SP2 TOOLKIT

for Calibration

DROPLET MEASUREMENT TECHNOLOGIES

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Trademark Information

Risks of Installing Additional Software

Instrument computers from DMT are configured to acquire data in a reliable, and robust manner. Typically, such instruments are either not connected to a network or are connected to a small, local network that is isolated from the internet, reducing the risk of viruses. Since anti-virus programs can cause erratic behavior when they run in the background on data acquisition computers, DMT does not install anti-virus, anti-spam, or anti-malware programs. If you choose to install these programs, you accept the risk associated with them in terms of potential performance degradation of the software installed by DMT.

For similar reasons, DMT recommends that you do not install or run other software on the dedicated instrument computer. Although the installation of some software may be unavoidable, it is particularly important not to run other software while the computer is acquiring data.

CONTENTS

Figures

1.0 Introduction

The SP2-XR calibration analysis toolkit is written in IGOR and allows the user to quickly analyze scattering and incandescence calibration data. The program analyzes particle ADC peaks within the Particle by Particle (PbP) data generated by the SP2-XR instrument. The software fits a Gaussian to the instrument response for each particle size. This response and the particle sizes are then fit to produce a threshold table, which is imported into the Labview interface of the SP2-XR. This allows for real-time conversion of the SP2-XR raw data to black carbon mass and particle size. The Toolkit is not intended to be used for detailed analysis of the SP2-XR data, but serves only as a tool for quickly processing calibration data.

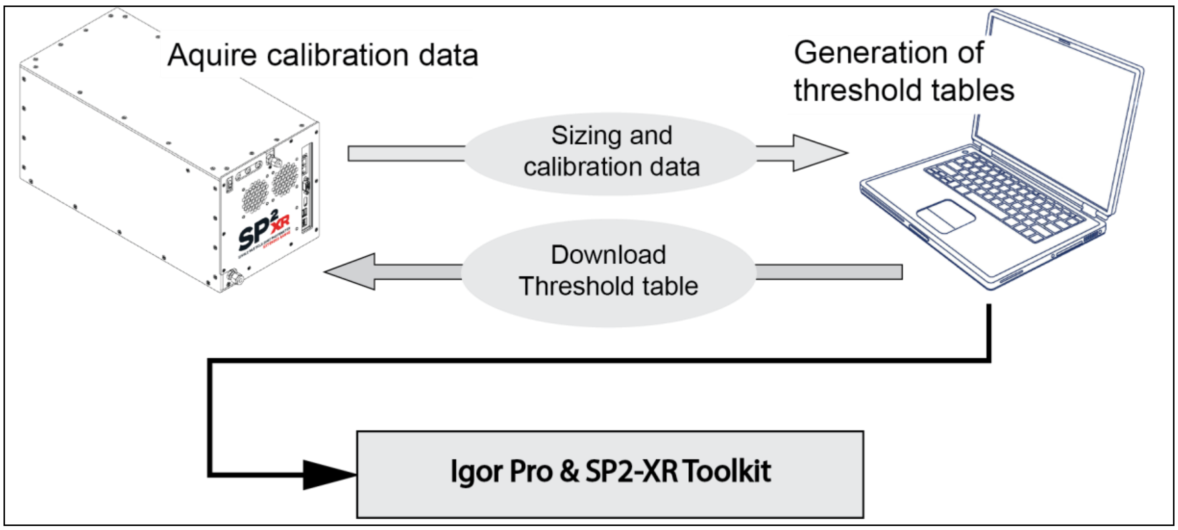

Figure 1: Flow diagram for SP2-XR Toolkit, (sizing and calibration).

1.1 Development Platform

The Toolkit was developed using Igor Pro (www.wavemetrics.com). Some familiarity with the Igor Pro environment, and programming language will aid in the use of the Toolkit, but a deep knowledge of Igor Pro is not necessary. This manual will adopt some terminology used in Igor Pro and users interested in learning more about Igor Pro are encouraged to visit the Wavemetrics website. There the user can examine the Igor Pro manual and explore the environment using widely available Igor Pro tutorials.

1.2 Toolkit Version Information

Version 1.013 is the first publicly released SP2-XR software from DMT.

2.0 Getting started

The SP2-XR toolkit requires a copy of Igor Pro which can be downloaded at:
https://www.wavemetrics.com.
An Igor Pro license and serial number is provided with each instrument.

NOTE: We recommend that data analysis not be performed using the SP2-XR onboard computer. Igor Pro, the SP2-XR Toolkit, and data analysis should use a dedicated computer workstation. Very large files can become truncated and/or corrupted unless the drive where the files are being saved has the appropriate amount of storage space.

2.1 SP2-XR Toolkit Installation Instructions.

A USB flash drive is shipped with the instrument, and has two files that will enable the toolkit to function within the Igor pro program. These files consist of two types, a Procedure file **(.ipf),** and a packed experiment file **(.pxt).** Both files should be copied to your desktop. These files will need to be placed in the proper folders to enable the Toolkit to function properly.

1. From the Igor Help menu, choose **"Show Igor Pro User Files"**, a file explorer window with the appropriate Igor folders should appear.
2. Place the **SP2-XR Toolkit_v1.015.ipf** (or a shortcut to it) in the **"User Procedures"** folder.
3. Place the **SP2-XR Toolkit_v1.015.pxt** (or a shortcut to it) on your desktop.

2.2 Starting the Toolkit and loading data

Double-click on the SP2-XR Toolkit packed experiment file (.pxt) or desktop shortcut to open the toolkit. The toolkit program main window should appear as shown in *Figure 2*.

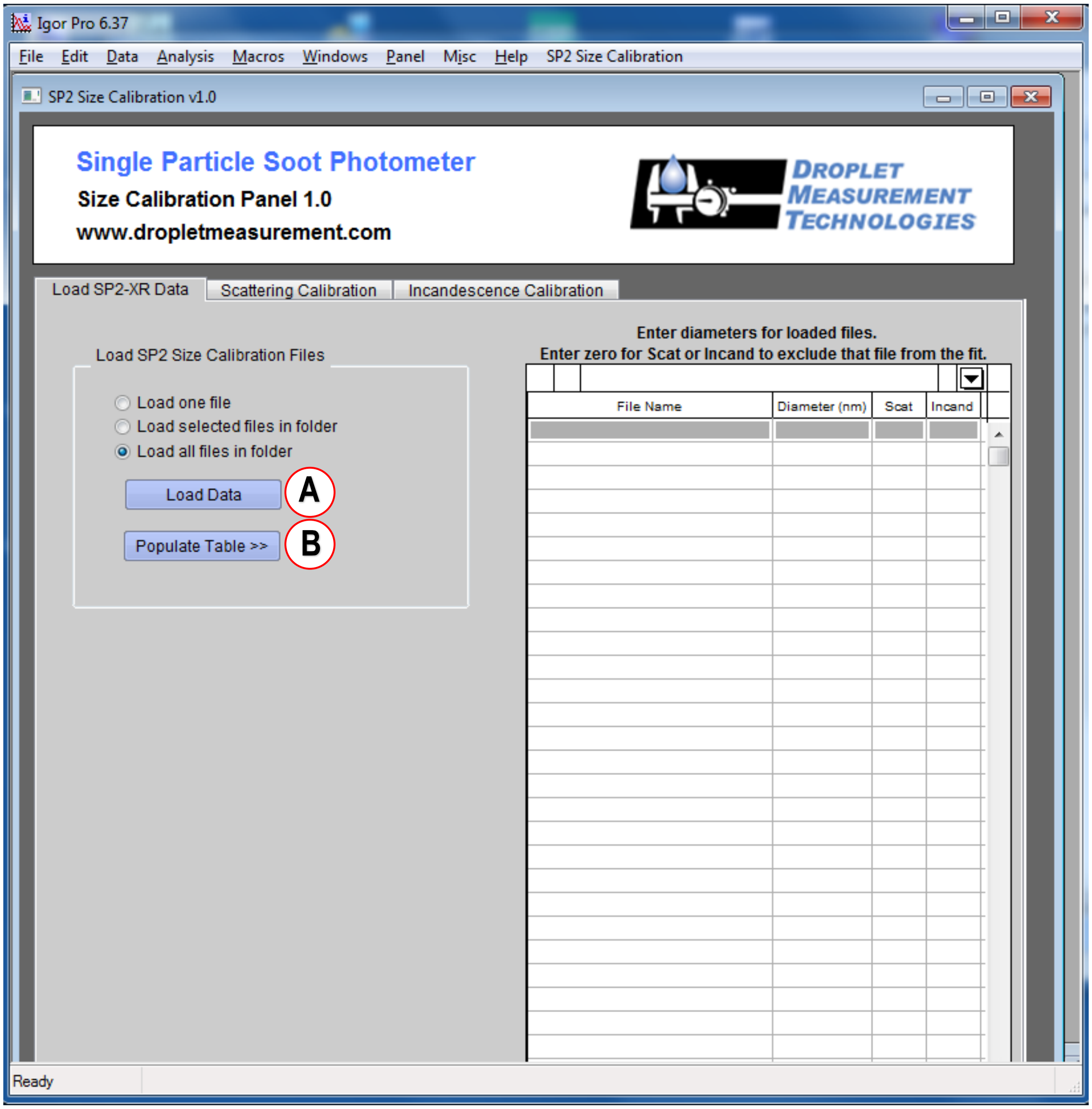

Figure 2: SP2-XR Toolkit dialog screen load data tab.

Calibration data can be loaded one file at a time, as a subset of files within a folder or an entire folder worth of files. After selecting how the data should be loaded click on **(A)** "**Load Data**", and direct the toolkit to the location of the stored PbP.csv calibration data. Once the data is loaded, clicking on **(B)** the **"Populate Table"** button will populate the table on the front panel.

3.0 Setting up calibration for individual particles

After the data table has been populated, the user must input the calibration size and type of particle for each file.

3.1 Designation of particle types and sizes

Particles must be defined as either **scattering**, or **incandescent** by entering either a (1=Select) or a (0 = deselect) in the corresponding column as shown in *Figure 3*. For SP2-XR calibrations we recommend using separate standards for the scattering and incandescence signals. A purely scattering aerosol such as polystyrene latex or ammonium sulphate should be used for the scattering calibrations. The black carbon proxy used for the incandescence calibration should be selected based on that which most closely resembles the ambient atmosphere in which you are measuring. For factory calibrations, Aquadag is used. The user must input the diameter (nm) corresponding to each file in the table.

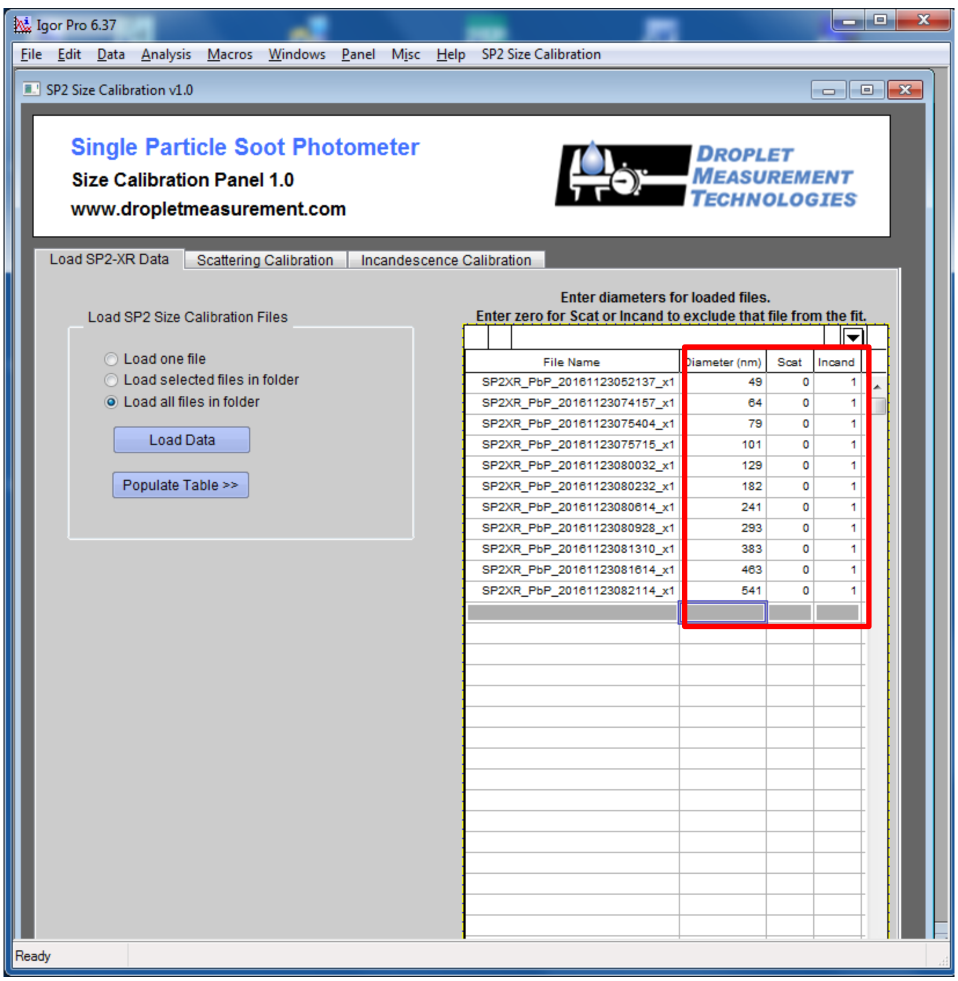

Figure 3: Designation of particle types.

3.2 Scattering Calibration Tab

The scattering calibration tab is used to analyze the calibration data and create a scattering threshold table to convert A/D counts to particle size (nm).

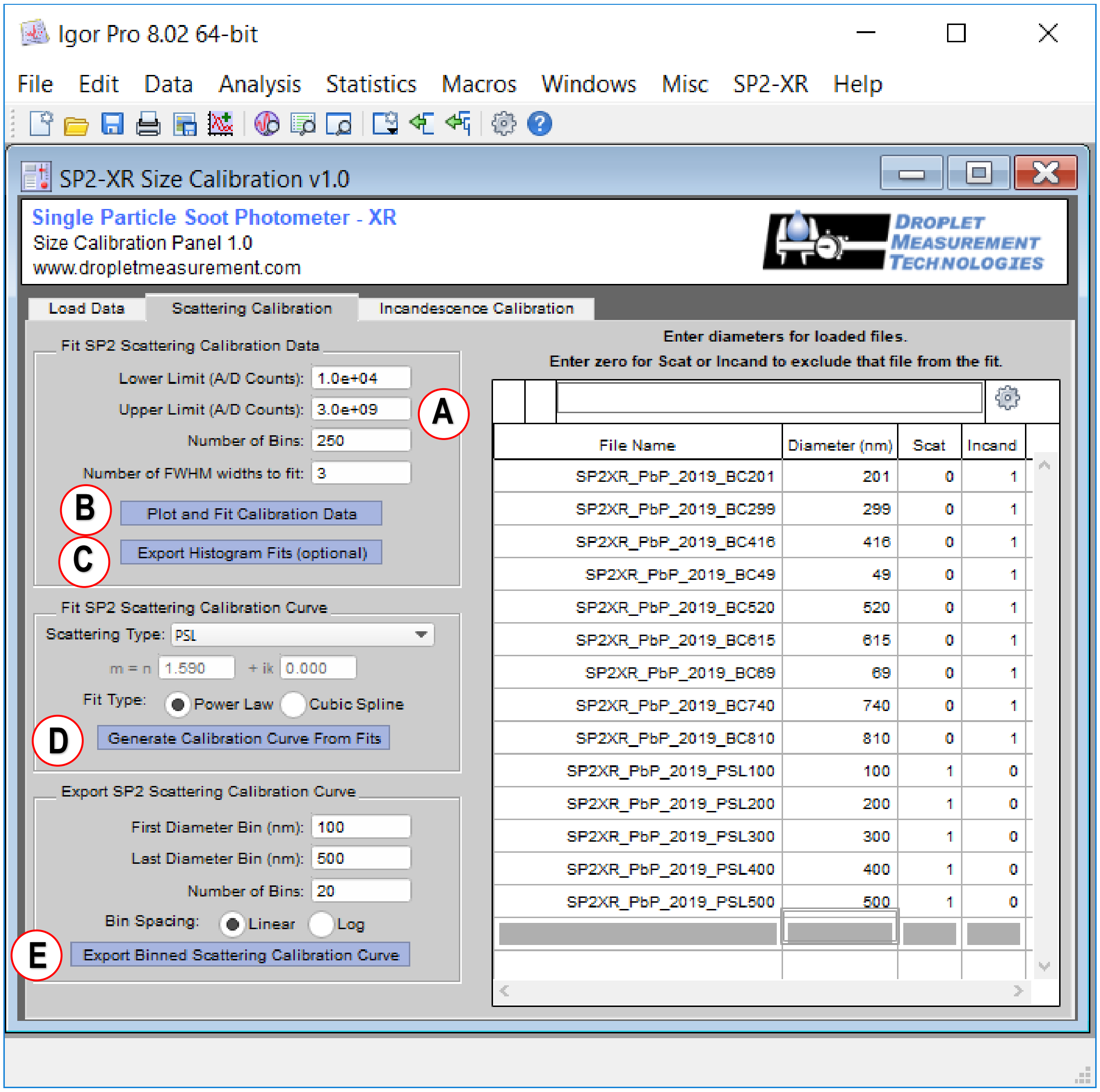

Figure 4: Scattering calibration tab.

3.3 Scattering Calibration Tools

The scattering calibrations fit will determine how the PBP files are processed for Gaussian fit. The important parameters **(A)** are:

- Lower Limit
- Upper Limit
- Number of bins
- Number of FWHM widths to fit

3.3.1 Lower/Upper Limit (A/D counts)

The Lower Limit and Upper Limit (A/D counts) relate to the Scatter Threshold values set in the SP2-XR software. This is designed to reject noise counts and oversized particles. Only A/D counts within the limits will be processed. The range for both limits is 1.0e+00 to 3.0e+09. The recommended values for the lower and upper limit respectively are 1.0e+04 and 3.0e+09.

3.3.2 Number of Bins

The number of bins parameter determines how many bins will be used to process the PBP peak for the Gaussian fit. More bins will increase the resolution of the Gaussian fit. Fewer bins will smooth out spikes in the particle data. Number of bins can be between 50 and 500.

The histogram for the gaussian fit will be determined by applying linear spacing of the number of bins between the A/D lower limit and A/D upper limit.

3.3.3 FWHM widths

The number of FWHM's to fit affects the width of Gaussian fit resolution. FWHM = 2.35482 * σ, where σ is the standard deviation of the distribution. This will determine how broad the Gaussian for the peak may be. The recommend value is 3.

3.4 Generate Fit for Particles

Clicking on the "**Plot and Fit Calibration Data**" button **(B)** generates the fit for individual particle sizes, and brings up a histogram as shown in *Figure 5*. This shows the fit for the selected scattering calibration data file. The window allows selection of individual data files and allows the user to assess the quality of the fit.

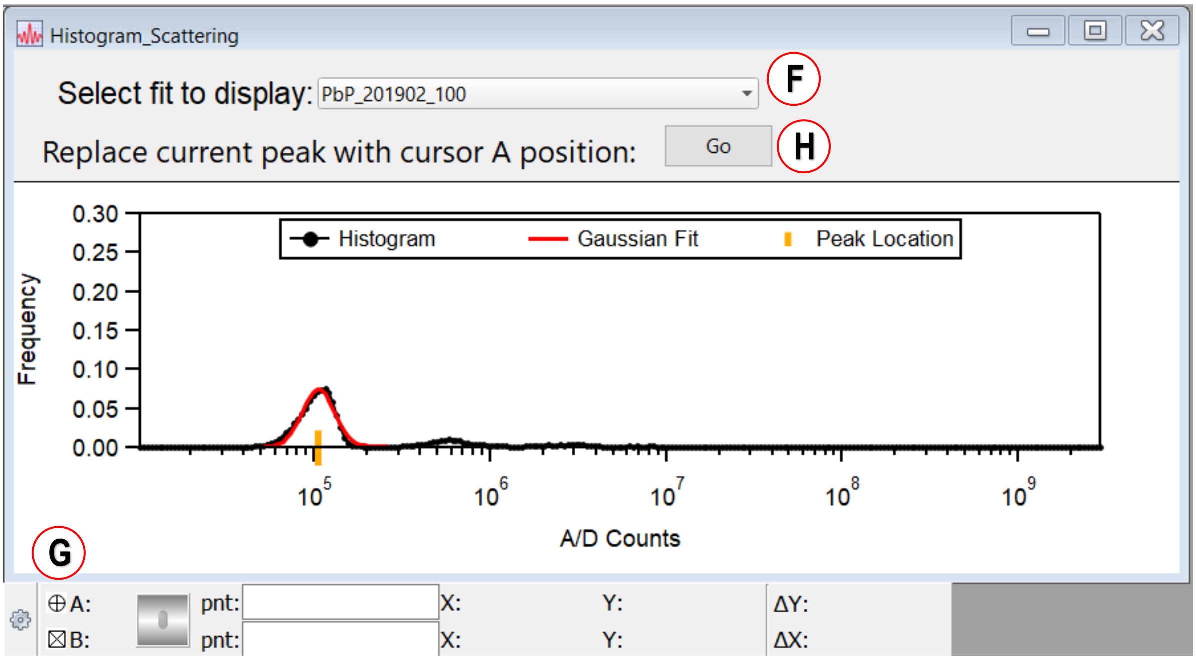

Figure 5: Analyzed response for scattering calibration.

The user should review all peaks and verify the peak location chosen by the software is the desired peak. The drop-down menu **(F)** selects the file to display. If an artifact exists in the file that causes the software to select an incorrect peak, the user may use the A cursor **(G)** to select the correct point. If a new peak has been selected with the A cursor, the "**Go**" button **(H)** is used to update the peak location.

3.4.1 Export Histogram Fits

If desired, the peak locations for each diameter can be exported to a CSV document with button **(C)**. An example output is shown in *Figure 6*.

	A	B
1	Diameter (nm)	A/D Counts from Gaussian Fit to Histogram
2	100	1.06E+05
3	150	1.12E+06
4	200	7.75E+06
5	269	4.17E+07
6	300	7.76E+07
7	400	3.72E+08
8	500	1.01E+09

Figure 6: Scattering histogram fit table.

3.5 Choosing the Scattering Type-RI

To Generate the calibration curve, the type of scattering particle used to generate the calibration data needs to be defined. In the Scattering Type drop-down menu, the software has built in refractive indexes for PSL and Ammonium Sulphate particles. If a different calibration standard is used to collect the calibration data, the user should set this value to Constant Refractive Index, then enter the refractive index information in the boxes below.

The Fit Type must then be selected. The fit type can be either Power Law fit, or Cubic Spline fit. For Ammonium Sulphate or PSL standards, the Power Law fit is recommended.

3.6 Generate Calibration Curve from fits

Clicking on the "**Generate Calibration Curve from Fits**" button, **(D)** takes the particle size data and the collected responses generating a plot and fit equation. This is shown in *Figure 7* below.

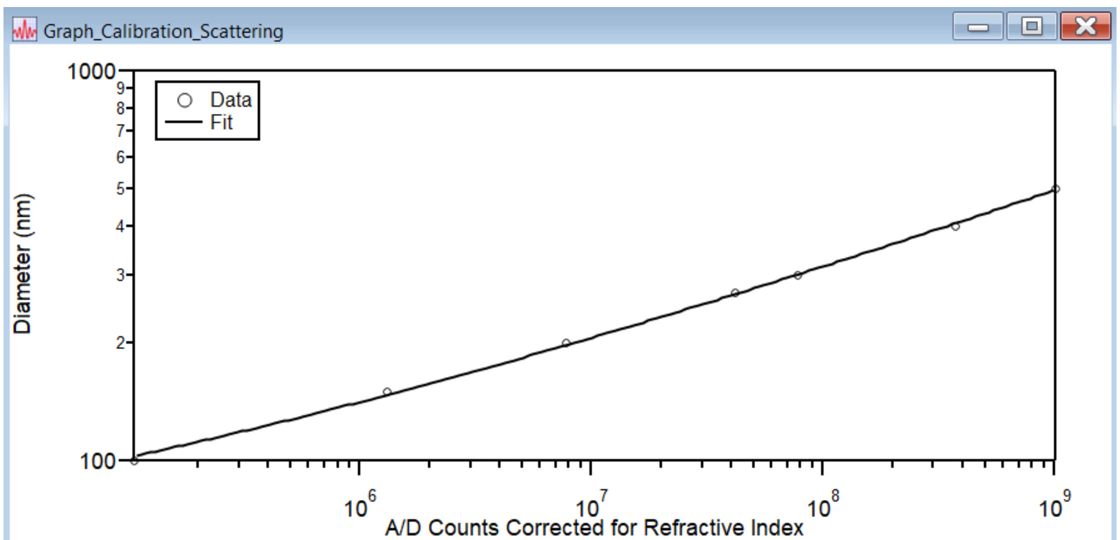

Figure 7: Plot showing calibration response as a function of particle size.

3.6.1 Export Binned Scattering Calibration Curve

To export the scattering calibration curve threshold table, the table values must first be defined. The factory settings for the first and last scattering bins are 100nm and 500nm respectively. The recommended number of bins is 20. The user may select the bins spacing to be linear or logarithmic. Linear is recommended for the scattering table. The button **(E)** will export the CSV threshold table that will be used by the instrument *Figure 8*. The SP2-XR software uses 20 bins for sizing and mass calculations. The first 20 values in the threshold table refer to the lower limit of the bin. The value of the 21st line is the maximum threshold value of the 20th bin. It is generated by the software automatically, and required by the SP2-XR for proper operation.

	A	B
1	100	1.65E+04
2	121.053	1.23E+05
3	142.105	4.85E+05
4	163.158	1.38E+06
5	184.211	3.23E+06
6	205.263	6.57E+06
7	226.316	1.21E+07
8	247.368	2.07E+07
9	268.421	3.35E+07
10	289.474	5.16E+07
11	310.526	7.65E+07
12	331.579	1.10E+08
13	352.632	1.53E+08
14	373.684	2.09E+08
15	394.737	2.80E+08
16	415.789	3.67E+08
17	436.842	4.75E+08
18	457.895	6.05E+08
19	478.947	7.62E+08
20	500	9.48E+08
21	inf	2.40E+09

Figure 8: Scattering threshold table.

3.7 Incandescence Calibration Tab

The incandescence calibration is used to review the calibration data and create an incandescence threshold table to convert A/D counts to particle mass (fg) for the SP2-XR instrument.

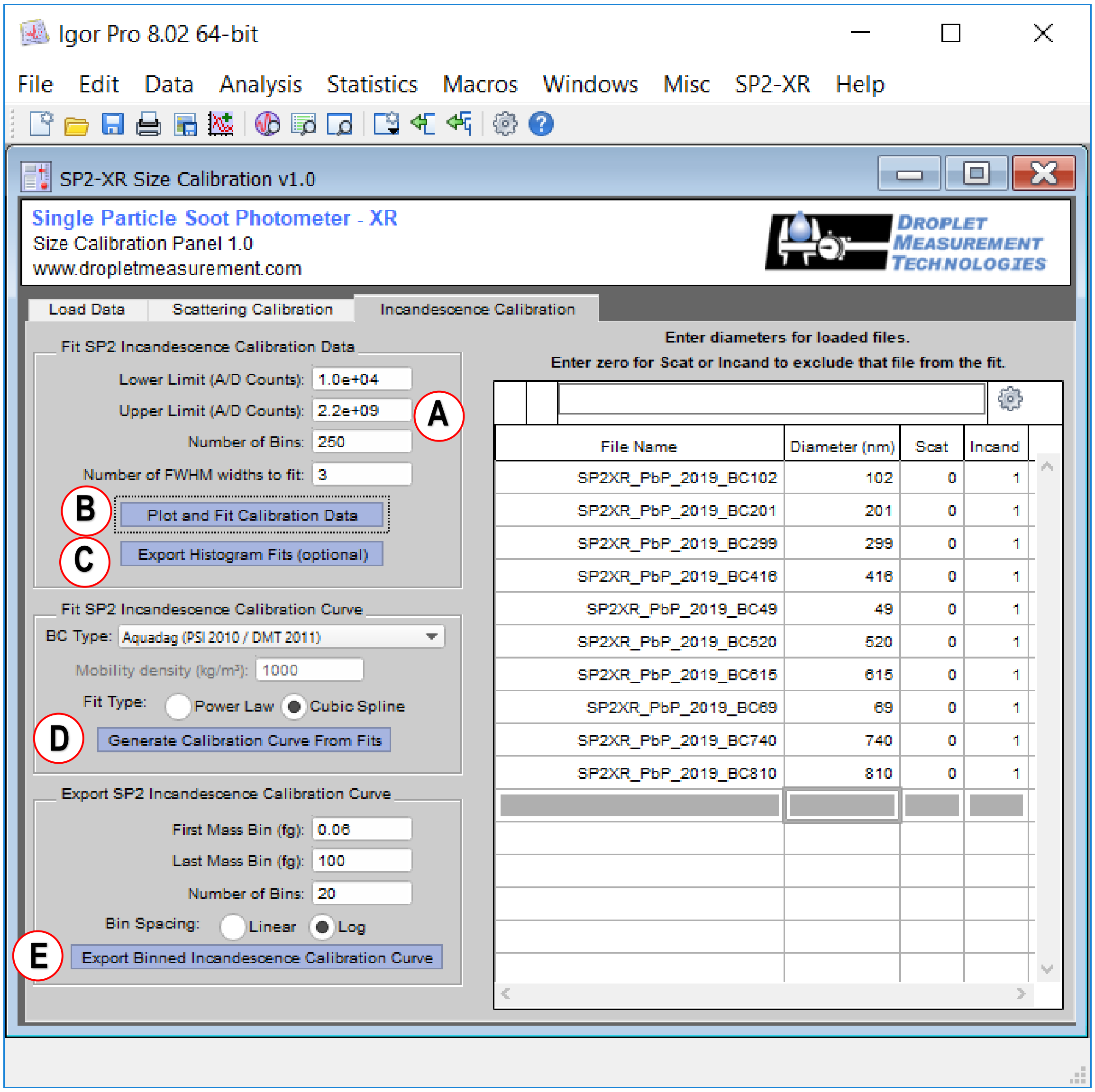

Figure 9: Incandescence calibration tab.

3.8 Incandescence Calibration tools for Black Carbon

The important parameters **(A)** are:

- Lower Limit
- Upper Limit
- Number of bins
- Number of FWHM widths to fit

3.8.1 Lower/Upper Limit (A/D counts)

The Lower Limit and Upper Limit (A/D counts) relate to the incandescence threshold values set in the SP2-XR software. This is designed to reject noise counts and oversized particles. Only A/D counts within the limits will be processed. The range for both limits is 1.0e+00 to 3.0e+09. The recommended values for the lower and upper limit respectively are 1.0e+04 and 3.0e+09.

3.8.2 Number of Bins

The number of bins parameter determines how many bins will be used to process the PBP peak for the Gaussian fit. More bins will increase the resolution of the Gaussian fit. Fewer bins will smooth out spikes in the particle data. Number of bins can be between 50 and 500.

The histogram for the gaussian fit will be determined by applying linear spacing of the number of bins between the A/D lower limit and A/D upper.

3.8.3 FWHM widths

The number of FWHM's to fit affects the width of Gaussian fit resolution. FWHM = 2.35482 * σ, where σ is the standard deviation of the distribution. This will determine how broad the Gaussian for the peak may be. The recommend value is 3.

3.9 Generate fit for particles

Clicking on the "**Plot and Fit Calibration Data**" button **(B)** generates the fit for individual particle sizes. And brings up a histogram as shown in *Figure 10* which shows the fit for the selected particle BC calibration. The window allows selection of individual data files and allows the user to assess the quality of the fit.

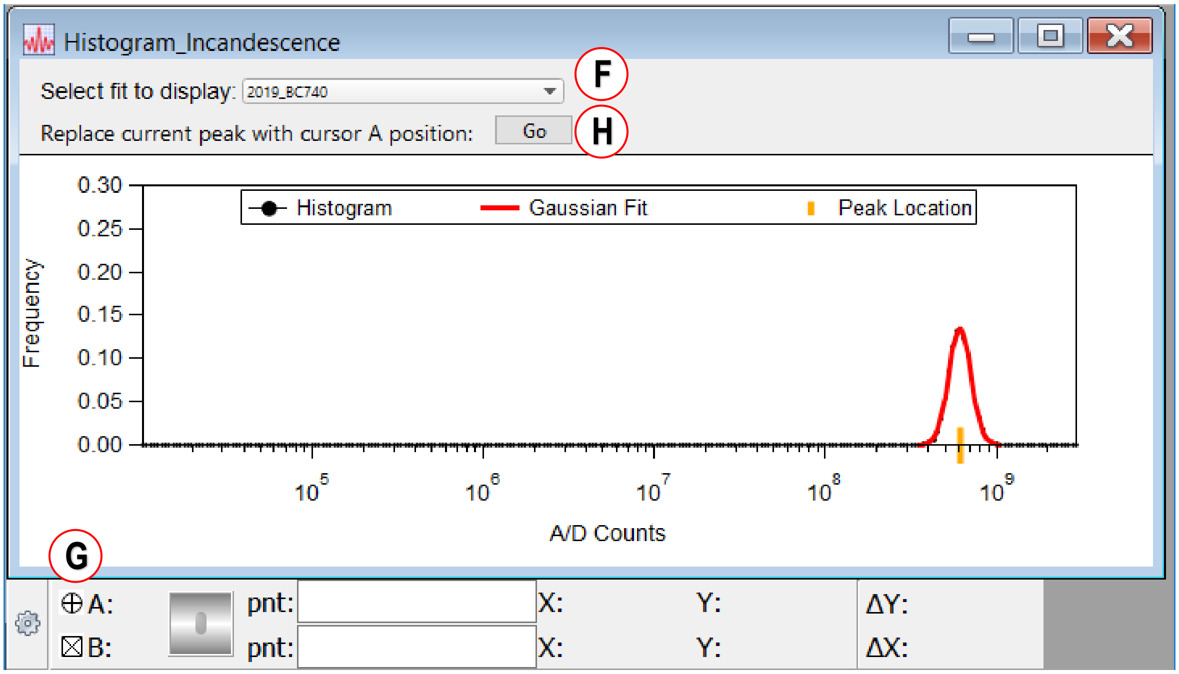

Figure 10: Analyzed response for incandescence calibration.

The user should review all peaks and verify the peak location chosen by the software is the desired peak. The drop-down menu **(F)** selects the file to display. If an artifact exists in the file that causes the software to select an incorrect peak, the user may use the A cursor **(G)** to select the correct point. If a new peak has been selected with the A cursor, the "**Go**" button **(H)** is used to update the peak location.

3.9.1 Export Histogram Fits

If desired, the peak locations for each diameter can be exported to a CSV document with button **(C)**. An example output is shown in *Figure 11*.

	A	B
1	Diameter (nm)	A/D Counts from Gaussian Fit to Histogram
2	102	2.20E+06
3	201	2.10E+07
4	299	6.53E+07
5	416	1.64E+08
6	49	1.51E+05
7	520	2.71E+08
8	615	3.92E+08
9	69	5.17E+05
10	740	6.09E+08
11	810	7.60E+08

Figure 11: Incandescence histogram fit table.

3.1 Choosing the BC type-RI

The software has built in refractive indexes for Glassy Carbon, Aquadag, and Fullerene Soot. If a different calibration standard is used then the BC Type should be set to Constant Density, and the mobility density for the calibration standard BC should be entered in the box below.

For incandescence calibration the recommended Fit Type is Cubic Spline.

3.2 Generate Calibration Curve from fits

Clicking on the "**Generate Calibration Curve from Fits**" button, **(D)** takes the particle mass data and the collected responses generating a plot and fit equation. This is shown in *Figure 12* below.

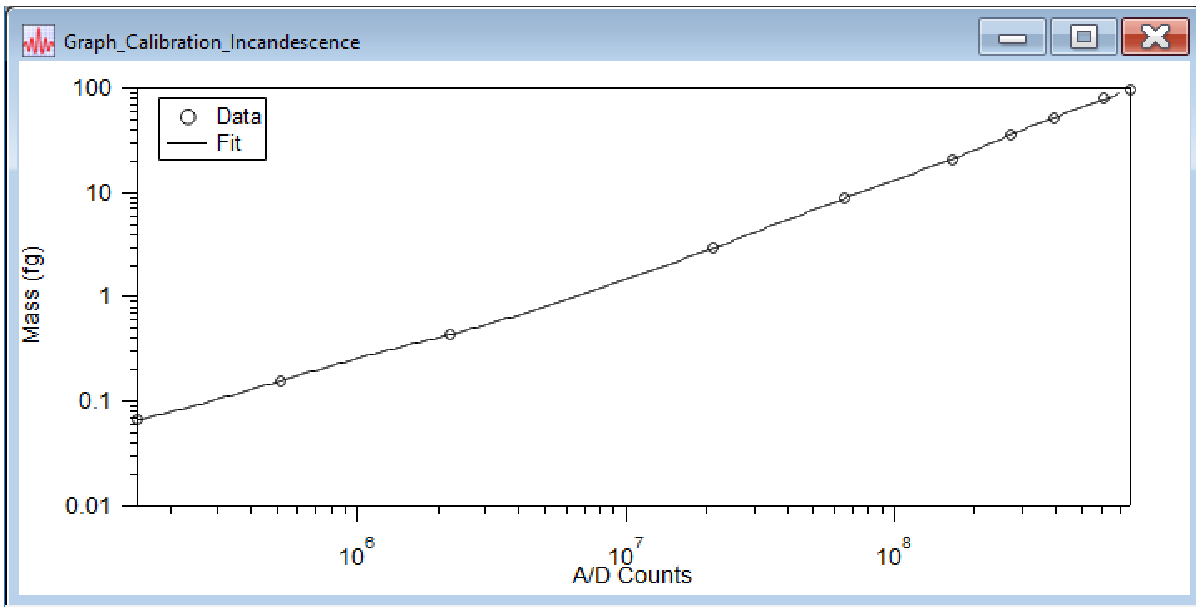

Figure 12: Plot showing calibration response as a function of particle mass.

3.2.1 Export Binned Incandescence Calibration Curve

To export the incandescence calibration curve threshold table, the table values must first be defined. The factory settings for the first and last scattering bins are 0.06fg and 100fg respectively. The recommended number of bins is 20. The user may select the bins spacing to be linear or logarithmic. Logarithmic is recommended for the Incandescence table. The button **(E)** will export the CSV threshold table that will be used by the instrument *Figure 13*. The SP2-XR software uses 20 bins for sizing and mass calculations. The first 20 values in the threshold table refer to the lower limit of the bin. The value of the 21st line is the maximum threshold value for the 20th bin. It is generated by the software automatically, and required by the SP2-XR for proper operation.

	A	B
1	0.06	1.46E+05
2	0.088659	2.41E+05
3	0.131007	3.81E+05
4	0.193582	6.12E+05
5	0.286046	1.02E+06
6	0.422675	1.62E+06
7	0.624564	2.55E+06
8	0.922886	4.07E+06
9	1.3637	6.32E+06
10	2.01507	9.64E+06
11	2.97756	1.46E+07
12	4.39979	2.17E+07
13	6.50134	3.13E+07
14	9.6067	4.54E+07
15	14.1953	6.61E+07
16	20.9757	9.44E+07
17	30.9947	1.36E+08
18	45.7992	1.88E+08
19	67.6751	2.53E+08
20	100	3.37E+08
21	inf	2.40E+09

Figure 13: Incandescence threshold table.

4.0 Additional Information

4.1 Tips for SP2-XR Data Calibration and Analysis

When collecting data:

- Manually decrease the lower limit threshold when collecting the smallest particle sizes.
- PSL Calibrations will typically be more accurate if the PSLs are size selected with a DMA.
- Increasing the sample flow rate will reduce the plumbing delay time.
- Adjust sample concentration for each size to reduce coincidence. In the SP2-XR 10% coincidence occurs at 3,000 particles per cubic centimeter.

5.0 Acknowledgements

This toolkit was developed by Rebecca Washenfelder.