent number concentration divided by the log of bin width in micrometers.
IncandMassByLogDp: The ensemble incandescent mass concentration divided by the log of the bin width in micrometers.

Appendix C: Fit Function Options (SP2 → Process Tab)

Descriptions for each of the supplied functions that can be used to convert raw SP2 data into peak height, peak width, etc. are found below.

SP2GaussianFit

This function is found in the DMTPAPIProcedures.ipf procedure file contained in DMT_PAPI_ExpTemplate.pxt. The function calls Igor's built-in Gaussian ("gauss") routine to fit a Gaussian curve to the data, mainly to determine the baseline. It generates eight waves containing the fitting results: **Base_ch#, PkHt_ch#, PkPos_ch#, PkFWHM_ch#, FtAmp_ch#, FtPos_ch#, GaussChiSq_ch#**, and **GaussErrorCode_ch#**. Channel number is determined from the data wave's name. **PkHt** is the peak value of the actual data (determined using Igor's WaveStats function (see SP2IncanAvgBaseFit for more information)), while **FtAmp** is the peak amplitude of the fitted Gaussian; both values are baseline-corrected. **PkPos** is the position of the actual data maximum, while **FtPos** is the position of the Gaussian peak amplitude. **FWHM** is full width at half max. This is calculated by the "width" parameter generated by Igor's gauss fitting routine, which is defined as $\sqrt{2} * \sigma$. The **FWHM** is $2*\sqrt{(2*\ln(2))}*\sigma$. This function is recommended for scattering data (usually Ch0).

SP2IncanAvgBaseFit

This function is found in the DMTPAPIProcedures.ipf procedure file contained in DMT_PAPI_ExpTemplate.pxt. The function averages the first 80% of the pre-trigger points to determine a baseline. It then uses that baseline to determine a peak height, peak position, start and end of the signal (useful to determine the peak width), and mid-points of the rise and decay sections of the signal. The number of points to average is determined from the configuration file info that was added to the wave note of the spectra waves (**Data_ch#**) upon loading. If the information cannot be found in the wave note, the default value is set to 20 points. This function generates seven result waves: **Base_ch#, PkHt_ch#, PkPos_ch#, PkStart_ch#, PkEnd_ch#, PkHalfRise_ch#,** and **PkHalfDecay_ch#**. Channel number is determined from the data wave's name. Peak height and peak position are determined by simply using V_max (corrected for the baseline) and V_maxloc results of Igor's WaveStats function. This function is recommended for incandescent data (typically **Ch1** and **Ch2**).

SP2IncandGaussBaseFit

This function is found in the DMTPAPIProcedures.ipf procedure file contained in DMT_PAPI_ExpTemplate.pxt. This is similar to the SP2IncanAvgBaseFit described above, except that this function calls Igor's built-in Gaussian ("gauss") curve-fitting routine to determine the baseline. The output is the same as SP2IncanAvgBaseFit except there is one additional wave, GaussErrorCode_ch#, which keeps track of any errors that may have occurred when applying the Gaussian fit.

SP2SplitScatterFit

This function is found in the DMTPAPIProcedures.ipf procedure file contained in DMT_PAPI_ExpTemplate.pxt, and is a preliminary step for processing the split detector data. The function averages the first 20 points of the event to determine a baseline. It then uses that baseline to determine a peak height, peak position and the split position. This function can be used to ensure the consistency of the gap between the split position and the center of the laser beam after running PSL particles.

User-Defined Processing Fit Functions

Users can generate their own fit functions by altering an existing file as needed. The file must be saved under a unique name that follows the **SP2*Fit** format.

Appendix D: Revision Notes

December 10, 2010: v0.31

1. Lag times included. Also non-LEO coating thickness. Waves generated: (AnalyzePAPI-SP2datav3.1.ipf)
ScatNumBCByLogDp[] = ScatNumEnsembleBC[p]/SpecSizeQuadLog[p]
ScatMassBCByLogDp[] = ScatMassEnsembleBC[p]/SpecSizeQuadLog[p]
Included particles that saturate the scattering detector, as the diameter at scattering.
ThickCoatTime - lag times (also see ThickCoatTimeStepSelected, ThickCoatTimeByLogDp, ThickCoatTimeSSByLogDp)
ThickCoatWidths - coating thickness (also see ThickCoatWidthsSelected, ThickCoatWidthsByLogDp, ThickCoatWidthsSSByLogDp)

2. Incandescent lag time: ScatPos is the mean position of the Gaussian fitted to the scattering signal; IncandPos is the peak position of the incandescent signal. Incandescent time lag = (ScatPos - IncandPos)*0.4, where we assume the NI card samples at 2.5 MHz. (If an older card is used, which samples at 5 MHz, replace 0.4 with 0.2.)

December 23, 2010: v0.32 STARTED - FINISHED November 1, 2011 as v0.35

Final procedure files: DMTPAPIprocedures.v1.2.ipf and AnalyzePAPI-SP2data.v03.5.ipf

1. Added a new SP2GaussianSatFit to replace saturated values with NaN, and fitting a Gaussian to remaining data points. (DMTPAPIprocedures.v1.15.ipf) This is now the default fitting option for Ch4, low-gain scattering.
2. In AnalyzePAPI-SP2data.v3.2.ipf, changed ScatPos and IncandPos to take Ch0 values if low-gain channels do not exist, even if high-gain signal is saturated.
3. Replaced Do-While loop for SpecSizeQuad and SpecSizeQuadImage with single-line Igor operation.
4. Removed unused ambient/chamber temperature/pressure loops, which speeds up processing significantly. SFlowStoreNow (which is saved in SFlowCycleArray) now moved inside SFlowCycleNow loop.
5. SFlowCycleArray now reports flows even if no particles were seen within a given time-step.
6. Quieten LoadWave operation (which loads individual *.dat files), so history is less cluttered.
7. Spectra based on scattering diameter now not limited to non-saturated particles (see #1).
8. Range for incandescent lag times increased to cover -10 to +10.5 microseconds, but coarser - bin widths now 0.5 microseconds.

9. If the number of *.dat files exceeded 999, Igor/Windows did not sort them correctly. Using SortList now fixes this problem, at least on Windows machines. Not tested on Macs (as of 10-18-2011.)
10. Replaced WaveStats with WaveStats/M=1 when calculating the average, max/maxloc, min/minloc (lower moment).
11. PAPI-SP2 now uses the first 300 lines of ConfigTextW to determine the number of pre-trigger points; in other words, only the first *.ini file loaded. (If there are more *.ini files in the folder, they are all concatenated into the ConfigTextW wave.)
12. Fixed: In pre-v0.35 PAPI-SP2, PAPILoadProcessButtonProc did not read-in the *.ini files, hence "Pre-Trig points" could not be found.
13. If "Pre-Trig Points" cannot be found, a default value of numBasePts2AvgBackup = 20 is used, assuming 25 pre-trigger points. If a specific SP2 uses a different number of pre-trigger points but this cannot be read-in by the program for whatever reason, the user can change numBasePts2AvgBackup to ~80% of their pre-trigger points. For example, if Pre-Trigger points = 100 (for 300 points/event), set numBasePts2AvgBackup = 80. (The algorithm uses 80% of the pre-trigger points to determine the baseline in SP2IncanAvgBaseFit; for Pre-trigger points = 25 (100 points/event), numBasePts2Avg = 20.)
14. PAPI-SP2 post-processing ("Analyze Data") now loads (SP2 v4.x-derived) configuration files. This creates three waves, with as many rows as number of INI files: TimeStampSecINI, OneOfEveryINI, OneOfWhatINI - these can be used to correct concentrations.
15. 1-of-N and 1-of-What (1-of-N applied to either scattering (TRUE) or all (FALSE) particles) data recording options now incorporated into PAPI-SP2.
16. Added explanatory notes for different counting variables, to assist the user in determining which filter affects the data set the most.
17. SP2 single-particle spectra graphs (from the Graph tab in PAPI) were hard-wired to 0.2 microseconds/point for the old, 4-channel, 5 MHz sampling PCI-6110 NI data acquisition card. New 8-channel SP2s use the PCI-6133, which samples at 2.5 MHz, so each point is 0.4 microseconds. "ElapsedTime" in DMTPAPIProceduresv1.2.ipf has been changed to default to the new PCI-6133 card times (0.4 microseconds/point.)
18. Note to the user on the SP2 "Filter" tab: The decision whether the peak location ("Peak Pos") should be used as to reject particles is left to the user (as is every other filter!) Generally, the peak location filter is used for scattering particles to remove "floaters" from the data set. Sometimes, noisy peaks in incandescence may also be removed with this method, though if there is a valid peak in the filtered event, that will also be lost. To disable any filter (e.g. only the incandescent peak offset filter without the incandescent temperature ratio filter), enter NaN into the relevant box.
19. Added "Should PAPI read-in a text file for calibration coefficients?" pop-up menu to PAPI-SP2 (under the "averaging intervals/bin widths pop-up). Please copy the text below (between the dashed lines) into a text file (values are exactly as the user enters into the "Calculate" tab), and modify the values as appropriate: (This file can have any name and can be stored anywhere.)

CalName	CalValue
c0Mass1	-0.143
c1Mass1	2.801e-4
c2Mass1	0
c0Mass2	-0.566
c1Mass2	2.829e-3
c2Mass2	3.109e-8
c0Scat1	0
c1Scat1	107.38
c2Scat1	0
c0Scat2	0
c1Scat2	1003.1
c2Scat2	0

----

20. By default, scattering signals are rejected if the incandescent signal (above the minimum peak height) does not meet other filtering criteria. The user can turn this off by UNchecking the "Remove scattering signal if BC invalid" box on the SP2\Filter subtab.
21. Added time-resolved scattering size distributions (ScatNumStepSelected & ScatMassStepSelected, as concentrations), and added ScatNumStepSelectedByLogDp graph to default SP2 graphs ("Plot Analyzed Data.")
22. Changes that (marginally) affect output:

    Previous if-else construct to write-out mass/number concentrations was equivalent to "TimeWave[i] > nxtime", which meant concentrations were only calculated if the particle time-stamp crossed "nxtime" (the end time for that time-step.). With PAPI-SP2 v0.35, explicitly stating mass/number concentration averages can be calculated if "TimeWave[i] >= nxtime".

    However, this means that *one* particle outside a given time-step may be included in the mass/number concentration averages for that time-step. (Earlier, this was *always* the case.)

    With PAPI-SP2 v0.35, the spectral averaging (size distributions, coating thicknesses etc.) if-else loop is moved OUT of the concentration-averaging loop. As in the case of the concentration-averaging loop, one particle outside a given time-step may or may not be included in the results for that particular time-step.
    Since both averaging loops are keyed off "TimeWave[i]", there appears to be no easy way to avoid the inclusion of *one* particle outside of a given time-step being included in the results for that time-step.

November 15, 2011: v0.351

Minor bug fix: Removed ConfigTextW from *.dat files.

December 14, 2011: v0.352

Minor bug fix: Replaced "Abort" with "printf" when converting *.sp2b files to *.dat files. If the folder includes empty *.sp2b files, "Abort" will stop processing; "printf" allows processing of non-empty files.

Appendix E: Revisions to Manual

Rev. Date	Rev No.	Summary	Section(s)
7-11-10	B	Inserted additional screen shots	2.2, 4.2
		Added overview at beginning of each step to explain its purpose	2.2, 4.2
11-9-10	C	Clarified data PAPI asks for after “Analyze Data” button is clicked	4.2
11-25-10	D	Updated manual to reflect PAPI update (v 0.30)	Throughout
10-11-11	D-1	Inserted recommended hardware guidelines	1.1.1
1-5-12	D-2	Updated manual to include Revision Notes	Appendix D