

ARM

CLIMATE RESEARCH FACILITY

Photoacoustic Soot Spectrometer HANDBOOK



January 2013

U.S. DEPARTMENT OF
ENERGYOffice of
Science

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Photoacoustic Soot Spectrometer (PASS) Handbook

January 2013

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Office of Science, Office of Biological and Environmental Research

1.0 Introduction

The photoacoustic soot spectrometer (PASS) measures light absorption by aerosol particles. As the particles pass through a laser beam, the absorbed energy heats the particles and in turn the surrounding air, which sets off a pressure wave that can be detected by a microphone. The PASS instruments deployed by ARM can also simultaneously measure the scattered laser light at three wavelengths and therefore provide a direct measure of the single-scattering albedo.

The Operator Manual for the PASS-3100 is included here with the permission of Droplet Measurement Technologies, the instrument's manufacturer.

Three-Wavelength Photoacoustic Soot Spectrometer (PASS-3) Operator Manual DOC-0163 Revision D



2545 Central Avenue
Boulder, CO 80301-5727 USA

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**2545 CENTRAL AVENUE
BOULDER, COLORADO, USA 80301-5727
TEL: +1 (303) 440-5576
FAX: +1 (303) 440-1965
WWW.DROPLETMEASUREMENT.COM**

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Warranty

The seller warrants that the equipment supplied will be free from defects in material and workmanship for a period of one year from the confirmed date of purchase of the original buyer. The probe owner will pay for shipping to DMT, while DMT covers the return shipping expense.

Consumable components, such as tubing, filters, pump diaphragms and Nafion humidifier are not covered by this warranty.

Software License

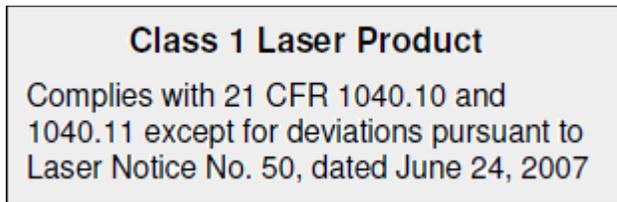
DMT licenses PASS-3 software only upon the condition that you accept all of the terms contained in this license agreement.

This software is provided by DMT “as is” and any express or implied warranties, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose are disclaimed. Under no circumstances and under no legal theory, whether in tort, contract, or otherwise, shall DMT or its developers be liable for any direct, indirect, incidental, special, exemplary, or consequential damages (including damages for work stoppage; computer failure or malfunction; loss of goodwill; loss of use, data or profits; or for any and all other damages and losses).

Some states do not allow the limitation or exclusion of implied warranties and you may be entitled to additional rights in those states.

Laser Safety

The PASS-3 is a Class I Laser Product.



CAUTION - Use of controls or adjustments or performance of procedures other than those specified herein may result in hazardous radiation exposure.

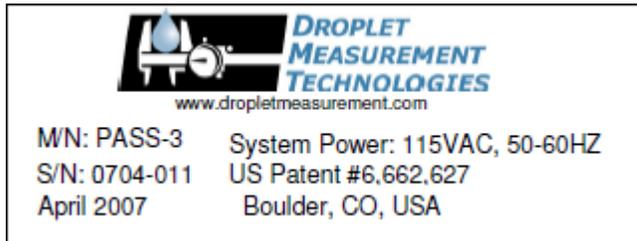
The following laser safety labels are located on the exterior and interior of the PASS-3 acoustic enclosure.



The three lasers embedded within the protective housings have the following beam characteristics:

Laser	Red	Green	Blue
Wavelength	781 nm	532 nm	405 nm
Maximum power	2 W	0.4 W	0.6 W

An identification label is located on the back panel of PASS-3.



CAUTION - Use of controls or adjustments or performance of procedures other than those specified herein may result in hazardous radiation exposure.

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PART I: Hardware

1.0 Product Description

1.1 Introduction

The Droplet Measurement Technologies (DMT) Three-Wavelength Photoacoustic Soot Spectrometer (PASS-3) is based on the design of W. Patrick Arnott of University of Nevada, Reno and Hans Moosmüller of Desert Research Institute.

The technology is patented and licensed for manufacturing from Desert Research Institute. Figure 1 shows the PASS-3 instrument.

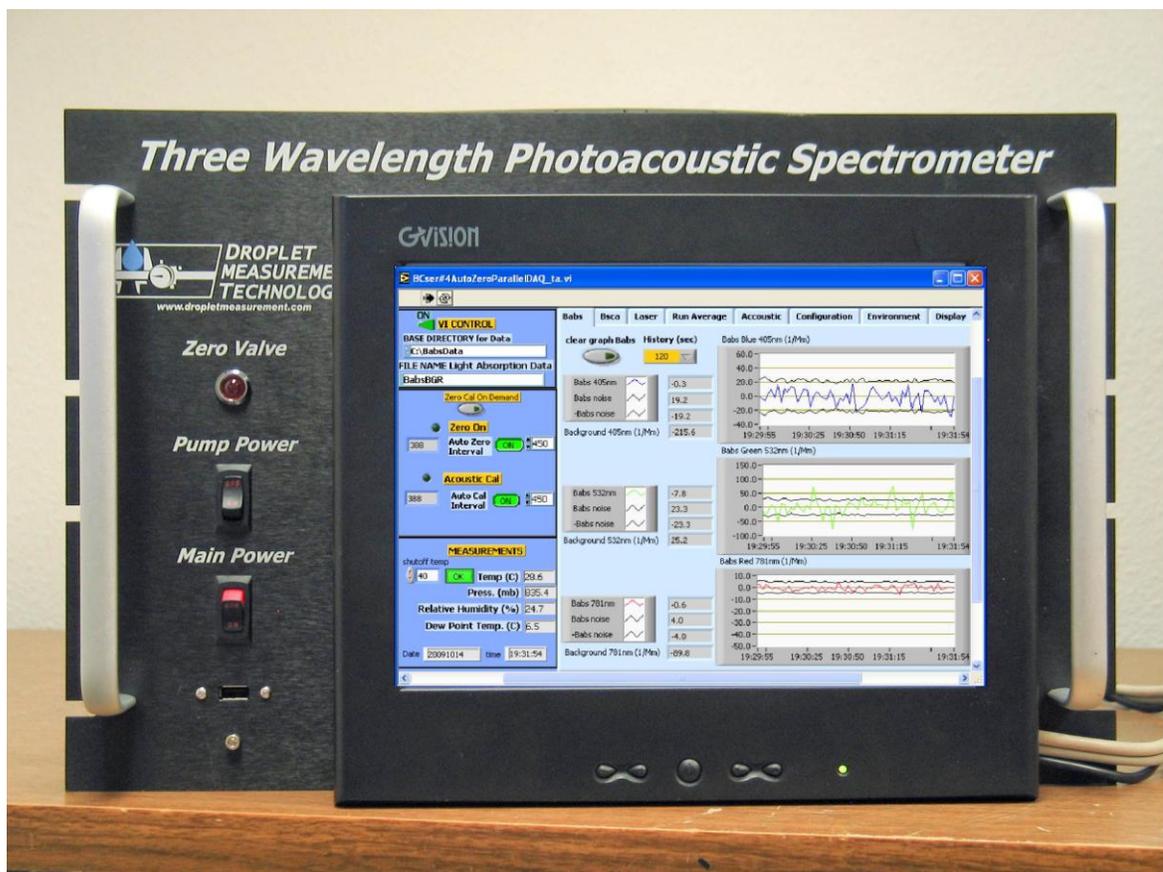


Figure 1: PASS-3 with Touch-Screen Display

1.2 PASS-3 Specifications

Technique:	Photoacoustic method for light absorption (B_{abs}) and integrated nephelometry for light-scattering (B_{scat}).
Sample Flow:	1 lpm
Modulation Frequency:	1500 Hz, square wave
Laser:	781 (2 W) , 532 nm (0.4 W) and 405nm (0.6 W)
Auxiliary Parameters:	Temperature, Pressure, Relative Humidity, Dew Point Temperature
Calibration:	Linear regressions applied to absorption, extinction and scattering coefficients

1.3 Electrical Specifications

Input Electrical Specifications:	105–125 V or 220–240 V (specify when ordering); 50-60 Hz
Power Consumption:	Electronics: 100 W
	AC Pump: 250 W

1.4 Physical Specifications

Weight:	33 kg, excluding pump
Dimensions:	Rack mount is 19" W x 24" L x 12" H / 48.3 cm W x 61 cm L x 30.5 cm H (7U)

1.5 Operating Limits

Temperature:	10 – 40 °C; temperatures above 40 °C may damage the laser
Relative Humidity:	Non-condensing; degraded performance above humidity level of 70%

2.0 Theory of Operation

2.1 PASS-3 Components and Data Outputs

The PASS-3 instrument measures light absorption by aerosols using the photoacoustic method. The instrument's main components are an acoustic resonator, lasers, microphone, piezo calibration source, and integrating sphere/photodetectors (Figure 2).

The primary quantity reported by the PASS-3 is the absorption coefficient B_{abs} . The instrument can also be ordered with an optional scattering sensor that uses a photomultiplier tube (PMT) detector; instruments with this option also report the scattering coefficient B_{scat} . For more information on data outputs, see section 11.2.

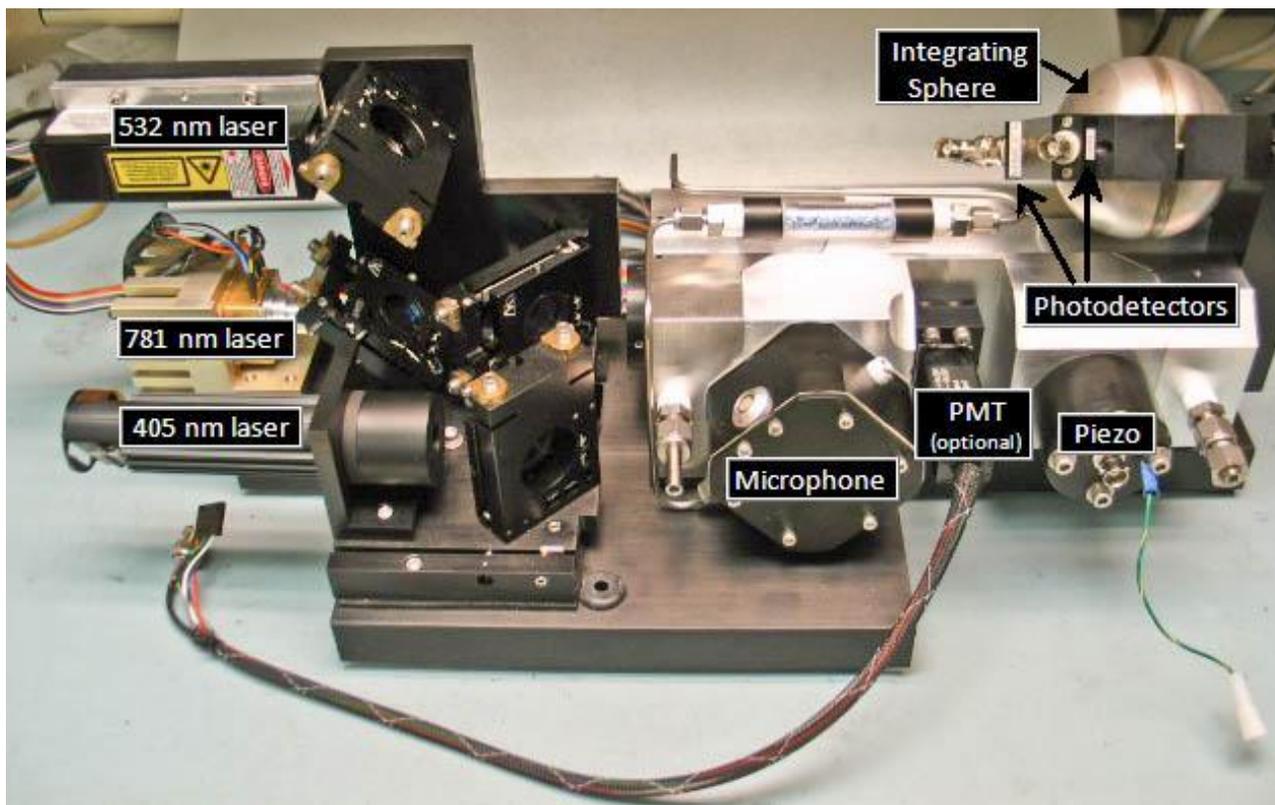


Figure 2: Main Components of the PASS-3

2.2 Overview of Photoacoustic Method

A brief description of the photoacoustic method is as follows. Sample air is drawn through the resonator at an approximate rate of 1 lpm. The laser beam is square-wave modulated at the frequency that matches the resonance acoustic frequency f_{res} of the resonator. Aerosols in the air stream absorb light, causing periodic heating of the gas in the resonator. The heated gas expands, creating a sound-source pressure wave. Since the heating is periodic, with frequency f_{res} , the resultant sound wave will have frequency f_{res} . A microphone attached to one end of the resonator measures this sound wave. The other end of the resonator contains a piezo electrical element used for finding the resonance acoustic frequency f_{res} of the resonator. The laser power is measured with the integrating sphere/photodetector. This information is then used to determine Babs and Bscat; see sections 2.2.1 and 2.2.2. With the PASS-3, light absorption for aerosol is measured *in situ*.

Figure 3 shows the sample flow diagram for the PASS-3. The sample flow goes directly into the resonator chamber or is diverted through the solenoid valve and filter to provide a particle-free zero for the resonator. A small flow of air is maintained at all times through the filter to keep it humidity equilibrated. The temperature and RH sensors are downstream of the filter after the resonator. A critical orifice controls the flows through the PASS-3.

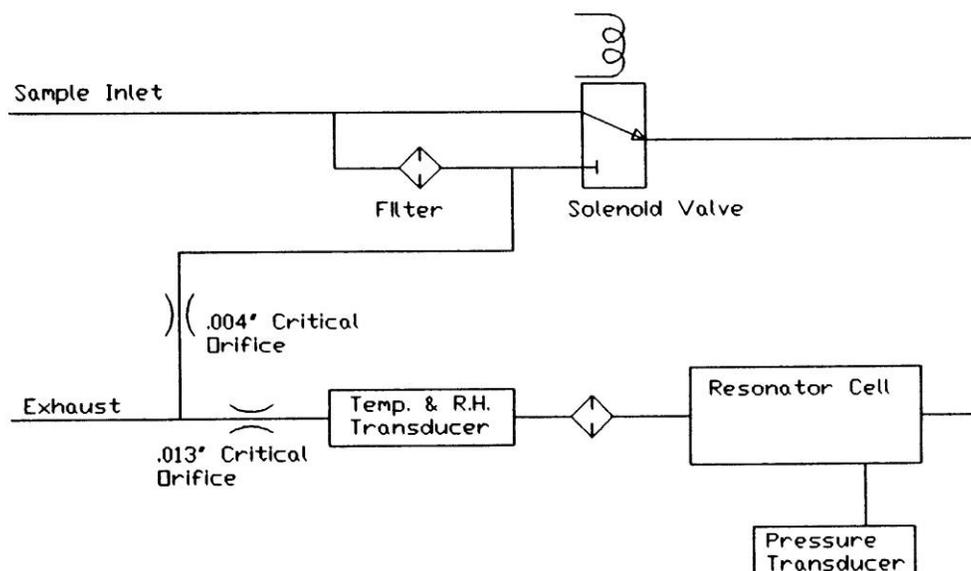


Figure 3: PASS-3 Sample Flow Diagram

2.2.1 Calculating B_{abs}

The absorption coefficient B_{abs} is calculated as follows. First, the raw signal $B_{abs,raw}$, which includes the B_{abs} background, is calculated according to the formula below:

$$B_{abs,raw} = \frac{P_{mic} \cdot A_{res} \cdot \pi^2 \cdot f_{res}}{P_L(\gamma - 1) \cdot Q}$$

where

P_{mic} = Microphone pressure at f_{res}

A_{res} = Cross-sectional area of the resonator

f_{res} = Resonance frequency in Hz (calculated from temperature, pressure, and RH)

P_L = Laser power

γ = Ratio of isobaric and isochoric specific heat

Q = Resonator quality factor (calculated from temperature, pressure, and RH)

Then B_{abs} is calculated as follows:

$$B_{abs} = B_{abs,raw} - B_{abs,bg}$$

where

$B_{abs,bg}$ is the background for B_{abs} on filtered air.

2.2.2 Calculating B_{scat}

The scattering coefficient B_{scat} is calculated as follows. First, the raw signal $B_{scat,raw}$, which includes the B_{scat} background, is calculated according to the formula below:

$$B_{scat,raw} = \frac{P_{scat}}{P_L}$$

where

P_{scat} = Calibrated readings from the photomultiplier tub

P_L = Laser Power

Then B_{scat} is calculated as follows:

$$B_{scat} = B_{scat,raw} - B_{scat,bg}$$

where

$B_{scat,bg}$ is the background for B_{scat} on filtered air.

3.0 Installation

The PASS-3 is a rack-mountable instrument designed for ground-based, mobile-platform or airborne applications. When installing in a rack, the back of the PASS-3 will need to be supported. A vibration isolation kit for rack-mounting the PASS-3 is available from DMT. The entire sampling system is sealed on the PASS-3, which means it can be used on a pressurized aircraft as long as the sample air inlet and outlet are at ambient pressure.

The connections for the power, keyboard, monitor, inlet air, and pump are located on the back panel of the PASS-3 (Figure 4). The power outlet on the back panel is for a sample pump with a maximum rating of 5 amps. The pump can be located any reasonable distance from the PASS unit itself. The pump must require the same voltage as the instrument input voltage, and it must maintain the orifice at critical conditions with a flow of 1 lpm.



Figure 4: Instrument Back Panel

4.0 Procedure for Initial PASS-3 Start-up

To ensure the unit is fully functional and operating properly, all customers should perform the following startup procedure before putting their instrument into service. The procedure involves emailing several screen shots to DMT, where technicians will analyze them to determine if the unit is operating properly.

If there is any concern that the unit is not functioning properly, shut down the unit and contact DMT before proceeding.

1. Set up the PASS-3 (see 0 for instructions).
2. Turn on the **MAIN POWER** and **PUMP POWER** switches. These are located on the front panel of the PASS-3.

3. After the computer has booted up, start the PASS-3 Control Program.
4. Let the instrument run for about 15 minutes before taking any screen shots.
5. Press the **Babs** tab on the Control Program so that the Babs screen will be displayed for the screen shot.
6. Press **Alt+PrtSc** and then paste the captured screen into **PAINT** program (under **Start > All Programs > Accessories**). Save the file.
7. Repeat steps 5 and 6 for the **Bscat, Laser, Acoustics, Configuration, and Environment** tabs.
8. Stop the PASS-3 control program by pressing the **VI CONTROL** toggle button (). The button will turn black and the indicator above will turn to **OFF**.
9. Email the 5 captured screen shots and the data file to:
PASS-INFO@dropletmeasurement.com.

5.0 Calibration

The following calibration procedure assumes that the scattering option is installed in the PASS-3. (All current versions of the PASS-3 are configured with scattering.) Otherwise, a nephelometer will need to be run in parallel with the PASS-3 during the absorption calibration. Figure 5 shows the typical flow system for PASS-3 calibration.

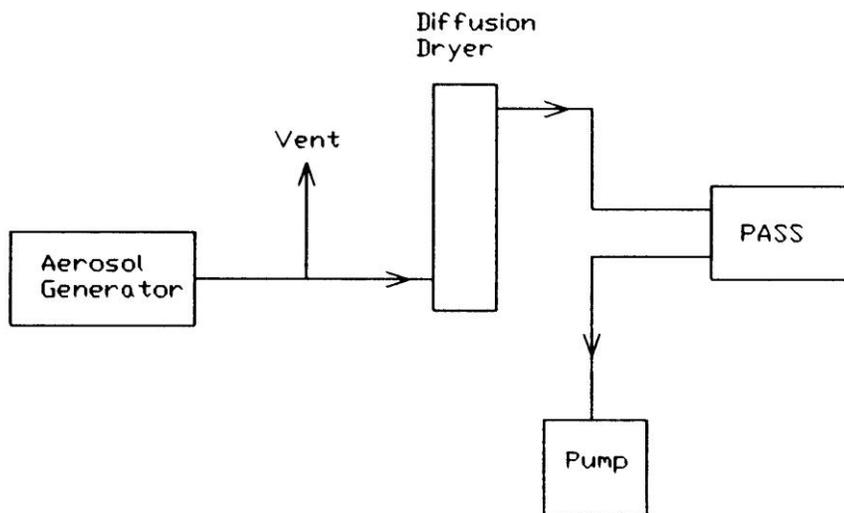


Figure 5: PASS-3 Flow Calibration Set-up

The aerosol generator may be purchased from DMT (part AAA-0005). The diffusion dryer may be purchased from PermaPure; visit permapure.com to see options. Tubing and fittings should be of an electrically conductive material such as brass, stainless steel, or carbon-impregnated silicone tubing.

5.1 Theory of Calibration

The PASS-3 is capable of measuring the scattering coefficient B_{scat} and absorption coefficient B_{abs} . For high concentrations of aerosol, it is also capable of independently measuring B_{ext} , the extinction coefficient. Since $B_{ext} = B_{abs} + B_{scat}$, and the PASS-3 can independently measure each of these three variables, the instrument can be easily calibrated.

Extinction is calculated as follows:

$$B_{ext} = -\frac{1}{.2486} \ln \frac{I}{I_0} \cdot 10^6 [Mm^{-1}]$$

where

B_{ext} is the extinction coefficient

0.2486 is the path length of the laser beam through the cavity in meters

10^6 is a conversion factor to express the extinction in Mm^{-1}

I_0 is the average laser power before and/or after calibration

and

I is laser power during calibration

Note that the PASS-3 should be calibrated with only one laser operating at a time for best results.

An overview of the calibration process is given below, while the following section provides specific step-by-step instructions.

- 1.) Calibrate the scattering measurement. First, run the PASS-3 using both clean air and a highly scattering aerosol sample. This process will generate measurements for B_{scat} and I , as well as for I_0 during clean-air sampling. Next, plot the calculated B_{ext} versus B_{scat} for each wavelength. Since absorption is negligible, the slope of a linear regression line represents the correction factor for the scattering calibration factor. Multiply the current **cal scattering** value (on the **Configuration Tab** in the control program) by the slope of the regression line to produce the new **cal scattering** value. Enter the new value for each wavelength into the PASS-3 calibration program.
- 2.) Calibrate the absorption measurement by doing one of the following:
 - *Nitrogen dioxide (NO_2) gas calibration (preferred):* Measure the actual and displayed laser power for each laser wavelength, and adjust the **photodiode cal** values accordingly. Calibrate the PASS-3 absorption measurement using NO_2 gas. Calculate the B_{ext} in the same manner as for scattering, plot B_{ext} versus B_{abs} , and use the regression coefficient from this analysis to adjust the **Microphone calibration factor**. *Note:* This method is more accurate than black carbon calibration because scattering is negligible and does not need to be estimated.
 - *Black carbon calibration:* Calibrate the absorption measurement using a black-carbon source. Calculate the B_{ext} in the same manner as for scattering, except now plot $(B_{ext} - B_{scat})$ versus B_{abs} for each wavelength. (Scattering is not negligible for this case, and thus must be factored into the equation.) Use the regression coefficient from this analysis to update the **cal Babs** value for each wavelength.
- 3.) Repeat the calibration process to ensure good results.

5.2 Step-by-Step Procedure for Calibrating the PASS-3

5.2.1 Scattering Calibration

5.2.1.1 Data Collection

1. Allow the instrument to warm up for 1 hour, sampling air with filter on the inlet. (If the room air is fairly clean, i.e. $B_{scat} < 20 Mm^{-1}$, you don't need the filter.) On the front panel of the PASS-3 control program, press the green **Zero On** and **Acoustic Cal** buttons to turn off these functions (Figure 6).

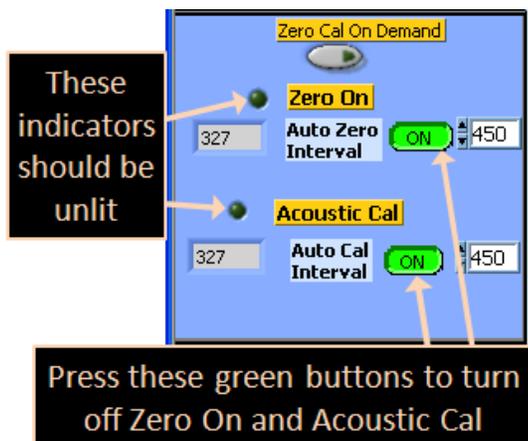


Figure 6: Preparing PASS-3 for Calibration

2. Turn off two of the three lasers. To turn lasers off:
 - a. The 532 nm laser is turned off by turning off the key on the black power supply box.
 - b. The 781 nm laser is turned off by unplugging the connector in the center of the electronics board labeled "781 nm lockout."
 - c. The 405 nm laser is turned off by unplugging the main power from the connector labeled "PJ8."
3. For the scattering calibration, prepare a high-concentration solution of approximately 200-260 nm PSL particles in an aerosol generator with the proper drying column.¹ The concentration should be high enough to give a scattering level of about 20,000 Mm^{-1} . Once the initial scattering aerosol concentration is high, it is best to avoid rapid fluctuations during this step.

¹ Other materials are also acceptable, so long as they are highly scattering and have low absorption.

4. Press the **Zero Cal On Demand** button and collect two minutes of data with the filter on the inlet of the PASS-3. This will allow the I_0 measurement. Wait for the zero and calibration cycle to finish before starting the data collection period.
5. Collect two to four minutes of data with the PSL particles into the PASS-3 with two of the three lasers shut off. Figure 5 gives a diagram of the setup for introducing the PSL particles into the PASS-3.
6. Remove the PSL particle stream from the PASS-3 and put the filter on the inlet.
7. Collect another 2 minutes of background data.
8. Repeat the calibration procedure for each of the 3 lasers, with the other two lasers off.

5.2.1.2 Data Analysis

1. Average approximately one minute of laser-power data collected with the filter on either before or after the scattering measurement. This average value will be the I_0 .
2. Calculate the extinction for both the filtered air periods and the period when the measurement of the PSL particles is stable. Use the following expression:

$$B_{ext} = -\frac{1}{.2486} \ln \frac{I}{I_0} \cdot 10^6 [Mm^{-1}]$$

3. Plot the calculated extinction from the equation in step 2 against the measured scattering as shown in Figure 7. Prepare a linear regression with calculated extinction as the y value and measured scattering as the x value.
4. Multiply the current **cal scattering** value (see **Configuration Tab** on the control program) by the slope of the regression line to produce the new **cal scattering** value. Update the cal scattering value in the Cal_write3.exe program (see software section).
5. Repeat steps 1-4 for each wavelength.

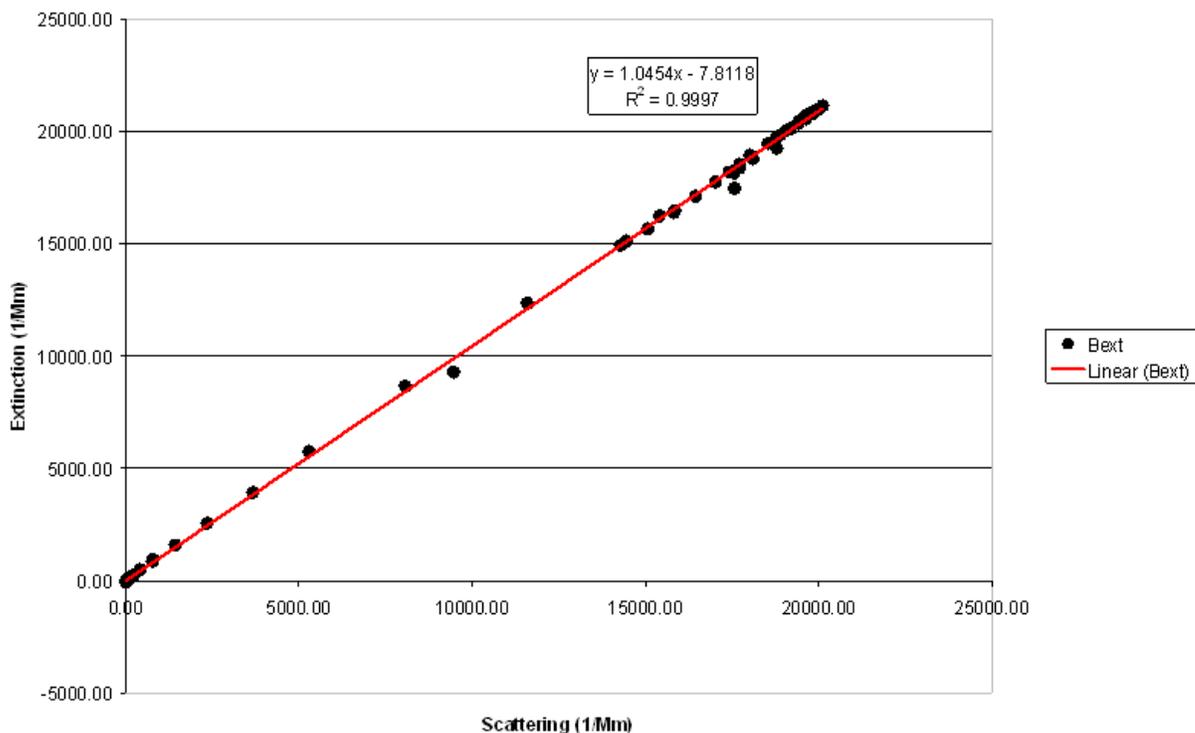


Figure 7: Regression Plot of Calculated Extinction Measurement against B_{scat} . This regression needs to be repeated for each wavelength.

5.2.2 Absorption Calibration – NO₂ Gas (Preferred Method)

This calibration method requires a laser power meter and a source for highly concentrated NO₂ gas (see below).

Light at the 532 nm wavelength is strongly absorbed by NO₂ gas. Each ppb of NO₂ gas will produce approximately 0.395 Mm⁻¹ absorption at standard temperature and pressure (STP) of 0°C and 1013.25 mBar. The recommended concentration of NO₂ gas for this procedure is 200,000 ppb, which will produce an absorption signal of 79,000 Mm⁻¹ at STP.

5.2.2.1 Relative Laser Calibration

1. **Shut down the PASS-3 before performing this step.** Remove the prism and integrating sphere combination and place the laser power meter in its place. Turn on the PASS-3. Measure the laser power of each laser individually, making sure the laser meter is properly placed. Note each laser's recorded power. Shut down the

PASS-3 once again. Replace the prism and integrating sphere combination. Turn on the PASS-3 and record the laser power readings on the front panel.

2. Adjust the **photodiode cal** values for each laser wavelength by multiplying the original values by the ratio of [laser power meter readings]/[front panel readings]. Use the **Cal_write3.exe** program to update these values.

5.2.2.2 Data Collection

Follow the same procedure as for the scattering calibration (see section 5.2.1.1), except use NO₂ gas instead of PSL particles and collect data for only the 532nm laser. The other two lasers should be off during this calibration. Measure I_0 before and after the data collection.

5.2.2.3 Data Analysis

The analysis is similar to that for scattering particles (section 5.2.1.2), except that the data plot uses B_{ext} on the Y axis and B_{abs} on the X axis.

After the data is plotted, divide the current **Microphone calibration factor** value (see **Configuration Tab** on the control program) by the slope of the regression line to produce the new **Microphone calibration factor** value. (Since scattering is negligible, the slope of the a linear regression represents the correction factor for the absorption measurement.) Update the **Microphone calibration factor** value in the Cal_write3.exe program (see software section). This will calibrate the absorption measurement at all wavelengths, since the response of the microphone is not dependent upon wavelength. Variations in calibration between individual lasers have already been corrected in the relative laser calibration (section 5.2.2.1).

5.2.3 Absorption Calibration – Black Carbon Source

5.2.3.1 Data Collection

For absorption calibration a high concentration of strongly absorbing aerosols is needed, preferably with a small amount of scattering. An ideal unit is a kerosene lamp that will run in a fuel-rich mode, producing large amounts of black smoke. Another option is glassy black carbon from Alfa-Aesar (alfa.com, stock# 38008), which can be dispensed in the same way as the PSL material. With any source of absorbing aerosol, the absorption should be greater than 5,000 Mm⁻¹, preferably closer to 10,000 Mm⁻¹.

1. If the kerosene lamp is used, it is suggested that a bag like a garbage bag be filled with smoke and the smoke allowed to mix in the bag for 5 minutes before sampling.
2. Follow the same procedure as for the scattering calibration above, except use the black-carbon source instead of PSL particles. Collect data for one laser at a time, and do a measurement of I_0 before and after the data collection.

5.2.3.2 Data Analysis

1. The analysis will be conducted similar to that for the scattering particles, except that the data plot will use $(B_{ext} - B_{scat})$ on the Y axis, as shown in Figure 8.
2. Multiply the current **cal Babs** value (see **Configuration Tab** on the control program) by the slope of the regression line to produce the new **cal Babs** value. Update the cal scattering value in the Cal_write3.exe program (see software section).
3. Repeat the procedure for each laser wavelength.

It is recommended that the entire calibration process be repeated to ensure accurate results.

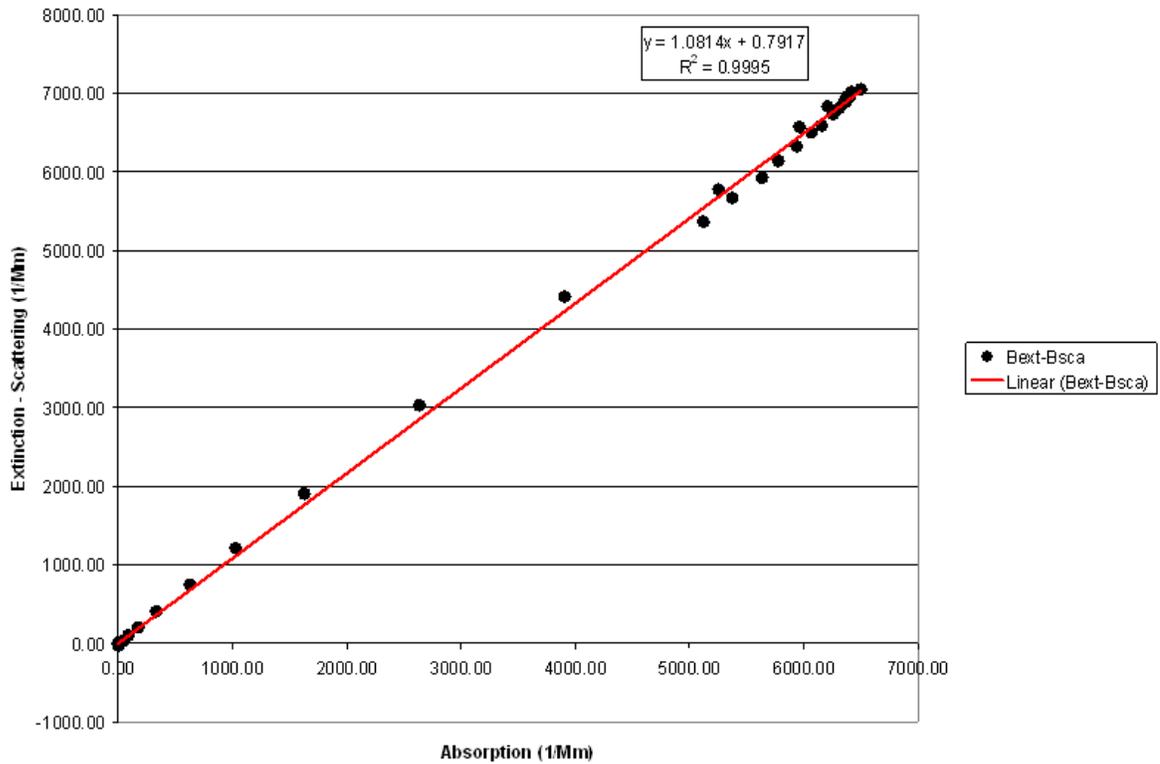


Figure 8: Regression Plot of Calculated [Extinction – Scattering] Measurement against B_{abs} .

6.0 Maintenance

Droplet Measurement recommends the following service and maintenance schedule for the PASS-3. This is only a guide based on ambient air sampling. If the PASS-3 is used for source sampling, then the maintenance frequency will have to be increased.

DANGER

The laser used in the PASS-3 is a CLASS 4 Laser

The lasers operate at 781, 532, and 405 nm and are rated up to 2 W.

Caution

The use of controls, adjustments, or procedures other than those specified in this document may result in hazardous radiation exposure. In particular, reflections caused by placing an object in the laser beam path can cause skin burns and/or blindness.

During maintenance, the PASS-3 should be powered down and power disconnected from the unit. The PASS-3 has two enclosures, an outer and inner isolation box with removable covers. Both covers will need to be removed before maintenance can be performed. A #2 Philips screw driver is needed to remove the outer cover (4 screws) and a 7/64 Allen wrench is required to remove the inner cover (16 screws). By removing the inner cover, the laser beam is exposed. There are two laser-interlock switches in the inner box that will shut down the lasers when the cover is removed. Do not depress these safety switches unless you have training in dealing with high-powered lasers.

6.1 Monthly Maintenance

1. Check the filter in front of the Temperature/RH sensor and the zero-air filter (Figure 10). These filters are accessed by removing the black panel on the underside of the PASS-3 enclosure (Figure 9). If material has accumulated on the filters, they should be replaced. They can be ordered from www.mcmaster.com and have the following specifications:
 - Part number 4795K3
 - Miniature inline thermoplastic filters
 - Smooth-end connection
 - 99.99% efficiency at .01 micron, 1" diameter
2. Check the DRIERITE in the tube on top of the acoustic resonator. If the color has turned from blue to pink, then the DRIERITE needs to be replaced. DRIERITE can be ordered from www.drierite.com.

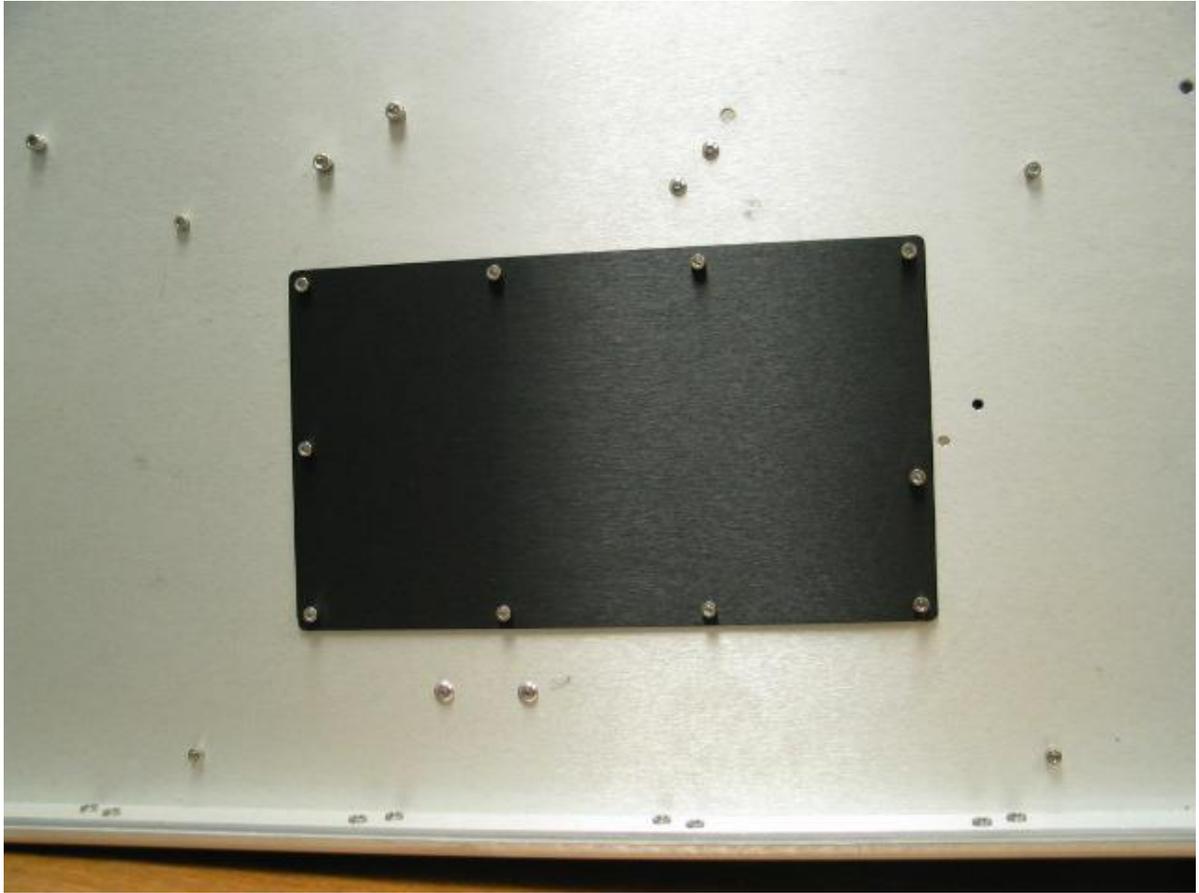


Figure 9: Filter Access Panel

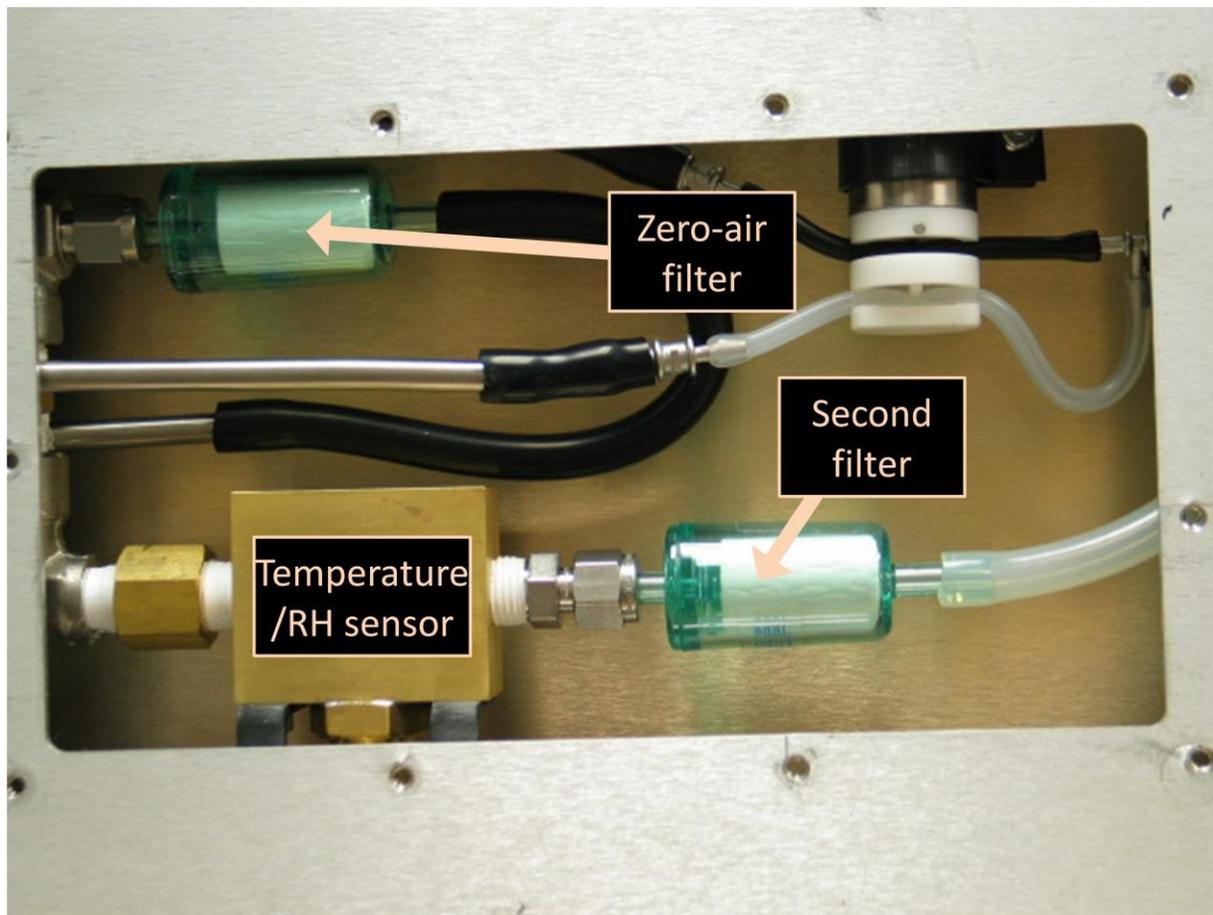


Figure 10: Filter Location

6.2 Bi-Monthly Maintenance

- Calibrate the absorption and scattering measurements (Section 5.0).
- Check the sample flow rate. **Note:** The sample flow rate cannot be measured at the sample inlet on the back of the instrument, as this reading includes the resonator flow as well as the bypass flow through the zero filter. The sample flow through the resonator needs to be made at the line immediately before the resonator.

6.3 Periodic Maintenance of Optic Components

The window and the prism on the acoustic resonator will periodically need to be cleaned. The frequency of cleaning the optics depends on type of aerosol that is sampled. For ambient sampling, the optics may need cleaning once every 3-12 months. Instruments

sampling diesel exhaust from a dilution tunnel may require cleaning once a week. An indication of dirty optics is a drop in laser-power readings.

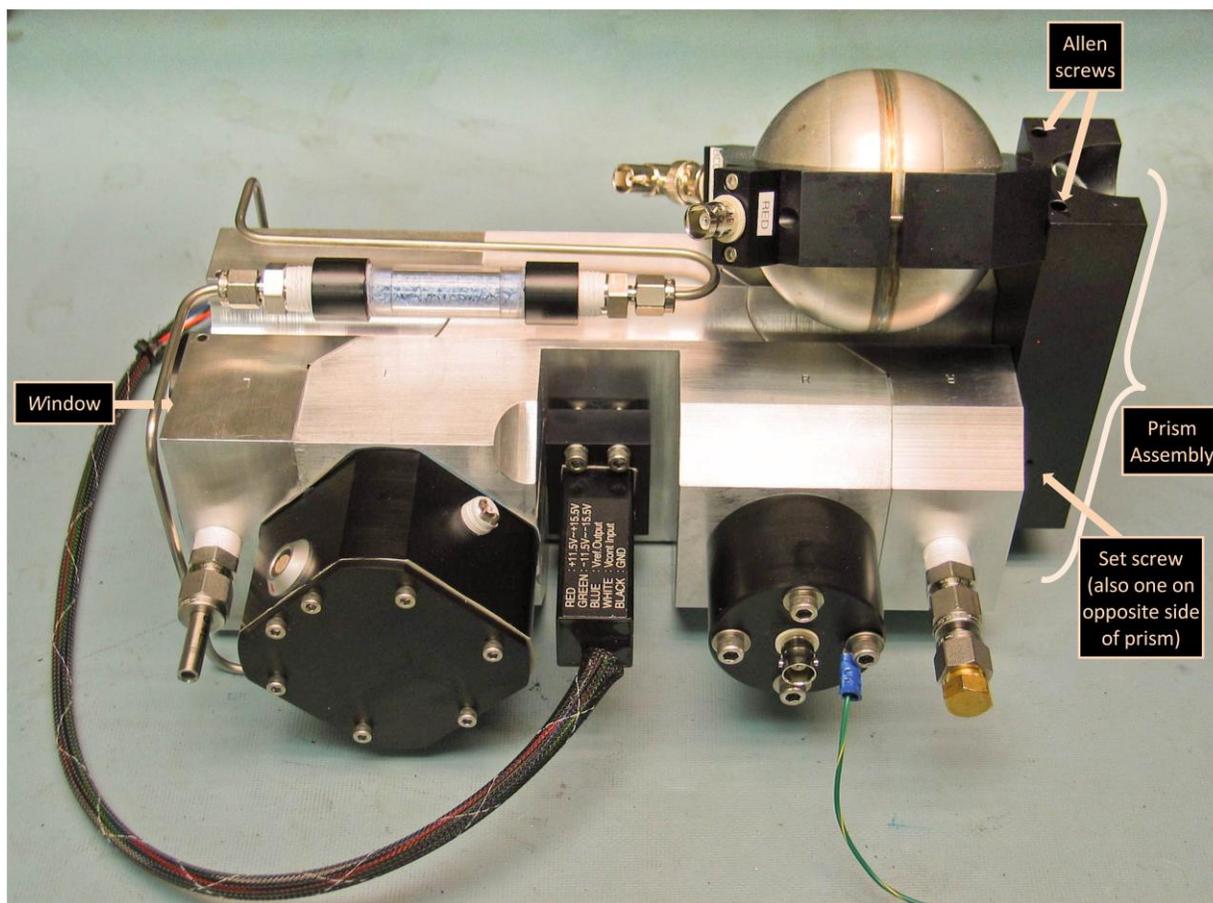


Figure 11: Window and Prism Location

6.3.1 Removing and Cleaning the Window

To remove and clean the window, follow the steps below. The use of optical gloves is recommended during this procedure.

1. Use the supplied 5/64 Allen wrench to loosen the screws that secure the window housing to the resonator. Take care as not to lose these screws, since they are custom-made and replacements will have to be ordered from DMT.
2. Inspect the window for any dirt or spots. If there is no visible accumulation on the window, then cleaning is not recommended. The optics should only be cleaned when needed, as excessive cleaning will damage the optical coating. If the window is dirty, continue with the steps below.

3. Blow off any large particles with clean dry air.
4. Remove the window from its holder and place the window on a clean, lint-free tissue or cloth. Lens paper will work.
5. Apply one or two drops of lens-cleaning solution on a piece of lens-cleaning tissue. Slowly drag the lens-cleaning tissue over the window surface, starting with the wet portion of the tissue. Continue moving the tissue across the window until the window is dry.
6. Inspect and repeat step 5 if necessary. If the window is still dirty, then wet a Q-tip in cleaning solution and place a lens-cleaning tissue over the Q-tip. Lightly swipe across the window where it is dirty. Generally, only the side facing the resonator will need cleaning.
7. Place the window in its holder and install the assembly on the resonator.

6.3.2 Removing and Cleaning the Prism

Removing and cleaning the prism involves the same procedure as used for the window, except the prism is held in place with two set screws.

1. Disconnect the BNC cables from the prism housing.
2. Remove the prism assembly from the resonator using the 5/64 Allen wrench. Place the prism assembly on a table with the prism facing up.
3. Loosen the two set screws on the side of the prism assembly, and remove the prism.
4. Use the same cleaning technique that was applied to the window.

Assembly is the reversal of removal.

7.0 Troubleshooting

Problem	Possible Cause	Solution
Monitor screen is blank.	Computer encountered an error during initial startup.	Occasionally, the computer will display an error message that is not seen on the touch screen. Attach a higher resolution monitor to see the displayed error. Generally, it is a request to press a key to continue.

Problem	Possible Cause	Solution
Pressure rises during a zero count.	Inlet tubing is clogged.	Open the access panel and check the small-diameter conductive tubing. Repace if necessary.
The Raw and Fit curves on the Acoustic tab do not overlap.	There is a cabling problem.	Make sure the resonator is grounded and the microphone cable is connected.

8.0 Housekeeping Channels

PO_dB: The peak acoustic pressure during acoustic calibration. If the instrument's microphone sensitivity changes, this channel is meant to reflect these changes. However, if measured pressure stays constant, **PO_dB** should remain stable.

Phase_deg: The relative phase between the microphone and the laser power modulation. The Phase_deg should always be very close to zero when there is a lot of signal. When there is no signal, this channel should be random between -180 and 180 degrees.

AverageBackgroundSubtractedBabs_1/Mm and **BscaBackGnd_1/Mm:** The background stability for absorption and scattering measurements, respectively. Background is determined during instrument zero. Background readings change with variables like temperature, but these channels should stay relatively constant during stable environmental conditions. Dramatic changes indicate a problem.

NoiseEqBabs_1/Mm: The uncertainty estimate for the measurement of Babs_1/Mm . This is a useful metric of instrument response. For the same laser power, the instrument should have the same NoiseEqBabs.

ADrange_v: The amplification factor in the programmable preamplifier. This should be around 200 (voltage gain on the mic preamp) and definitely greater than 50.

PhotoDiodeCal_mWperVolt: The calibration factor used for the laser power measurement. This should be a constant.

LaserPower_mW: The laser power at the operating frequency. This channel is used when calibrating the instrument by extinction measurement. It should remain fairly constant unless heavy aerosol loadings are found. Even in heavy-loading conditions, LaserPower_mW should not fluctuate by more than 5% in a short period of time.

Other housekeeping channels are used to gauge the thermodynamic properties of the sample air (temperature, pressure, and RH), and to indicate when the instrument is zeroing. The remaining channels are for seldom-used features like running averaged data, which averages data during specific user-chosen episodes.

PART II: Software

8.1 Introduction

The computer system for the Three Wavelength Photoacoustic Spectrometer (PASS-3) is a CyberResearch CZEG Single-Board Computer. It has the following features:

- A Pentium 2.4 GHz processor
- 1024 MB of RAM
- A National Instruments PCI-6601 timing card
- A National Instruments PCI-6143 DAQ interface card
- 80-GB hard drive for program and data storage
- One USB 2.0 port on the front panel
- Ethernet 100/10Mbps LAN controller (RJ-45 connector) on the rear of the unit

Users can communicate with the instrument through either the provided touch screen or a standard keyboard and mouse.

Software for the PASS-3 is written in LabVIEW and is provided as an executable program that allows no user modifications. The software revision level is shown on the **Configuration** tab of the PASS-3 program.

Two programs are provided:

- **PASS-3.exe** is the main program for operating the PASS instrument.

- **Cal_write3.exe** allows the user to set the calibration coefficients used by the **PASS-3.exe** program

9.0 PASS Control Program, PASS-3.exe

9.1 PASS-3.exe Startup

The PASS-3 program normally loads during startup after the computer has booted. In the event the program does not load, double-click on the PASS-3.exe icon on the desktop. Press or left-click the white arrow in the upper left corner of the program window (Figure 12) to start the program. When the program is running, the arrow will turn black.

Stop program execution by pressing the green **VI CONTROL** toggle button (). The button will turn black and the indicator above will turn to OFF. Using this button rather than pressing the black arrow above it will ensure that the instrument shuts down properly.

To restart the program, first make sure the **VI CONTROL** button is **ON**, and then press the white arrow above the button.

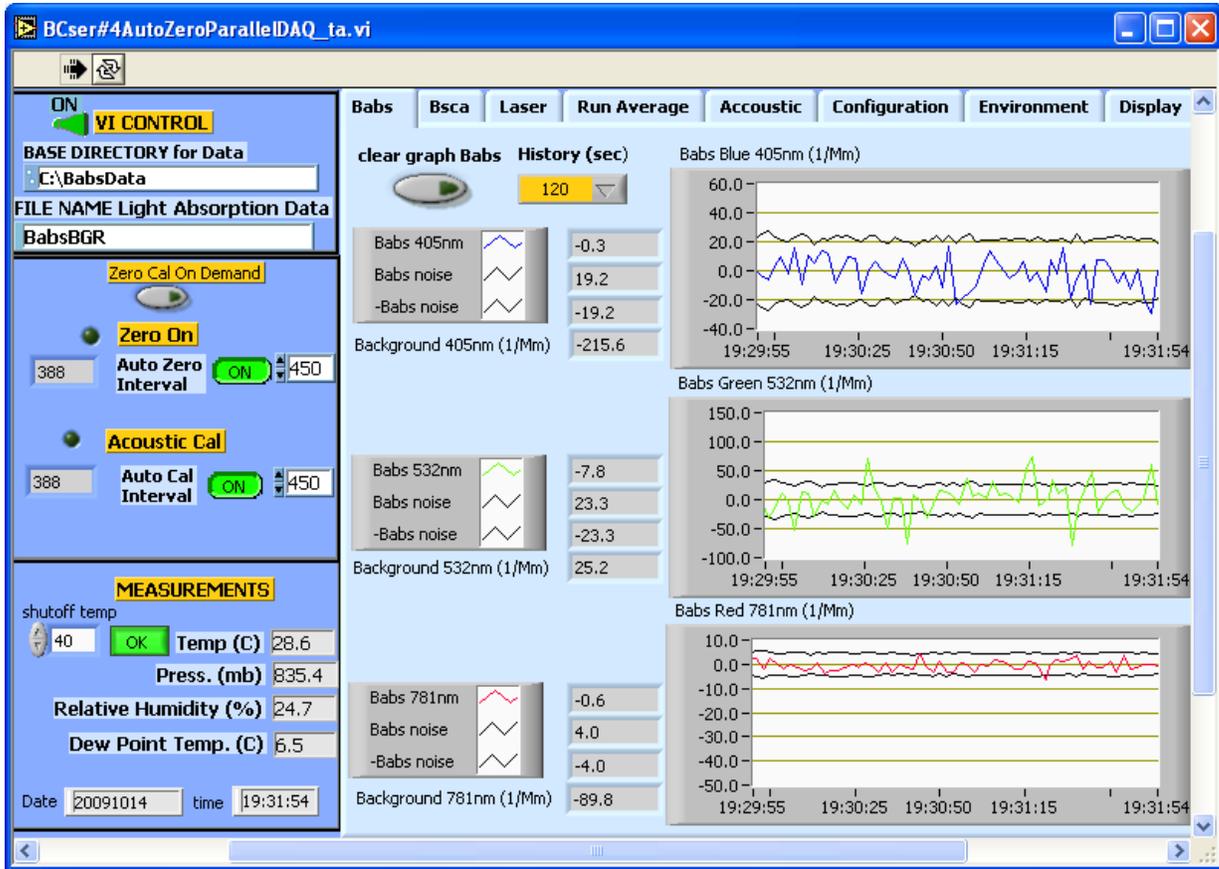


Figure 12: PASS-3 Control Program on Startup (Babs Tab)

The PASS-3 screen features a program control panel on the left side of the screen. This panel appears whenever PASS-3.exe is running. On the right side of the screen is a tab-based display that allows the user to access different features of the PASS-3 programs. More information about each of these displays is provided below.

9.2 Program Control Panel

The Program Control Panel on the left side of the PASS-3 display window is shown below.

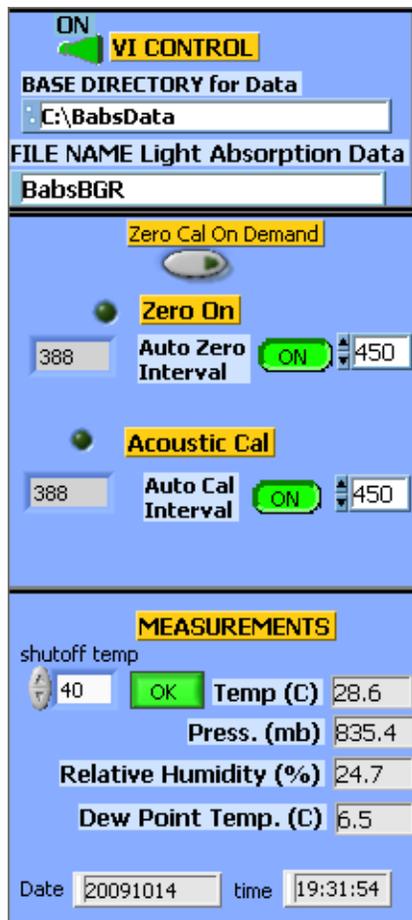


Figure 13: Program Control Panel

The top section of the panel lists the file that the PASS-3 is recording data to, along with the directory where the file is located.

The middle section of the panel allows users to control zeroing and acoustic calibration. Zeroing determines the B_{scat} and B_{abs} background readings, i.e. the readings with no aerosols present. Acoustic calibration determines the resonance frequency finding, f_{res} , and Q , which is the resonator quality factor. During normal ambient conditions, these two processes occur at cyclic intervals determined by the **Auto Zero Interval** and the **Auto Cal Interval**. These intervals control the number of regular measurements that occur in between zeroing and calibration. In Figure 13, for example, both **Auto Zero Interval** and the **Auto Cal Interval** are set to 450 measurements, so $450 * 2 = 900$ seconds = 15 minutes would elapse between every zeroing and calibration process. The number of measurements between auto zero and auto calibration should be set to between 200 and 1800.

The count-down times until the next zeroing and calibration begins are listed on the left of the middle panel. In Figure 13, for example, both zeroing and calibration will begin after the PASS-3 has taken 388 more measurements.

If the PASS-3 is operated in an environment with stable temperature, pressure, and humidity, then more time can elapse between zeroing and calibrations. If these conditions are fluctuating rapidly, however, the elapsed time should be relatively short.

Occasionally, an acoustic calibration and zero may want to be performed on demand. Press the **Zero Cal On Demand** button, and both an acoustic calibration and zero will be performed after the completion of the current measurement. The count-down displays will be reset after the operations are completed.

The bottom section of the Program Control panel displays sample air temperature, pressure, relative humidity and dew point temperature. These measurements are taken before the sample air stream exits the instrument. The current date (in yyymmdd format) and time are displayed below these variables. In the upper left of this section is the **shutoff temp** control, which allows users to specify a temperature threshold above which the instrument turns off.

9.3 Babs Tab

The **Babs** tab (Figure 12) displays absorption coefficient data for the three wavelengths. For each laser frequency, the program displays current tabular data and time-series data.

The first row of tabular data is the absorption coefficient (**Babs [laser frequency]**) in 1/Mm, which is followed by the noise level (**Babs Noise** and **-Babs Noise**) of the current reading. The last row displays the background absorption value (**Background [laser frequency]**). This value represents the background signal caused by stray laser light hitting the resonator.

The laser modulation frequency is displayed for each laser wavelength above its respective graph.

At the top of the **Babs Tab** is a button to clear the graph displays (**clear graph Babs**). There is also a **History (sec)** control, which allows users to specify how far back in time graph data should be displayed. In Figure 12, for instance, the program is set to display data acquired in the previous 120 seconds = three minutes.

9.4 Bsca Tab

The **Bsca** tab (Figure 14) displays scattering data. The format is similar to the **Babs** tab. There are indicators for the scattering coefficient (**Bsca**), scattering background (**Background**), a graph of the recent scattering values, and a button to control chart history and one to clear the graph. These buttons work similarly as the ones described in section 9.3.

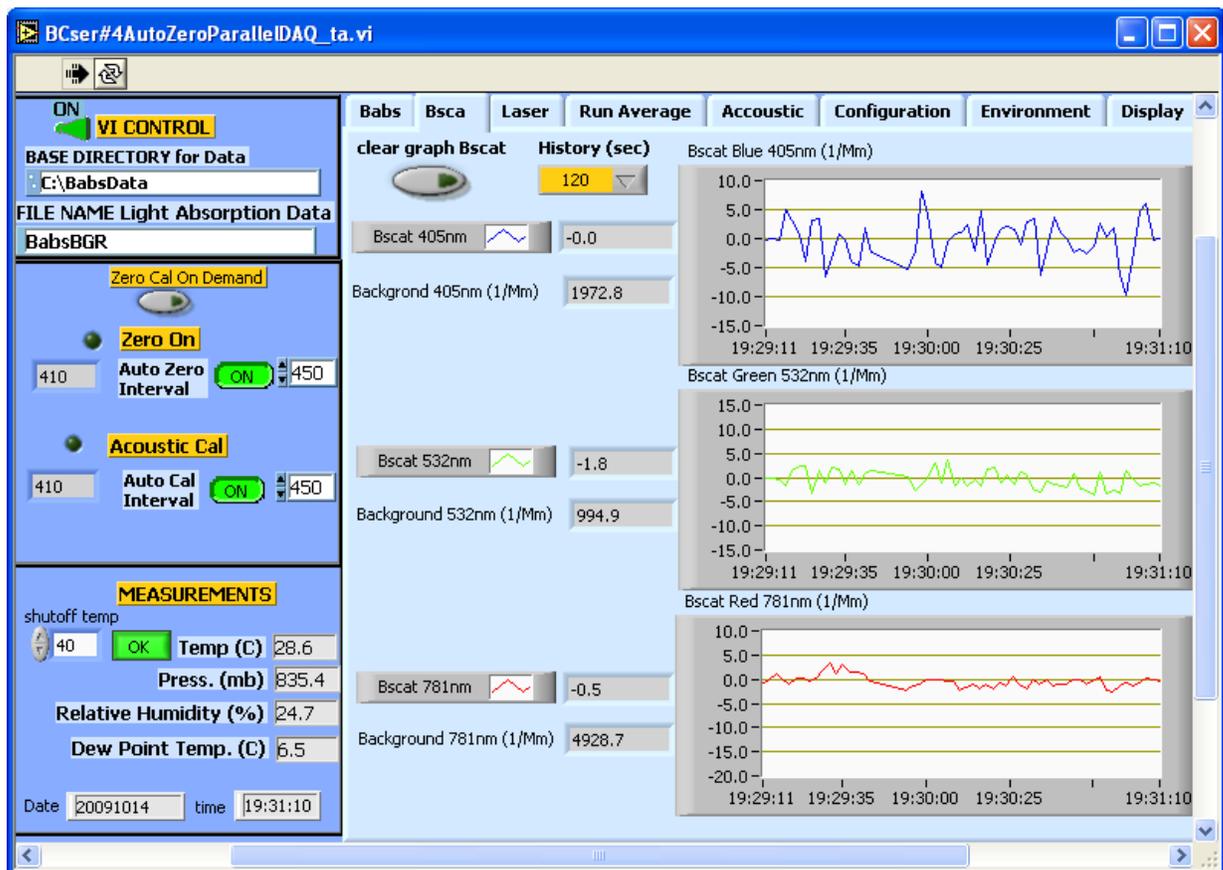


Figure 14: Bsca Tab

9.5 Laser Tab

The Laser tab (Figure 15) monitors laser power for the PASS-3's three lasers.

The clear graph Laser button allows the user to clear the graph displays, while the History (sec) indicator lets users specify how many seconds of previously acquired data the graphs should display.

Tabular data for the current moment in time is displayed on the left side of the Laser tab. The program displays three channels for each laser frequency:

- Laser Power in mW (117.4 for the 405-nm laser in Figure 15)
- The phase in degrees of the current Babs reading (**Babs Phase**)
- The phase in degrees of the Babs background (**background phase**)

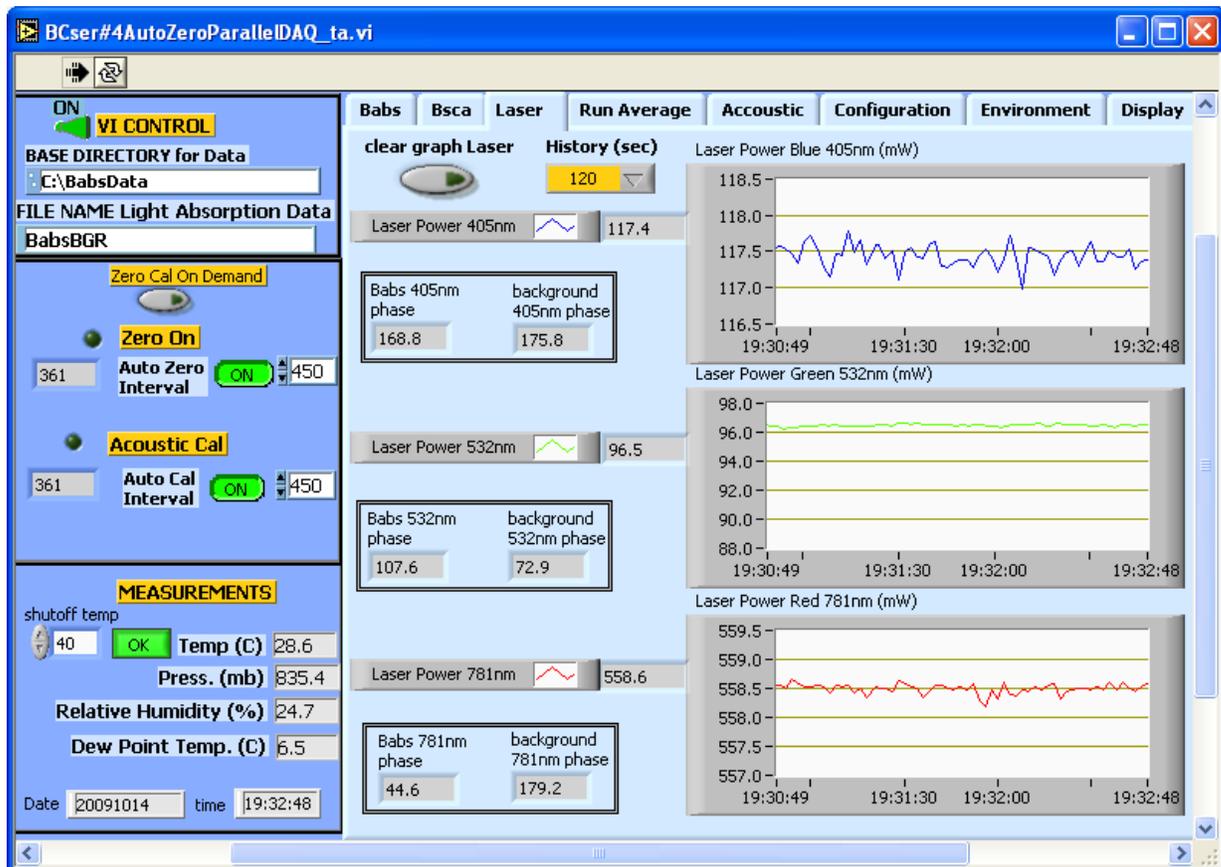


Figure 15: Laser Tab

9.5.1 Calculation of Phase and Background Phase

Background phase ϕ_{bg} is calculated during the auto-zeroing process and represents the phase of the background signal relative to the phase of the laser power signal. The resulting phase of the B_{abs} signal, ϕ , is calculated as follows. The B_{abs} signal can be viewed as a complex number $re^{i\phi}$ where $r = B_{abs} / \cos\phi$. (B_{abs} reported by the PASS-3 is the real part of $re^{i\phi}$.) Background signal is expressed as $r_{bg}e^{i\phi_{bg}}$, where $r_{bg} = B_{abs,bg} / \cos\phi_{bg}$. ($B_{abs,bg}$ reported by the PASS-3 is the real part of $r_{bg}e^{i\phi_{bg}}$.) Let ϕ_{sig} represent the phase of the B_{abs} raw signal relative to the phase of the laser power signal, and let $B_{abs,sig}$ represent the real part of the complex representation of the raw signal $r_{sig}e^{i\phi_{sig}}$. Then the resulting B_{abs} background-subtracted value is calculated as $re^{i\phi} = r_{sig}e^{i\phi_{sig}} - r_{bg}e^{i\phi_{bg}}$.

When no absorption signal is present, e.g., a filter is on the inlet, the phase ϕ will be random ($-180 < \phi \leq 180$). On the other hand, during sampling of high concentrations of absorbing aerosol, the phase ϕ will approach zero.

9.6 Run Average Tab

The **Run Average** tab (Figure 16) allows the user to start and stop an averaging time period. This can be done either manually or automatically at user-specified time intervals.

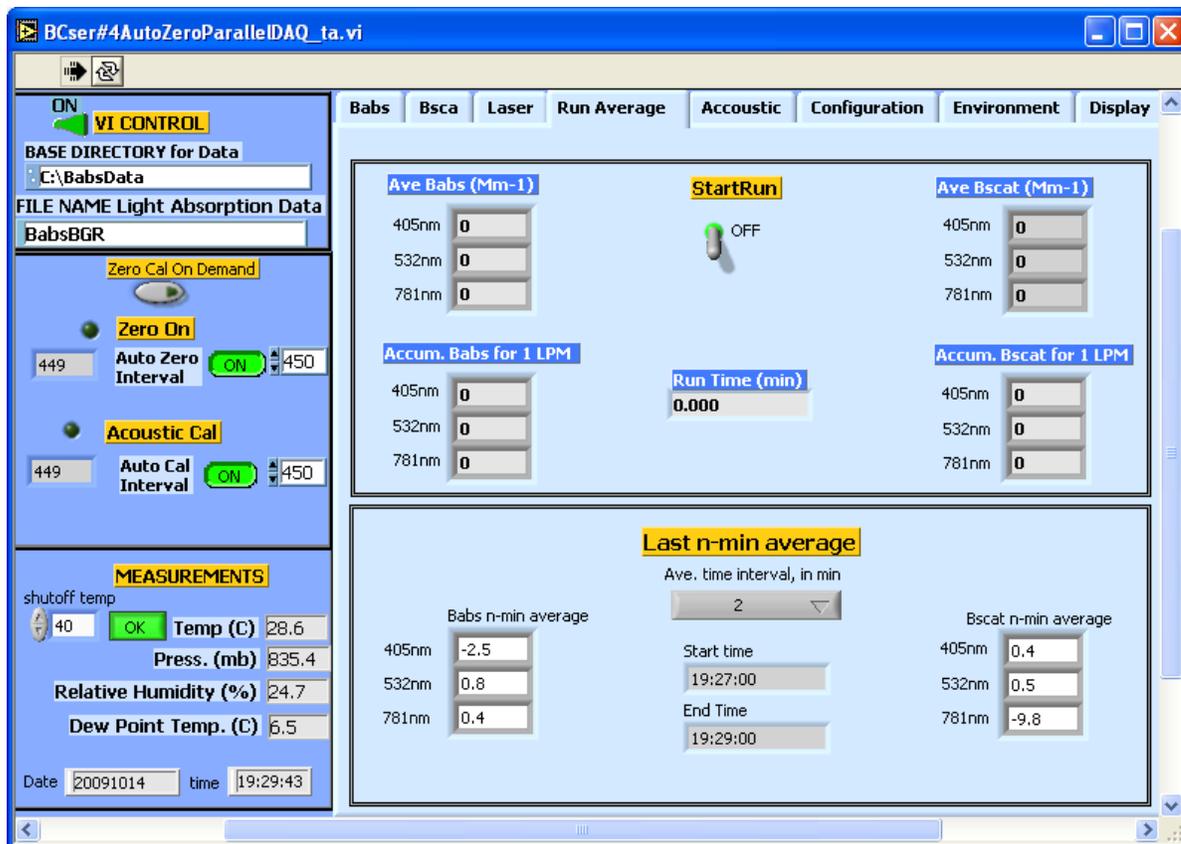


Figure 16: Run AverageTab

9.6.1 Starting a Data-Averaging Session Manually

To start an averaging period manually, use the top panel on the **Run Average** tab. Switch the **StartRun** switch to the **ON** position. The fields in the panel will display the following information:

- Average values in 1/Mm for Babs and Bsca
- Accumulated values in (m³)(1/Mm) for Babs and Bsca, assuming sampling at 1 liter per minute (LPM)
- Run time of the averaging session

Note that multiplying the accumulated values for Babs by the user-determined efficiency factor for the given laser wavelength will produce an estimated of black carbon accumulated during the run.

To stop averaging data, change the **StartRun** switch to the **OFF** position.

Averaged data will be stored in the regular PASS-3 output file, i.e. the file path and name displayed in the top left corner of the program window. Note that averaged data are for the current averaging session only; they are not a running average from all previous averaging sessions.

9.6.2 Setting up Automatic Data-Averaging Sessions

The PASS-3 program also allows users to average data automatically at specified intervals. To start averaging data automatically, use the gray control labeled **Ave. time interval, in min** to select the desired time of the run. The program will then start averaging data. The panel will display the following information:

- Average values in 1/Mm for Babs and Bsca for the most recently completed averaging session
- Start and end times of the last completed session. These will occur on the minute.

Unlike the manually acquired averaged data, automatically acquired data are written to a separate output file. This file is located in the same directory as the main PASS-3 output file, and its name has the format `n-minAve_[Mainfile]_yyyymmdd`. If the user initiates more than one averaging session, results from later sessions are appended to the existing file.

9.7 Acoustics Tab

Information about the last acoustic calibration is found on the **Acoustic tab** (Figure 17). The data and time of last calibration is located in the center top part of this tab. Below the date and time is the initial guess used for finding the resonance frequency of the acoustic chamber. A graph of the resonance curve is displayed in the middle of this tab with three indicators about the graph. They are the resonance frequency (f_0 (Hz)), quality factor (Q) of the resonance curve, and the pressure on resonance (P_0 (dB)). The lower part of the **Acoustic** has a box displaying the frequency in Hz that the PASS-3's three lasers are modulated at.

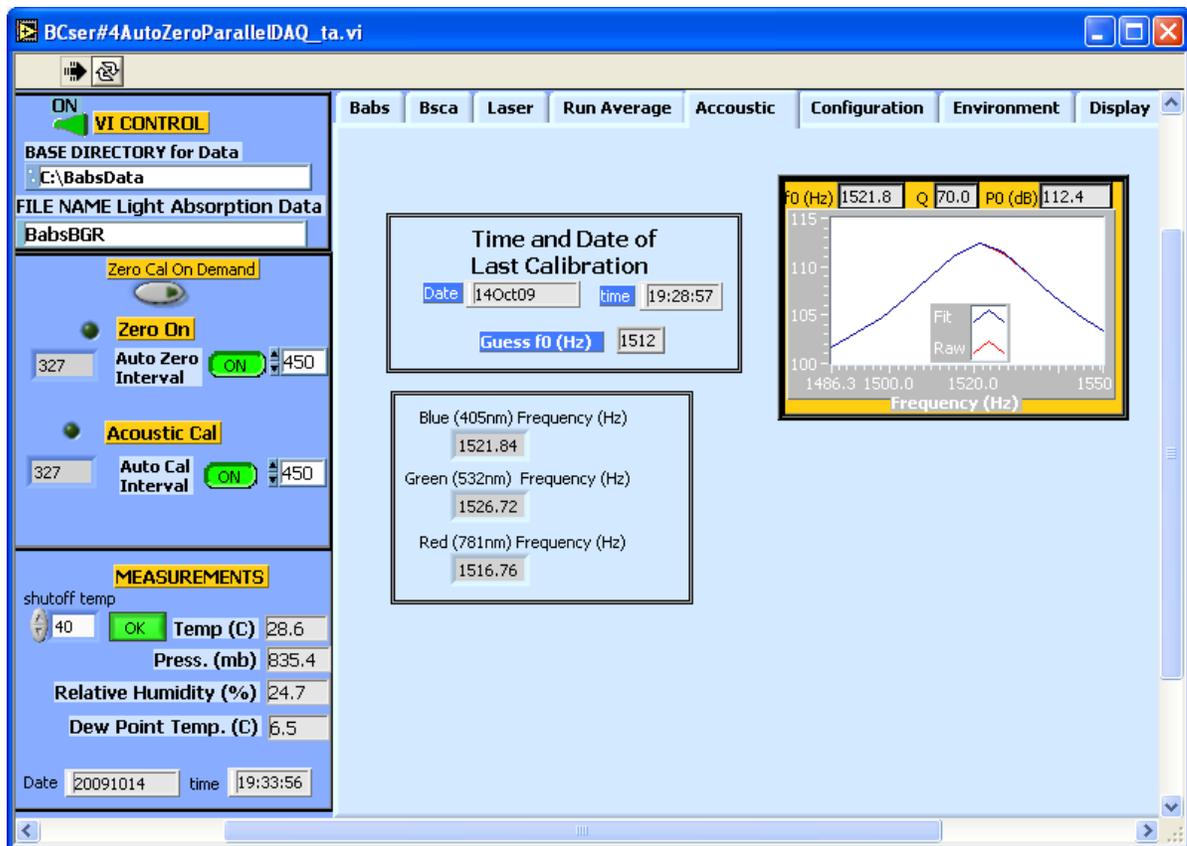


Figure 17: Acoustic Tab

9.8 Configuration Tab

The **Configuration** tab contains calibration and configuration information as well as the version number of the PASS-3 software. This information is only valid after the program has been started. The calibration values displayed in the gray fields cannot be changed on this screen; to modify them, use the **Cal_write3.exe** program (see section 10.0). Values displayed in white fields can be changed on the **Configuration** screen.

Microphone Calibration Factor (mVolts/Pascal): This value determines how the sound wave measured by the microphone determines the B_{abs} values generated by all three lasers.

Amp Gain Factor: The amplification gain factor currently being used by the microphone. The PASS-3 will automatically lower this gain if the measurement is out of range; in this case, the outlier measurement gets thrown out. **Amp Gain Factor** will not rise above the value the user stipulates in **AMP Max Gain**.

Phase Corr: The correction factor for the phase of the laser power signal. Each of the PASS-3's lasers has its own correction factor. These can be changed during calibration using the **Cal_write3.exe**, but this normally will not need modification.

Cal Babs: The laser-specific correction factor for the B_{abs} measurement. This value is determined by the linear regression performed during calibration.

Cal scattering: The laser-specific correction factor for the B_{scat} measurement. This value is determined by the linear regression performed during calibration.

Photodiode Cal: The laser-specific correction factor for the photodiode measurement. This may be changed during calibration if the laser calibration is being changed, and it must be done separately for each laser wavelength.

Test Acoustic Performance Button: A rarely used feature occasionally employed during DMT-assisted troubleshooting measures. This button should be **OFF** (green) during normal operation.

AMP Max Gain: The maximum gain amplification used by the microphone, which should not exceed 200. **Amp Gain Factor** should never exceed the Max Gain.

Microphone Measuring Time (sec): The time in seconds that it takes the microphone to make one measurement. The default value is 2.0.

Df(Hz): The difference in modulation frequencies of the lasers. Typically this is set to five Hz.

Make Current Values Default button: An option that allows the user to save the current configuration parameters as the defaults. These parameters are saved in the file `C:\BabsData\PASS-3_Config.ini`.

UDP Settings: The User Datagram Protocol settings used by the PASS-3. The factory defaults for these settings are as follows:

- Data Stream = UDP Data Stream
- Local Port = 58431
- Time-to-live (TTL) = 1
- Multicast Address = 234.5.6.7
- Send to Port = 58432

Number of zero averages: The number of measurements used in each average during zeroing. The PASS-3 does not average raw 16K Hz data, but during zeroing it is desirable to average processed data to decrease the noise in the Babs background measurement. Microphone measuring time during zeroing will equal to $2 * (\text{Number zero averages})$ seconds. The factory default is 16, but this can be changed for greater accuracy (more measurements) or faster turnaround (fewer measurements).

Press slope and Press offset: Coefficients used in calculating the pressure reading from the pressure transducer, as follows:

$$\text{Pressure (mBar)} = [\text{Pressure voltage from transducer}] * \text{Press slope} + \text{Press offset}$$

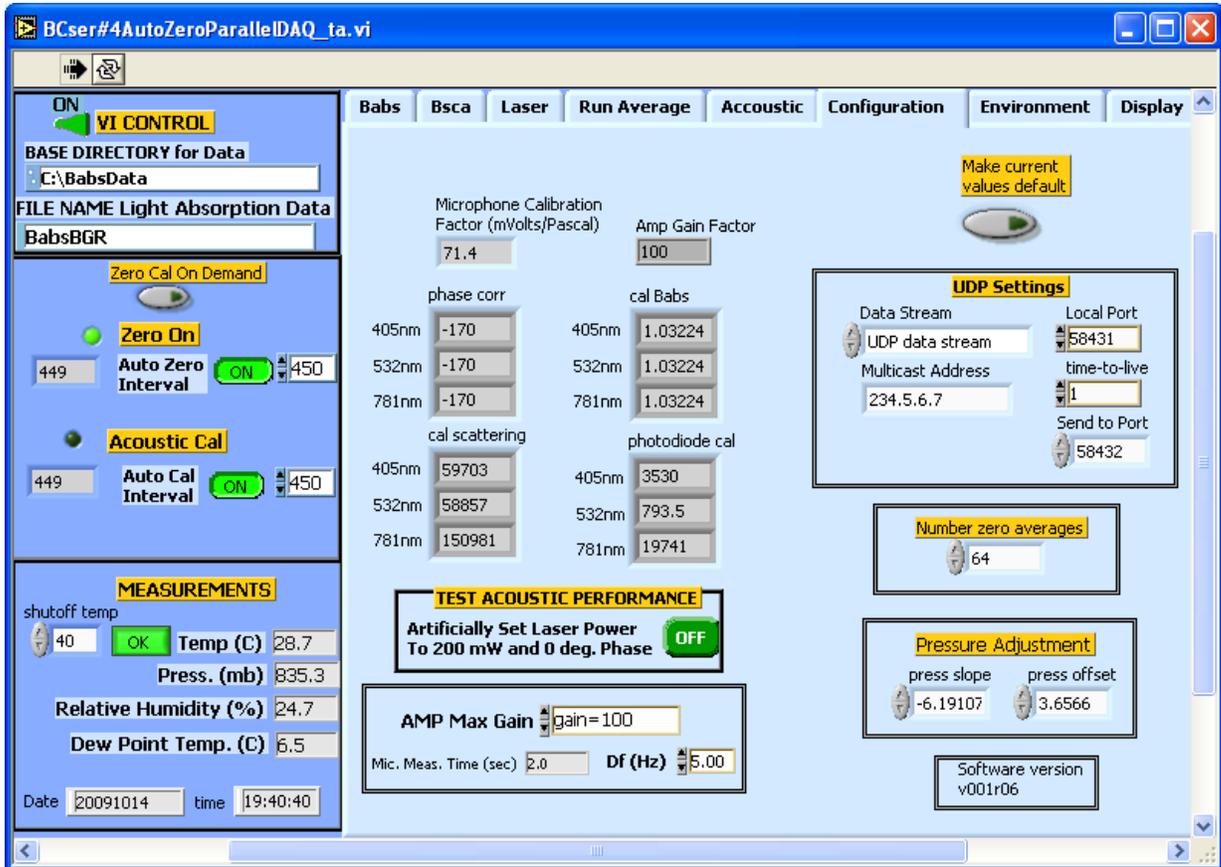


Figure 18: ConfigurationTab

9.9 Environment Tab

The Environment tab (Figure 19) provides time-series information about ambient conditions such as temperature, pressure, and relative humidity. Pressing the **clear Graph Environment** clears the data from the display, while the **History** drop-down box allows the user to select the length of time for which historical data are displayed. In Figure 19, for instance, data are displayed for the previous 20 minutes (1200 seconds).

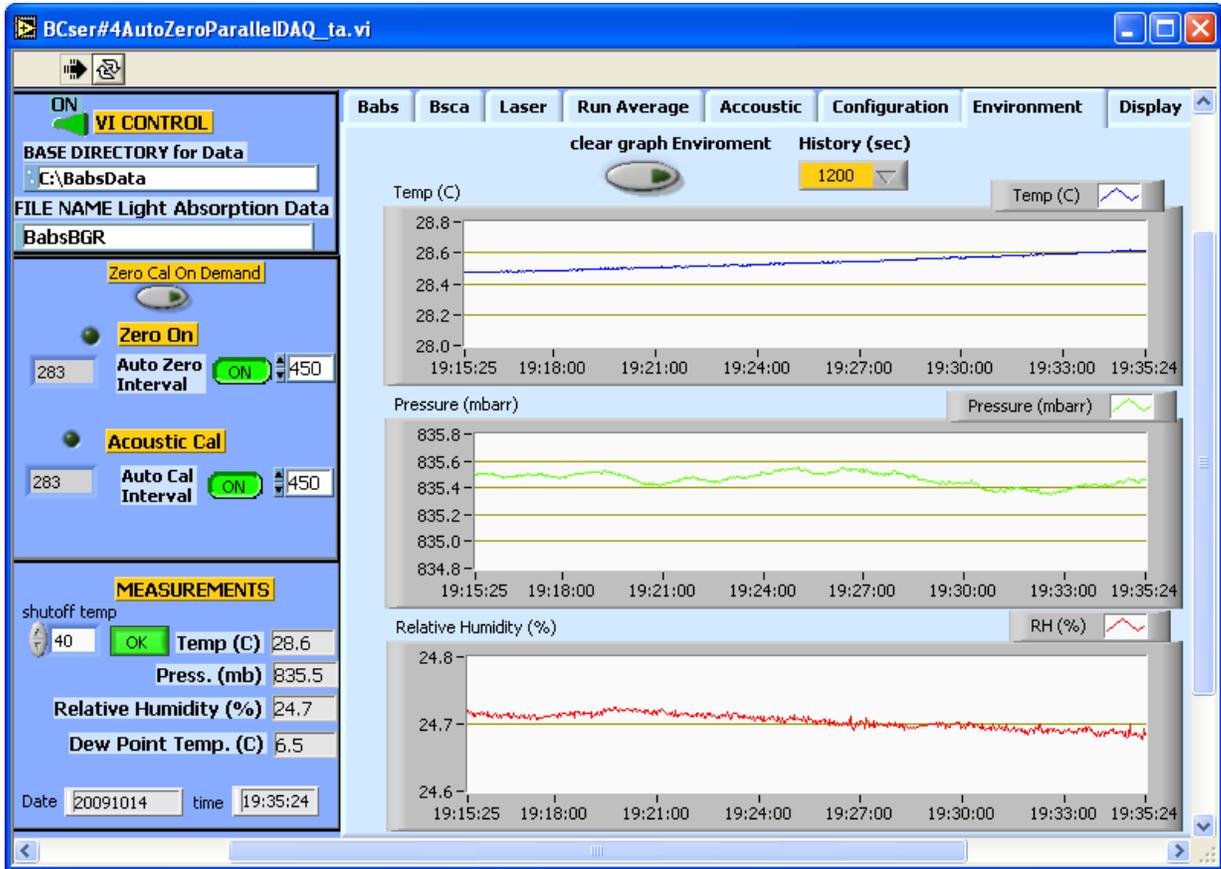


Figure 19: Environment Tab

9.10 Display Tab

The Display tab (Figure 21) allows the user to display the front panels of some of the control program's sub-vis or sub-programs. They are mainly used in diagnosing problems with the instrument and normally are not opened.

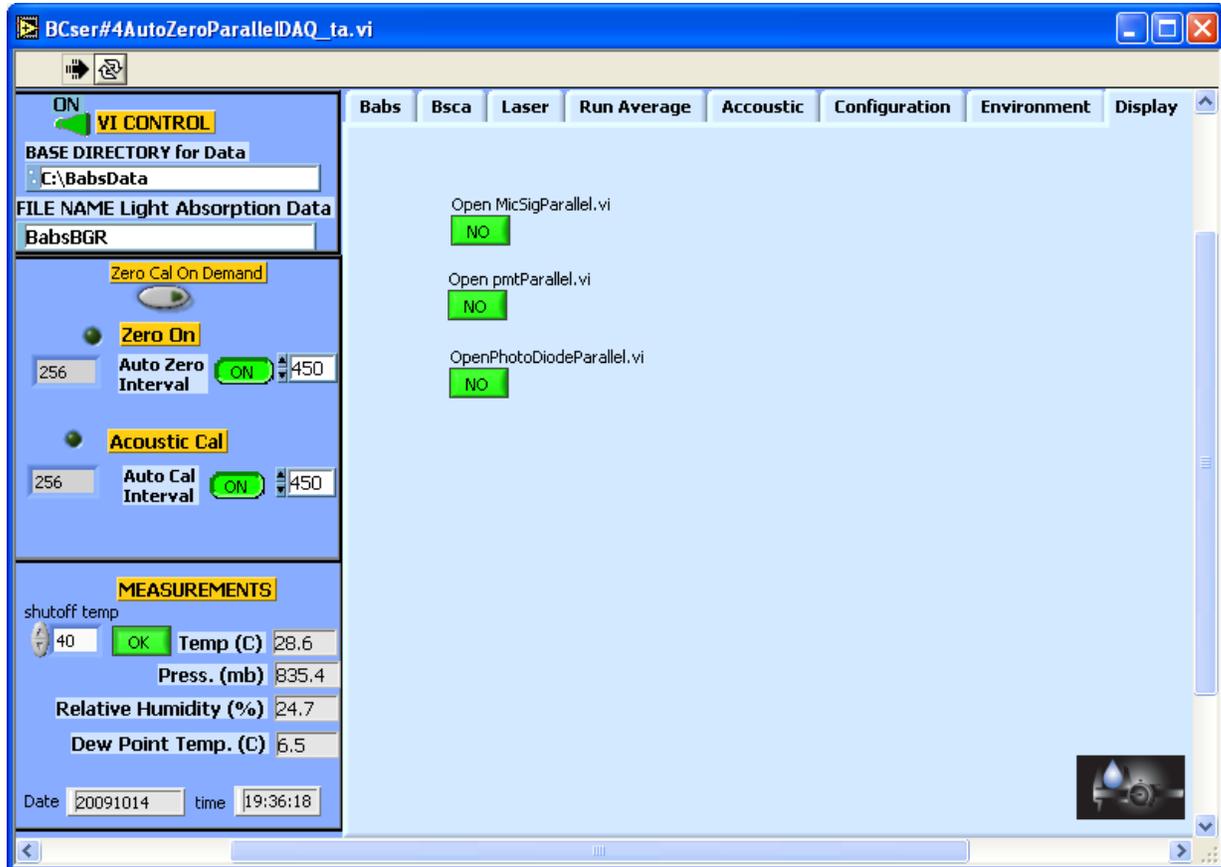


Figure 20: DisplayTab

10.0 Calibration Program Cal_write3.exe

10.1 PASS calibration program

The program *Cal_write3.exe* is used to change the various calibration parameters and can be found on the desktop. These calibration values are stored in the file C:\Babsdata\calibration_PASS-3.txt. Just double click on the *Cal_write3.exe* icon on the desktop to bring up the front panel (see Figure 21). Start the program by pressing on the white arrow in the upper left corner of the program window. The arrow will change to black while the program is running.

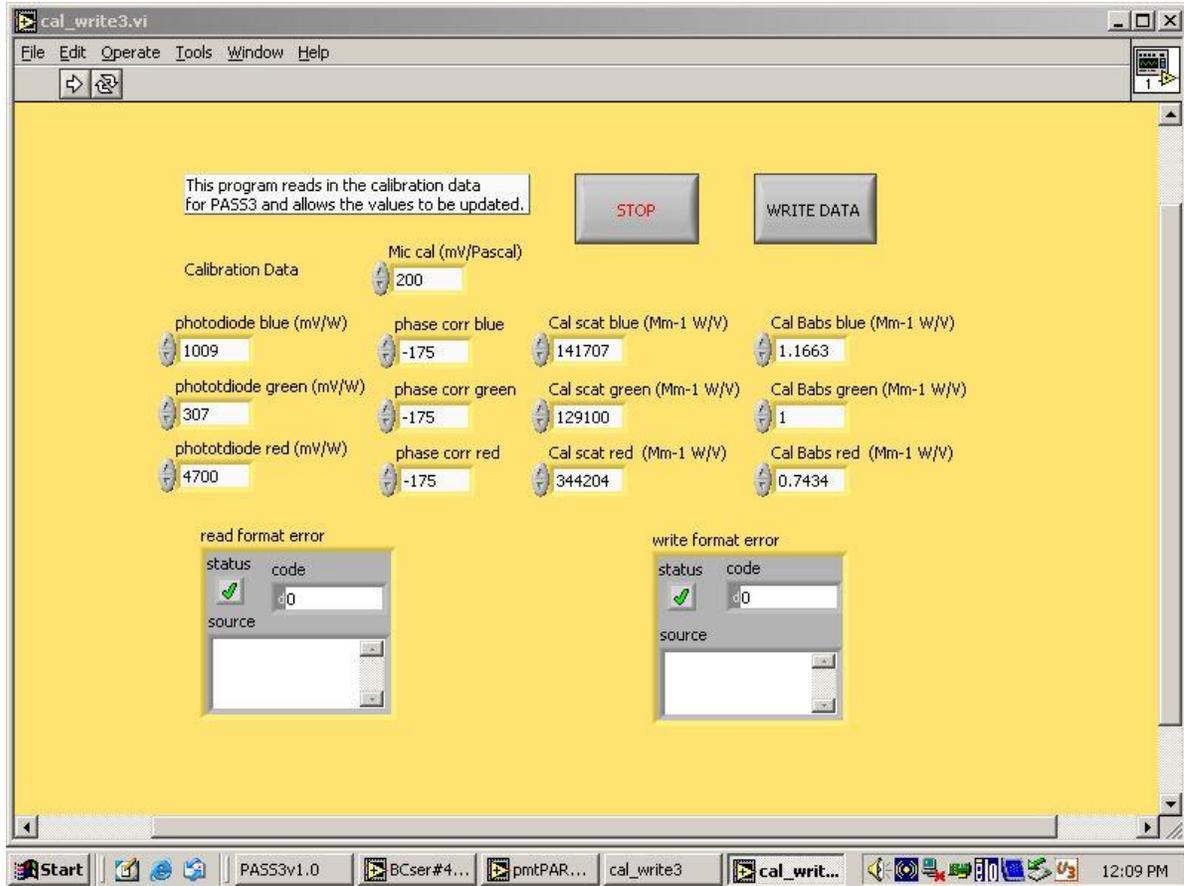


Figure 21: Cal_write3.exe Program

10.2 Updating Calibration Parameters

When **Cal_write3.exe** starts up, it displays the calibration parameter values stored in the file `C:\Babsdata\calibration_PASS-3.txt`. Clicking on a corresponding indicator changes a calibration parameter. When all the changes have been made, click on the **WRITE DATA** button to update the calibration file. A system prompt (Figure 22) will appear; press the **Replace** button to overwrite the old values. The program will stop execution after the file has been updated or the **Cancel** button has been pressed.

Pressing the **STOP** button will terminate the program and no calibration parameters will be updated.

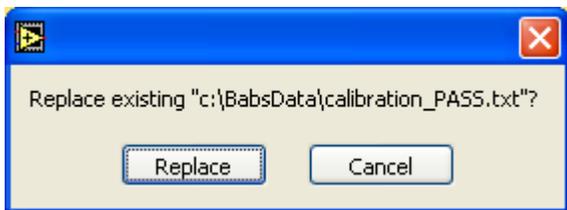


Figure 22: Replacement Prompt

11.0 PASS-3.exe Output File Format

11.1 Overview

Output from the *PASS-3.exe* program will be stored in the default text file `c:\Babsdata\yyyy_mm_dd\BabsBGR_yyyymmdd.txt` where **yyyymmdd** represents the current data (yyyy=four-digit year, mm=two-digit month, and dd=two-digit day). To change the default output file, type a new file name and/or path into the relevant fields in the PASS-3 control program, as shown in Figure 23. Then click on the check mark in the menu bar in order for the changes to take effect. **Note:** These changes will only be in effect while the program window is opened. If you close the window, then the default values will appear the next time the *PASS-3.exe* program is opened.

If PASS-3 is used in multiple sampling sessions during one day, the data from later sessions will be appended to the already existing file.



Figure 23: Changing Base Directory and/or File Name for Output Data

11.2 File Format and Data Channel Definitions

The output file of the *PASS-3.exe* program has 38 comma-delimited columns. Each column stores the results of one PASS-3 data channel, and each row in the file contains

data for a particular sampling instance. Sampling instances are normally two-seconds apart, but data gaps will appear when the PASS-3 is zeroing.

The PASS-3 channels are defined below. *Note: In many cases, the same data gets reported for all three PASS-3 laser wavelengths. In such instances, the definitions below have been generalized so that [Color] in the channel definition indicates the definition pertains to three possible channels, one each for the blue, green, and red lasers. For instance, the entry for Babs[Color]_1/Mm applies to BabsBlue_1/Mm (at 405 nm), BabsGreen_1/Mm (at 532 nm), and BabsRed_1/Mm (at 781 nm).*

AccumulatedBabsfor1LPM[Color]_1/Mm: The accumulated B_{abs} values in $(\text{m}^3)(1/\text{Mm})$ collected during a manually instigated averaging session (see section 9.6.1). These accumulated values assume sampling occurs at 1 liter per minute (LPM), and they tally the reported values only from the current averaging session.

AccumulatedBscafor1LPM[Color]_1/Mm: The accumulated B_{scat} values in $(\text{m}^3)(1/\text{Mm})$ collected during a manually instigated averaging session (see section 9.6.1). These accumulated values assume sampling occurs at 1 liter per minute (LPM), and they tally the reported values only from the current averaging session.

ADrange_v: The range in volts for the analog-to-digital converter. This is normally 5 V.

AmpGain: The amplifier gain on the microphone. This is normally 200.

AverageBackgroundSubtractedBabs[Color]_1/Mm: The average of the absorption coefficient B_{abs} measurements (1/Mm), which have been adjusted for the background signal.

AverageBackgroundSubtractedBscat[Color]_1/Mm: The average of the absorption coefficient B_{scat} measurements (1/Mm), which have been adjusted for the background signal.

AveragePhaseSubtracted[Color]_deg: The average phase in degrees of Babs for the relevant laser wavelength.

Babs[Color]_1/Mm: The absorption coefficient in 1/Mm, B_{abs} , measured at the relevant laser wavelength.

Bsca[Color]_1/Mm: The scattering coefficient in 1/Mm, B_{scat} , measured at the relevant laser wavelength.

BscatCal[Color]_mWperVolt: The B_{scat} calibration factor for the relevant laser wavelength.

CurrentAveBabs[Color]_1/Mm: The averaged B_{abs} values in 1/Mm collected during a manually instigated averaging session (see section 9.6.1). These values assume sampling occurs at 1 liter per minute (LPM), and they average only values from the current averaging session.

CurrentAveBscat[Color]_1/Mm: The averaged B_{scat} values in 1/Mm collected during a manually instigated averaging session (see section 9.6.1). These values assume sampling occurs at 1 liter per minute (LPM), and they average only values from the current averaging session.

DATE: The date in *yyyymmdd* format.

DewPointTemp_C: The dew point of the sample air in °C.

DoingARunIFunity: A Boolean channel that indicates whether the PASS-3 is doing a run average. Yes if = 1, otherwise = 0

f0_(Hz): The resonance frequency in Hz.

GMTJulianDateBeforeMeas: The Greenwich Mean Time Julian Date before measurement.

GMTJulianDateAfterMeas: The Greenwich Mean Time Julian Date after measurement.

LaserPhase[Color](deg): The phase of the laser power reading for the relevant laser.

LaserPower_[Color]mW: The power in mW used by the relevant laser.

MicCalFactor_mV/Pascal: The microphone calibration factor.

NoiseEqBabs[Color]_1/Mm: The B_{abs} noise equivalent for the relevant laser.

Phase[Color]_deg: The phase of the B_{abs} for the relevant laser.

PhotoDiodeCal[Color]_mWperVolt: The photodiode calibration for the relevant laser.

P0_dB: The acoustic pressure at resonance.

Pressure_mb: The pressure in the acoustic resonator in mBar—i.e., sample inlet pressure.

Q: The quality factor, normally around 75 @ 1013 mBar.

RH_%: The relative humidity of the sample air measured inside the instrument. This should stay below 70% for optimum performance.

Temperature_C: The temperature in °C of sample air measured inside the instrument. This temperature should stay in the 10-40° range for optimum performance.

TIME: The time in *HH:MM:SS* format.

TIMESECatWRITE: The seconds since midnight at the time of the data write.

Tlaser_C: This channel is unused.

ZeroAirFilterInIfUnity: A Boolean channel that indicates whether the PASS-3 is currently performing a zero air background measurement. If this indicator is 1, the instrument is doing a zero; if it is 0, no zero is currently being performed.

12.0 UDP Output Stream Format

12.1 Overview

There are two options for sending a data stream out over the internet via UDP multicast. Either no data are sent, or the instrument sends the complete data stream. To send no data, set the **Configuration** tab's **Data Stream** control to **No UDP Data Stream** (see Figure 18). To send the entire stream, set this control to **UDP Data Stream**. For more information about UDP parameters, see section 9.8.

On the receiving computer, the Multicast Address and Send to Port must match the values set on the configuration tab. Time to Live (TTL) is decremented by 1 when intercepted by a router. If the value is greater than 1 after being decremented, then the router will pass the UDP data stream on; otherwise, it will ignore the data stream. A value of 0 will cause the data stream not to be sent out anywhere (LAN or internet), while a 1 will cause the data stream to be sent out only to the local area network.

The output format of the UDP data stream is the same as the file output—namely, 38 comma-delimited columns (see section 11.2).

Appendix A: Revisions to Manual

Rev. Date	Rev No.	Summary	Section
10-28-09	B	Updated and revised sections on specifications, calibration procedures, housekeeping	Various
		Revised and expanded list of PASS-3 output channels	11.2
		Updated screen shots of PASS-3 program to reflect new software	Part II
4-5-10	B-1	Corrected "Technique" field in specifications table	1.2
		Updated Laser Safety Information	Frontmatter
8-4-10	C	Added information on NO ₂ absorption calibration method	5.2
8-22-11	D	Expanded Laser Safety information	Frontmatter, 6.0