

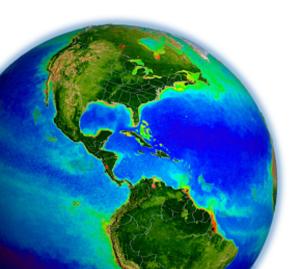
# **Updated Submission Reporting Requirements**



New "Checklist" documents are being designed for commonly submitted data types

### Outline

- 1) Quick overview of SeaBASS metadata
- 2) Briefly describe new requirements & page
- 3) Feedback?



Violeta is spearheading the development of a new algorithm development dataset (i.e., NOMAD) using SeaBASS datasets. With the need to add uncertainties, she has also been leading review of QC standards



# Background, updated community protocols



New "Checklist" documents will help organize methods and processing details related to protocols best practices

- Inherent Optical Property Measurements and Protocols: Absorption Coefficient (November 2018)
- Beam Transmission and Attenuation Coefficients: Instruments, Characterization, Field Measurements and Data Analysis Protocols (April 2019)
- Protocols for Satellite Ocean Color Data Validation: In situ Optical Radiometry (In Press)
- Best Practices for the Collection and Processing of Ship-Based Underway Flow-Through Optical Data (In Press)
- Measurement Protocol of Absorption by Chromophoric Dissolved Organic Matter (CDOM) and Other Dissolved Materials (DRAFT)
- Noteworthy and Supplemental Topics on Ocean Colour Radiometry Protocols (DRAFT) (led Sanjuan & Craig)

# **SeaBASS**

# **Requirements for PACE algorithm development**



- Protocols updates need to be reflected on SeaBASS submission updates
- Tighter QA/QC in view of PACE cal/val and algorithm development
- Possibility of classification of datasets according to special characteristics (Optically shallow waters, HAB, NOMAD dataset)
- Uncertainty traceability on all validation products
- Measurement uncertainty up to 5%

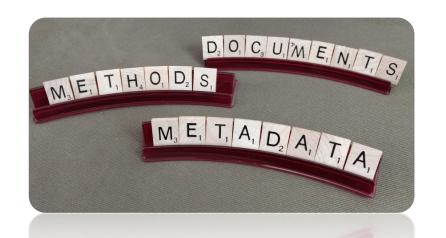
Updated checklists and reporting requirements come as a result of community updates on measurements protocols as well as PACE mission requirements for validation, algorithm development and NOMAD

## **Documentation and metadata**



### Types of metadata in SeaBASS submissions

- 1. Metadata headers within data files
  - i. Keyword-value pairs (machine interpretable)
  - ii. Comments (short text)
- 2. External Documents and Calibration Files
  - i. Explain how raw instrument measurements were collected and processed into your reported values (open-ended format)



# **Current documents requirements**



Existing documentation requirements are written flexibly since there's no one size-fits-all approach

- Should describe calibration equations and values, how the instruments were calibrated, and what types of corrections and data analysis were applied to create your reported values
- No specific file formats are required

Due to open-ended format, essential details are often spread out in descriptions, or sometimes not provided...

= often time consuming or difficult to evaluate data quality details

## **Data submission special requirements**



https://seabass.gsfc.nasa.gov/wiki/data\_submission\_special\_requirements

For commonly submitted measurements:

- 1) **Checklists** new documentation templates
- 2) **Special Notes** reminders & tips
- 3) Example Submissions

### Goals:

- improve SeaBASS data quality & consistency
- make quality easier to assess
- clarify reporting requirements to reduce unnecessary back and forth during data submission process



# SeaBASS

# **Data submission special requirements**



- Filter pad absorption (community protocol)
- CDOM absorption (community protocol)
- POC (community protocol draft)
- HPLC and pigments
- Radiometry (community protocol)

Developed with Field Support Group from Ocean Biology Processing Group, leading community protocols

# SeaBASS

# Filter pad absorption



#### **Sample collection**

- Water bottles, underway
- Filtration vacuum
- Blank filters
- Replicates
- Samples measured fresh, frozen,
- Storage conditions (container, preservation method, temperature)

#### Sample measurement

- Instrument make, model and accessories
- Instrument calibration, performance tests and maintenance performed
- Measurement method: transmittance, transmittance-reflectance, inside sphere...
- Measurement protocol references (if any)
- Air scans

#### **Data analysis**

- Blank and air scans
- Correction or null methods applied
- Beta factor used with reference

### **CDOM**



#### **Sample collection**

- Niskin bottle, surface pump, bucket...
- Location (coastal, offshore, estuarine, etc.) and depths
- Filtration system: vacuum pump, peristaltic, syringe, vacuum jar, etc.) type of filter and pore size
- Sample storage (e.g. refrigerated, frozen, acidified, etc.) and in what type of bottle (e.g. amber glass, high or low density poly-ethylene (HDPE, LDPE), Nalgene, etc.)

#### Sample measurement

- Spectrophotometer used (dual or single beam, waveguide, integrating sphere, etc.), cuvette size (benchtop), effective pathlength (on waveguide)
- Instrument settings: (integration time, scan speed, slit width, smoothing, wavelength range and increment, etc.)
- Samples re-filtered before the spectrophotometric analysis?

## **CDOM**



#### Reporting

- Raw scans of absorbance should be reported for each all measurements. When multiple scans measured, the average absorbance can be reported along with their standard deviation
- Documentation file should be provided describing the methods for collection, filtration, analysis protocols
- Absorption coefficient may be reported after null correction, smoothing, truncated wavelengths, etc.
   has been applied... Fully documented
- Standardization on variable names for CDOM: wavelength, abs\_ag, abs\_ag\_sd, ag

## POC



#### Filter diameter and nominal pore size

Make and type (e.g., Whatman GF/F), filter pre-treated?

#### Sampling and processing

 Method of filtration: filtration volume (volfilt), sample replicates, Standard deviation or % cv of replicates reported

#### Post sampling processing

- Acidification step: Mode of application (i.e., fumes vs. solution)
- Drying method and temperature (length of time in oven, desiccator, etc)

#### **Elemental analysis**

 Instrument make and model, Calibration standard, Reference material used and performance metric results relative to reference

#### **Blank corrections**

DOC/DON adsorption ("filtrate") blank correction should be measured and applied (Moran et al. 1999).
 Were samples blank corrected?

## **HPLC**



#### Filled out by data submitter

#### Sample collection method

- Filter type/pore size, Vacuum pressure, Replicates collected, Flash frozen?, Long term storage conditions

#### Filled out by HPLC Lab

#### Sample measurement and analysis

- Extraction, solvent, volume added/delivery method, disruption method, time, soak time, clarification method

#### **HPLC** analytical method

- Method reference, column temperature, mobile phase, Flow rate, Gradient, wavelengths monitored, spectra collected? If so, what wavelengths, Internal standard used, name

**Instrument**: Make and model, Injector type, Pump type, sample compartment refrigerated?, Heated/thermostatted column compartment? Detector type

**Instrument calibration**: Frequency, Source of standards, Single point or multi-point calibration, How are calibration factors (or response factors. RF) calculated? Is calibration accuracy monitored between calibrations? If so, how and how often? Noise at each wavelength

## Radiometry



#### Instrument

- Model and manufacturer, instrument characteristics including spatial, spectral electrical and physical.
- Report instrument characterization including spectral range, spectral resolution, spectral accuracy, field
  of view, linearity, cosine response, thermal response, immersion effects
- Calibration: report absolute radiometric calibration for radiance and equation, and absolute calibration for irradiance and equation.

#### **Deployment conditions**

- Deployment type: buoy mode, profiler (single cast), profiler (multi cast).
- Deployment strategy, pressure tare, dark readings.

Remember to include "optional" metadata headers: Wind speed, Cloud cover, (Ship heading & SZA)

## Radiometry



#### **Data analysis**

- Conversion data counts to engineering units: conversions from raw binary optical data into counts. Apply calibration equation.
- Dark correction: specify the correction scheme used to correct light values for dark values.
- Deglitch shutter data: specify deglitching scheme used for dark values, if any
- Smooth shutter darks: specify, if any.
- Interpolate shutter darks as a function of measurement time to match the number of dark and light data measurements.
- Dark correction of light data
- Temperature correction of light data. Report temperature correction equation.
- Time interpolation if any (better not interpolated). Detail interpolation scheme applied.

## Feedback



Please refer to SeaBASS website for detailed requirement on submission guidelines for each validation product.

- Enforced QA/QC is required for algorithm development within PACE for uncertainty estimates.
- Data collection and processing can account for significant error budget.
- SeaBASS will require a full traceability on acquisition methods and data processing to ensure quality standards.

Submission guidelines open for feedback and suggestions from the community to revisit according to protocols update.

https://seabass.gsfc.nasa.gov/wiki/data\_submission\_special\_requirements