Argo data management

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Processing Bio-Argo nitrate concentration at the DAC Level

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**Preamble**

This document does NOT address the issue of nitrate quality control (either real-time or delayed mode). As a preliminary step towards that goal, this document seeks to ensure that all countries deploying floats equipped with nitrate sensors document the data and metadata related to these floats properly. We produced this document in response to action item 11 from the first Bio-Argo Data Management meeting in Hyderabad (November 12-13, 2012).

If the recommendations contained herein are followed, we will end up with a more uniform set of particle backscattering data within the Bio-Argo data system, allowing users to begin analyzing not only their own particle backscattering data, but also those of others, in the true spirit of Argo data sharing.

# Introduction

The only method used to date to measure dissolved nitrate concentration (NITRATE) with sensors mounted on profiling floats is based on the absorption of light at ultraviolet wavelengths by nitrate ion (Johnson and Coletti, 2002; Johnson et al., 2010; 2013; D’Ortenzio et al., 2012). Nitrate has a modest UV absorption band with a peak near 210 nm, which overlaps with the stronger absorption band of bromide, which has a peak near 200 nm. In addition, there is a much weaker absorption due to dissolved organic matter and light scattering by particles (Ogura and Hanya, 1966). The UV spectrum thus consists of three components, bromide, nitrate and a background due to organics and particles. The background also includes thermal effects on the instrument and slow drift. All of these latter effects (organics, particles, thermal effects and drift) tend to be smooth spectra that combine to form an absorption spectrum that is linear in wavelength over relatively short wavelength spans. If the light absorption spectrum is measured in the wavelength range around 217 to 240 nm (the exact range is a bit of a decision by the operator), then the nitrate concentration can be determined.

Two different instruments based on the same optical principles are in use for this purpose. The In Situ Ultraviolet Spectrophotometer (ISUS) built at MBARI or at Satlantic has been mounted inside the pressure hull of a Teledyne/Webb Research APEX and NKE Provor profiling floats and the optics penetrate through the upper end cap into the water. The Satlantic Submersible Ultraviolet Nitrate Analyzer (SUNA) is placed on the outside of APEX, Provor, and Navis profiling floats in its own pressure housing and is connected to the float through an underwater cable that provides power and communications. Power, communications between the float controller and the sensor, and data processing requirements are essentially the same for both ISUS and SUNA.

There are several possible algorithms that can be used for the deconvolution of nitrate concentration from the observed UV absorption spectrum (Johnson and Coletti, 2002; Arai et al., 2008; Sakamoto et al., 2009; Zielinski et al., 2011). In addition, the default algorithm that is available in Satlantic sensors is a proprietary approach, but this is not generally used on profiling floats. There are some tradeoffs in every approach. To date almost all nitrate sensors on profiling floats have used the Temperature Compensated Salinity Subtracted (TCSS) algorithm developed by Sakamoto et al. (2009), and this document focuses on that method.

It is likely that there will be further algorithm development and it is necessary that the data systems clearly identify the algorithm that is used. It is also desirable that the data system allow for recalculation of prior data sets using new algorithms. To accomplish this, the float must report not just the computed nitrate, but the observed light intensity.

Then, the rule to obtain only one NITRATE parameter is, if the spectrum is present then, the NITRATE should be recalculated from the spectrum while the computation of nitrate concentration can also generate useful diagnostics of data quality.

# Compute Nitrate concentration from the spectrum

## Parameters

|  |  |  |
| --- | --- | --- |
| UV\_INTENSITY\_NITRATE | Intensity of ultra violet flux from nitrate sensor | count |
| UV\_INTENSITY\_DARK\_NITRATE | Intensity of ultra violet flux dark measurement from nitrate sensor | count |
| NITRATE | Nitrate | micromole/kg |
| MOLAR\_NITRATE | Nitrate | micromole/l(\*) |
| FIT\_ERROR\_NITRATE | Nitrate fit error | dimensionless |
| HUMIDITY\_NITRATE | Relative humidity inside the SUNA sensor (If > 50% There is a leak) | percent |
| TEMP\_NITRATE | Internal temperature of the SUNA sensor | degree\_Celsius |
| TEMP\_SPECTROPHOTOMETER\_NITRATE | Temperature of the spectrometer | degree\_Celsius |

Table 1. Parameters related to Nitrate sensor. (\*), the NITRATE parameter should be recalculated from the spectrum, anyway some floats only report MOLAR\_NITRATE computed on board, in this case MOLAR\_NITRATE should be considered as an “i” parameter reported in the b-file.

|  |  |  |
| --- | --- | --- |
| *E\_NITRATE* | *Sea water absorptivity* | liter.µmol-1.cm-1 |
| *E\_SWA\_NITRATE* | *Molar absorptivity of nitrate* |  |
| *OPTICAL\_WAVELENGTH\_UV* | *Wavelength* | *nm* |
| *TEMP\_CAL\_NITRATE* | *Calibration temperature* | degree\_Celsius |
| *UV\_INTENSITY\_REF\_NITRATE* |  |  |

Table 2. Coefficients related to calibration

## Calibration file

Each nitrate sensor is individually calibrated at the builder and a calibration file accompanies each instrument. The calibration file must be present on the sensor to allow nitrate concentration to be computed. The calibration file should also be archived in the data system to allow nitrate to be recomputed if improved algorithms are developed.

The calibration file is a comma delimited, ASCII text file. It consists of a series of Header lines, which begin with the character H, and a series of calibration data lines, which begin with the character E. The last header line describes the contents of the data lines. There is one calibration data line for each of the 256 pixels on the detector array. The contents of the calibration files from different builders are similar, but the number of header lines and the order of the contents on the data lines differs for MBARI and Satlantic instruments. The last header line is essential to decipher the contents. An example of a Satlantic calibration file, including the last header line and first 5 calibration data lines is shown in Table 2.

|  |
| --- |
| Table 2. Partial calibration file from Satlantic showing last header line and first 5 data lines. |
| H,Wavelength,NO3,SWA,TSWA,Reference  E,189.17,0.00274308,-0.00902953,-0.01006273,22.00000000  E,189.97,0.00872217,-0.01496882,-0.01635747,22.00000000  E,190.76,0.01199933,-0.01635049,-0.01752441,12.00000000  E,191.56,0.02000221,-0.00239762,-0.00251983,39.00000000  E,192.35,0.00703844,-0.00795972,-0.00820488,21.00000000 ……… |

The 6 columns of the above calibration file are:

1. Letter, H is for header lines, E is for data lines.

2. Wavelength corresponds to *OPTICAL\_WAVELENGTH\_UV*(N):

Wavelength (nm) of pixel N based on calibration reported by manufacturer (Zeiss).

3. NO3 corresponds to *E\_NITRATE*(N):

Molar absorptivity of nitrate determined during laboratory calibration at pixel N. Units are liter.µmol-1 path length-1. The optical path length is nominally 1 cm, but ISUS and SUNA units have been built with path lengths from 0.5 to 4 cm. To date only 1 cm path lengths have been used on profiling floats (thus units is liter.µmol-1.cm-1),

4. SWA corresponds to *E\_SWA\_NITRATE*(N):

The sea water absorptivity (absorbance of seawater with no nitrate/salinity (PSS)) determined during laboratory calibration at the pixel N and the calibration temperature (*TEMP\_CAL\_NITRATE*). The sea water absorptivity is due primarily to the bromide ion with a few other minor contributions.

5. TSWA:

Satlantic proprietary and not used.

6. Reference corresponds to *UV\_INTENSITY\_REF\_NITRATE*(N):

Light intensity reaching detector array through ultrapure water minus detector counts with the lamp turned off or the lamp shutter closed at pixel N. It is determined in the laboratory during calibration.

In the header part, another line is essential for the TCSS algorithm.

For Satlantic systems, the line which contains “T\_CAL\_SWA”:

H,T\_CAL\_SWA 20.01068750053828,,

For MBARI ISUS systems, the line which contains “CalTemp”

H,CalTemp,20.07

This line provides the laboratory temperature at which the E\_SWA\_NITRATE values were determined. This value will be stored in *TEMP\_CAL\_NITRATE*.

## Computing nitrate concentration

### 2.3.1 Input data

The sensor returns:

UV\_INTENSITY\_NITRATE(Ntrans): a subset of continuous pixels of UV\_INTENSITY\_NITRATE(N), N = 1 to 256

UV\_INTENSITY\_DARK\_NITRATE.

The Ntrans indices span the interval [PIXEL\_START, PIXEL\_END] subset of the original array (1 to 256). Thus Ntrans(i) refers to pixel N = (PIXEL\_START+i-1)

PIXEL\_START and PIXEL\_END are defined from calibration data so that the [PIXEL\_START, PIXEL\_END] interval is the smallest interval of pixels that correspond to the [217 nm, **250 nm**] interval of wavelengths.

Only a subset of the [PIXEL\_START, PIXEL\_END] interval is processed to compute nitrate concentration. This subset is defined as the [PIXEL\_FIT\_START, PIXEL\_FIT\_END] interval which is the smallest interval of pixels that correspond to the [217 nm, **240 nm**] interval of wavelengths (thus PIXEL\_FIT\_START = PIXEL\_START).

In the following equations the data are computed for each pixel R = PIXEL\_FIT\_START to PIXEL\_FIT\_END.

### 2.3.2 Nitrate concentration processing

The nitrate concentration is computed using the TCSS algorithm following three steps, which are described in more detail by Sakamoto et al. (2009).

***Step i:Compute absorbance spectrum of seawater***

Absorbance is calculated over pixel range R:

ABSORBANCE\_SW(R) = - log10[(UV\_INTENSITY\_NITRATE(R) – UV\_INTENSITY\_DARK\_NITRATE) / *UV\_INTENSITY\_REF\_NITRATE*(R)]

(Eq. 1)

***Step ii:Remove spectrum due to bromide and other sea salt components***

Calculate the spectrum due to Bromide and other sea salt components, with a correction of the in situ temperature :

E\_SWA\_INSITU(R) = *E\_SWA\_NITRATE*(R) \* F(R, TEMP) / F(R, *TEMP\_CAL\_NITRATE*)

(Eq. 2)

With two calculations of F, for TEMP (temperature sampled by the CTD (cf 3.1)) and for *TEMP\_CAL\_NITRATE* following:

F(R, T) = (A + B\*T)

\*exp[(C + D\*T)\*(*OPTICAL\_WAVELENGTH\_UV*(R) – *OPTICAL\_WAVELENGTH\_OFFSET*)]

(Eq. 3)

A = 1.1500276, B = 0.02840, C = -0.3101349, D = 0.001222

*OPTICAL\_WAVELENGTH\_OFFSET* = 208.5 nm (\*)

(\*) Experience with many ISUS units deployed on floats in tropical waters suggests that there are deficiencies in the temperature compensation scheme used in equation 2. These may arise from uncertainty in the wavelength registration of the diode array spectrometer. These uncertainties lead to a generally positive bias in nitrate concentrations above about 20°C. It has been found that these biases can be eliminated by small adjustments in the *OPTICAL\_WAVELENGTH\_OFFSET* parameter (typically in the range from 206 to 212 nm). The operator may choose to treat *OPTICAL\_WAVELENGTH\_OFFSET* as a tunable parameter for each float to eliminate these biases in near surface nitrate. Thus, the value of *OPTICAL\_WAVELENGTH\_OFFSET* should be reported.

The predicted absorbance spectrum due to nitrate and the baseline is then

ABSORBANCE\_COR\_NITRATE(R) = ABSORBANCE\_SW(R) – E\_SWA\_INSITU(R) \* PSAL

(Eq. 4)

Where PSAL is the salinity sampled by the CTD (cf 3.1).

***Step iii:Compute nitrate concentration***

Nitrate in units of µmol.l-1, MOLAR\_NITRATE is then computed by a multiple linear regression, least squares fit:

ABSORBANCE\_COR\_NITRATE(R) = BASELINE\_INTERCEPT

+ BASELINE\_SLOPE\**OPTICAL\_WAVELENGTH\_UV*(R)

+ MOLAR\_NITRATE\**E\_NITRATE*(R)

(Eq. 5)

This yields three regression constants: MOLAR\_NITRATE, the intercept (BASELINE\_INTERCEPT) and slope (BASELINE\_SLOPE) of a baseline linear in wavelength that is due to light absorption and scattering by organics, particles and instrumental drift.

Finally, as the Argo unit for nitrate is µmol/kg density (ρ) is used to compute the final value (cf 3.1):

NITRATE = MOLAR\_NITRATE / ρ

(Eq. 6)

# Nitrate concentration adjustment

Some studies reported in Pasqueron de Fommervault et al., 2015, highlight the need for extra adjustment during the computation of the nitrate concentration.

## Vertical offset

A bias in the TCSS correction is induced if at a given time, the SUNA and the CTD are not sampling the same water. For example, on PROVORIII (which are used in NAOS and remOcean), SUNA are located on the outside of the float, around 1.5m under the CTD intake. This distance between the CTD intake and the SUNA should be reported in the METADATA file (cf 4.1.2)

This vertical offset (Δ) is to be considered in the TCSS algorithm. Temperature (in Eq. 3) and salinity (in Eq. 4) from the CTD are then linearly interpolated at the depth of the SUNA. This allows measurement to be properly handled especially in depth of strong temperature and salinity gradient.

## Pressure effect

Some studies conducted in low nutrient concentrations highlighted a possible pressure dependency of the bromide absorption spectrum (Pasqueron de Fommervault et al., 2015). Some experiments in lab will be performed soon at MBARI.

The equation 4 is changed in:

ABSORBANCE\_COR\_NITRATE(R) = ABSORBANCE\_SW(R)

– (E\_SWA\_INSITU(R) \* PSAL)\*[1 – (0.02 \* PRES / 1000)]

(Eq. 7)

# Data processing

## Sensor METADATA and Configuration parameters

### Sensor and parameter metadata

This section contains information about the sensors of the profiler and the parameters measured by the profiler or derived from profiler measurements that need to be filled. All the reference tables can be found in the Argo user’s manual.

|  |  |
| --- | --- |
| Sensor metadata | |
| SENSOR | SPECTROPHOTOMETER\_NITRATE |
| SENSOR MAKER | Satlantic |
| SENSOR\_MODEL | SUNA\_V2 *(or ISUS\_V3)* |
| SENSOR\_SERIAL\_NO | *To be filled* |

The SUNA and the ISUS spectrophotometers were developed at MBARI and commercialized by Satlantic (SUNA\_V2, ISUS\_V3)

|  |  |
| --- | --- |
| Parameter metadata | |
| PARAMETER | UV\_INTENSITY\_NITRATE |
| PARAMETER\_SENSOR | SPECTROPHOTOMETER\_NITRATE |
| PARAMETER\_UNITS | count |
| PARAMETER\_ACCURACY |  |
| PARAMETER\_RESOLUTION |  |
|  |  |
| PARAMETER | UV\_INTENSITY\_DARK\_NITRATE |
| PARAMETER\_SENSOR | SPECTROPHOTOMETER\_NITRATE |
| PARAMETER\_UNITS | count |
| PARAMETER\_ACCURACY |  |
| PARAMETER\_RESOLUTION |  |
|  |  |
| PARAMETER | FIT\_ERROR\_NITRATE |
| PARAMETER\_SENSOR | SPECTROPHOTOMETER\_NITRATE |
| PARAMETER\_UNITS | dimensionless |
| PARAMETER\_ACCURACY |  |
| PARAMETER\_RESOLUTION |  |
|  |  |
| PARAMETER | HUMIDITY\_NITRATE |
| PARAMETER\_SENSOR | SPECTROPHOTOMETER\_NITRATE |
| PARAMETER\_UNITS | percent |
| PARAMETER\_ACCURACY |  |
| PARAMETER\_RESOLUTION |  |
|  |  |
| PARAMETER | TEMP\_NITRATE |
| PARAMETER\_SENSOR | SPECTROPHOTOMETER\_NITRATE |
| PARAMETER\_UNITS | degree\_Celsius |
| PARAMETER\_ACCURACY |  |
| PARAMETER\_RESOLUTION |  |
|  |  |
| PARAMETER | TEMP\_SPECTROPHOTOMETER\_NITRATE |
| PARAMETER\_SENSOR | SPECTROPHOTOMETER\_NITRATE |
| PARAMETER\_UNITS | degree\_Celsius |
| PARAMETER\_ACCURACY |  |
| PARAMETER\_RESOLUTION |  |
|  |  |
| PARAMETER | MOLAR\_NITRATE(\*) |
| PARAMETER\_SENSOR | SPECTROPHOTOMETER\_NITRATE |
| PARAMETER\_UNITS | umol/L |
| PARAMETER\_ACCURACY |  |
| PARAMETER\_RESOLUTION |  |
|  |  |
| PARAMETER | NITRATE |
| PARAMETER\_SENSOR | SPECTROPHOTOMETER\_NITRATE |
| PARAMETER\_UNITS | umol/kg |
| PARAMETER\_ACCURACY | 2 umol/kg |
| PARAMETER\_RESOLUTION | * 1. mol/kg |
|  |  |

(\*), the NITRATE parameter should be recalculated from the spectrum, anyway some floats only report MOLAR\_NITRATE computed on board, in this case MOLAR\_NITRATE should be considered as an “i” parameter reported in the b-file.

### 4.1.2 Configuration parameters

The distance between the CTD intake and the SUNA should be reported in the METADATA file. For example for the PROVORIII:

CONFIG\_SunaVerticalPressureOffset\_dbar = 1.5

Vertical pressure offset due to the fact that the sensor is not exactly at the CTD pressure

CONFIG\_SunaWithScoop\_LOGICAL

Suna with scoop which redirects flow through Suna optics. Values: Yes = 1, No = 0.

CONFIG\_SunaInPumpedStream\_LOGICAL

Bio Argo sensors can either be mounted separately to the CTD or mounted within the CTD pumped stream. Values: Yes = 1, No = 0.

CONFIG\_SunaApfFrameOutputPixelBegin\_NUMBER

The Apf frame definition allows for a variable number of spectrometer pixels (also called channels) to be included in the frame. The two pixel values are configured indirectly via the wavelength range of the spectrum to be output (Suna Hardware Manual, section 4.2.3, input/output configuration parameters, data wavelength low/high.) The firmware converts the wavelength values to spectrometer pixels.

CONFIG\_SunaApfFrameOutputPixelEnd\_NUMBER

The Apf frame definition allows for a variable number of spectrometer pixels (also called channels) to be included in the frame. The two pixel values are configured indirectly via the wavelength range of the spectrum to be output (Suna Hardware Manual, section 4.2.3, input/output configuration parameters, data wavelength low/high.) The firmware converts the wavelength values to spectrometer pixels.

## Nitrate concentration data related parameters

During the ADMT13, the decision to separate data files for floats with biogeochemical sensors was taken. Then for biogeochemical floats, there are three files: one (c-file) for P,T,S, one (b-file) containing P, intermediate parameters and ocean state variables and one merged file (m-file) containing P, T, S and ocean state variables.

### 4.2.1 Nitrate concentration related parameters for the b-file

Raw data from the Suna sensor is output in counts (UV\_INTENSITY\_NITRATE) from the sensor.

**PARAMETER** = "UV\_INTENSITY\_NITRATE"

**PREDEPLOYMENT\_CALIB\_EQUATION** = "none"

**PREDEPLOYMENT\_CALIB\_COEFFICIENT** = "none"

**PREDEPLOYMENT\_CALIB\_COMMENT** = " Intensity of ultra violet flux from nitrate sensor"

**PARAMETER** = "UV\_INTENSITY\_DARK\_NITRATE"

**PREDEPLOYMENT\_CALIB\_EQUATION** = "none"

**PREDEPLOYMENT\_CALIB\_COEFFICIENT** = "none"

**PREDEPLOYMENT\_CALIB\_COMMENT** = "Intensity of ultra violet flux dark measurement from nitrate sensor"

**PARAMETER** = "HUMIDITY\_NITRATE"

**PREDEPLOYMENT\_CALIB\_EQUATION** = "none"

**PREDEPLOYMENT\_CALIB\_COEFFICIENT** = "none"

**PREDEPLOYMENT\_CALIB\_COMMENT** = "Relative humidity inside the SUNA sensor (If > 50% There is a leak)"

**PARAMETER** = "TEMP\_NITRATE"

**PREDEPLOYMENT\_CALIB\_EQUATION** = "none"

**PREDEPLOYMENT\_CALIB\_COEFFICIENT** = "none"

**PREDEPLOYMENT\_CALIB\_COMMENT** = "Internal temperature of the SUNA sensor"

**PARAMETER** = "TEMP\_SPECTROPHOTOMETER\_NITRATE"

**PREDEPLOYMENT\_CALIB\_EQUATION** = "none"

**PREDEPLOYMENT\_CALIB\_COEFFICIENT** = "none"

**PREDEPLOYMENT\_CALIB\_COMMENT** = "Temperature of the spectrometer"

**PARAMETER** = "FIT\_ERROR\_NITRATE"

**PREDEPLOYMENT\_CALIB\_EQUATION** = "none"

**PREDEPLOYMENT\_CALIB\_COEFFICIENT** = "none"

**PREDEPLOYMENT\_CALIB\_COMMENT** = "Nitrate fit error (dimensionless)"

**PARAMETER** = "MOLAR\_NITRATE"(\*)

**PREDEPLOYMENT\_CALIB\_EQUATION** = "none"

**PREDEPLOYMENT\_CALIB\_COEFFICIENT** = "none"

**PREDEPLOYMENT\_CALIB\_COMMENT** = "Molar nitrate concentration(umole/L)"

(\*), the NITRATE parameter should be recalculated from the spectrum, anyway some floats only report MOLAR\_NITRATE computed on board, in this case MOLAR\_NITRATE should be considered as an “i” parameter reported in the b-file.

### 4.2.2 Nitrate data for the b-file and the merged file

**PARAMETER** = "NITRATE"

**PREDEPLOYMENT\_CALIB\_EQUATION**=”The sensor returns UV\_INTENSITY\_DARK\_NITRATE and UV\_INTENSITY\_NITRATE(Ntrans), a subset of continuous pixels of UV\_INTENSITY\_NITRATE(N), N = 1 to 256. The Ntrans indices span the interval [PIXEL\_START, PIXEL\_END] subset of the original array (1 to 256). Thus Ntrans(i) refers to pixel N = (PIXEL\_START+i-1). PIXEL\_START and PIXEL\_END are defined from calibration data so that the [PIXEL\_START, PIXEL\_END] interval is the smallest interval of pixels that correspond to the [217 nm, 250 nm] interval of wavelengths. Only a subset of the [PIXEL\_START, PIXEL\_END] interval is processed to compute nitrate concentration. This subset is defined as the [PIXEL\_FIT\_START, PIXEL\_FIT\_END] interval which is the smallest interval of pixels that correspond to the [217 nm, 240 nm] interval of wavelengths (thus PIXEL\_FIT\_START = PIXEL\_START). In the following equations the data are computed for each pixel R = PIXEL\_FIT\_START to PIXEL\_FIT\_END; ABSORBANCE\_SW(R)=-log10[(UV\_INTENSITY\_NITRATE(R)-UV\_INTENSITY\_DARK\_NITRATE)/UV\_INTENSITY\_REF\_NITRATE(R)]; F(R,T)=(A+B\*T)\*exp[(C+D\*T)\*(OPTICAL\_WAVELENGTH\_UV(R)-OPTICAL\_WAVELENGTH\_OFFSET)]; E\_SWA\_INSITU(R)=E\_SWA\_NITRATE(R)\*F(R,TEMP)/F(R,TEMP\_CAL\_NITRATE); ABSORBANCE\_COR\_NITRATE(R)=ABSORBANCE\_SW(R)-E\_SWA\_INSITU(R)\*PSAL; Perform a multilinear regression to get MOLAR\_NITRATE with estimated ABSORBANCE\_COR\_NITRATE(R) with ABSORBANCE\_COR\_NITRATE(R)=BASELINE\_INTERCEPT+BASELINE\_SLOPE\*OPTICAL\_WAVELENGTH\_UV(R)+MOLAR\_NITRATE\*E\_NITRATE(R); NITRATE=MOLAR\_NITRATE/rho, where rho is the potential density [kg/L] calculated from CTD data”

**PREDEPLOYMENT\_CALIB\_COEFFICIENT**=" PIXEL\_START=35, PIXEL\_END=76, PIXEL\_FIT\_START=35, PIXEL\_FIT\_END=63; UV\_INTENSITY\_REF\_NITRATE(Ntrans)=[37412.29166667,40030.25000000,42741.87500000,45432.04166667,47890.45833333,49953.58333333,51429.37500000,52159.79166667,52094.54166667,51315.25000000,49942.04166667,48128.08333333,46205.12500000,44256.25000000,42533.33333333,41047.29166667,39920.79166667,39100.20833333,38672.62500000,38492.00000000,38619.91666667,39051.95833333,39662.29166667,40537.66666667,41657.75000000,42952.08333333,44479.45833333,46200.91666667,48060.00000000,50055.08333333,52105.70833333,54106.50000000,56017.12500000,57668.50000000,58959.04166667,59763.41666667,60041.45833333,59659.79166667,58671.41666667,57137.45833333,55076.62500000,52773.04166667]; A=1.1500276, B=0.02840, C=-0.3101349, D=0.001222, OPTICAL\_WAVELENGTH\_OFFSET=208.5; OPTICAL\_WAVELENGTH\_UV(Ntrans)=[217.07,217.86,218.65,219.44,220.23,221.02,221.81,222.60,223.39,224.18,224.97,225.76,226.55,227.34,228.13,228.93,229.72,230.51,231.30,232.10,232.89,233.68,234.47,235.27,236.06,236.85,237.65,238.44,239.24,240.03,240.83,241.62,242.42,243.21,244.01,244.80,245.60,246.39,247.19,247.99,248.78,249.58]; TEMP\_CAL\_NITRATE=20.155; E\_SWA\_NITRATE(Ntrans)=[0.00677218,0.00534786,0.00422602,0.00333490,0.00262609,0.00205092,0.00160600,0.00127921,0.00097924,0.00079266,0.00062711,0.00050231,0.00039663,0.00032128,0.00024922,0.00019977,0.00019884,0.00014188,0.00012114,0.00009859,0.00008577,0.00006516,0.00007669,0.00004643,0.00003962,0.00002723,0.00002678,0.00001013,0.00002632,0.00001246,0.00002210,0.00000134,0.00001108,0.00000517,-0.00000143,-0.00002175,-0.00000076,-0.00000170,-0.00001359,-0.00000694,-0.00000647,-0.00001461]; E\_NITRATE(Ntrans)=[0.00472355,0.00437718,0.00403355,0.00368769,0.00338022,0.00309584,0.00281598,0.00253733,0.00228849,0.00203116,0.00179797,0.00157366,0.00137826,0.00119483,0.00104755,0.00089762,0.00074843,0.00063593,0.00054625,0.00045669,0.00037110,0.00030405,0.00023806,0.00020015,0.00016474,0.00013242,0.00009841,0.00007981,0.00004412,0.00003956,0.00001899,0.00001948,-0.00000380,-0.00000297,-0.00000461,-0.00000211,-0.00001947,-0.00002003,-0.00000616,-0.00001470,-0.00000748,-0.00001192]”

**PREDEPLOYMENT\_CALIB\_COMMENT** = " Nitrate concentration in umol/kg; see Processing Bio-Argo nitrate concentration at the DAC Level, Version 1.0, May 3rd 2016"

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# Annexe A

We present here a complete calibration file of a SUNA. The yellow highlighted text is the part of the file that is used for the computation of nitrate concentration. The yellow +pink highlighted text is the part of the spectrum transmitted by the float.

H,SUNA 0201 Cal A extinction coefficients and reference spectra,,,

H,File generated by SUNACom 3.0.0

H,File format version 3

H,File creation time 12-Sep-2012 17:50:15

H,File generated by Internal Software Suite Version 1.8.5\_83 (2012/08/09 10:30) Copyright (c) 2012\, Satlantic LP,,,

H,File format version 3,,,

H,File creation time 14-Sep-2012 13:32:09,,,

H,Operator Jenn,,,

H,T\_S\_CORRECTABLE ,,,

H,T\_CAL\_SWA 20.15499577132076,,,

H,NitrateFile G:\SUNA0201\SUNA\_0201\_001.xml,,,

H,TFile G:\MPRO-SUNA\_P1\_001.xml,,,

H,DIW Log file G:\SUNA0201\Cal\_001\SUNA201\_Cal01\_DIW\_1.raw,,,

H,LNSW Log file G:\SUNA0201\Cal\_001\SUNA201\_Cal01\_LNSW\_1.raw,,,

H,Nitrate in LNSW Log file G:\SUNA0201\Cal\_001\SUNA201\_Cal01\_NO3\_1.raw,,,

H,Wavelength,nm,,

H,NITRATE,uM,,

H,AUX1,none,,

H,AUX2,none,,

H,Reference,counts,,

H,Wavelength,NO3,SWA,TSWA,Reference

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E,194.30,-0.00391184,-0.00048775,-0.00047939,9.25000000

E,195.08,-0.00769102,-0.01492974,-0.01439481,15.41666667

E,195.86,-0.00955434,0.01774702,0.01678557,13.50000000

E,196.64,-0.00016024,0.00364657,0.00338339,7.83333333

E,197.43,-0.00015769,-0.00047421,-0.00043151,8.45833333

E,198.21,-0.00529922,-0.00580219,-0.00517924,13.41666667

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E,199.78,-0.00015011,0.04082710,0.03506140,297.41666667

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E,205.27,-0.00013240,-0.00044031,-0.00033031,24498.25000000

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