Volume title:

Inherent Optical Property Measurements and Protocols: Best practices for the collection and processing of ship-based underway flow-through optical data

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1. Introduction

Continuous, flow-through measurements of temperature and salinity have been collected with thermo-salinographs for decades (e.g. Henin and Grelet, 1996), which has led to well-established protocols for quality control, archiving and distribution of such underway data (e.g. http://www.gosud.org/, http://ocean.ices.dk/data/underway/underway.htm). Chlorophyll fluorescence has also been integrated into such systems, with the first underway flow-through fluorometry dating back to the late 1960s (Lorenzen, 1966).

More recently, several research groups have begun collecting additional optical data using the flow-through systems installed on research vessels and ships of opportunity to take advantage of the availability of sea water pumped into the vessel (we do not discuss tethered systems). These “in-line” or “underway” data are able to provide data at spatial resolutions of 10-100 m. These measurement scales are not accessible with standard hydrographic surveys and enable characterization of sub-pixel variability in satellite ocean color (OC) data. Thus, data collected using this approach are useful for targeted science questions, but also for large-scale calibration/validation of satellite OC products (Werdell et al., 2013).

As the number of research groups making these measurements grows, there is a need to provide coordinated data collection and processing protocols to standardize methodology and data quality. In 2015, a NASA-sponsored workshop was organized to share such knowledge. Here, we discuss the essential issues associated with in-line data collection, provide recommendations on best practices for collection and processing and report on available software.

This report is organized as follows: First, we address the instruments and hardware associated with deploying an in-line system and discuss a number of considerations that can affect data Quality Assurance/Quality Control (QA/QC). Second, we address issues associated with processing of data from specific optical sensors that have been deployed in-line and software that is available for their use.

2 Optical sensors used in in-line systems.

The easiest optical sensors to integrate into underway systems are those designed for flowing or pumped sample (for example, flow-through fluorometers and transmissometers Other optical sensors can be integrated into underway systems using flow cells available as options from manufacturers, or custom-built. Common sensors included in underway systems are included in the list below.

Table: sensors deployed in flow-through systems

Transmissometers (beam attenuation):	Spectrophotometers (measurements of absorption)	Scattering meters	Fluorometers (CDOM, Chlorophyll)
WET Labs C-Star	WET Labs ac-9	WET Labs ECO series (2)	WET Labs ECO series (2)
WET Labs ac-9	WET Labs ac-s	HOBI Labs	HOBI Labs

		HydroScat sensors (2)	HydroScat sensors (2)
WET Labs ac-s		Sequoia LISST 100X (1)	WET Labs ALFA
Sequoia LISST 100X (1)			Seapoint (1)

Notes:

1. *Requires manufacturer-supplied flow cell or chamber*
2. *Requires custom-built chamber or tank to contain instrument sample volume*

It is assumed that a thermo-salinograph (typically a SeaBird SBE 45 or SBE 21) or equivalent is part of the in-line system, as well as a GPS, and that all instruments are synchronized in time. Daily synchronization is necessary to ensure all instrument data is merged appropriately in post processing; a time server can be set to facilitate this. It is also assumed that logging software and computer(s) are available to which data is transferred from the optical sensor(s) for time stamping and storage.

3 Water system consideration

3.1 Water source

Sample seawater typically enters a vessel from a "sea chest", a rectangular or cylindrical recess in the hull of the vessel providing an intake reservoir from which seawater is drawn; or directly via a thru-hull fitting. In either case, location at the ship's bow is preferred. In the case of a sea chest, a metal grating separates the open ocean from the sea chest, dampening the exchange of water and excluding large debris (centimeters in size) that might clog any downstream pump or plumbing. In order to measure properties with the in-line system that are as close as possible to those in the water outside the ship, it is critical that the sea chest is clean and not biofouled by filter-feeding organisms. We note that this can be difficult to assess without inspection by a diver. Vessels with thru-hull intakes (e.g., R/V Atlantis or schooner Tara) typically pump through a strainer basket (mesh size ~ 3-4 mm) and a vent loop to release accumulated air.

3.2 Feeding pump

Impeller pumps are the most common pump used in UNOLS vessels (US academic fleet) and can adversely affect particle assemblages (Cetinic et al., 2016). Diaphragm and peristaltic pumps are recommended in order to minimize artifacts introduced by the pump. Past comparison (Fig. 3B-C in Westberry et al., 2010), as well as recent comparisons between particle images collected from underway systems and Niskin bottles found very good agreement between the two water sources when using diaphragm pumps.

We have experience with the following pumps:

1. ARO air-operated diaphragm pumps (SABOR, NAAMES) http://www.arozone.com/en/products/diaphragm-pumps.html.
2. Shurflo electric pump (Tara). https://www.svb24.com/en/shurflo-pressurized-water-pump-aqua-king-ii-standard-3-0.html.

3. Graco Husky 1050E pump (NAAMES). http://www.graco.com/content/dam/graco/ipd/literature/flyers/345088/345088ENEU-A.pdf
4. Tapflo air-operated pump (KORUS, Falkor) http://www.tapflo.com/en/diaphragm-pumps/pe-ptfe-pumps/t100

Note that new or modified installations of feeding pumps and downstream scientific instruments often have initial problems with bubbles in the sample flow, a condition that severely affects the measurements of (mostly) particulate optical properties. Typically, adjustment of the flow such as increasing flow rates through instruments, increased application of debubbler(s), and addition of slight backpressure downstream of instruments solves the bubble problem entirely. However, vigilance is required as ship operations (e.g., maintaining station, bow thrusters) or increase in sea state while underway may also introduce bubbles in the flowing seawater. Note also that the flow from peristaltic, and especially diaphragm pumps, may be pulsed. Semi-rigid and softer tubing tends to damp this pulsation, and we have not found it to adversely affect optical measurements (i.e., we have not observed fluctuations in raw measurements at the pulsation frequency, nor significant particle breakage).

3.3 Plumbing

Similar to the sea chest, plumbing needs to be cleaned prior to cruises, typically by running water with a bleach solution through them or, if possible, by replacing the tubing system. Reducing the amount of contact between the input seawater and plumbing (including sea chest, pump, and plumbing to labs) leads to less opportunity to affect the optical properties of measured particles or introduce dissolved substances to the stream. Larger diameter pipes (i.e., sizing plumbing to favor laminar flow conditions) are also expected to reduce turbulent flow and potential consequent particle breakage. Thus, we anticipate better agreement between underway and in situ samples for short and wide pipes compared to long and narrow.

4. General considerations

4.1 Flow rate

Flow rate between 2-10 L/min has been found to work well, depending on instruments being deployed in the underway system and how much water is vented in de-bubbler(s) upstream of the instruments (see below). Flow rate considerations are important to assess delays between different instruments installed in series along the water path. It is a good idea to monitor the flow rate as well as the pressure within the system as it provides a diagnostic to check (especially when examining data post-deployment) when measurements change with no apparent reason.

4.2 Bubbles and debubbling

In addition to bubbles introduced by turbulence in the plumbing system, warming of the water and/or cavitation through the path can cause bubble formation. Further, during rough seas we experience significantly more bubbles in the system, likely due to exposure of the sea chest to hull turbulence.

In addition to the solutions to bubbles described in the pump section, we have found that the installation of a vortex debubbler (Ocean Instrument Laboratory, Stony Brook University, MSRC Vortex Debubbler, Model VDB-1, e.g. http://www.seabird.com/pdf_documents/VortexDebubbler_Oct2012.pdf) upstream of the instruments is necessary to remove bubbles. The debubblers are manufactured in two sizes: either 2- or 3-inch diameter models designed for flow rates of 10 or 20 liters per minute, respectively. Using multiple debubblers in series does reduce the bubble impact in rough seas; however it increases residence time in the plumbing system and increases exposure of particles to shear, possibly leading to particle breakage.

In addition, adding a constriction (i.e., valve or section of smaller diameter tubing) at the outlet of the system to create a slight backpressure has been found to help alleviate bubble issues. The backpressure may expose water leaks elsewhere in the system, however such leaks are important to identify as before introduction of the backpressure, they were likely points where air could leak into the system. Additionally, the use of a wye or tee fitting placed at a high point in the system with a valve to release trapped air (a “degassing Y”) is useful, especially if positioned between the particle filter and instruments to bleed air introduced into the system when changing the filter.

4.3 In-line filters

It is sometimes of interest to measure the properties of specific size ranges of particles or to use measurements performed with a specific filtered fraction as the blank for larger particles (see calibration below). We have found that industrial filters (similar to ones used for drinking water, but typically with tighter specifications, i.e., “absolute-rated”) work well, providing a large filter surface area which does not excessively constrict the flow (e.g., flow would go down by O(40%) between total and filtered). An alternative is to use the industrial filter as pre-filter, then into 0.2 um capsule filter (e.g. PALL Maxi Capsule 12112). Frequent switching between filtered and non-filtered operation after following a filter change helps reduce bubble problems associated with a new filter. Letting the new filter sit in water overnight before putting it in the flow system also helps alleviate bubble problems. Note that immediately after switching to filtered measurement, there may be a transient in measured optical properties as the slug of water trapped in the filter housing is flushed through the system (for example, scattering and fluorescence measurements may increase due to material that was produced in/on the filter). Such contamination needs to be removed and one has to be sure to take sufficiently long filter measurements for this artifact to be accounted for. This artifact (in addition to reduction in flow rate during filtered measurements as function of time) should also be used to evaluate the need to replace the in-line filter, such that if it takes several minutes to clear or the flow rate is excessively reduced (e.g., less than 60% of the non-filtered flow) it is time to replace the filter.

It is also possible to use a valve (either manual or automated) to periodically divert the sample seawater through a particle filter (typically 0.2-μm pore size) in order to measure filtered seawater, and by difference obtain “calibration independent” particulate optical properties (assuming the interpolation between the dissolved measurement provides a good estimate of the properties of the dissolved fraction when measurements of unfiltered seawater are made, which could be confirmed/assessed/interpolated using a CDOM fluorometer). In turbid waters, an additional pre-filter with a wider pore-size (e.g. 5-μm) can assist in preventing rapid filter clogging. This method of particulate measurements can provide highly sensitive and high-quality measurements of particulate optical properties (Balch et al., 2004; Slade et al., 2010; Werdell et al., 2013). Commercial systems for automating filtered seawater measurements are available (FlowControl-Lab, Sequoia Scientific, Inc.) which also include measurements of flow, useful to evaluate when to change filters and QC data post-deployment. Flow meters can also be custom built (e.g. http://www.instructables.com/id/How-to-Use-Water-Flow-Sensor-Arduino-Tutorial/). Similarly, if the backscattering sensor is placed after the valve/filter, measurements of the backscattering by the <0.2-μm fraction in addition to the bulk water can be made. A fluorometer in-line after the switch is also able to assess the contribution of CDOM to the measured chlorophyll (see below) and the validity of the use of interpolation between measurements of the dissolved fraction. It is also beneficial to increase the frequency of filtered measurements if working in regions where dissolved optical properties are expected to be more variable, such as in shelf waters or along frontal boundaries. Typically, 12-24 filtered measurement intervals per day (10-15 minutes per measurement) are more than sufficient in open-ocean waters.

For 0.2-μm filtration Sequoia and UMaine uses:
1. Filter housing, Cole Parmer part EW-01508-24
2. Spacer “sump extension adapter” for filter, Cole Parmer part EW-01508-96
3. Filters, Cole Parmer part EW-06479-18

Other filters used (with appropriate housing) are: PALL AcroPak Supor Membrane and the GE Osmonics Memtrex NY.

4.4 In situ vs. instrument temperature

Differences between the in situ water temperature and the instrument temperature can affect optical measurements in several ways. For example, ac-meter calibration tables rely on the instrument temperature being within a predetermined range of temperatures to apply the correct calibration coefficients (this range is found in the device file). We have also found that ac-meters that have not been properly purged for humidity can develop condensation on the interior of the instrument windows further contaminating the measurements when cold waters flow through them. To avoid these problems, immerse all or part of the instrument (especially detector-end pressure housing) in a bucket or other enclosure with flowing water (e.g., outflow from the instrument).

4.5 Contamination by ambient light

Instruments such as the LISST and the ac-meter absorption measurements are sensitive to ambient light. One needs to make sure that no ambient light can reach an instrument detector, e.g. by putting opaque black electric tape on plumbing entering/exiting the instrument, using black opaque tubing, and/or covering the setup with blackout material.

4.6 Enclosures for flat-faced instruments

Commercial backscattering meters and some fluorometers perform open path measurements. Therefore, they require an enclosure of known (and minimal) effect on the measurement in order to deploy them in-line. To determine accurate measurements it is also critical to assess (and later remove) the impact of reflections from the internal walls of the flow-through chamber on the measured signals. This can be accomplished by computing the difference between a measurement of pure water at a given temperature and salinity (obtained by filling the enclosure with high quality DIW water[1]). A large curved PVC elbow (septic clean-out), with the interior painted flat black, also can be used to minimize internal wall reflectance for backscattering measurements and is relatively inexpensive to fabricate.

4.7 Cleaning

Periodic cleaning is required to remove bacterial films from instrument windows and particles that may not get flushed out of the flat-faced instrument enclosure. We have found, for typical oligotrophic, open-ocean conditions, that weekly cleaning is sufficient while in meso- and eutrophic conditions, more frequent cleaning is needed. If, following cleaning, a significant change (drop) in signal is observed, fouling has likely degraded the previous data, which should be flagged accordingly and, if possible, corrected (for example by removing a trend). It is still unclear, however, whether it is better to assume a linear trend or an exponential trend, given that fouling organisms typically grow exponentially (Manov et al., 2004). For cleaning details (e.g., suggested solvents and/or detergents to be used) for specific sensors, refer to manufacturer protocols. We recommend using lens paper on all optical surfaces (e.g., windows, flow sleeves) to ensure that their properties do not change it time due to scraping with harsher materials. More careful procedures are warranted when cleaning heavily-fouled instruments, as optical surfaces can be damaged if grit is scraped across them. More frequent cleaning (e.g. daily) is recommended for the enclosures of flat-faced sensors (such as employed with WET Labs ECO-type sensors) as the slower flow within the chamber allows for particles to more easily settle onto the instrument optical surface.

4.8 Calibration

Pre- and post-cruise calibration of optical instruments is highly recommended to help establish measurement uncertainty. For example, some optical instruments - in particular, the ac-9, ac-s, backscattering and transmissometers with 660 nm red LEDs - are known to drift significantly throughout a single cruise. It is therefore recommended, if high quality DIW is available and conditions are adequate, to calibrate these instruments throughout the cruise (e.g. Dall’Olmo et al., submitted). Taking discrete water samples to measure CDOM absorption/attenuation on the vessel or back in shore, if following correct protocol, can be used to vicariously calibrate the in-line ac-meter, as long as it is sufficiently close in time (as reported in Matsuoka et al., 2017), to provide hourly CDOM estimates (in this mode the ac-meter is used to interpolate between the discrete samples).

If absolute calibration is not feasible, a valve can be used to measure “calibration independent” particulate optical properties, as discussed above (Section 2.3). Long term changes in the 0.2-μm filtered water fraction can also provide a diagnostic of drift due to

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[1] Note that by high quality DIW we mean deionized water that has a resistance of 18.2MΩ and has been radiated with a UV lamp to photo oxidize organics.

accumulation of material on the instrument's face, and those measurements can be used to correct for it (though the best strategy is to clean sufficiently often to avoid the drift).

4.9 Ancillary data

In many instances, optical measurements are used as proxies for biogeochemical parameters (e.g. Chlorophyll a, POC, TSM, DOC, HPLC pigments, size distribution). Often, the proxies are of much wider utility than the IOPs. While global proxy relationships exist, it is highly desirable that biogeochemical measurements are made periodically along the cruise to establish the cruise-specific or regional relationship.

4.10 QA/QC

To assess that the in-line system does not bias the measurements, it is critical to make measurements on both in-line as well as surface waters and contrast the two. These may include different IOP measurements as well as biogeochemical measurements (to check for consistency). In addition, we expect certain relationships between parameters measured by different instruments. For example: transmissometers should agree within a consistent difference due to their design differences (e.g., acceptance angle); beam-attenuation, backscattering and chlorophyll are all related in the surface ocean and relationships between them have been derived (e.g., Westberry et al., 2010); and crossing of oceanic fronts is generally observed in both physical and optical measurements. Significant deviations from these relationships may point out a problem in the data. In general, measurements should evolve smoothly with the exception of spikes due to large particles. Instability in the signal might reveal that bubbles, light, or other unrealistic elements are perturbing the observations. Ancillary measurements such as underway system flow rate and pressure, changes in ship's course or speed, and sea state can also be used to flag regions of data requiring more detailed examination. A more general QA/QC manual for optical data is the QARTOD manual (https://ioos.noaa.gov/project/qartod/).

5 Acquisition software, logging data

A general recommendation for data logging software is that it should be stable and write data frequently to the hard drive of the computer instead of buffering large amounts of data in memory. Small digestible files that are simple to read will ease your data processing. For example, for the ac-9 and ac-s, a custom version of Compass (r2.1) was provided by the manufacturer to write hourly files, avoiding the generation of gigabyte-sized files that are hard to open and process. Other sensors can be logged with software such as Haëntjens' Inlinino (http://inlinino.readthedocs.io/) a simple data logger and visualizer built specifically for acquisition of underway system data; alternatively, Wetlabs' host program (with or without their DH-4) is useful to record hourly files, with individual instrument ported to their native software using virtual ports for real-time visualization. Also, Terminal software such as TeraTerm (version >1.9.5) can be used to save data from any serial sensor, timestamped robustly, however it does not provide a plot of the data. When possible, visualization of the data in real-time will help to monitor the inline system and to troubleshoot issues.

Automated backup clock synchronization across instruments and computers used for data logging should be set up at the beginning of the cruise. It is preferable multiple copies of the data are located in different rooms of the ship and are synchronized frequently (every few hours). Many software options exist to do backups, we have had good experiences with SyncToy from Microsoft that we run every 4 hours using the Task Scheduler of Windows.

6. Considerations for specific instruments/measurements

6.1 Chlorophyll fluorescence and non-photochemical quenching

Phytoplankton decrease their fluorescence within seconds of exposure to high light. Hence, measurements of chlorophyll fluorescence will be dependent upon the short-term light-acclimation state of the phytoplankton, which in turn will be affected by the residence time of the water within the dark plumbing system, clear tubing, or within an illuminating instrument. Look (and if needed correct) for differences between day and night as well as effects of lights within the ship/lab.

6.2 Chlorophyll fluorescence measurement and CDOM

It is also known that fluorescence by CDOM, if significant in the water, contaminates the measurements by chlorophyll fluorometers (e.g., Proctor and Roesler, 2010). To assess this problem, one may do the measurement periodically through a 0.2μm filter to provide a baseline (see Sections 2.3 and 2.5 on In-line filters and Calibration).

6.3 Absorption and attenuation

Instruments commonly-used to measure absorption and attenuation in ocean optics are designed for in situ deployment but can be adapted to underway systems (the WET Labs ac-s and ac-9, and C-Star are built with flow cells, and the Sequoia Scientific LISST-100X has a flow chamber accessory that allows for flow-through measurements). As indicated above, calibration is key to good measurements; or, if particulate measurements are primarily of interest, periodic filtration with a 0.2-μm filter can be used to provide "calibration independent" particulate measurements by difference of total and dissolved measurements. This is particularly important when calibration (and other instrumental) uncertainties become a significant part of the signal, such as the LISST-100X or LISST-200X whose pathlengths are short (5 or 2.5 cm) and therefore less sensitive in very clear water (meaning calibration uncertainties become a large part of the signal); or even when measuring particulate absorption in extremely clear open ocean water (Slade et al., 2010). If dissolved or total absorption/attenuation are of interest, at least a daily pass of DIW through the system (Dall'Olmo et al., submitted), or a daily sample of CDOM absorption (Matsuoka et al., 2017), is required.

7. Processing flow-through data

7.1 Binning

In-line data allows one to bin, a process that increases signal to noise. Using a median bin or a specific percentile helps in reducing contamination by spikes due to bubbles or rare large particles. The longer the bin, however, the more smeared the resulting spatial signal and hence we do not advise for binning beyond a minute (providing a spatial scale of 309 m for a vessel moving at 10 kn), unless increased signal/noise is required and the lower spatial resolution is acceptable.

7.2 Removal of data contaminated by bubbles

Periods with enhanced bubble contamination are easy to visualize and need to be removed from the data. These periods are characterized by increased variance and "spiky" data.

7.3 Merging

Quantifying the delays between instruments (if significant) is important when merging data from multiple sensors. This may be more important for some measurements, such as temperature and salinity correction of absorption. Generally, it is advised to merge prior to processing.

7.4 Interpolating

When using periodic calibrations and/or periodic filtered periods for particulate measurements, it is important to view all of them to assess their consistency and remove obvious outliers (e.g. large change in values not associated with fronts or change in total measurements). We have found that application of interpolated blanks derived from linearly interpolating 'good' blanks provide for consistent data.

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9 Picture gallery

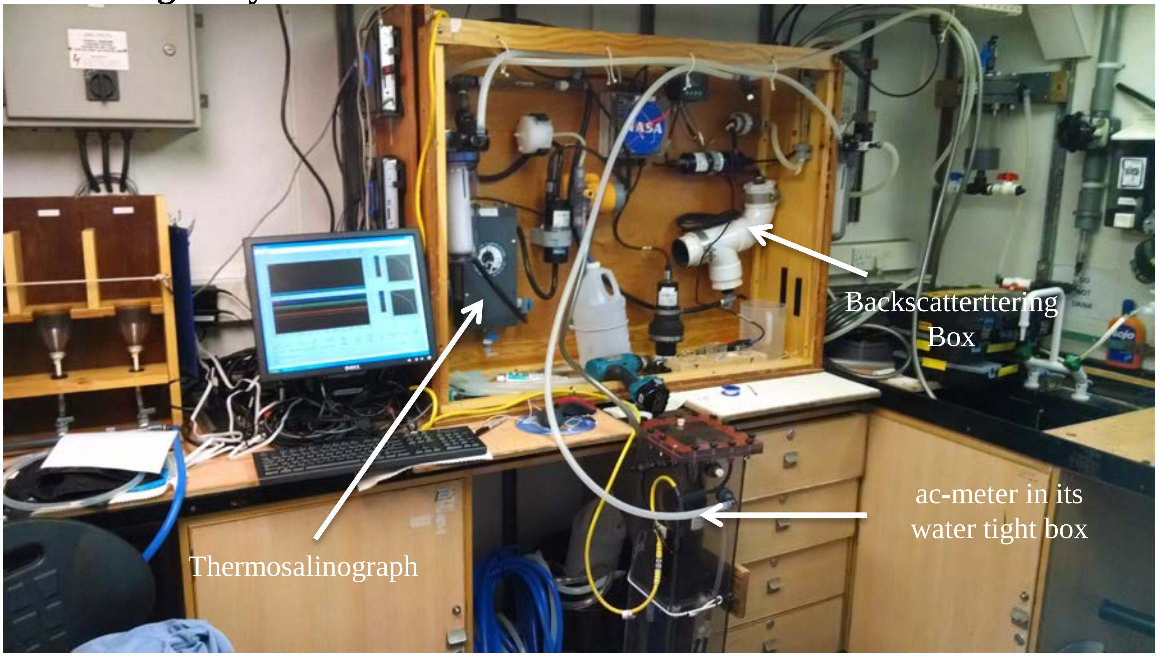


Figure 1. In-line set-up of B. Balch in a container.

Figure 2. Moon pool aka Straza Tower (center and left), custom intake (center) and the compressed air driven diaphragm pump and hose installed for the flow through system on the Atlantic Explorer by Norm Nelson.

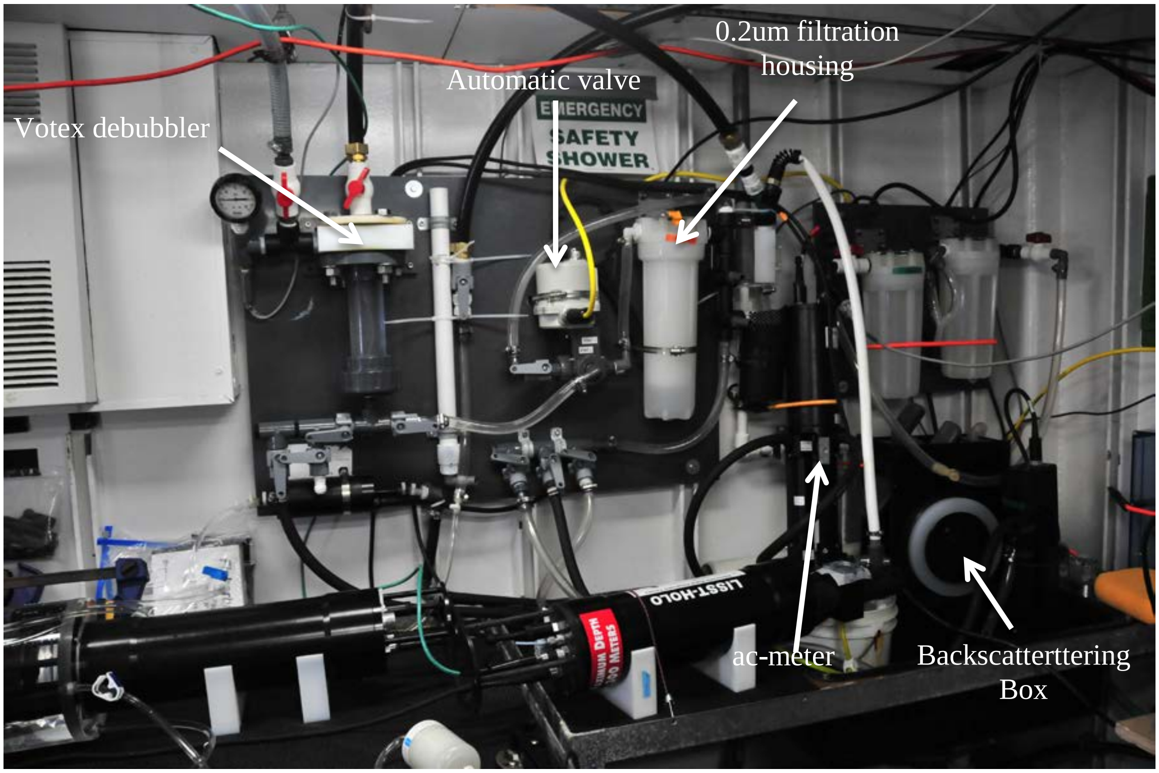


Figure 3. In-line set-up of W. Slade in a UNOLS vessel lab.

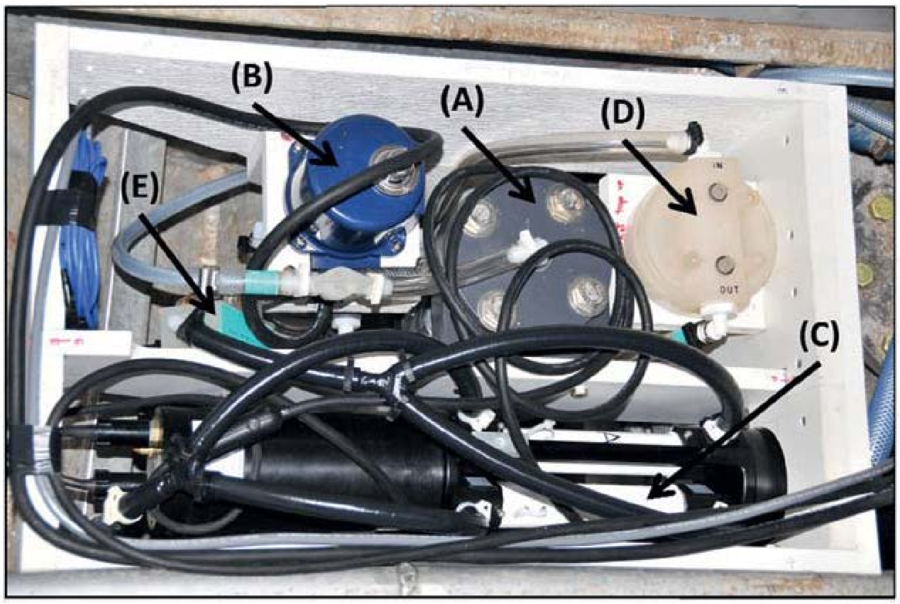


Figure 4. Flow through installed in the bilge of the S/V Tara. Flowing seawater enters system at (a) a Vortex debubbler, before (b) the three-way electrically actuated valve, which sends flow directly to (c) the ac-meter instrument, or diverts it through (d) a 0.2μm cartridge filter, before entering the ac-s instrument. Seawater flow is measured using (e) a paddle-wheel flow sensor. The valve controller and logging computer are located in dry laboratory space (From Slade et al., 2010).

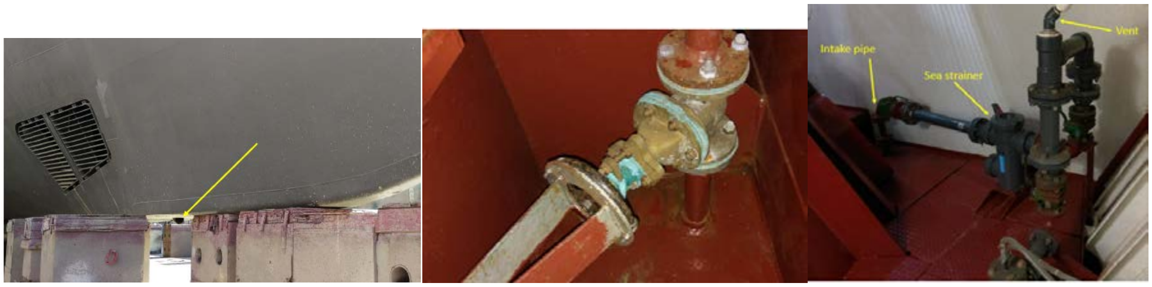


Figure 5. Intake scoop on the bottom of the vessel (left), intake pipe (center) and sea strainer debubbling and venting loop(right) of the R/V Atlantis.

Figure 6. Underway instrument loop and pump on the R/V Atlantis during NAAMES03.

Figure 7. Front (left) and top (right) views of the sink on the R/V Atlantis where the inline system was set up. The water carboy on the left side was used for daily calibrations. In the sink there are a bb-box and the ac-S sitting in a plastic bin with ambient waters. The LISST is on the edge of the sink. The long white tube from the roof is the source of seawater which is routed through the debubbler. From there water flow into the automated switch (connected with yellow power/control cable) and from there to the instrument either through the 0.2µm filter or unfiltered.

Appendix I: Pre-cruise checklist

- Contact the ship regarding pump and cleaning of in-line pipes.
- Contact the ship regarding adequate DIW source (UV lamp, 18.2MΩ, sufficient quantity) and replacement filters for it.
- Contact ship regarding possibility to visit or get pictures of the lab + sink where you will install your system. Know in advance how you will connect to the intake pump and bring several possible adapters.
- Make sure the ship's personnel know how much water (from instruments and debubbler) will go into the sink – some sinks empty directly into the sea, some empty into a hold.
- Check all instruments and cables are packed *including* spares. Bring spare power supplies, serial to USB converters and required drivers. Plan for each electronic element to be splashed with seawater; think about what would need replacing?
- Check you have sufficient filters to last the whole expedition (pack for extras in case you encounter productive waters).
- Sufficient tubing + replacement tubing. Hose clamps, connectors, valves.
- Tool box.
- Cleaning supplies (soap, isopropyl alcohol, wipes, sponges).

Appendix II: Schedule

Throughout the day

- Note flow rate and compare to previous day.
- Look for bubbles by viewing the output of the AC-S and bb3 and noticing the variance in the signal (in AC-S bubbles will result in noticeable disruption in the middle of the spectra).
- Make sure filtration periods occur when scheduled and are long enough for value to stabilize.
- Check that data are backed up.
- Check that all software is recording data.
- Check date and time of computer (must be UTC).
- Check power supply is set to 12-13.5 V.
- Check that the number of records lost on Compass r2.1 is not too high (>20). If it is reboot software, consider defragmenting hard drive and restarting logging computer.

Once a day

- Clean bb-box and LISST flow cell. Clean bb meter.
- Run DIW through the whole system until you reach a steady-state value in all instrument. Record at least 1min of these conditions.
- Analyze some data to make sure it is reasonable.

Weekly (more frequent in eutrophic waters or if you notice a significant jump in the data following the cleaning)

- Clean ac-S.
- Replace 0.2μm filter.

- Once filter replaced, run the system switching back and forth between filtered and unfiltered mode until no more bubbles get into the system from the filter housing (this can be accelerated using the purging valve in the filter housing).

Appendix III: Processing Software for ac-meters in flow-through

The ac-meter Data Processing Software processes data collected with a WETLabs ac-S In-Situ Spectrophotometer (ac-9 will be included in a future release). The intended audience of the software is members of the optical oceanography community looking for standardized, extensible, maintainable software to process their data with. The goal of having a standard data processing code is to ensure uniformity in the processing of data submitted to SeaBASS.

The goal for this software project was to create a usable, modifiable, community software package with a long lifespan that would change and grow with researcher's needs, but not be dependent long-term on any one individual. Therefore, the code is publicly available on the online code repository GitHub at the following at: https://github.com/OceanOptics/ACCode

For those preferring a faster, more streamlined, code, try Haëntjens' code at: https://github.com/OceanOptics/InLineAnalysis.

Description

The ac-meter Data Processing Software has been written in Matlab and takes Level 1 (one step above 'raw') data from an ac-meter and processes it to a set of standards determined by the workshop held at the Bigelow Labs, Maine on March 13, 2015. A future version of the code will be written in (ported to) Python. The software is a rewrite of existing Matlab procedural code used to process in-line ac-meter data collected to date. The existing code was typically shared by physically transferring code between users (with pieces of codes contributed by W. Slade, G. Dall'Olmo, T. Leeuw, E. Boss, and W. Neary). Cutting and pasting working sections of code into new code mostly facilitated reuse or commenting in/out sections of code as needed. A few functions were used, but most of the logic was contained in a single procedural file. QA and QC need to be performed before submitting processed data to SeaBASS.

The current ac-meter Data Processing software has a *flexible and extensible* design, allowing for future changes to be made without breaking the old code. Additional processing can be added at each processing step. This flexible design is built on a series of procedural Matlab scripts, which in turn calls object-oriented Matlab code. The combination of objects and scripts/functions provides the reusability and extensibility required of a project of this scope. There are only a few steps to set up a new project, documented in the software README.txt, on GitHub.

The ac-meter Data Processing software runs in Matlab on both Windows and OSX, on a standard current desktop/laptop system.

Software Overview

The software is divided into four sections: Ingest, Pre-processing, Processing, and Output (Fig. 1). The Ingest phase reads in all the necessary data files for processing. The

Pre-processing phase separates the total from filtered data, preparing it for the processing phase. The Processing phase applies the main processing rules to the data. The Output phase creates the data files necessary for SeaBASS submission, as well as any desired plots.

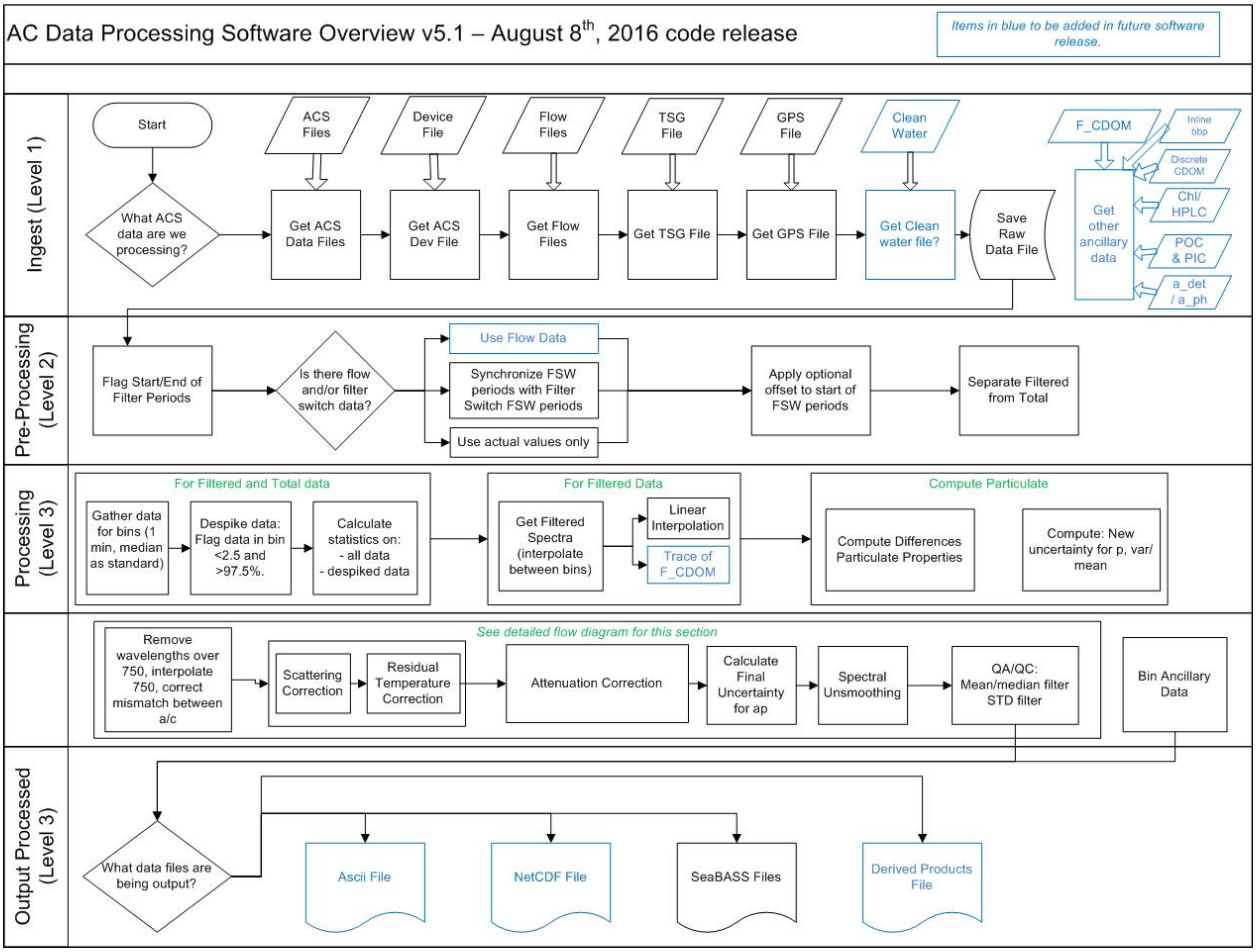


Figure A1. Schematics of the in-line ac-meter processing software.

Ingest

The software stores data processing parameters from the user in a text-based .ini file, allowing customization of the processing. All the necessary data files (ac-meter data files, device files, etc.) to process ac-meter data are ingested, allowing for differences in file formats or file availability. It is flexible enough to allow for *new* file types to be added, such as those for post-processing (F_CDOM, HPLC, etc.)

Pre-Processing

The data is processed by first differencing the filtered from total data. The software automatically identifies the start and end of each filtered/unfiltered period. Users decide to either use the valve on/off data or detects the transitions automatically within the data itself. The transitions between filtered/unfiltered can also be manually edited and saved. Once the transitions have been identified and checked, the data is ready for separation into ‘total’ and ‘filtered’ data sets and for “Processing”.

Processing

Both attenuation and absorption data are median minute-binned. Data values between 2.5% and 97.5% percentiles are used (to remove rare outliers). It is also possible to use the mean for binning.

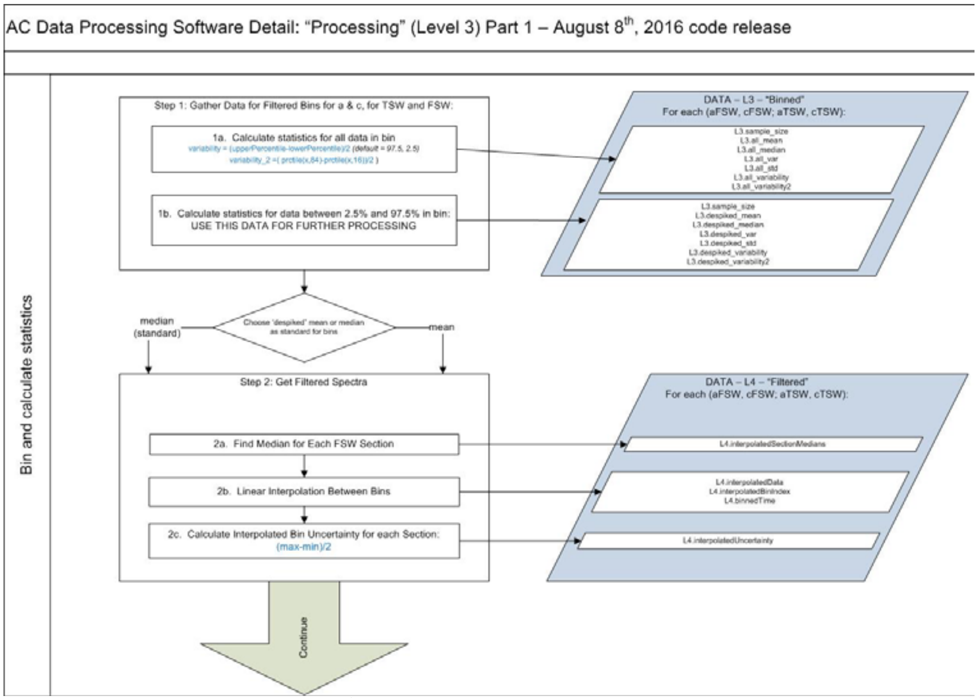


Figure A2. Schematic of 1st part of processing software which separates segments where water were piped through the 0.2μm filter.

Dissolved values needed to obtain the particulate values are linearly interpolated to the time of particulate measurements. Wavelengths over 750nm are then removed and a 750 wavelength is linearly interpolated. Spectral band of absorption are interpolated to those of attenuation.

The 3rd method of Zaneveld et al., 1994 is typically used to correct for scattering with 730nm as the null wavelengths simultaneously performing a residual temperature correction (see Slade et al., 2010). Attenuation is also corrected for residual temperature. Other types of scattering corrections are also possible to choose from (e.g. Rottgers et al., 2013).

Then, a spectral unsmoothing based on the method in Chase, A., et al., 2013 is used. Finally, data is filtered out based on two criteria:

1. If the bin fails the check:

(abs(TSW_bin_median - TSW_bin_mean))./(TSW_bin_median-FSW_interp_median) > max(0.3 , 0.001./(TSW_bin_median-FSW_interp_median));

2. If the bin fails the check:

TSW_bin_std > stdThreshold

where the stdThreshold is .015 for a, and .030 for c.

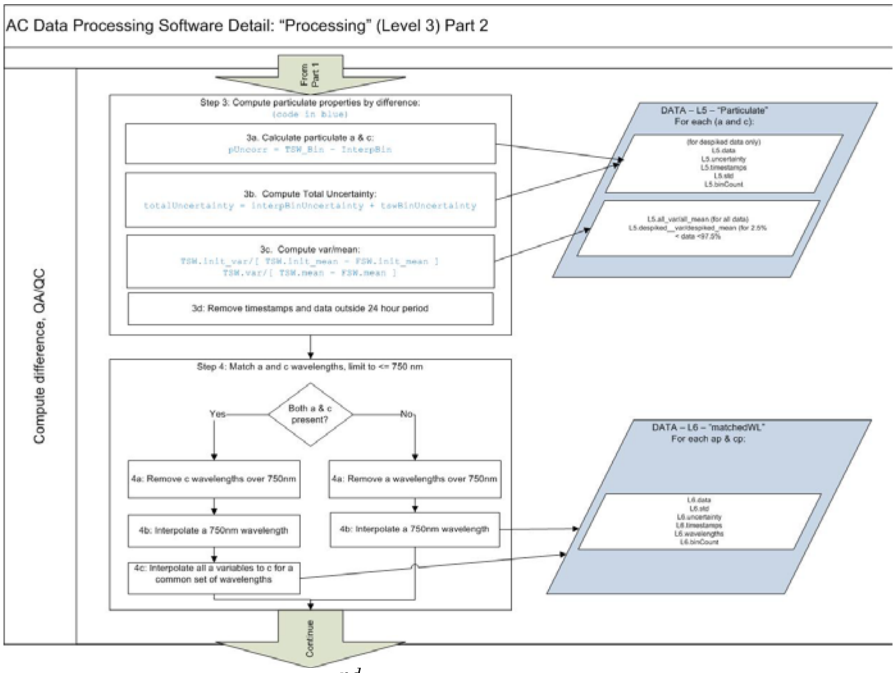


Figure A3. Schematic of 2nd part of processing software which compute the particulate attenuation and absorption as the difference of the two total and filtered measurements.

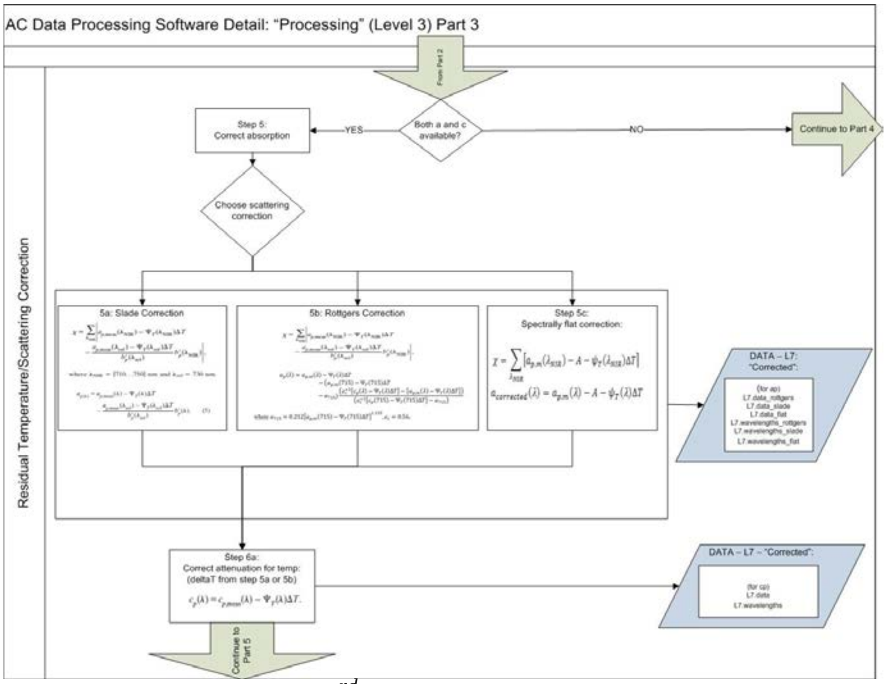


Figure A4. Schematic of 3rd part of processing software in which absorption and attenuation are corrected for residual temperature effects and in which the absorption is scatter corrected.

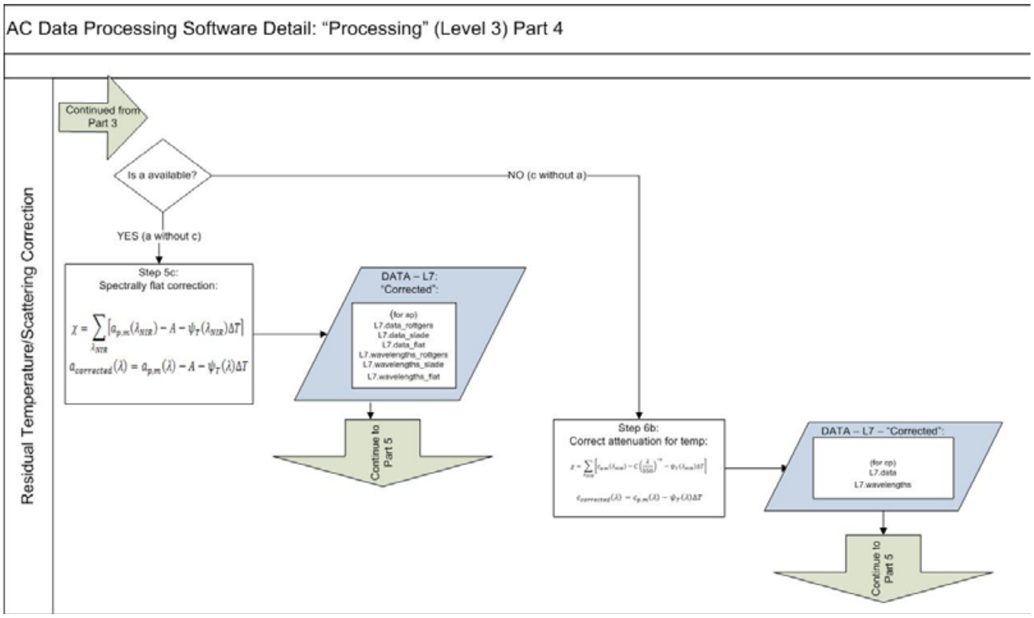
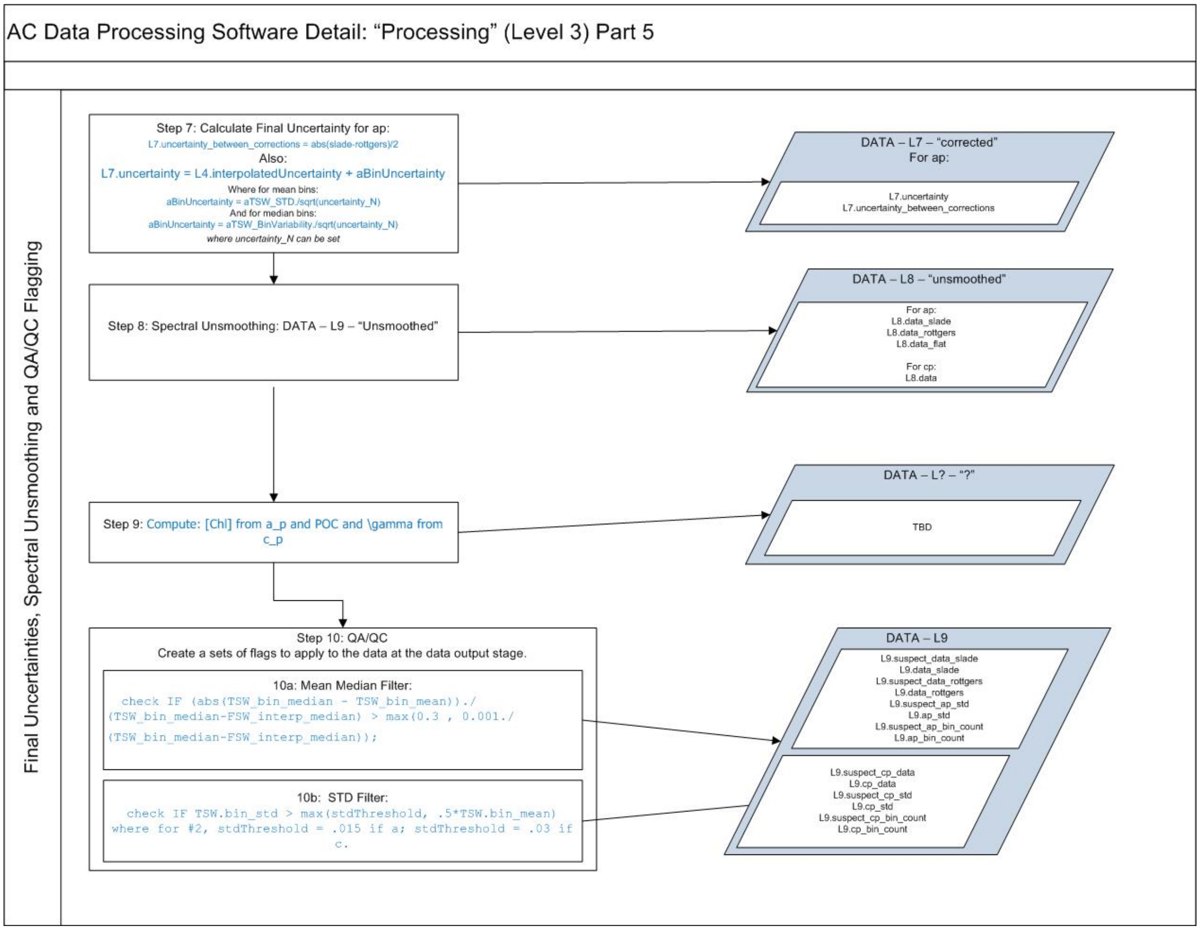


Figure A5. Schematic of 4th part of processing software in corrected IOPs are derived.



```
 check IF (abs(TSW_bin_median - TSW_bin_mean))./
(TSW_bin_median-FSW_interp_median) > max(0.3 , 0.001./
(TSW_bin_median-FSW_interp_median));
```

```
 check IF TSW.bin_std > max(stdThreshold, .5*TSW.bin_mean)
where for #2, stdThreshold = .015 if a; stdThreshold = .03 if
                              c.
```

Figure A6. Schematic of the final part of processing software in corrected in which spectral smoothing and final automated QA/QC is done.

Output
SeaBASS-compatible files are the standard output of the software, for both spectral particulate absorption (a_p) and attenuation (c_p). Date, time, latitude, longitude, temperature, salinity, standard deviation and bin count are included in each file, along with either the absorption or attenuation data. Spectra with negative absorption in the blue regions are kept, as these values are not significantly different from zero. In extreme cases bad values are replaced with -9999.

To facilitate human-in-the-loop QA/QC, many plots are also produced as the software runs, with final plots of the SeaBASS data produced at the end (Fig. A7).

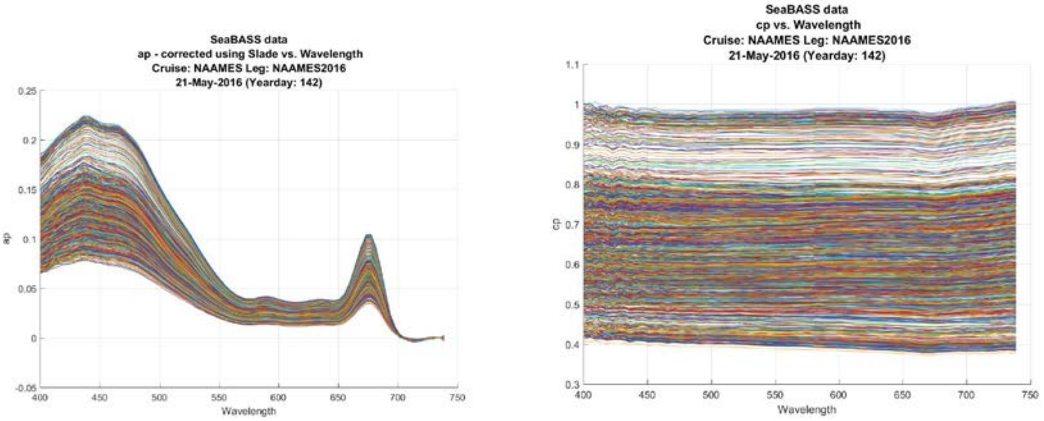


Figure A7. One-day of particulate absorption and attenuation spectra generated for human-in-the-loop QA/QC of the data generated to be submitted to SeaBASS.