Recommendations for Production Centers and Data Providers

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Introduction

Data provided to CMEMS must be provided in a way ensuring that their use in quality control but also for the community is obvious. While this is most often understood for physical parameters, it is not always the case for biogeochemical (BGC) data.

Issues Observed

In general, there are two categories of issues regarding these data that should be corrected as soon as possible for incoming data:

1. Name and (especially) units are not given in the appropriate way. Data that are provided to CMEMS should be related to a physical parameter that makes sense. See table below for standards that should be used.
2. Make sure parameters are registered for the adequate platform.

Parameter Standardization

It seems some data is provided to the community without being related to the physical unit they are supposed to represent. Therefore, the following table gives standard names and units that should be used for some BGC data. These are compatible with the conventions used in CORIOLIS and CF-Names.

Table 1 Standardized naming for parameters.

Short Name	Long Name	Unit	Description
CDOM	Cdom	ppb	
CPHL	total chlorophyll-a	milligram/m3	mass_concentration_of_chlorophyll_a_in_sea_water
FLU2	Fluorescence	milligram/m3	

DOXY	Dissolved oxygen	millimole/m3	mole_concentration_of_dissolved_molecular_oxygen_in_sea_water
NTRA	nitrate (no3-n)	millimole/m3	mole_concentration_of_nitrate_in_sea_water
PHOS	phosphate (po4-p)	millimole/m3	mole_concentration_of_phosphate_in_sea_water
SLCA	silicate (sio4-si)	millimole/m3	mole_concentration_of_silicate_in_sea_water
TUR4	Turbidity	NTU	sea_water_turbidity
TSMP	total suspended matter	gram/m3	mass_concentration_of_suspended_matter_in_sea_water
ALKW	total alkalinity	micromole/kg	
PCO2	co2 partial pressure	microatmosphere	surface_partial_pressure_of_carbon_dioxide_in_sea_water
PHPH	Ph	none	sea_water_ph_reported_on_total_scale

Note that millimole/m3 is equivalent to µmole/l or µM. Similarly, milligram/m3 is equivalent to µg/l.

CDOM can also be given 1/m.

Parameters considered

In the rest of this document we will consider the special case of Chl-a fluorescence and O2 concentration. The main reasons for choosing these two parameters are the following

1. Field sensors for these parameters have been available for quite a long time and there is therefore a high data volume.
2. Sensors have been installed almost all platforms
3. Due to the larger amount of data there is also more knowledge about these parameters.

Moreover, Chl-a fluorescence is a complicated parameter and O2 concentration requires knowledge of auxiliary data for their interpretation. In a repository consisting purely on data, solving these issues will provide solutions for other parameters.

Scientific Background Summary

The information provided here tries to clarify some misunderstandings concerning the measured parameters and should not be solely considered as a description of the involved processes. More information can be found in the MyOcean reports *Real Time Quality Control of biogeochemical measurements v2.5* (Jaccard, Norli et al. 2015) and *R&D Reference Report, WP15 (Garau, Vizoso et al. 2012)*.

Chl-a Fluorescence and Chl-a Concentration

When algae absorb light, a part of this light will be re-emitted as fluorescence. Fluorescence is mainly emitted from the pigment Chl-a and can therefore be used as a proxy for to get an estimation of the biomass. However, this measure is not completely equivalent to Chl-a concentration. This is due to the conditions affecting *in vivo* or *in situ* Chl a fluorescence emission:

- Light regime (night/day, day length)
- Self-shading and dense blooms
- Different species and groups

- Regional variability
- Nutrient status
- Quenching (ie photosaturation of the pigment that limits the fluorescence)

Light Conditions

High variation in fluorescence is a result of varying light conditions (irradiance, spectral composition and day length) and different algae groups and species. In low light conditions, light harvesting pigments efficiently transfer the light energy in order to give maximum light harvesting. This efficiency is reduced in high light conditions, because of production increase and of the saturation of pigment by incoming light.

Groups and Species

Different groups/species of phytoplankton contain different additional pigments.

Regional Variability

In some regions cyanobacteria can dominate the phytoplankton biomass. They have a different allocation of energy regarding the photosystems. In cyanobacteria the most of Chl-a is located in the non-fluorescing photosystem I. However this Chl-a is included in the extracted Chl-a yield. On the other hand phycobilin pigments such as phycocyanin (specific for filamentous cyanobacteria) provide strong in vivo fluorescence. Consequently during abundant cyanobacteria blooms occurring annually in the Baltic Sea, the phycocyanin fluorescence should be used as auxiliary parameter to correct the ratio of in vivo Chl-a fluorescence against extracted Chl a (Seppälä, Ylöstalo et al. 2007).

Chl-a Fluorescence and Chl-a Concentration

Chl-a concentration is determined in laboratory from water samples using HPLC or spectrophotometry methods. There are other methods providing satisfying results, however not all of them have been recommended for satellite validation.

The ratio of *in vivo* fluorescence against extracted Chl-a may vary remarkably. This is a result of certain processes in algae such as regulation, acclimation or adaptation to different environmental conditions in order to optimize their evolutionary fitness (Raven and Geider 2003). One example from the Ferrybox system in Norway is shown in **Erreur ! Source du renvoi introuvable.**-3. Chl-a fluorescence often appear too high at low concentrations and too small at high concentrations using a calibration of the sensor based on algal cultures.

In practice, water samples are taken for laboratory analysis and an average relation between Chl-a concentration and Chl-a fluorescence is generated. Averages can be computed over different time ranges and geographical extent. This is up to the data provider to determine. However, distributed data should only include measurements corrected in this way.

The factory calibration of new sensors should be considered as a preliminary calibration. Users have to perform a final calibration that is suited to the water masses in which sensors will be used.

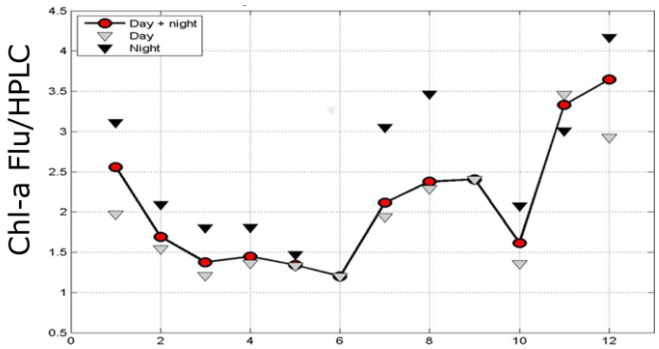


Figure 1 Seasonal plot of Chl-a_fl/Chl-a_HPLC ratio based on a yearly calibration of the data.

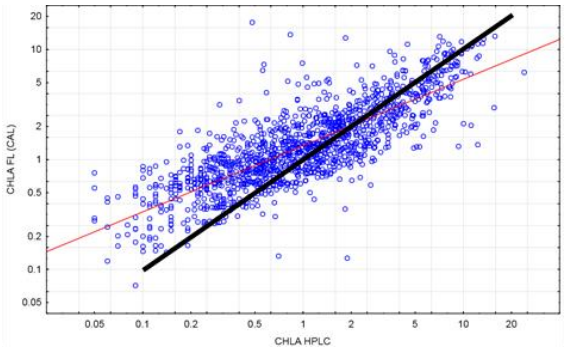


Figure 2 Regression plot between Chl-a fluorescence and HPLC Chl a concentration (from Ferrybox data during the years 2003-2008).

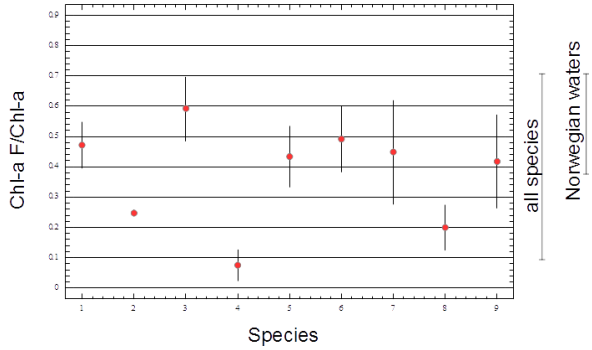


Figure 3 Relation between Chl-a fluorescence and HPLC Chl a concentration for different algae species (see table)

No	Alga
1	Chrysochromulina polylepis
2	Dunaliella tertiolecta
3	Emiliania huxleyi
4	Oscilatoria agardii
5	Prorocentrum minimum
6	Prymnesium parvum
7	Phaeodactylum tricornutum
8	Selenastrum capricornutum
9	Skeletonema costatum

O2 Concentration

Oxygen optodes measure oxygen saturation but output oxygen concentration. The latter is usually calculated from seawater temperature, salinity and pressure. In practice, salinity and pressure are constants while temperature is given by an internal sensor. Unfortunately, this sensor does not give an accurate value and varies from sensor to sensor, as shown in Figure 4 to Figure 6.

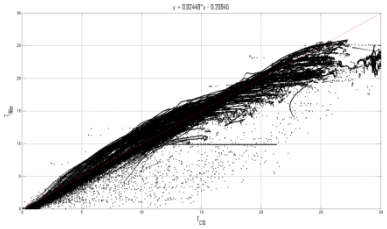


Figure 4 inlet temperature (SBE38) on y-axis versus temperature from STD (SBE45) on x-axis.

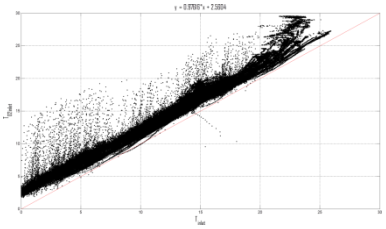


Figure 5 Inlet temperature from oxygen optode (AADI3835) on y-axis versus inlet temperature (SBE38) on x-axis.

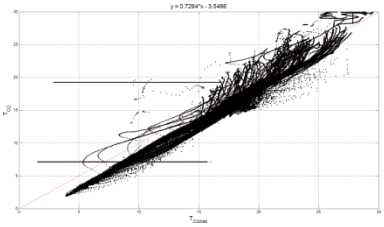


Figure 6 Temperature from both oxygen optodes (AADI3835), inlet sensor on x-axis.

An error of 1°C will lead to an error of about 4µM oxygen concentration. For salinity, an error of 2ppm yields a difference close to 3µM on oxygen concentration. Therefore, measurements must be corrected with more accurate temperature, salinity and pressure values.

In general, O2 concentration measurements should be compensated for depth and better temperature and salinity measurements. Whether this step has been performed or not should be provided together with data as well as which values have been used for compensation.

Requirements

List by parameters, one per page.

Chl-a Fluorescence

As a consequence of the scientific background for this parameter, we distinguish to types of Chl-a fluorescence

1. Chl-a fluorescence related to Chl-a concentration. This is parameter is for Chl-a fluorescence measurements that have been post-modified by the data provider to relate to a Chl-a concentration. These can be considered as a proxy for Chl-a concentration and used further in the quality control.
2. Unrelated Chl-a fluorescence. This parameter is to be used for Chl-a fluorescence measurements provided directly by the sensors.

Chl-a Fluorescence related to Chl-a concentration

CPHL is for Chl-a fluorescence that is related to Chl-a concentration. In this case, the following attributes must also be set

STEP 1. **sensing_method** must be *fluorescence*

STEP 2. **proxy_method** must provide a description or a link to the method used for relating the fluorescence measurements to the Chl-a concentration. This attribute should normally not change often and relate to laboratory methods like water samples analysis or algal cultures.

Names, units, vocabulary

CPHL	total chlorophyll-a	milligram/m3	mass_concentration_of_chlorophyll_a_in_sea_water

Required Attributes

proxy_method	A description or a link to the method used to relate the fluorescence measurements to Chl-a concentration
sensing_method	fluorescence

If any of these attributes are not set or invalid, the quality control must flag these values with 4 (bad data).

Optional Attributes

last_proxy_method_date	last time the relation to Chl-a concentration was applied

Required Auxiliary Parameters

Optional Auxiliary Parameters

DPAR	downwelling photosynthetic active radiation	micromol m-2 s-1	downwelling_photosynthetic_photon_flux_in_sea_water

Field Control

Calibration method

Unrelated Chl-a Fluorescence

FLU2 must be used for these measurements. Quality control flags for these values must be set to 3 (bad data that are potentially correctable). As such, parameters FLUO and FLU3 are also accepted and fall in the same category. However, they should be avoided.

Names, units, vocabulary

FLU2	Fluorescence	milligram/m3	
FLUO	fluorescence	relative unit	
FLU3	fluorescence	FFU	

Required Attributes

Optional Attributes

Required Auxiliary Parameters

Optional Auxiliary Parameters

Field Control

Calibration method

Chl-a Concentration

Chl-a concentration is described with **CPHL**. In this case, variable attribute *sensing_method* must be set to *HPLC*, *spectrophotometry* or some other name describing the method used in the laboratory. For example *fluorometry_analysis*

Names, units, vocabulary

CPHL	total chlorophyll-a	milligram/m3	mass_concentration_of_chlorophyll_a_in_sea_water

Required Attributes

sensing_method	HPLC, spectrophotometry, …

If this attribute is not set or invalid, the quality control must flag these values with 4 (bad data).

Optional Attributes

Required Auxiliary Parameters

Optional Auxiliary Parameters

Field Control

Calibration Method

O2 Concentration

O2 concentration comes in different unit flavors. These can be related to each other provided the auxiliary parameters for depth, temperature and salinity have been provided. The standard name to be used here is **DOXY**, but we accept also DOX1 and DOXY2.

Names, units, vocabulary

DOXY	dissolved oxygen	millimole/m3	mole_concentration_of_dissolved_molecular_oxygen_in_sea_water
DOX1	dissolved oxygen	ml/l	volume_fraction_of_oxygen_in_sea_water
DOX2	dissolved oxygen	micromole/kg	moles_of_oxygen_per_unit_mass_in_sea_water

Required Attributes

salinity	Constant value or short name of variable containing salinity values used to compensate concentration measurements
temperature	Constant value or short name of variable containing temperature values used to compensate concentration measurements
pressure	Constant value or short name of variable containing pressure values used to compensate concentration measurements
compensated	yes or no

If attributes depth, temperature and salinity are provided as the name of another variable, values for these variables must of course be provided.

Some sensors perform compensation in real time during measurements when all auxiliary sensors are available (note: this is not the case of optodes). In this case attribute compensated can be set to yes, and other auxiliary attributes must be set to the appropriate values.

If any of these parameters is missing or invalid, the quality control must flag these data with 3 (bad data that are potentially correctable).

Optional Attributes

Required Auxiliary Parameters

Temperature	Temperature values used for compensation
Salinity	Salinity values used for compensation
Pressure	Pressure values used for compensation

Note that if the associated attributes is set to a constant (as it could the case for a platform at constant depth), the related parameter is not required.

Optional Auxiliary Parameters

Field Control

Calibration Method

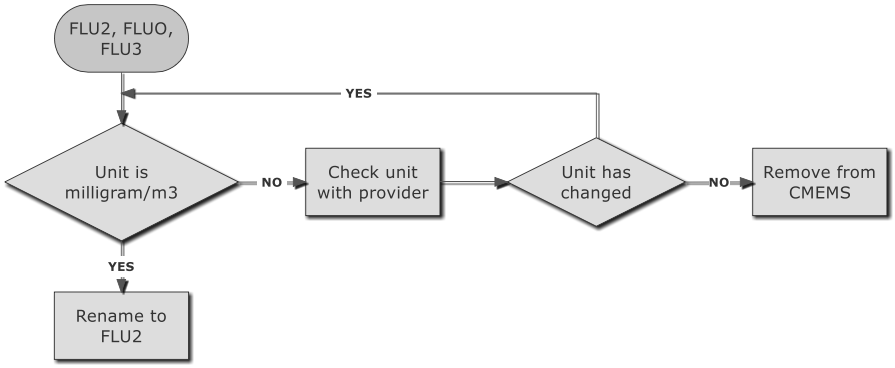
Actions

Things to check before creating new files:

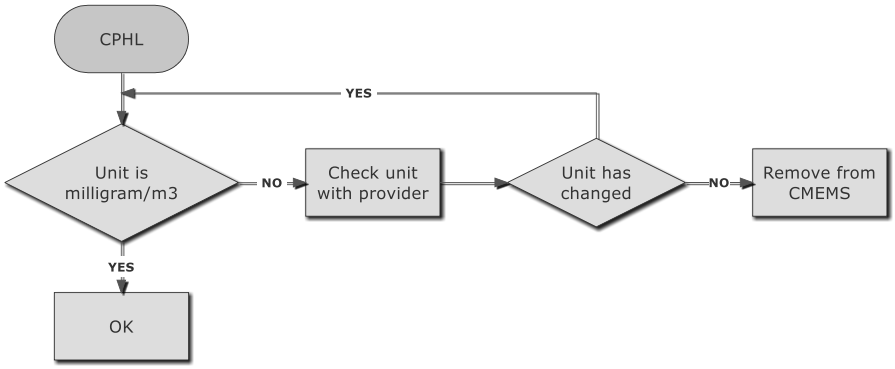
1. Oxygen is given as concentration
2. Oxygen has been compensated or not
3. With oxygen, there is information about temperature, salinity and depth that were used for compensation
4. Chl-a concentration is mapped to CPHL in milligram/m3
5. CPHL data from a sensing platform have attribute sensing_method set fluorescence and have undergone a correction by the data provider in order to give a better proxy for Chl-a concentration. This correction is defined in attribute proxy_method.
6. CPHL data from laboratory analysis have attribute sensing_method set to HPLC, spectrophotometry, or some other name describing the method used in laboratory.
7. Any other Chl-a related measurement in milligram/m3 is mapped to parameter FLU2.
8. Chl-a measurements that are not given in milligram/m3 should be refused.

In addition to implement the rules above, the following steps should be performed at DU/PU level in order to correct the existing files. A list of files to be corrected can be provided to DU/PU once these corrections have been agreed by the BioGroup at DU/PU level.

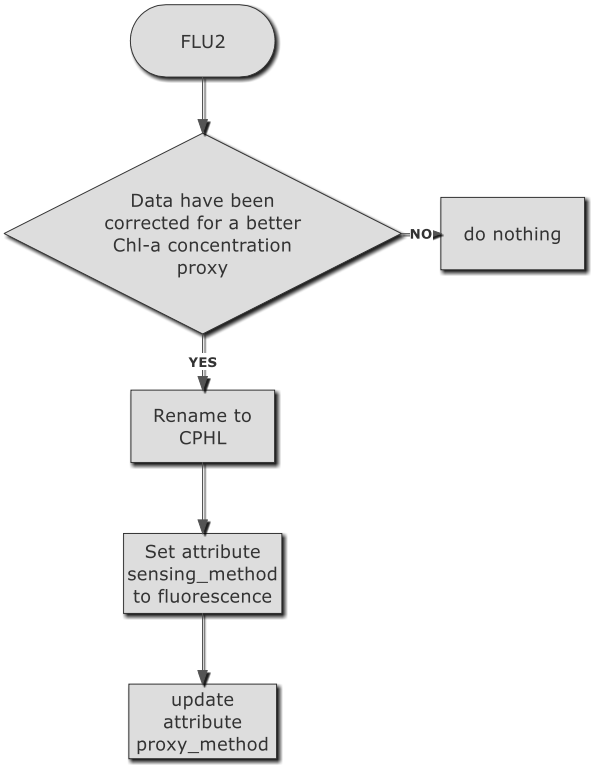
STEP 1. Correct Chl-a fluorescence units



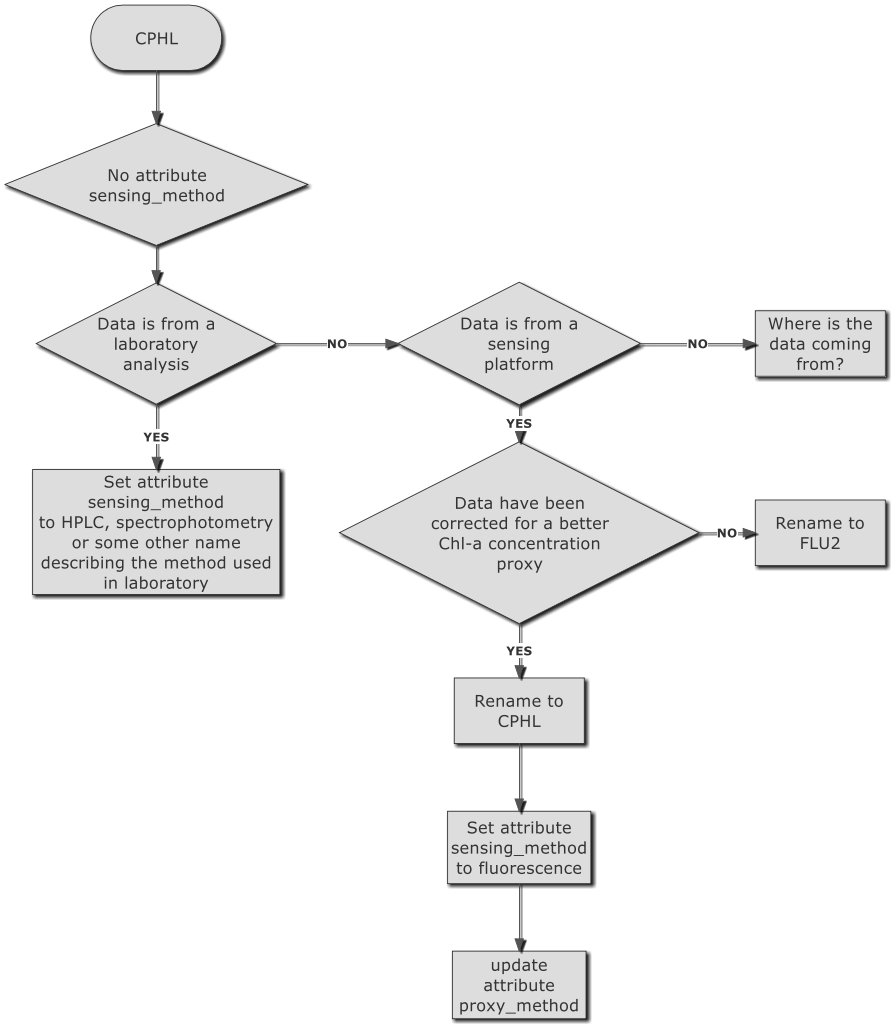
STEP 2. Correct Chl-a concentration units



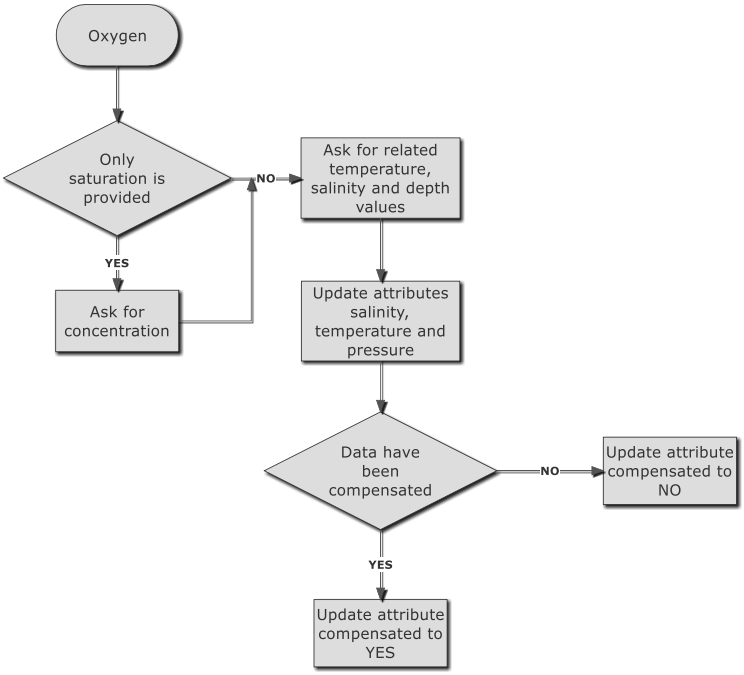
STEP 3. Check if Chl-a fluorescence has been corrected by the data provider to obtain a better proxy for Chl-a concentration



STEP 4. Update Chl-a concentration values



STEP 5. Correct Oxygen parameters



References

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Raven, J. and R. Geider (2003). Adaptation, Acclimation and Regulation in Algal Photosynthesis. Photosynthesis in Algae. A. D. Larkum, S. Douglas and J. Raven, Springer Netherlands. **14:** 385-412.

Seppälä, J., et al. (2007). "Ship-of-opportunity based phycocyanin fluorescence monitoring of the filamentous cyanobacteria bloom dynamics in the Baltic Sea." Estuarine, Coastal and Shelf Science **73**(3–4): 489-500.

See also reports from European projects Jerico (http://www.jerico-ri.eu/) and Ferrybox (http://www.ferrybox.com/).

Templates

Parameter Template

Use this template to give a common structure to document.

Keep each paragraph as short as possible so it can be used as a check list by users. More scientific or technologic background can be added in section background.

Description of parameter

Names, units, vocabulary

Required Meta Data

Required Auxiliary Parameters

Optional Auxiliary Parameters

Field Control

Calibration Method