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Processing BGC-Argo nitrate concentration at the DAC Level

Version 1.2.2
March 4, 2024

ARGO
part of the integrated global observation strategy

Argo data management
Processing BGC-Argo nitrate concentration at the DAC Level

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History of the document

Version	Date	Authors	Modification
1.0	May 2016	Ken Johnson, Orens Pasqueron de Fommervault, Romain Serra, Fabrizio D'Ortenzio, Catherine Schmechtig, Hervé Claustre, Antoine Poteau	Initial version
1.1	March 2018	Ken Johnson, Orens Pasqueron de Fommervault, Romain Serra, Fabrizio D'Ortenzio, Catherine Schmechtig, Hervé Claustre, Antoine Poteau	Carole Sakamoto reference added
1.2	September 5, 2023	Ken Johnson, Josh Plant, Carole Sakamoto, Tanya Maurer, Orens Pasqueron de Fommervault, Romain Serra, Fabrizio D'Ortenzio, Catherine Schmechtig, Hervé Claustre, Antoine Poteau	Calculate the spectrum due to Bromide and other sea salt components, with an updated correction for the effect of in situ temperature. Also a rewrite of much of the document for clarity
1.2.1	September 28, 2023	Ken Johnson, Josh Plant, Carole Sakamoto, Tanya Maurer, Orens Pasqueron de Fommervault, Romain Serra, Fabrizio D'Ortenzio, Catherine Schmechtig, Hervé Claustre, Antoine Poteau	Fixed a couple errors in the check values in Annexe 5.2 & 5.3 reported by R. Scott and C. Schallenberg from CSIRO
1.2.2	March 4, 2024	Ken Johnson, Josh Plant, Carole Sakamoto, Tanya Maurer, Orens Pasqueron de Fommervault, Romain Serra, Fabrizio D'Ortenzio, Catherine Schmechtig, Hervé Claustre, Antoine Poteau	Figure 1 incorrectly plotted the nitrate absorbance spectrum. The bromide sea salt spectrum was accidentally plotted twice

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. This document was produced 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, the nitrate data set within the Bio-Argo data system will be more uniform, allowing users to begin analyzing not only their own nitrate concentration data, but also those of others, in the true spirit of Argo data sharing.

1 Introduction

The primary method used to date to measure the concentration of dissolved nitrate (NITRATE) in seawater with sensors mounted on profiling floats is based on the absorption of light at ultraviolet wavelengths by nitrate ions (Johnson and Coletti, 2002; Johnson et al., 2010; 2013; D'Ortenzio et al., 2012). These sensors measure the intensity of returned light after passing through the seawater sample in the optical path. These intensity values are then used to calculate absorbance. If the light absorption spectrum is measured in the wavelength range between 217 to 240 nm, then the nitrate concentration can be determined. 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 (Figure 1). In addition, there is a much weaker absorption due to dissolved organic matter and light scattering by particles (Ogura and Hanya, 1966). In order to estimate the nitrate concentration a model seawater absorbance spectrum is used. This model consists of three components, bromide (and other sea salts), nitrate and a background due to dissolved organics and particles. The background absorbance can also include thermal effects on the instrument as well as slow changes in absorption due to fouling of the optics. All of these latter effects contributing to the baseline absorbance tend to combine to form an absorption spectrum that is linear in wavelength over relatively short wavelength spans. In anoxic waters, bisulfide and nitrite ions can also contribute noticeably to the measured UV spectrum (Johnson and Coletti, 2002; Stanev et al., 2018) and custom data processing may be required for these cases.

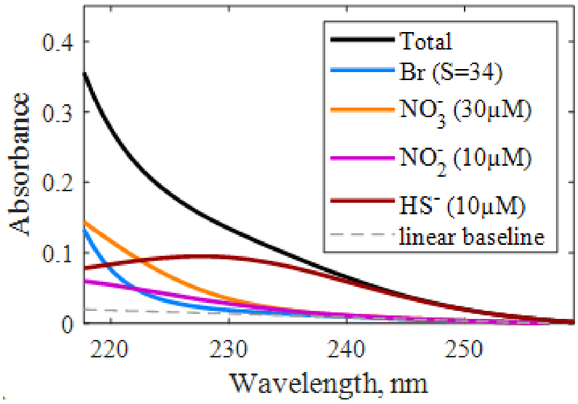


Figure 1. Potential constituent spectra to the total measured absorbance of sewater

Two different instruments based on the same optical principles are presently used on biogeochemical (BGC) floats. The In Situ Ultraviolet Spectrophotometer (ISUS), built at the Monterey Bay Aquarium Research Institute (MBARI) (Johnson and Coletti, 2002), is mounted inside the pressure hull of Teledyne/Webb Research APEX profiling float and the optics penetrate through the upper end cap into the water. The second instrument is Seabird Scientific's (SBS) version called the Deep Submersible Ultraviolet Nitrate Analyzer (Deep SUNA) which was originally commercialized by Satlantic. It is attached to the outside of a profiling float hull (APEX, Provor, Navis, SOLO-II) in its own pressure housing and is connected to the float through an underwater cable that provides power and communications. Power and communications between the float controller and the sensor, as well as 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; Wang et al., 2021). There are some tradeoffs in every approach. To date, almost all nitrate sensors on profiling floats use a modified version of the Temperature Compensated Salinity Subtracted (TCSS) algorithm developed by Sakamoto et al. (2009) with an added pressure correction (Sakamoto et al.,2017). This approach requires complementary PRES TEMP and PSAL data from the float's CTD. Starting with version 1.2 of this manual, an update to the 2009 temperature correction is included (Plant et al., 2023), which improves the accuracy for measurements in waters warmer (and colder) than the calibration temperature (usually 20C). It is likely that there will be future algorithm developments so it is necessary that the data systems clearly indicate the algorithm that has been applied via the PREDEPLOYMENT_CALIB_COMMENT field in the Argo meta file. 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 also the measured UV light intensity spectra for the samples. While the calibration file usually reports values for all pixels measured by the spectrophotometer, the data returned by the float (and stored at the GDAC) are a subset of these pixels in the range of interest to calculate nitrate as described below due to data storage & transmission concerns. When nitrate is calculated this returned subset is usually subsetted once again to optimize the accuracy of the nitrate estimate. For example the calibration file contains all 256 spectrophotometer pixels spanning the wavelength range round 190 to 394 nm. The float returns a pixel subset in the wavelength range between 215 to 250 nm and nitrate is usually calculated on a further subset spanning the wavelengths between 217 and 240 nm.

It is strongly recommended that if the sample intensity spectra are available, then nitrate concentrations should be recalculated from these spectra and the NITRATE parameter populated with these resulting values. Recomputing the nitrate concentration ensures consistent processing with the latest methods and also has a side benefit of producing diagnostic data that can guide the quality control of the measured sample.

2 Compute Nitrate concentration from the Intensity spectrum

2.1 Parameters

During the ADMT13, the decision was made that floats with biogeochemical sensors would have separate data files. This means that are four relevant data files for biogeochemical floats: (1) the core or "c-file" containing PRES, TEMP and PSAL; (2) the biogeochemical or "b-file" containing PRES, intermediate BGC parameters and BGC ocean state variables; (3) the float metafile which contains sensor calibration and configuration information and (4) a merged file (synthetic or "Sprof") containing P, T, S and ocean state variables all merged onto a common pressure axis to ease data usability for scientific purposes. For nitrate there are many paramters involved in its determination from raw intensity measurements. Some of these parameters are stored in the "b-file", others are store in the float metafile, and some are just mentiond in this document. The following tables break these paramters into groupings. Table 1 lists parameters that can be found in the individual cycle Bfiles while Tables 2 and 3 list parameters found in the float meta files and Table 4 lists paramters that are used in this document but not stored at the GDAC.

NOTE: All arrays in the following tables correspond to wavelengths from a subset of the manufacturer's 256 element calibration data from PIXEL_START through PIXEL_END (see Table 3). This is the data subset returned by the float.

Table 1. B file parameters related to the nitrate sensor. Type "i" refers to intermediate parameters and type "b" refers to the ocean state variable receiving quality control and adjustment. Type "i" parameters may be found in the B files but are not found in the merged synthetic (Sprof) files on the GDAC. All arrays are data array subsets from PIXEL_START through PIXEL_END.

Parameter	Description	Type	Units
UV_INTENSITY_NITRATE	Intensity array for the ultra violet light flux returning to the sensor's spectrophotometer after passing through a seawater sample	i	count
UV_INTENSITY_DARK_NITRATE	Intensity for the ultra violet light flux returning to the sensor's spectrophotometer when the lamp is off or the shutter is closed. This can be an array or scalar value (sensor set up dependent)	i	count
NITRATE	Computed nitrate concentration	b	umol/kg
MOLAR_NITRATE	Computed nitrate concentration	i	umol/L
FIT_ERROR_NITRATE	Root mean square error of the multiple linear regression used to calculate nitrate (Very helpful for sensor trouble shooting and QC)	i	dimensionless
HUMIDITY_NITRATE	Relative humidity inside the SUNA sensor (If > 50% there is a leak)	i	percent
TEMP_NITRATE	Internal housing temperature of the sensor	i	degree Celsius
TEMP_SPECTROPHOTOMETER_NITRATE	Temperature at the spectrophotometer	i	degree Celsius

Table 2 . Calibration parameters determined by the sensor manufacturer. All arrays are data array subsets of the manufacturer's calibration file from PIXEL_START to PIXEL_END (the pixel subset returned by the float). These indices are described in Table 3 below and are stored in the PREDEPLOYMENT_CALIB_EQUATION and PREDEPLOYMENT_CALIB_COEFFICIENT parameters found in the floats meta file. See section 3.4

Parameter	**Description**	**Units**
OPTICAL_WAVELENGTH_UV	Wavelength array	nanometer
E_SWA_NITRATE	Absorptivity array for nitrate free seawater in terms of salinity (absorptivity is mostly due to bromide with minor contributions from other salts which are all proportional to salinity)	L/psu/cm
E_NITRATE	Molar absorptivity array for nitrate (for convenience this is reported per umol vs. per mole)	L/umol/cm
UV_INTENSITY_REF_NITRATE	Dark count corrected intensity array measured through a sample of ultra pure water. Dark counts (lamp off or shutter closed intensity counts) have already been subtracted during the manufacturer's calibration process	count
TEMP_CAL_NITRATE	Calibration temperature during manufacturer's calibration of the sensor	degree Celsius

Table 3. Parameters related to nitrate calculation. All PIXEL indices are relative to the manufacturer reported pixel count in the calibration file (1 to 256). **NOTE: With the updated temperature correction (Plant et al., 2023) the OPTICAL_WAVELENGTH_OFFSET is now discouraged for use as a tuning parameter.**

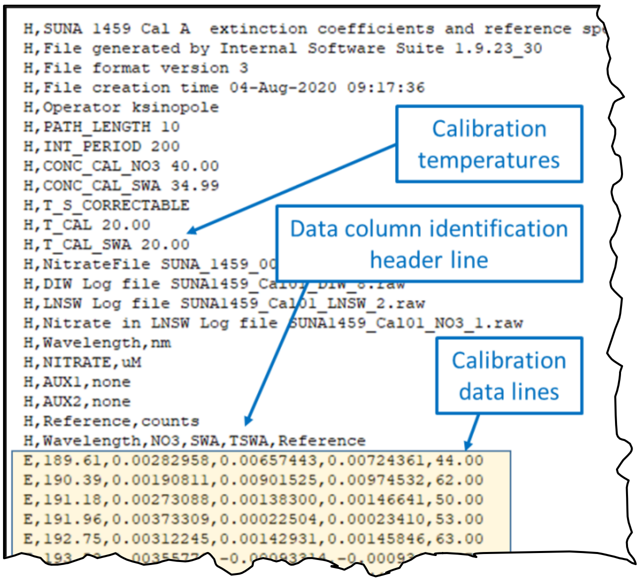
Parameter	**Description**	**Units**
PIXEL_START	Starting pixel index of UV_INTENSITY_NITRATE subset returned by the sensor. Usually the pixel mapped to the first wavelength >= 215 nm. For SUNA sometimes first wavelength >=217.	count
PIXEL_END	Ending pixel index of UV_INTENSITY_NITRATE subset returned by the sensor. Usually the pixel mapped to the first wavelength <= 250 nm.	count
PIXEL_FIT_START	Starting pixel index of the data subset used to compute NITRATE. Usually the pixel mapped to the first wavelength >= 217 nm. (Always >= PIXEL_START)	count
PIXEL_FIT_END	Ending pixel index of data subset used to compute NITRATE. Usually the pixel mapped to the first wavelength <= 240 nm. (Always <= PIXEL_END)	count
OPTICAL_WAVELENGTH_OFFSET	A scaling parameter used in the temperature correction (default = 210). It was also used with the Sakamoto et al. (2009) temperature correction to compensate for warm water bias of the E_SWA_NITRATE temperature correction.	nanometer

Table 4. Parameters used in this document but not found in any GDAC files. All arrays are data array subsets from PIXEL_START to PIXEL_END (the pixel subset returned by the float).

Parameter	Description	Units
START_IND	Starting pixel of UV_INTENSITY_NITRATE used to compute nitrate relative to the data subset returned by the float	count
END_IND	Ending pixel of UV_INTENSITY_NITRATE used to compute nitrate relative to the data subset returned by the float	count
R, R' and R''	Pixel index array used to calculate nitrate (R), excluding saturated pixels (R'), and excluding saturated pixels and negative intensity pixels (R'')	count
UV_INTENSITY_NITRATE_DC	Dark corrected sample intensity array	count
ABSORBANCE_SW	Absorbance spectrum of the sea water sample	unitless
$PRES_{NO3}$, $TEMP_{NO3}$, $PSAL_{NO3}$	Pressure temperature and salinity values at the nitrate sensor optics (may be offset from the CTD values)	dbar, degree Celsius, psu
WL	Scaled wavelength array used in temperature correction	nanometer
E_SWA_INSITU	Absorptivity array for nitrate free seawater in terms of salinity corrected for in situ temperature and pressure	L/psu/cm
ABSORBANCE_TCSS_NITRATE	Absorbance spectrum of the sea water sample after the absorbance due to sea salts has been removed	unitless
BASELINE_INTERCEPT	Linear baseline absorbance intercept resulting from the least squares solution.	unitless
BASELINE_SLOPE	Linear baseline absorbance slope resulting from the least squares solution.	1/nanometer
NITRATE_SENSOR_OFFSET	The vertical offset between the CTD and the optical sample window of the SUNA sensor. A value >= 0. PROVOR=1.5, NAVIS=1.26, SOLO=1.1, APEX=0	dbar

2.2 Calibration file

Each nitrate sensor is individually calibrated by the builder and a calibration file should accompany each instrument. The calibration file should be archived in the data system to allow nitrate to be easily computed from the raw sample intensity spectra (or recomputed if improved algorithms become available). The calibration data should also be stored on board the sensor to allow nitrate concentration to be computed onboard the float. Ideally this would also allow calibration data to be reported by the float if a request is sent.



```
H,SUNA 1459 Cal A  extinction coefficients and reference sp
H,File generated by Internal Software Suite 1.9.23_30
H,File format version 3
H,File creation time 04-Aug-2020 09:17:36
H,Operator ksinopole
H,PATH_LENGTH 10
H,INT_PERIOD 200
H,CONC_CAL_NO3 40.00
H,CONC_CAL_SWA 34.99
H,T_S_CORRECTABLE
H,T_CAL 20.00
H,T_CAL_SWA 20.00
H,NitrateFile SUNA_1459_00
H,DIW Log file SUNA1459_Ca
H,LNSW Log file SUNA1459_Cal01_LNSW_2.raw
H,Nitrate in LNSW Log file SUNA1459_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
E,189.61,0.00282958,0.00657443,0.00724361,44.00
E,190.39,0.00190811,0.00901525,0.00974532,62.00
E,191.18,0.00273088,0.00138300,0.00146641,50.00
E,191.96,0.00373309,0.00022504,0.00023410,53.00
E,192.75,0.00312245,0.00142931,0.00145846,63.00
```

Figure 2. Screen capture of SUNA calibration file identifying the important sections (WMO # 5906311).

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 (Figure 2). There should be one data line for each of the 256 spectrophotometer pixels. In the header part of the calibration file there is line that reports the temperature at which the calibration was performed. This value is essential for the TCSS algorithm and will be stored as TEMP_CAL_NITRATE

For SUNA sensors, there are often two calibration temperatures header lines in the calibration files:

H,T_CAL 20.00
H,T_CAL_SWA 20.00

When possible, the temperature found in the header line containing "T_CAL_SWA" should be used. In some situations (mostly older sensor calibration files) this line is missing from the calibration file and the temperature found in the header line containing "T_CAL" should be used instead. For MBARI ISUS sensors, the calibration temperature is found in the header line that contains "CalTemp":

H,CalTemp,20.07

Each calibration data line corresponds to one of the 256 pixels on the detector array and each pixel corresponds to a unique wavelength based on a calibration reported by the spectrophotometer manufacturer (Zeiss). These 256 pixels roughly span the wavelength range from 190 to 394 nm. The last header line describes the contents of the data lines. The contents of the calibration files from different builders are similar. However the number of header lines and the order of the contents on the data lines may be different. Additionally the column header names also vary between manufactures. This last header line is essential to decipher the calibration data. Table 5 matches equivalent column header names between sensors to the Argo parameter used in this document.

Table 5. Equivalent calibration file data column header names for SUNA and ISUS sensors and the corresponding Argo processing document parameter name**. The Argo parameters are a subset of the full 256 pixel calibration file from PIXEL_START through PIXEL_END (described in Table 3)**

SUNA Data column header	ISUS Data column header	Argo parameter from Table 2	Comment
Wavelength	WaveLen	OPTICAL_WAVELENGTH_UV	
NO3	New ENO3	E_NITRATE	
SWA	New ESW	E_SWA_NITRATE	
TSWA	--	--	SBS SUNA proprietary parameter. Not used for nitrate determination
--	EHS	--	ISUS Bisulfide molar absorptivity placeholder. Not used for nitrate calculation
Reference	DI DC Corr	UV_INTENSITY_REF_NITRATE	Dark counts have already been subtracted during the manufacturer's calibration procedure

2.3 Computing nitrate concentration

2.3.1 Required data

The nitrate sensor returns:

PIXEL_START and **PIXEL_END**: The starting and ending pixel indices indicating the subset of spectrophotometer pixels measured and returned by the sensor in the range [1, 256]. Only a subset of the total spectrophotometer pixels are usually returned by the float due to data transmission and storage concerns. See Table 3. Usually set at the factory but also configurable by the float owner.

UV_INTENSITY_NITRATE: A continuous array of spectrophotometer intensity counts from PIXEL_START through PIXEL_END for a seawater sample measured at pressure P of the sensor PRES profile array. See Table 1.

UV_INTENSITY_DARK_NITRATE: Spectrophotometer intensity counts at pressure P of the sensor PRES profile array when the lamp is turned off or the shutter is closed. This can be a pixel subset array from PIXEL_START through PIXEL_END or it can be a scalar value averaged over the mentioned pixel subset range depending upon how the sensor is configured. See Table 1.

The CTD returns:

PRES, PSAL and TEMP: Pressure, temperature and salinity measurements from the float's CTD at the time (pressure) of the nitrate sensor reading are required to calculate nitrate. If salinity and temperature values are not reported at the nitrate sample pressure levels they should be interpolated to these levels prior to computing nitrate. The reported pressure associated with nitrate samples will differ between float types and can also be changed via post deployment modifiable firmware within a float type. The accuracy of this nitrate-associated pressure varies and may require different interpolation schemes. It is recomended for the float to return a pressure reading recorded at the time of the Nitrate sensor measurement (e.g. PROVOR, SOLO) if it has the ability to do so. In contrast other floats (Navis and APEX) assign a common pressure value for all sensor measurements taken at a target pressure level. Finally, in some cases only the target sampling pressure is known (e.g. SOLO). Knowledge of how the pressure and nitrate readings are related are necessary for the most accurate nitrate calculation.

Calibration and meta data:

OPTICAL_WAVELENGTH_UV: Continuous wavelength array subsetted from the manufacturer's calibration file from PIXEL_START through PIXEL_END. See Table 2.

E_SWA_NITRATE: Continuous absorptivity array for nitrate free seawater in terms of salinity subsetted from the manufacturer's calibration file from PIXEL_START through PIXEL_END. Absorptivity is mostly due to bromide in seawater with minor contributions from other sea salts which are all proportional to salinity. See Table 2.

E_NITRATE: Continuous molar absorptivity array for nitrate subsetted from the manufacturer's calibration file from PIXEL_START through PIXEL_END. See Table 2.

UV_INTENSITY_REF_NITRATE: Array of dark count corrected intensity counts measured through ultra pure water and subsetted from the manufacturer's calibration file from PIXEL_START through PIXEL_END. Data reported in the calibration file have already had the dark subtracted during the sensor manufacturer's calibration process. See Table 2.

TEMP_CAL_NITRATE: Calibration solution temperature during manufacturer's calibration of the sensor. See Table 2.

OPTICAL_WAVELENGTH_OFFSET: A scaling parameter and tunable parameter once used to compensate for warm water bias of the E_SWA_NITRATE temperature correction (default = 210). With the improved temperature correction of Plant et al. (2023), it is best to use the default value of 210. It's use as a tuning parameter should be used sparing if at all. See Table 3.

NITRATE_SENSOR_OFFSET: This is the offset in dbar between the CTD sensor and the optical path of the SUNA sensor attached to the float hull (a distance really). This offset is used to adjust the temperature and salinity values used to calculate nitrate for PROVOR, Navis and SOLO floats which all have SUNA sensors attached to the lower portions of the float hull. PROVOR=1.5, NAVIS=1.26, SOLO=1.1.

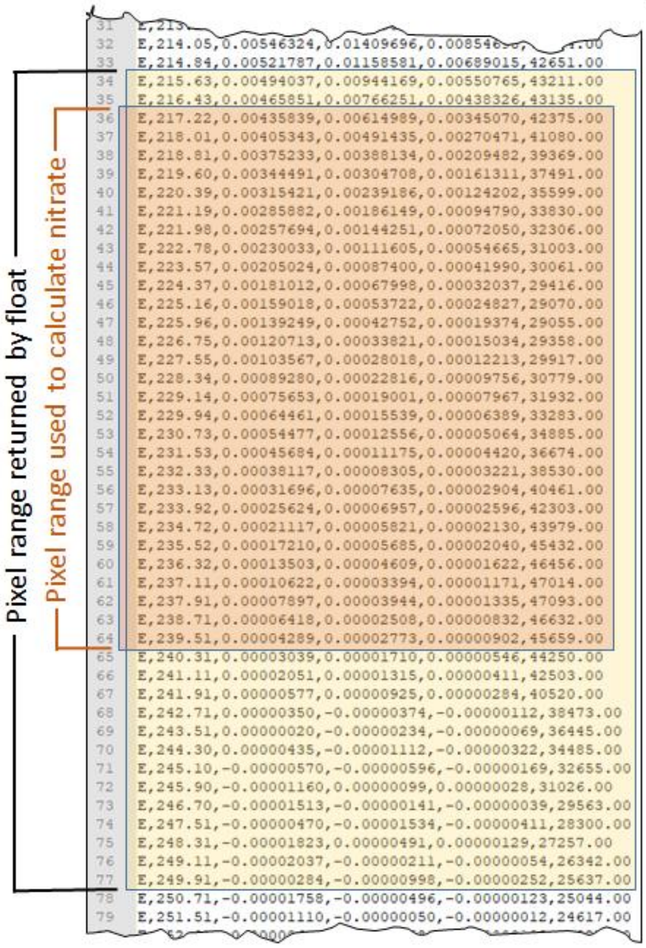
2.3.2 Nitrate concentration processing

Only a subset of the intensity data returned by the float is used to compute the nitrate concentration. The continuous array of pixel indices, R, defines this computation subset where:

R = [PIXEL_FIT_START… PIXEL_FIT_END]

The default indices corresponds to the calibration file wavelengths >= 215nm and <= 240 nm. See Table 3 and Figure 3. In rare instances it may be advantageous to modify these bounds. Sometimes extending the upper bound a few pixels can improve calculation performance if the calculated absorbance spectrum exhibits an abnormal "hump" at higher wavelengths.

In the processing steps that follow, the equations are applied to each pixel indexed in R. It is often more convenient to use indices relative to the pixel subset returned by the float to define the computation subset. In that case the following indices can be used to define the indices in R:



```
31  E,213
32  E,214.05,0.00546324,0.01409696,0.008546
33  E,214.84,0.00521787,0.01158581,0.00689015,42651.00
34  E,215.63,0.00494037,0.00944169,0.00550765,43211.00
35  E,216.43,0.00465851,0.00766251,0.00438326,43135.00
36  E,217.22,0.00435839,0.00614989,0.00345070,42375.00
37  E,218.01,0.00405343,0.00491435,0.00270471,41080.00
38  E,218.81,0.00375233,0.00388134,0.00209482,39369.00
39  E,219.60,0.00344491,0.00304708,0.00161311,37491.00
40  E,220.39,0.00315421,0.00239186,0.00124202,35599.00
41  E,221.19,0.00285882,0.00186149,0.00094790,33830.00
42  E,221.98,0.00257694,0.00144251,0.00072050,32306.00
43  E,222.78,0.00230033,0.00111605,0.00054665,31003.00
44  E,223.57,0.00205024,0.00087400,0.00041990,30061.00
45  E,224.37,0.00181012,0.00067998,0.00032037,29416.00
46  E,225.16,0.00159018,0.00053722,0.00024827,29070.00
47  E,225.96,0.00139249,0.00042752,0.00019374,29055.00
48  E,226.75,0.00120713,0.00033821,0.00015034,29358.00
49  E,227.55,0.00103567,0.00028018,0.00012213,29917.00
50  E,228.34,0.00089280,0.00022816,0.00009756,30779.00
51  E,229.14,0.00075653,0.00019001,0.00007967,31932.00
52  E,229.94,0.00064461,0.00015539,0.00006389,33283.00
53  E,230.73,0.00054477,0.00012556,0.00005064,34885.00
54  E,231.53,0.00045684,0.00011175,0.00004420,36674.00
55  E,232.33,0.00038117,0.00008305,0.00003221,38530.00
56  E,233.13,0.00031696,0.00007635,0.00002904,40461.00
57  E,233.92,0.00025624,0.00006957,0.00002596,42303.00
58  E,234.72,0.00021117,0.00005821,0.00002130,43979.00
59  E,235.52,0.00017210,0.00005685,0.00002040,45432.00
60  E,236.32,0.00013503,0.00004609,0.00001622,46456.00
61  E,237.11,0.00010622,0.00003394,0.00001171,47014.00
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63  E,238.71,0.00006418,0.00002508,0.00000832,46632.00
64  E,239.51,0.00004289,0.00002773,0.00000902,45659.00
65  E,240.31,0.00003039,0.00001710,0.00000546,44250.00
66  E,241.11,0.00002051,0.00001315,0.00000411,42503.00
67  E,241.91,0.00000577,0.00000925,0.00000284,40520.00
68  E,242.71,0.00000350,-0.00000374,-0.00000112,38473.00
69  E,243.51,0.00000020,-0.00000234,-0.00000069,36445.00
70  E,244.30,0.00000435,-0.00001112,-0.00000322,34485.00
71  E,245.10,-0.00000570,-0.00000596,-0.00000169,32655.00
72  E,245.90,-0.00001160,0.00000099,0.00000028,31026.00
73  E,246.70,-0.00001513,-0.00000141,-0.00000039,29563.00
74  E,247.51,-0.00000470,-0.00001534,-0.00000411,28300.00
75  E,248.31,-0.00001823,0.00000491,0.00000129,27257.00
76  E,249.11,-0.00002037,-0.00000211,-0.00000054,26342.00
77  E,249.91,-0.00000284,-0.00000998,-0.00000252,25637.00
78  E,250.71,-0.00001758,-0.00000496,-0.00000123,25044.00
79  E,251.51,-0.00001110,-0.00000050,-0.00000012,24617.00
```

Figure 3. Screen capture of a partial calibration file indicating the typical wavelengths and pixel ranges returned by a float and the computation subset used to calculate nitrate (WMO # 5906311).

START_IND = PIXEL_FIT_START – PIXEL_START + 1
END_IND = PIXEL_FIT_END - PIXEL_FIT_START +1

The nitrate concentration is computed using a modified version of the Sakamoto et al. (2009) TCSS algorithm. A pressure correction is included following Sakamoto et al. (2017) and an updated temperature correction is applied following Plant et al. (2023) which replaces the temperature correction found in Sakamoto et al. (2009). Nitrate is calculated in three steps: (1) An absorbance spectrum is calculated from the measured sample intensities, (2) The temperature and pressure corrected absorbance due to bromide and other sea salts is subtracted from the sample absorbance spectrum, and (3) Nitrate and the linear baseline coefficients are calculated by solving an over determined multiple linear regression (MLR).

2.3.2.1 Compute the absorbance spectrum of the seawater sample

Check UV_INTENSITY_NITRATE(R) for saturated pixels and remove these indices from R:

Each spectrophotometer pixel saturates at 2^{16} or 65,536 counts. Saturated pixels will not produce usable absorbance measurements and must be excluded from all future calculations. At pixel counts near saturation, the detector response to the light flux may deviate from expected. A somewhat arbitrary limit of 64,500 counts is set for the valid upper limit of UV_INTENSITY_NITRATE(R). Quite often a valid NITRATE measurement can still be determined even when some of the pixels are saturated in the intensity spectrum but these samples should be flagged for extra scrutiny during quality control procedures.

$$\mathrm{R'} = \mathrm{R \ for \ UV\_INTENSITY\_NITRATE(R)} \ < \ 64{,}500 \ \mathrm{counts}$$

Check for UV_INTENSITY_NITRATE(R) <= UV_INTENSITY_DARK_NITRATE(R)

Under conditions of low sample light throughput returned to the sensor spectrophotometer the measured sample intensity counts for a given pixel can be less than the measured dark counts. This will result in zero or negative dark corrected sample intensities in the next step which in turn will result in taking the log of a negative or zero value when calculating absorbance. These pixels, if they exist, must also be excluded from all future calculations. This situation can occur if the optics become heavily fouled, the alignment of the optical light path shifts or becomes damaged, or the light source itself has problems. Valid NITRATE measurement can still be determined even when some of the pixels are flagged by this test but again these samples will need a higher degree of scrutiny

$$\mathrm{R''} = \mathrm{R \ for \ UV\_INTENSITY\_NITRATE(R')} \ > \mathrm{UV\_INTENSITY\_DARK\_NITRATE(R')}$$

If *UV_INTENSITY_DARK_NITRATE* is a scalar value this constant value replaces the *UV_INTENSITY_DARK_NITRATE(R)* array.

Calculate dark count corrected seawater sample intensities:

$$\begin{aligned}&\mathrm{UV\_INTENSITY\_NITRATE\_DC(R'')}\\&\qquad = \mathrm{UV\_INTENSITY\_NITRATE(R'')} - \mathrm{UV\_INTENSITY\_DARK\_NITRATE(R'')}\end{aligned}$$

Calculate the seawater absorbance spectrum over pixel range R'':

$$\mathrm{ABSORBANCE\_SW(R'')} = -log_{10}\left[\frac{\mathrm{UV\_INTENSITY\_NITRATE\_DC(R'')}}{\mathrm{UV\_INTENSITY\_REF\_NITRATE(R'')}}\right]$$

2.3.2.2 Remove the absorbance spectrum due to bromide and other sea salt components

Do temperature and salinity measurements exist at each level of the nitrate sensor pressure axis?

To date this is true for ISUS sensors on APEX floats and SUNA sensors on BGC Navis floats. This may not necessarily be the case for PROVOR or SOLO floats which have individual pressure axes for each float sensor. If the answer is no, the missing measurements must first be interpolated from the float's primary pressure axis before proceeding to the next steps.

Is the NITRATE_SENSOR_OFFSET different from zero?

YES for all SUNA sensors and NO for all ISUS sensors.

If yes, this means the nitrate sensor is measuring at a different pressure level than the CTD despite reporting the CTD pressure for the nitrate sensor pressure axis. In regions of strong temperature gradients this can induce a noticeable error in the nitrate calculation because the absorptivity of sea salts in seawater (mostly due to bromide) is temperature dependent. In these cases salinity and temperature measurements must first be determined for the actual pressure at the optical sample path of the nitrate sensor. This can be accomplished by interpolating temperature and salinity from the primary or NITRATE pressure axis to the offset corrected nitrate pressure axis ($PRES_{NO3}$). Interpolation can impart one complication for the deepest $PRES_{NO3}$ value: it could be greater than the largest value measured by the float. In these situations it is sufficient to pad with the original value as the temperature gradients tend to be low at depth. This parameter name should be listed in the CONFIG_PARAMETER_NAME/VALUE parameter pair in the metafile as CONFIG_SunaVerticalPressureOffset_dbar and the value should be listed in the CONFIG_PARAMETER_VALUE parameter (see 3.3).

$PRES_{NO3}$ = PRES + NITRATE_SENSOR_OFFSET

$TEMP_{NO3}$ = TEMP at PRES = $PRES_{NO3}$

$PSAL_{NO3}$ = PSAL at PRES = $PRES_{NO3}$

Calculate a scaled wavelength array:

WL(R'') = (OPTICAL_WAVELENGTH_UV(R'') – OPTICAL_WAVELENGTH_OFFSET)

The scaled wavelength was first used by Sakamoto et al. (2009) to improve the numerical stability when solving for the coefficients used in their nonlinear temperature correction model and remained as an input for their resulting model. In the past the OPTICAL_WAVELENGTH_OFFSET was also used as a tuning parameter in specific situations. This was in conjunction with the Sakamoto et al. (2009) temperature correction to account for some noted minor deficiencies which were most noticeable when warm surface waters were several degrees higher than the calibration temperature. The temperature correction found in Sakamoto et al. (2009) is now superseded by Plant et al. (2023) and the use of OPTICAL_WAVELENGTH_OFFSET as a tuning parameter is now discouraged and the default value of 210 should be used. This is discussed in more detail in Plant et al. (2023). If older data are reprocessed with the newer temperature correction it is recommended to ensure that the OPTICAL_WAVELENGTH_OFFSET is reset to the default value of 210 nm and to also re-asses any delayed mode quality control corrections and flagging of the data.

While the updated temperature correction greatly minimizes the biases observed with the original Sakamoto et al. (2009) correction scheme, a data manager may still choose to use OPTICAL_WAVELENGTH_OFFSET at times if nitrate data cannot be adequately corrected with standard quality control adjustments. In rare cases small biases may still be observed in the nitrate concentration profile due to uncertainty in the wavelength registration of the diode array spectrometer, small errors in the calibration coefficients, or shifts in the instrument response. These biases can sometimes be minimized through small adjustments in the OPTICAL_WAVELENGTH_OFFSET parameter (210 ± 2 nm) but these adjustments should be performed by data managers well experienced with nitrate sensor operational principals and a good understanding of what the true nitrate concentration profiles should look like.

Calculate the in situ absorptivity spectrum of seawater due to bromide and other sea salt components at the sample temperature and pressure

Most of this absorbance is due to the bromide molecule. Bromide’s molar absorptivity decreases as temperature decreases (Sakamoto et al., 2009; Plant et al., 2023) and pressure increases (Pasqueron de Fommervault et al., 2015; Sakamoto et al., 2017). For example the absorptivity of seawater due to sea salts at 225 nm decreases by 60% as the temperature changes from 25 to 7 degrees C. The pressure response is not as dramatic but it reduces the absorptivity by an additional 5% at 2000 dbar. If left uncorrected these factors would result in the underestimation of nitrate in the colder waters of the deep ocean. Therefore each calibration value in E_SWA_NITRATE(R") must be adjusted for the in situ sample conditions found in $TEMP_{NO3}$ and $PRES_{NO3}$. The temperature correction follows Plant et al. (2023) while the pressure correction follows Sakamoto at al. (2017). In Sakamoto et al. (2017) the pressure coefficient was rounded to 0.026. Here we include one more significant figure: 0.0265.

$$\mathrm{E\_SWA\_INSITU}(\mathrm{R}'') = \mathrm{E\_SWA\_NITRATE}(\mathrm{R}'') * \mathrm{Tcorr}(\mathrm{R}'') * \mathrm{Pcorr}$$

Where:

$$\mathrm{Tcorr}(\mathrm{R}'') = \exp(\ \mathrm{TcorPoly}(\mathrm{R}'') \ * [TEMP_{NO3} - \mathrm{TEMP\_CAL\_NITRATE}\,]\ )$$

$$\mathrm{TcorPoly}(\mathrm{R}'') = A + B * \mathrm{WL}(\mathrm{R}'') + C * \mathrm{WL}(\mathrm{R}'')^2 + D * \mathrm{WL}(\mathrm{R}'')^3 + E * \mathrm{WL}(\mathrm{R}'')^4$$

A= 1.46380e-02; B= 1.67660e-03; C= 2.91898e-05; D= -7.56395e-06; E= 1.27353e-07

$$\mathrm{Pcorr} = 1 - \left(\frac{PRES_{NO3}}{1000} * 0.0265\right)$$

Tcor(R") represents the most recent temperature correction model from Plant et al. (2023) and is the preferred correction. The following equation redefines Tcor(R") in terms of the Sakamoto et al. (2009) nonlinear correction model. Its use is now discouraged but it is presented for backwards compatibility related to older floats equipped with nitrate sensors. F = A/B and A= 1.1500276, B= 0.02840, D= 0.001222

$$\mathrm{Tcor}(\mathrm{R}'') = \frac{(F + TEMP_{NO3})}{(F + \mathrm{TEMP\_CAL\_NITRATE})} * exp\big(D * WL(R'') * (TEMP_{NO3} - \mathrm{TEMP\_CAL\_NITRATE})\big)$$

Subtract the absorbance due to sea salts from the sample absorbance

$$\mathrm{ABSORBANCE\_TCSS\_NITRATE}(\mathrm{R}'') = \mathrm{ABSORBANCE\_SW}(\mathrm{R}'') - \mathrm{E\_SWA\_INSITU}(\mathrm{R}'') * PSAL_{NO3}$$

2.3.2.3 Compute the nitrate concentration

Solve for the unknown parameters

MOLAR_NITRATE (umol/L) and the background linear absorbance coefficients (BASELINE_INTERCEPT, BASELINE_SLOPE) are calculated by solving for these three unknowns in a multiple linear regression using an ordinary least squares fit.

$$\begin{aligned} ABSORBANCE\_TCSS\_NITRATE(R'') = {} & BASELINE\_INTERCEPT \\ & + \mathrm{BASELINE\_SLOPE} * OPTICAL\_WAVELENGTH\_UV(\mathrm{R}'') \\ & + \mathrm{MOLAR\_NITRATE} * E\_NITRATE(\mathrm{R}'') \end{aligned}$$

For example, in the Matlab® compuation envirnonment the linear algebra solution depicted in Figure 4 can be solved with one line using their backslash operator: B hat = X\Y .

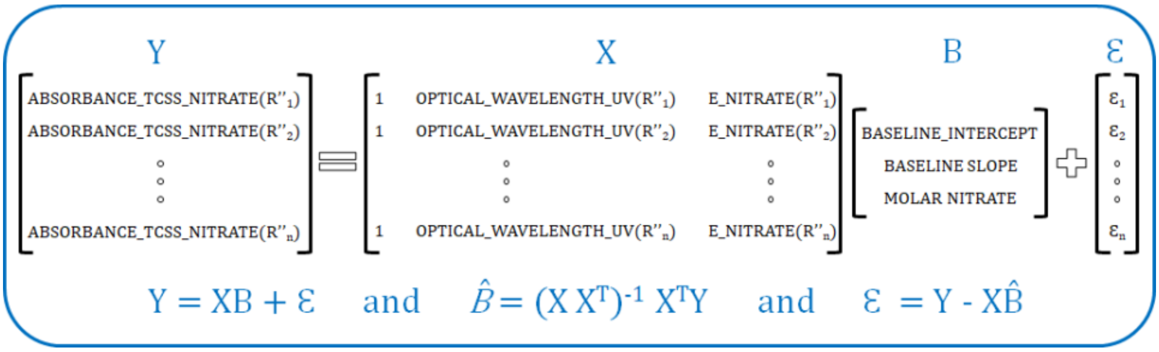

Figure 4. A cartoon depicting the linear algebra matrix set up and the least squares solution to solve for nitrate and the linear absorbance baseline coefficients. The Y vector respresents the independant measurements, the X matrix the dependant variables, and the B vector the unknowns. The B hat vector contains the estimates of the unknowns and the Ɛ vector the error or residuals to the model fit.

Convert to Argo approved units

Finally the nitrate concentration needs to be converted to Argo aproved units (umol/kg) by dividing by the density of the seawater sample.

$$NITRATE\ = MOLAR\_NITRATE / \rho * 1000$$

Where ρ is the potential density of the seawater (kg/m^3) calculated at zero pressure and at potential temperature using $TEMP_{NO3}$, $PSAL_{NO3}$ as starting inputs and following Millero & Poisson (1981) for density.

Determine the fit error

The root mean square error of the model fit can be calculated as follows:

$$FIT\_ERROR\_NITRATE = \sqrt{\frac{1}{n}\sum_{R''=1}^{n} \mathcal{E}^2}$$

Where n equals the number of elements in R” and

$$\begin{aligned}\mathcal{E}(R'') = {} & ABSORBANCE\_TCSS\_NITRATE(R'') \\ & - (BASELINE\_INTERCEPT + BASELINE\_SLOPE * OPTICAL\_WAVELENGTH\_UV(R'')) \\ & - MOLAR\_NITRATE * \mathrm{E\_NITRATE}(R'')\end{aligned}$$

The baseline coefficents and the model fit residuals are not stored at the GDAC. While not required, it is strongly recomended that the data mangers store these parameters in their data system. These diagnostic data are incrediably usuful for later quality control and for trouble shooting any pontential sensor issues that may arise

3 Metafile data

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

3.1 Sensor metadata

Table 6. Sensor metadata	
SENSOR	SPECTROPHOTOMETER_NITRATE
SENSOR MAKER	SATLANTIC, MBARI or Seabird Scientific
SENSOR_MODEL	SUNA_V2 *(or ISUS_V3)*
SENSOR_SERIAL_NO	*To be filled*

3.2 Parameter metadata

Table 7. 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	3
PARAMETER_RESOLUTION	0.01

3.3 Configuration metadata

The following information can be stored within the CONFIG_PARAMETER_NAME string array and each entry has an associated value entered in the CONFIG_PARAMETER_VALUE numeric array

Table 8. Sensor configuration metadata

CONFIG_PARAMETER_NAME	UNITS	COMMENT
CONFIG_SunaApfFrameOutputPixelBegin_NUMBER	count	Equal to PIXEL_START in Table 3. 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	count	Equal to PIXEL_END in Table 3. See additional comments in above row of this table
CONFIG_SunaVerticalPressureOffset_dbar	dbar	The between the SUNA optical sample window and the CTD. See Table 4 and section 2.3.2.2
CONFIG_SunaWithScoop_LOGICAL	logical	Now obsolete. Default = 0. 1 = SUNA with scoop, which redirects flow through the optical sample path
CONFIG_SunaInPumpedStream_LOGICAL	logical	Now obsolete. Default = 0. 1 = SUNA in CTD's pumped flow stream

3.4 Calibration metadata

Each of the eight parameters potentially found in the "b-file" can have can have associated predeployment calibration information stored in the following metafile string arrays: PREDEPLOYMENT_CALIB_EQUATION, PREDEPLOYMENT_CALIB_COEFFICIENT, PREDEPLOYMENT_CALIB_COMMENT. The calibration cooeficient data from aoml float WMO # 5906311 are used as an exmple in the following table.

Table 9. Sensor calibration metadata

PARAMETER = NITRATE	
PREDEPLOYMENT_CALIB_EQUATION (Plant et al. (2023) temperature correction)	The sensor returns UV_INTENSITY_DARK_NITRATE and UV_INTENSITY_NITRATE from PIXEL_START to PIXEL_END, a continuous subset of the 256 pixel array returned by the spectrophotometer. A subset of these pixels returned by the float, R, is used to calculate nitrate (PIXEL_FIT_START >=R<= PIXEL_FIT_END) corresponding to 217nm >= WAVELENGTH_UV <= 240nm. The following equations are computed across all R: ABSORBANCE_SW(R)= -log10[(UV_INTENSITY_NITRATE(R)-UV_INTENSITY_DARK_NITRATE(R))/UV_INTENSITY_REF_NITRATE(R)]; ABSORBANCE_TCSS_NITRATE(R)= ABSORBANCE_SW(R) -E_SWA_INSITU(R)*PSAL); E_SWA_INSITU(R)= E_SWA_NITRATE(R) * Tcorr(R) * Pcorr; Tcorr(R)= exp(TcorPoly(R) *[TEMP-TEMP_CAL_NITRATE]); TcorPoly(R)= A+B*WL(R) + C*WL(R)^2+D*WL(R)^3+E*WL(R)^4; WL(R) = (OPTICAL_WAVELENGTH_UV(R) – OPTICAL_WAVELENGTH_OFFSET); Pcorr = 1 – (PRES/1000*0.0265). Set up a multiple linear regression and solve for MOLAR_NITRATE and baseline coefficients: ABSORBANCE_TCSS_NITRATE(R)= BASELINE_INTERCEPT +BASELINE_SLOPE*OPTICAL_WAVELENGTH_UV(R) + MOLAR_NITRATE*E_NITRATE(R). NITRATE= MOLAR_NITRATE/rho*1000, where rho is the potential density [kg/m^3] calculated from the CTD data.

PREDEPLOYMENT_CALIB_EQUATION (original Sakamoto et al. (2009) temperature correction)	The sensor returns UV_INTENSITY_DARK_NITRATE and UV_INTENSITY_NITRATE from PIXEL_START to PIXEL_END, a continuous subset of the 256 pixel array returned by the spectrophotometer. A subset of these pixels returned by the float, R, is used to calculate nitrate (PIXEL_FIT_START >=R<= PIXEL_FIT_END) corresponding to 217nm >= WAVELENGTH_UV <= 240nm. The following equations are computed across all R: ABSORBANCE_SW(R)= -log10[(UV_INTENSITY_NITRATE(R)-UV_INTENSITY_DARK_NITRATE(R))/UV_INTENSITY_REF_NITRATE(R)]; ABSORBANCE_TCSS_NITRATE(R)= ABSORBANCE_SW(R) -E_SWA_INSITU(R)*PSAL); E_SWA_INSITU(R)= E_SWA_NITRATE(R) * Tcorr(R) * Pcorr; Tcorr(R)= (F+TEMP)/(F+TEMP_CAL_NITRATE]) * exp(D* WL(R)*(TEMP-TEMP_CAL_NITRATE));WL(R)= (OPTICAL_WAVELENGTH_UV(R) – OPTICAL_WAVELENGTH_OFFSET); Pcorr= 1 – (PRES/1000*0.0265). Set up a multiple linear regression and solve for MOLAR_NITRATE and baseline coefficients: ABSORBANCE_TCSS_NITRATE(R)= BASELINE_INTERCEPT +BASELINE_SLOPE*OPTICAL_WAVELENGTH_UV(R) + MOLAR_NITRATE*E_NITRATE(R). NITRATE= MOLAR_NITRATE/rho*1000, where rho is the potential density [kg/m^3] calculated from the CTD data.
PREDEPLOYMENT_CALIB_COEFFICIENT (Plant et al. (2023) temperature correction)	PIXEL_START=36, PIXEL_END=77, PIXEL_FIT_START=36, PIXEL_FIT_END=63; OPTICAL_WAVELENGTH_OFFSET=210; A= 1.46380e-02, B= 1.67660e-03, C= 2.91898e-05, D= -7.56395e-06, E= 1.27353e-07; OPTICAL_WAVELENGTH_UV(R)= 217.22,218.01,218.81,219.6,220.39,221.19,221.98,222.78,223.57,224.37,225.16,225.96,226.75,227.55,228.34,229.14,229.94,230.73,231.53,232.33,233.13,233.92,234.72,235.52,236.32,237.11,237.91,238.71,239.51,240.31,241.11,241.91,242.71,243.51,244.3,245.1,245.9,246.7; E_NITRATE =4.358E-03,4.053E-03,3.752E-03,3.445E-03,3.154E-03,2.859E-03,2.577E-03,2.300E-03,2.050E-03,1.810E-03,1.590E-03,1.392E-03,1.207E-03,1.036E-03,8.928E-04,7.565E-04,6.446E-04,5.448E-04,4.568E-04,3.812E-04,3.170E-04,2.562E-04,2.112E-04,1.721E-04,1.350E-04,1.062E-04,7.897E-05,6.418E-05,4.289E-05,3.039E-05,2.051E-05,5.770E-06,3.500E-06,2.000E-07,4.350E-06,-5.700E-06,-1.160E-05,-1.513E-05,-4.700E-06,-1.823E-05,-2.037E-05,-2.840E-06; E_SWA_NITRATE (R)= 6.150E-03,4.914E-03,3.881E-03,3.047E-03,2.392E-03,1.861E-03,1.443E-03,1.116E-03,8.740E-04,6.800E-04,5.372E-04,4.275E-04,3.382E-04,2.802E-04,2.282E-04,1.900E-04,1.554E-04,1.256E-04,1.118E-04,8.305E-05,7.635E-05,6.957E-05,5.821E-05,5.685E-05,4.609E-05,3.394E-05,3.944E-05,2.508E-05,2.773E-05,1.710E-05,1.315E-05,9.250E-06,-3.740E-06,-2.340E-06,-1.112E-05,-5.960E-06,9.900E-07,-1.410E-06,-1.534E-05,4.910E-06,-2.110E-06,-9.980E-06; UV_INTENSITY_REF_NITRATE(R)= 42375,41080,39369,37491,35599,33830,32306,31003,30061,29416,29070,29055,29358,29917,30779,31932,33283,34885,36674,38530,40461,42303,43979,45432,46456,47014,47093,46632,45659,44250,42503,40520,38473,36445,34485,32655,31026,29563;
PREDEPLOYMENT_CALIB_COEFFICIENT (original Sakamoto et al. (2009) temperature correction)	PIXEL_START=36, PIXEL_END=77, PIXEL_FIT_START=36, PIXEL_FIT_END=63; OPTICAL_WAVELENGTH_OFFSET=210; F = A/B and A= 1.1500276, B= 0.02840, C= -0.3101349, D= 0.001222; OPTICAL_WAVELENGTH_UV(R)= 217.22,218.01,218.81,219.6,220.39,221.19,221.98,222.78,223.57,224.37,225.16,225.96,226.75,227.55,228.34,229.14,229.94,230.73,231.53,232.33,233.13,233.92,234.72,235.52,236.32,237.11,237.91,238.71,239.51,240.31,241.11,241.91,242.71,243.51,244.3,245.1,245.9,246.7; E_NITRATE =4.358E-03,4.053E-03,3.752E-03,3.445E-03,3.154E-03,2.859E-03,2.577E-03,2.300E-03,2.050E-03,1.810E-03,1.590E-03,1.392E-03,1.207E-03,1.036E-03,8.928E-04,7.565E-04,6.446E-04,5.448E-04,4.568E-04,3.812E-04,3.170E-04,2.562E-04,2.112E-04,1.721E-04,1.350E-04,1.062E-04,7.897E-05,6.418E-05,4.289E-05,3.039E-05,2.051E-05,5.770E-06,3.500E-06,2.000E-07,4.350E-06,-5.700E-06,-1.160E-05,-1.513E-05,-4.700E-06,-1.823E-05,-2.037E-05,-2.840E-06; E_SWA_NITRATE (R)= 6.150E-03,4.914E-03,3.881E-03,3.047E-03,2.392E-03,1.861E-03,1.443E-03,1.116E-03,8.740E-04,6.800E-04,5.372E-04,4.275E-04,3.382E-04,2.802E-04,2.282E-04,1.900E-04,1.554E-04,1.256E-04,1.118E-04,8.305E-05,7.635E-05,6.957E-05,5.821E-05,5.685E-05,4.609E-05,3.394E-05,3.944E-05,2.508E-05,2.773E-05,1.710E-05,1.315E-05,9.250E-06,-3.740E-06,-2.340E-06,-1.112E-05,-5.960E-06,9.900E-07,-1.410E-06,-1.534E-05,4.910E-06,-2.110E-06,-9.980E-06; UV_INTENSITY_REF_NITRATE(R)= 42375,41080,39369,37491,35599,33830,32306,31003,30061,29416,29070,29055,29358,29917,30779,31932,33283,34885,36674,38530,40461,42303,43979,45432,46456,47014,47093,46632,45659,44250,42503,40520,38473,36445,34485,32655,31026,29563;
PREDEPLOYMENT_CALIB_COMMENT	Nitrate concentration in umol/kg; see Processing Bio-Argo nitrate concentration at the DAC Level, Version 1.2, March 31st 2023. Data was processed using the [Plant et al., 2023 OR, original Sakamoto et al, 2009] temperature correction algorithm. Data manager to specify which algorithm was used in processing.
PARMETER = MOLAR_NITRATE	
PREDEPLOYMENT_CALIB_EQUATION	none
PREDEPLOYMENT_CALIB_COEFFICIENT	none
PREDEPLOYMENT_CALIB_COMMENT	Molar nitrate concentration, umol/L
PARMETER = UV_INTENSITY_NITRATE	
PREDEPLOYMENT_CALIB_EQUATION	none
PREDEPLOYMENT_CALIB_COEFFICIENT	none
PREDEPLOYMENT_CALIB_COMMENT	Intensity of ultra violet flux dark measurement from nitrate sensor
PARMETER = 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
PARMETER = TEMP_NITRATE	
PREDEPLOYMENT_CALIB_EQUATION	none
PREDEPLOYMENT_CALIB_COEFFICIENT	none
PREDEPLOYMENT_CALIB_COMMENT	Internal temperature of the nitrate sensor
PARMETER = TEMP_SPECTROPHOTOMETER_NITRATE	
PREDEPLOYMENT_CALIB_EQUATION	none
PREDEPLOYMENT_CALIB_COEFFICIENT	none
PREDEPLOYMENT_CALIB_COMMENT	Temperature of the spectrophotometer
PARMETER = FIT_ERROR_NITRATE	
PREDEPLOYMENT_CALIB_EQUATION	none
PREDEPLOYMENT_CALIB_COEFFICIENT	none
PREDEPLOYMENT_CALIB_COMMENT	Nitrate fit error (dimensionless)
PARMETER = 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)

4 References

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5 Annexe

5.1 Example Calibration File

Example calibration for SUNA sensor on board aoml Navis float 5906311

```
H,SUNA 1459 Cal A  extinction coefficients and reference spectra
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H,File format version 3
H,File creation time 04-Aug-2020 09:17:36
H,Operator ksinopole
H,PATH_LENGTH 10
H,INT_PERIOD 200
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H,CONC_CAL_SWA 34.99
H,T_S_CORRECTABLE
H,T_CAL 20.00
H,T_CAL_SWA 20.00
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H,DIW Log file SUNA1459_Cal01_DIW_8.raw
H,LNSW Log file SUNA1459_Cal01_LNSW_2.raw
H,Nitrate in LNSW Log file SUNA1459_Cal01_NO3_1.raw
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H,NITRATE,uM
H,AUX1,none
H,AUX2,none
H,Reference,counts
H,Wavelength,NO3,SWA,TSWA,Reference
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E,367.48,0.00040521,0.00043560,0.00000621,9511.00
E,368.28,0.00044893,0.00042137,0.00000589,9268.00
E,369.08,0.00045264,0.00040207,0.00000551,8990.00
E,369.89,0.00046278,0.00040284,0.00000542,8731.00
E,370.69,0.00047759,0.00037901,0.00000500,8474.00
E,371.49,0.00046037,0.00040423,0.00000523,8275.00
E,372.30,0.00043534,0.00042444,0.00000538,8072.00
E,373.10,0.00046453,0.00038424,0.00000478,7880.00
E,373.90,0.00046545,0.00041610,0.00000507,7749.00
E,374.70,0.00046534,0.00044152,0.00000528,7631.00
E,375.50,0.00046421,0.00041991,0.00000492,7504.00
E,376.31,0.00048278,0.00044239,0.00000508,7421.00
E,377.11,0.00047870,0.00049364,0.00000556,7338.00
E,377.91,0.00044283,0.00047704,0.00000527,7271.00
E,378.71,0.00047063,0.00048917,0.00000530,7229.00
E,379.51,0.00047758,0.00048171,0.00000512,7184.00
E,380.31,0.00048916,0.00043819,0.00000457,7068.00
E,381.12,0.00048520,0.00042048,0.00000430,6965.00
E,381.92,0.00042243,0.00046974,0.00000471,6866.00
E,382.72,0.00050694,0.00045968,0.00000452,6790.00
E,383.52,0.00043909,0.00051019,0.00000492,6728.00
E,384.32,0.00046291,0.00048126,0.00000455,6644.00
E,385.12,0.00048983,0.00048235,0.00000447,6603.00
E,385.92,0.00048005,0.00048949,0.00000445,6560.00
E,386.72,0.00052317,0.00047020,0.00000419,6527.00
E,387.52,0.00051586,0.00049325,0.00000431,6514.00
E,388.32,0.00050026,0.00053141,0.00000455,6515.00
E,389.12,0.00053400,0.00049008,0.00000412,6482.00
E,389.92,0.00056924,0.00045116,0.00000372,6437.00
E,390.72,0.00055163,0.00052061,0.00000421,6341.00
E,391.52,0.00052875,0.00049032,0.00000389,6123.00
E,392.31,0.00051342,0.00055539,0.00000432,5865.00
E,393.11,0.00053142,0.00047851,0.00000365,5440.00
E,393.91,0.00051760,0.00053219,0.00000398,4825.00
```

5.2 Deep Check value

This deep check value is from aoml Navis float 5906311 cycle 5 and PRES = 1749.6 dbar and includes wavelength dependent intermediate calculations

```
OPTICAL_WAVELENGTH_OFFSET,210
CONFIG_SunaVerticalPressureOffset_dbar,1.26

PIXEL_START,36
PIXEL_END,77
PIXEL_FIT_START,36
PIXEL_FIT END,64

DC, 857
PRES, 1749.6
TEMP, 2.8267
PSAL, 34.5250
PRES_NO3, 1750.9
TEMP_NO3, 2.8254
PSAL_NO3, 34.5254
MOLAR_NITRATE, 38.38
FIT_ERROR, 6.5962e-04

OPTICAL_WAVELENGTH_UV(R"),ABSORBANCE_SW(R"),Tcorr(R" ),E_SWA_INSITU(R")
,ABSORBANCE_TCSS_NITRATE(R" )

217.22,0.3549,0.64244,3.7711E-03,0.2247
218.01,0.3159,0.63353,2.9716E-03,0.2133
218.81,0.2822,0.62604,2.3193E-03,0.2022
219.60,0.2532,0.62022,1.8038E-03,0.1909
220.39,0.2290,0.61602,1.4064E-03,0.1805
221.19,0.2083,0.61345,1.0899E-03,0.1707
221.98,0.1899,0.61262,8.4348E-04,0.1608
222.78,0.1743,0.61357,6.5360E-04,0.1518
223.57,0.1612,0.61631,5.1413E-04,0.1434
224.37,0.1494,0.62096,4.0302E-04,0.1355
225.16,0.1392,0.62747,3.2174E-04,0.1281
225.96,0.1308,0.63606,2.5955E-04,0.1218
226.75,0.1236,0.64659,2.0873E-04,0.1164
227.55,0.1172,0.65939,1.7634E-04,0.1111
228.34,0.1121,0.67421,1.4683E-04,0.1071
229.14,0.1078,0.69153,1.2542E-04,0.1034
229.94,0.1036,0.71124,1.0549E-04,0.0999
230.73,0.1009,0.73315,8.7864E-05,0.0978
231.53,0.0985,0.75788,8.0838E-05,0.0957
232.33,0.0959,0.78526,6.2247E-05,0.0937
233.13,0.0943,0.81536,5.9419E-05,0.0923
233.92,0.0933,0.84780,5.6296E-05,0.0913
234.72,0.0923,0.88343,4.9084E-05,0.0907
235.52,0.0922,0.92187,5.0023E-05,0.0905
236.32,0.0915,0.96310,4.2368E-05,0.0900
237.11,0.0910,1.00645,3.2604E-05,0.0899
237.91,0.0913,1.05290,3.9636E-05,0.0899
238.71,0.0910,1.10170,2.6373E-05,0.0901
239.51,0.0912,1.15258,3.0506E-05,0.0901
```

5.3 Shallow Check Value

This shallow check value is from aoml Navis float 5906311 cycle 5 and PRES = 36.8 dbar and includes wavelength dependent intermediate calculations

```
OPTICAL_WAVELENGTH_OFFSET,210
CONFIG_SunaVerticalPressureOffset_dbar,1.26

PIXEL_START,36
PIXEL_END,77
PIXEL_FIT_START,36
PIXEL_FIT END,64

DC, 806
PRES, 36.8
TEMP,1 3.6680
PSAL, 34.4072
PRES_NO3, 38.0
TEMP_NO3, 13.5537
PSAL_NO3, 34.4129
MOLAR_NITRATE, 7.98
FIT_ERROR, 4.1982e-04

OPTICAL_WAVELENGTH_UV(R''),ABSORBANCE_SW(R''),Tcorr(R'' ),E_SWA_INSITU(R'')
,ABSORBANCE_TCSS_NITRATE(R'' )

217.22,0.2213,0.84698,5.2037E-03,0.0422
218.01,0.1822,0.84255,4.1365E-03,0.0399
218.81,0.1496,0.83880,3.2524E-03,0.0376
219.60,0.1230,0.83586,2.5444E-03,0.0355
220.39,0.1020,0.83373,1.9922E-03,0.0334
221.19,0.0850,0.83242,1.5480E-03,0.0317
221.98,0.0715,0.83200,1.1990E-03,0.0302
222.78,0.0602,0.83248,9.2818E-04,0.0282
223.57,0.0519,0.83388,7.2809E-04,0.0268
224.37,0.0448,0.83624,5.6806E-04,0.0252
225.16,0.0400,0.83952,4.5056E-04,0.0245
225.96,0.0360,0.84381,3.6039E-04,0.0236
226.75,0.0329,0.84903,2.8687E-04,0.0231
227.55,0.0304,0.85530,2.3940E-04,0.0221
228.34,0.0285,0.86246,1.9659E-04,0.0217
229.14,0.0268,0.87071,1.6528E-04,0.0211
229.94,0.0257,0.87995,1.3660E-04,0.0210
230.73,0.0248,0.89002,1.1164E-04,0.0210
231.53,0.0244,0.90118,1.0061E-04,0.0209
232.33,0.0233,0.91326,7.5771E-05,0.0207
233.13,0.0231,0.92624,7.0649E-05,0.0207
233.92,0.0231,0.93991,6.5325E-05,0.0208
234.72,0.0227,0.95455,5.5509E-05,0.0208
235.52,0.0231,0.96993,5.5086E-05,0.0212
236.32,0.0230,0.98599,4.5399E-05,0.0214
237.11,0.0227,1.00242,3.3988E-05,0.0215
237.91,0.0230,1.01954,4.0171E-05,0.0216
238.71,0.0227,1.03702,2.5983E-05,0.0218
239.51,0.0231,1.05475,2.9219E-05,0.0221
```