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Bio-Argo quality control manual for Chlorophyll-A concentration
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ARGO
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Bio-Argo quality control manual for Chlorophyll-A concentration

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History of the document

Version	Date	Authors	Modification
1.0	December 2014	Schmechtig Catherine, Claustre Herve, Poteau Antoine, D'Ortenzio Fabrizio	CS: creation of the document
1.0	January 2015	Schmechtig Catherine, Claustre Herve, Poteau Antoine, D'Ortenzio Fabrizio	TC: apply the Argo document style
1.1	March 2018	Schmechtig Catherine, Claustre Herve, Poteau Antoine, D'Ortenzio Fabrizio	CS: QC Flag 5 for NPQ, Roesler factor 2.

Preamble

In this document, we present the rules applied to control and adjust the chlorophyll-A concentration.

Users should be aware that although biogeochemical data are now freely available at the Argo Global Data Assembly Centres (GDACs) along with their CTD data, the accuracy of these biogeochemical data at their raw state is not suitable for direct usage in scientific applications. Users are warned that the raw biogeochemical data should be treated with care, and that often, adjustments are needed before these data can be used for meaningful scientific applications.

Any user of these biogeochemical data that would develop a specific and dedicated adjustment improving their accuracy is welcome to exchange with ADMT on the developed and applied method

1 Introduction

TBD

2 Bio-Argo real-time quality control test procedures on vertical profiles for the chlorophyll-A parameter

2.1 Generalities

The general calibration equation for the Chlorophyll-A, as obtained by fluorometer, is

- CHLA=(FLUORESCENCE_CHLA-DARK_CHLA) * SCALE_CHLA (Equation 1)

Where FLUORESCENCE_CHLA is the Chlorophyll-A signal from the fluorescence sensor, DARK_CHLA is the dark value and SCALE_CHLA is the slope of the calibration equation.

DARK_CHLA and SCALE_CHLA are provided by manufacturer. They are stored in the metadata file.

Presently, SCALE_CHLA value is not checked in the RTQC tests.

When DARK_CHLA value is not reliable, a specific procedure will be presented, in details, as part of the quality control tests. This procedure is based on the assumption that at depths and when water column is not mixed, the chlorophyll-A should be zero. Consequently, if a non-zero value at depth is collected after application of equation 1, a bad calibration or a drift of the chlorophyll-A sensor is possible and, eventually, corrigible.

Warning: In most cases, this assumption is true. Anyway, for some specific regions with an oxygen minimum, the signal can increase with depth (Black Sea). Setting up a regional test is in discussion.

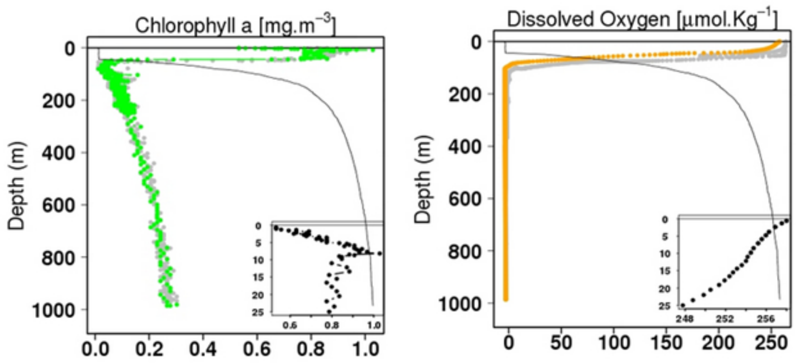

Figure 1.a

Figure 1.b

Figure 1: Illustration with profiling float 7900591, in the Black Sea. The signal assigned to chlorophyll-a increase with depth (Figure 1.a) in anoxic conditions (Figure 1.b).

2.2 LAST_DARK_CHLA and first profile

We introduce LAST_DARK_CHLA, which will be stored for each profile in the technical file and which is defined as the last DARK_CHLA considered as good for calibration.

For the first profile and before the beginning of the RTQC procedure:

- LAST_DARK_CHLA=DARK_CHLA (Equation 2)

2.3 Quality control Tests

The RTQC of the Chlorophyll-A parameter is described in the following in a sequential way (i.e. each step is described in the order of its application).

Control of the calibration equation

The first test is to compare the DARK_CHLA (factory calibration) to the LAST_DARK_CHLA (the last DARK_CHLA considered as good for calibration) in order to identify any eventual deviation.

- DARK_CHLA ≠ LAST_DARK_CHLA (Test 1)

If Test 1 is true, CHLA_QC=3. As a change in the calibration was identified for the previous profiles, the Chlorophyll-A calculated with the factory calibration is certainly bad.

If Test 1 is false CHLA_QC=1

Mixed Layer Depth estimation

To evaluate DARK_CHLA, an estimation of the mixed layer depth is required (MLD, considered here as a proxy of the mixing conditions of the water column) is required.

The calculation of the MLD is based on the CTD measurements (PRES, TEMP, PSAL), assuming that the RT density inversion test is already done.

For each profile, the MLD is the depth where the potential density exceeds the potential density at 10m of 0.03 Kg/m3 (de Boyer Montégut et al., 2004):

$$\sigma(MLD)-\sigma(10m)>0.03\ Kg/m^3 \quad \text{(Equation 3)}$$

Profile depth

Only profiles sufficiently deep could be corrected /evaluated. A specific test is then introduced, by comparing the depth of the last available observation (Depth_Last_Obs) with a threshold depth depending of the MLD.

$$Depth\_Last\_Obs > MLD + \Delta depth + \Delta depthdark \quad \text{(Test 2)}$$

With ($\Delta depth = 200m$, $\Delta depthdark = 50m$),

➔ Test 2 is false: Mixing situations and/or shallow profiles

A new dark value at depth cannot be estimated. DARK'_CHLA is assumed to be equal to the last "good" estimation:

- DARK'_CHLA = LAST_DARK_CHLA (Equation 7)

CHLA_QC and CHLA_ADJUSTED_QC are assumed to have value =2.

We also raise the flag, FLAG_MLD. This Flag will be used to ignore the Non Photochemical Quenching correction in the next steps.

➔ Test 2 is true: Non mixing situation and no shallow profiles :

The DARK'_CHLA parameter is then calculated following equation 4 and round to be consistent with counts:

DARK'_CHLA=median(FLUORESCENCE_CHLA[Depth_Last_Obs,Depth_Last_Obs-Δdepthdark]) (Equation 4)

Using the actual value of DARK'_CHLA, the DARK_CHLA parameter is checked:

- |DARK'_CHLA-DARK_CHLA|>0.2*DARK_CHLA (Test 3)

If Test 3 is true , that means that the new dark estimated has dramatically changed compared to the factory calibration, then we assume that there might be an issue with the sensor and CHLA_QC=3, CHLA_ADJUSTED_QC=3 and equation 7 is applied.

If Test 3 is false, we test:

DARK_CHLA ≠ DARK'_CHLA (Test 4)

If test 4 is true, CHLA_QC=3, CHLA_ADJUSTED_QC=1 and we store the new value of the LAST_DARK_CHLA.

- LAST_DARK_CHLA=DARK'_CHLA(Equation 5)

Then, we calculate the value of the CHLA_ADJUSTED:

- CHLA_ADJUSTED=(FLUORESCENCE_CHLA-DARK'_CHLA)*SCALE_CHLA (Equation 6)

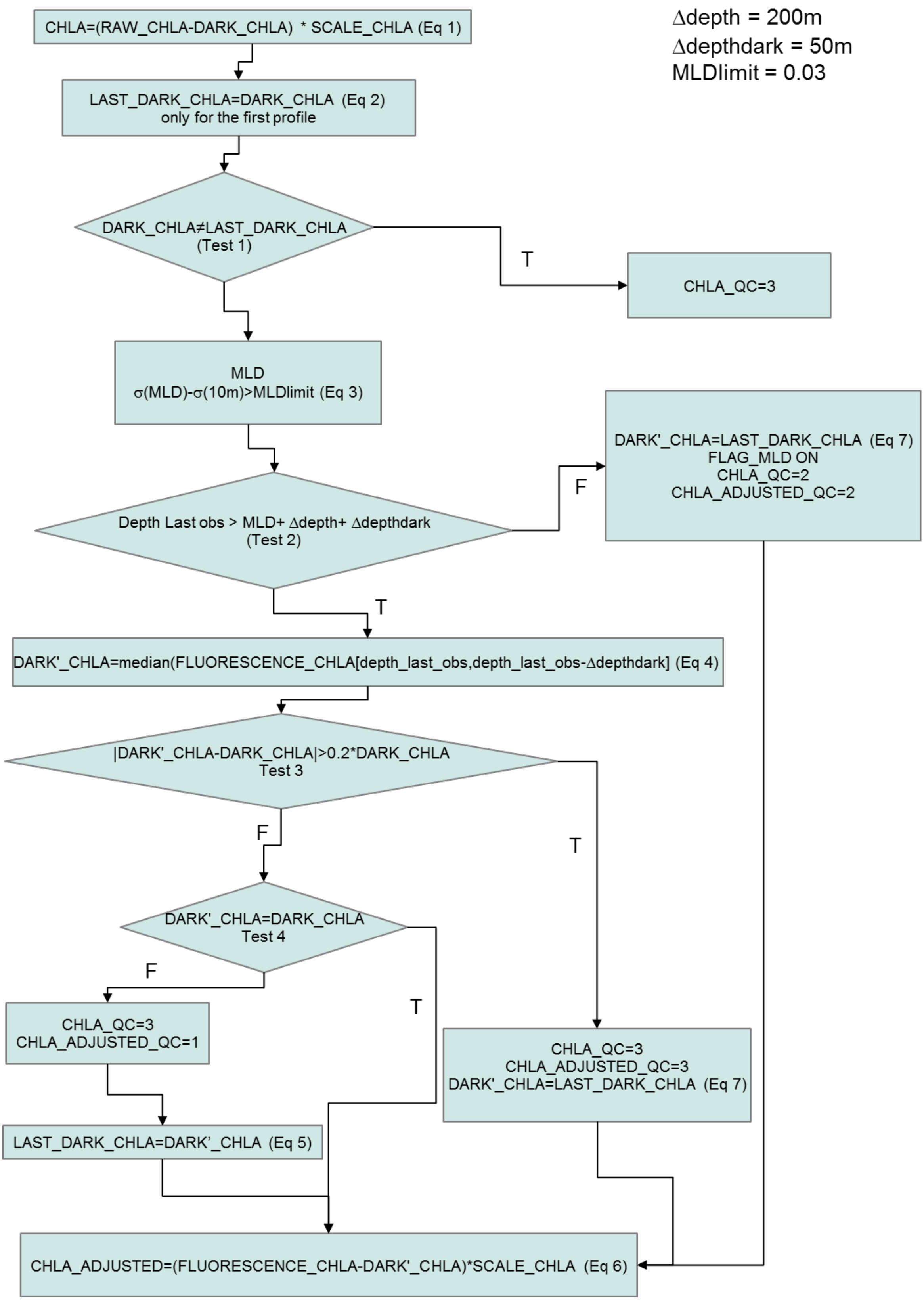

Figure 2: We illustrate with a flow chart the first part of the RTQC for the Chlorophyll-A.

Range test

This test applies a gross filter on observed values. It needs to accommodate all of the expected extremes encountered in the oceans. On the figure 3, from Antoine et al., 1996, we see that up to 90 % of the global waters have a Chlorophyll concentration lower than 1mg/m3.

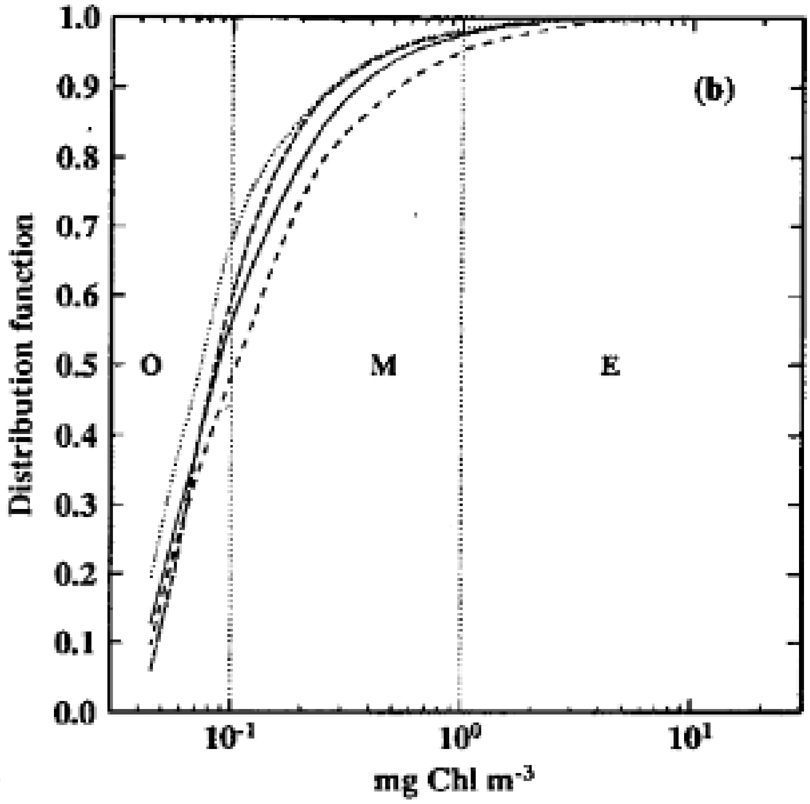

Figure 3.

O is for oligotrophic waters , Mesotrophic waters et eutrophic waters

--- is Atlantic, …. Is Pacific, long dash Indian and plain is global

Then, we assume that a correct value of chlorophyll-A should be within the range of -0.1-50mg/m3. If not, CHLA_QC=4, CHLA_ADJUSTED_QC=4.

- -0.1 < CHLA_ADJUSTED < 50 (Test 5)

Spike Test

Difference between sequential measurements, where one measurement is quite different than adjacent ones, is considered as a spike. With respect to biogeochemistry, most of the time, spikes contain information, mainly in case of positive spikes. This is the reason why we set up a test to discriminate negative spikes.

We calculate the difference between the chlorophyll-A at a certain depth (V2) and a running median (5 values, V0, V1, V2, V3, V4) along the whole profile.

- RES=V2-median(V0,V1,V2,V3,V4) (Equation 8)

Then we calculate the percentile10 and the percentile90 of this difference. If the difference between the chlorophyll-A and the running median is smaller than 2*percentile10 (Test 6), then it is considered as a spike.

- RES< 2*percentile10 (RES) (Test 6)

then it is considered as a spike.

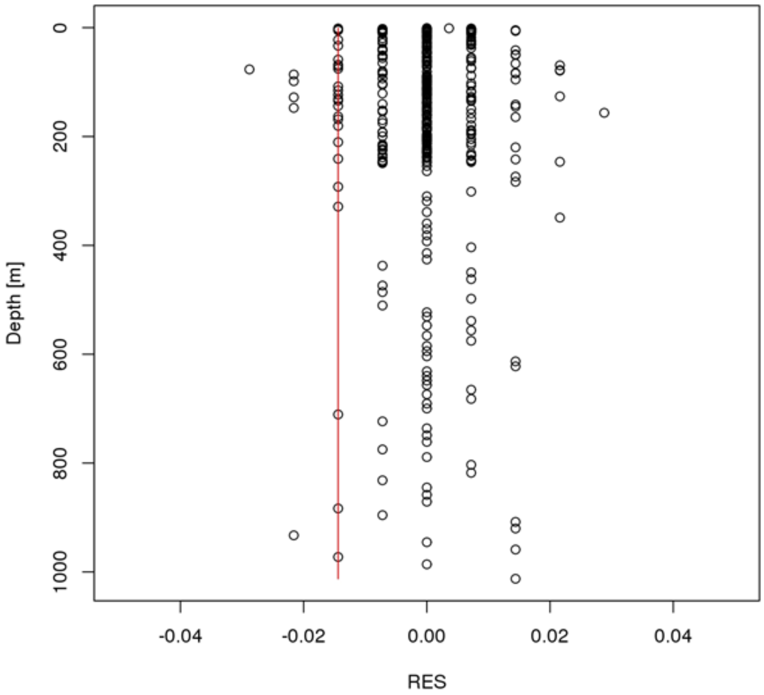

Figure 4. Illustration of RES calculation on profiling float 6901511, 2*percentile10 is represented by the red line.

Non Photochemical Quenching (Xing, 2012)

The Non-Photochemical Quenching (NPQ) is a mechanism employed by plants and algae to protect themselves from the adverse effects of high light intensity. In case of Non-Photochemical Quenching, the Chlorophyll fluorescence is no longer proportional to the chlorophyll-A concentration. Non Photochemical Quenching occurs in non mixing situations, this is the reason why we will test the FLAG_MLD (Test 7) before accounting for the NPQ correction.

In Xing et al., 2012 it appears that the daytime fluorescence maximum (MaxFluo) and its depth ZMaxFluo within MLD, is a good proxy to identify depthNPQ, the thickness of the layer potentially affected by the quenching. We slightly revise this criteria by choosing ZMaxFluo within the layer between surface and 0.9*MLD. To estimate MaxFluo and ZmaxFluo, we run a median filter on 5 values on the CHLA_ADJUSTED profile and we eliminate depths for which RES (calculated in equation 8) is over 2*Percentile90, to avoid positive spikes in the determination of Maxfluo (Test 8)

- RES> 2*percentile90 (RES) (Test 8)

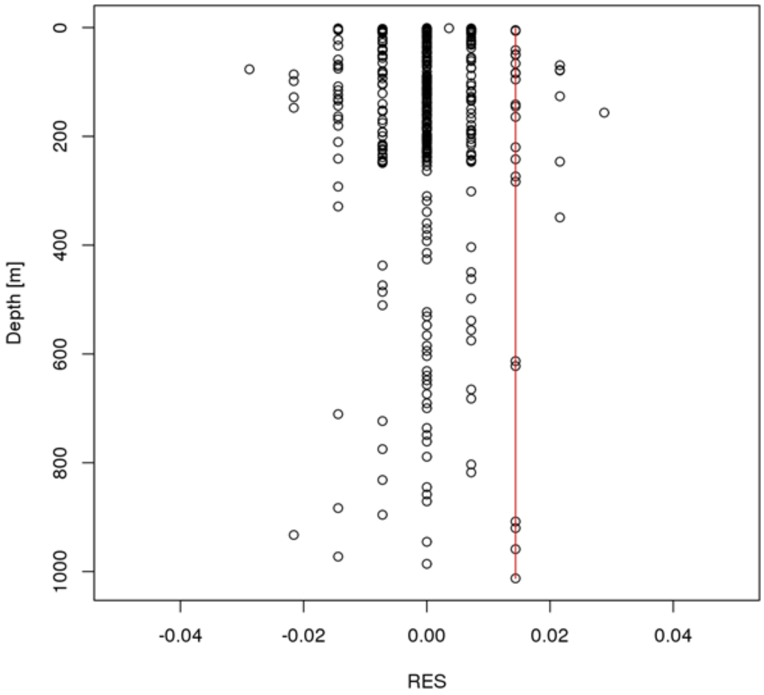

Figure 5. Illustration of RES calculation on profiling float 6901511, 2*percentile90 is represented by the red line

Finally,

- depthNPQ=depth[max[median(CHLA_ADJUSTED(V0,V1,V2,V3,V4))]] (Equation 9)

Then, to adjust the chlorophyll-A concentration between depthNPQ and the surface, it is proposed to extrapolate the adjusted chlorophyll concentration at depthNPQ toward the surface as a way to correct for the quenching effect (equation 10).

- CHLA_ADJUSTED[0,depthNPQ]=CHLA_ADJUSTED(depthNPQ) (Equation 10)

From the surface to depthNPQ, CHLA_QC=3 and CHLA_ADJUSTED_QC=5.

The value of 5, “changed” for the QC was decided after ADMT17, in the previous version the QC value was 8, “interpolated”

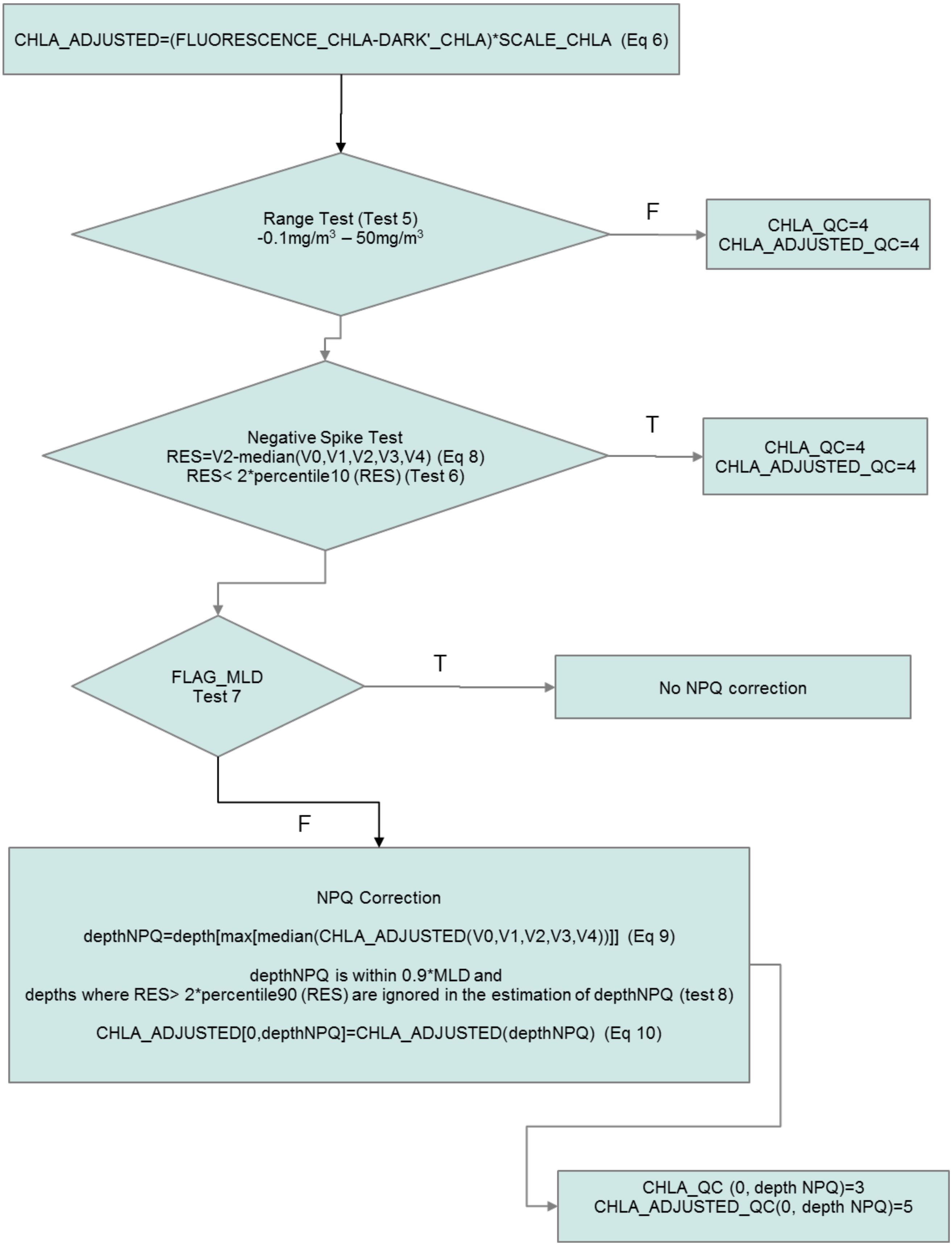

Figure 4: We illustrate the following part of the flowchart of the RTQC for the Chlorophyll-A. (Following equation 6, on the Figure 2)

2.4 Calibration issue

In Roesler et al.2017, a recommendation is made to account for a factor of 2 as a global bias correction to be applied for the WET Labs ECO sensors, this should improve the global accuracy of chlorophyll concentration estimates and products derived from them. This result was presented and discussed in ADMT17 and ADMT18 and approved for application.

- CHLA_ADJUSTED=CHLA_ADJUSTED/2 (Equation 11)

This should be recorded in the SCIENTIFIC_CALIB_xxx fields.

2.5 Quality control Flag application policy

The Argo quality control flag application policy is used. Then, the QC flag value assigned by a test cannot override a higher value from a previous test. A value with QC flag '4' (bad data) or '3' (bad data that are potentially correctable) is ignored by the quality control tests.

3 References

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CHLA Chlorophyll-A concentration (mg/m3)

CHLA_QC Quality flag for the Chlorophyll-A concentration

CHLA_ADJUSTED Adjusted chlorophyll-A concentration (mg/m3)

CHLA_ADJUSTED_QC Quality flag for the adjusted Chlorophyll-A concentration

DARK_CHLA Dark count of the calibration equation to transform the fluorescence signal into chlorophyll-A concentration (Counts)

DARK'_CHLA Estimated/adjusted Dark Count of the calibration equation to transform the fluorescence signal into adjusted chlorophyll-A concentration (counts)

□depth Interval between the end of the mixed layer depth and the depth at which the estimation of the dark value begins (200m)

□depthdark Interval of depth on which the dark value is estimated (50m)

Depth_Last_Obs Depth of the deepest measurements of a profile

depthNPQ the thickness of the layer potentially affected by quenching

FLUORESCENCE_CHLA Counts for the fluorescence signal

LAST_DARK_CHLA Stored value of the Last dark count to estimate the evolution of the dark count from the beginning of the mission. This value can come either from the factory calibration or from the estimated value at depth

MLD Mixed Layer Depth

MLDlimit Threshold of the difference on potential density between MLD and 10m (0.03)

RES Difference between Chlorophyll-A concentr

SCALE_CHLA Slope of the calibration equation to transform the fluorescence signal into chlorophyll-A concentration