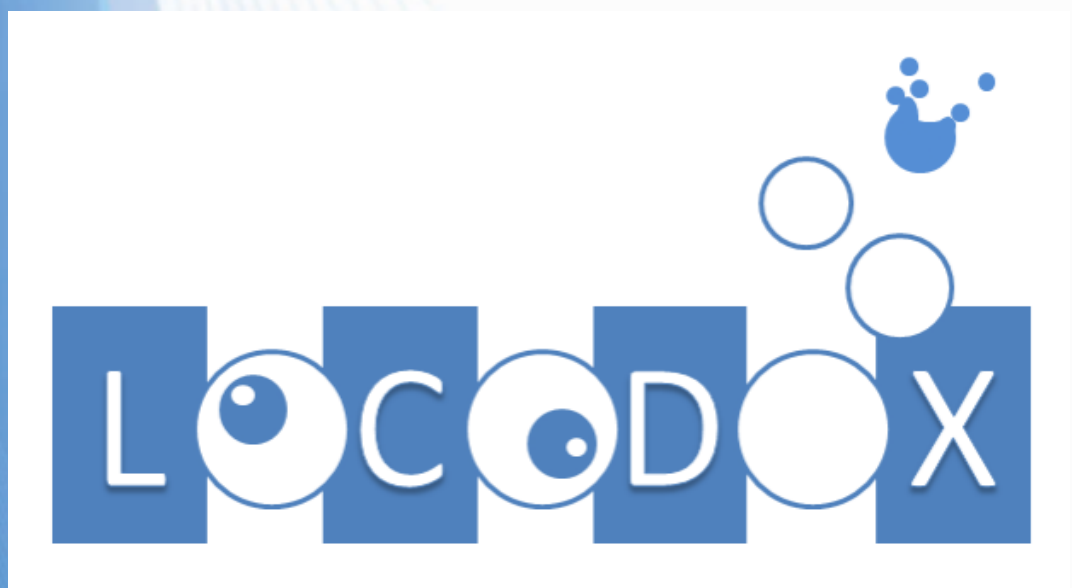


LOCODOX: a Software for Argo Oxygen data correction - User Manual

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LOCODOX : a tool for ARGO Oxygen correction

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Acronyms		
Name	Description	unit
DOXY	Dissolved oxygen concentration	μmol/kg
PSAT	Percentage of oxygen saturation	%
PPOX	Partial Pressure of Oxygen	mBar
PRES	Pressure	dBar
TEMP	Temperature	°C
PSAL	Salinity	none
WOA	DOXY correction based on the comparison to the WOA climatology	none
REF	DOXY correction method based on a comparison to an In Situ Reference profile	none
INAIR	DOXY correction based on in-air oxygen measurement and atmospheric reference NCEP	none
NCEP	Reference atmospheric PO2	none
CTD	Probe measuring Conductivity, Temperature and Depth	none
WMO	Float identification number	none
NAOS	Novel Argo Ocean observing System	none
LOPS	Laboratoire d'Océanographie Physique et Spaciale (Laboratory of Physical and Spatial Oceanography)	none

1 Introduction

LOCODOX is a MATLAB based interactive software that corrects dissolved oxygen concentration data acquired by Argo profiling floats. It works with Argo v3.1 netcdf files and provides files with corrected and well formatted delayed mode Argo data compliant with the Argo format (Argo Data Management Team, 2019).

LOCODOX corrects only oxygen data available in the vertical profiles. Data acquired during drifting phases (at parking depth or at the surface) and available in the trajectory files are not corrected by LOCODOX.

Three types of correction are proposed:

- a pressure dependent correction
- a time drift correction
- a slope and/or offset correction

The above correction schemes are based on Takeshita et al (2013) and Bittig and Kortzinger (2018) proposed methods.

This document describes the methodology and the strategy followed by the tool, and it explains how to install and use LOCODOX.

LOCODOX has been tested under Matlab R2021b and uses

- M_MAP 1.4m with the GSHHG package (<https://www.ngdc.noaa.gov/mgg/shorelines/data/gshhs/>)
- Seawater 330 matlab library (seawater_330_its90_lpo)
- Etopo2 bottom topography

2 Methodology

The 6 steps followed by LOCODOX are summarized below and detailed hereafter:

1. Argo data reading and processing
2. Reference data reading and processing; Colocalization of reference data with the argo trajectory, interpolation of reference profile data to the argo levels;
3. Application of a pressure dependent correction if necessary
4. Computation of the oxygen sensor time drift computed and application (2 methods available)
5. Computation of the slope/offset correction of the oxygen profiles and application (3 methods available);
6. Correction application and computation of the error: Update of the NetCDF files following the the Argo format v3.1.

Data provided by the Argo floats are *dissolved oxygen concentration* (DOXY) in $\mu\text{mol/kg}$. When needed, LOCODOX works with the *percentage of saturation* (PSAT) in percentage (%) or with the *partial pressure of oxygen* (PPOX) in mBar. The conversion equations between DOXY, PSAT and PPOX are those of Bittig et al. (2016). Note that the conversion between DOXY and PSAT requires pressure (PRES), temperature (TEMP) and salinity (PSAL) values. If the PRES, TEMP or PSAL values are bad data, then the converted oxygen value (PSAT) will also be bad, even though DOXY was good.

The time drift and slope/offset gains estimated by LOCODOX rely on a comparison between the float data and reference data.

Atmospheric data can be used to compare PPOX measured by the float in the air when surfacing to the theoretical value based on the atmospheric pressure. LOCODOX proposes to use this comparison to (1) estimate the sensor time drift and to correct it (step 4); and (2) to estimate the slope/offset correction in step 5. The latter correction is refer to hereinafter to **INAIR method**.

Climatological in situ data can be compared to PPOX values to (1) estimate the sensor time drift and to correct it (step 4); and (2) to estimate the slope/offset correction in step 5. The latter correction is refer to hereinafter to **WOA method**.

In situ calibrated ship-based reference profiles can be compared to PPOX data from different float profiles to estimate the main gain (slope/offset correction) in step 5. The latter correction is refer to hereinafter to **REF method**.

The matlab file `locodox_config.m` in the main LOCODOX directory allow the choice of different options to run LOCODOX and defines the path to the `m_map1.4`, seawater directories and input dataset (WOA, ARGO, in situ profiles database).

2.1 Step 1: Argo data reading and processing

To correct dissolved oxygen concentration (DOXY) measured by Argo floats, LOCODOX requires many parameters : of course the oxygen parameter measured *in situ* and also in air when available, the

pressure, the temperature and salinity (to compute density), the QC associated to each of those parameters, the date and position of the considered profiles.

The input and output format of the Argo Data in LOCODOX is the NetCDF Argo 3.1, following the recommendations of the Argo Data Management described in the Argo User's Manual v3.2 (ADMT 2017). For a given Argo float, LOCODOX works with the corresponding Argo monoprofile files and the Argo trajectory files. This latter file contains all the timing information, the argos localization, and the in air oxygen measurements acquired during surfacing.

2.1.1 The Argo profile files

The monoprofile contains the data during one cycle of the Argo float. PRES, TEMP and PSAL are provided in the C file, while biogeochemical parameters, including DOXY, are provided in the B files. The correspondence between the C and B files is done through PRES because it is common to the two files. The profile can be ascending or descending. In each monoprofile file (C or B), the data are organized such that parameters measured with the same sampling method are grouped in the same vertical profile. Those data are associated to a specific vertical sampling scheme (see Argo User's Manual for more details).

Four types of Vertical Sampling Scheme (VSS) exist: Primary sampling, Secondary sampling, Near-surface sampling, Bounce sampling.

- The **Primary Sampling scheme** corresponds to the typical core Argo sampling: profile down to 2000 dbar or more, TEMP and PSAL data acquired with the CTP pump on. PRES, TEMP and PSAL that feeds the Argo data stream are available in this profile.
- The **Near-Surface Sampling scheme** corresponds to shallow profiles (less than 5 dBar) acquired when the CTD pump is off. PSAL is generally bad for such profiles.
- The **Secondary Vertical Sampling scheme** concerns all other profiles acquired with VSS that differs from the Primary or the Near-Surface Sampling Scheme.
- The **Bounce Vertical Sampling scheme** corresponds to data acquired during several ascending /descending profiles during a single cycle. **Be aware that this case has not been tested in LOCODOX.**

2.1.2 Profile data recovery

2.1.2.1 DOXY data

LOCODOX works only with DOXY, the raw oxygen data, even if DOXY_ADJUSTED already exists in the file.

Using the STATION_PARAMETERS variable, LOCODOX determines the profiles in which DOXY is found, typically one in a profile with CTD pump activated (either the primary or the secondary sampling), and one in the unpumped profile (Near-Surface sampling). For a given cycle, DOXY data can be found in at most 2 profiles with different VSS: either in the Primary sampling and maybe the Near-surface sampling, or Secondary sampling and maybe Near-surface sampling.

The associated QC fields are retrieved.

LOCODOX separates profiles data as function of their sampling schemes into four structures:

- A **primary** structure (one profile/cycle) that contains CTD data and DOXY if available
- A **secondary** structure (one profile/cycle) that contains the full depth DOXY profile if it is not available in the Primary structure.
- A **nearsurf** structure (one profile/cycle) that contains DOXY when it is acquired in the near surface sampling profile
- An **other** structure that aggregates all the profiles that do not carry the DOXY parameter

If there is no profile in a given structure (for instance secondary and other), the structure is not used by LOCODOX.

LOCODOX identifies the structure (called “main profile”) that contains the data used to compute the correction. Once estimated, the same correction will be applied to the oxygen data available in the other structures. Depending on the correction type, the main profile could be either the primary or the secondary structure (WOA and REF methods), or the near-surface one (INAIR).

2.1.2.2 PRES data

Pressure values associated with CTD data are retrieved in the Primary profile of the C-File. Pressure values associated to the profiles carrying DOXY data are also retrieved.

The user can choose (see the configuration file) :

- to work only with PRES data, even if PRES_ADJUSTED exist
- to work with PRES_ADJUSTED if it exists. In that case, PRES will be used instead of PRES_ADJUSTED if PRES_ADJUSTED is filled with FillValues and the corresponding DATA_MODE is set to “R” (real time).

2.1.2.3 TEMP and PSAL data

The TEMP and PSAL data are retrieved the primary profile in the C-file. As for PRES, the user can choose (see the configuration file) to work only with TEMP (PSAL) or to work with TEMP_ADJUSTED (PSAL_ADJUSTED).

The associated QC field are retrieved.

PSAL and TEMP are interpolated on the pressure levels found in the profile bearing DOXY, if it is different from the primary profile.

2.1.2.4 PSAL, TEMP and PRES recovery for the INAIR correction

When in air oxygen measurements are used to compute the correction, LOCODOX needs the PSAL and TEMP values just below the sea surface. Those data are used to compute surface water vapor pressure and the possible influence of waves on air PPOX measurements. As salinity data is only valuable when the CTD pump is on, salinity data available in the near-surface profile are not usable. PSAL data are thus retrieved in the primary profile, at the shallower valid data encountered by cycle. TEMP is retrieved in the Near-Surface profile, or in the primary one if no valid data could be found in the near surface profile. The PRES associated to TEMP is used, even if it is not at the same level than PSAL.

The values of TEMP and PSAL are looked for in a layer whose maximum depth (typically 10 dbar) defined in the configuration file (see Section 3.2). If no value is found, a message warns the user and LOCODOX stops.

Moreover, the in-water PTS thus recovered are also used to compute the PPOX in-water data, only for float with in-air measurement with no distinction between Near-Surface and In Air data. For those floats, the in-water part measurements are taken in the profile data and not in the trajectory data.

2.1.2.5 Date and position

The date and the position of the profiles are retrieved in the monopfiles files (DATE, LATITUDE and LONGITUDE).

2.1.3 Trajectory data recovery

The trajectory file is read only when in-air oxygen measurements are used for the correction.

To get the partial pressure of oxygen measured during surfacing (PPOX) and its associated datation, pressure, temperature and salinity, LOCODOX relies on the measurement codes (MC), in agreement to the argo v3.1 format. The measurement code corresponding to the in-air measurement is defined by the operator. Note that based on the document "Near surface and in air data processing at Coriolis V2.0", the current measurements code for in-air measurements are 699, 711 or 799. For the in-water data, the measurements code are 690 or 710.

The salinity associated to PPOX data is not taking into account during the correction process because it was acquired either when the CTD pump was cut off or when the sensor was in the air.

The date and position of the trajectory data are get in the Core-trajectory file. LOCODOX follows the hereafter strategy:

- All the measurement marked with an in-air or in-water measurement are taken (the MC could be modified in the configuration file)
- The datation is kept except if NaN values have been detected. In this case, the Ascent End Time is preferred
- The localization corresponds to the first available argo localization, selected between the transmission Start Time, the First message transmitted, the argos localization, the Last Message transmitted.

For float with in-air measurement with no distinction between Near-Surface & In Air, LOCODOX considers that all the PPOX_DOXY measurements have been taken in-air. The needed in-water measurements are picked up in the profile (see Section 2.1.2.4).

2.1.4 Data selection for the correction computation

Before computing the correction, LOCODOX processes a simple quality control on the float data to select the data to be considered for the correction computation. This quality control does not change the QC flag of the data and is not reported in the final NetCDF corrected files.

Data are discarded for the correction computation when:

- The pressure is negative
- The pressure is constant on the vertical
- The QC flag are not allowed by the operator (see the configuration file)

2.2 Step 2: Reference data reading and processing

2.2.1 Climatological data

Monthly climatological field can be used for correcting Argo oxygen data. The data should be provided as a unique netcdf file with the following variables.

Netcdf WOA_monthly_5500_1deg {

dimensions:

```
lat = 180 ;  
lon = 360 ;  
Depth = 33 ;  
time = 12 ;
```

variables:

```
double latitude(lat) ;  
    latitude :long_name = « latitude » ;  
    latitude :units = « °N » ;  
double longitude(lon) ;  
    longitude:long_name = "longitude" ;  
    longitude:units = "°E" ;  
double Depth(Depth) ;  
    Depth:long_name = "Depth" ;  
    Depth:units = "day" ;  
double time(time) ;  
    time:long_name = "time" ;  
    time:units = "day" ;  
double doxywoa(time, Depth, lat, lon) ;  
    doxywoa:long_name = "DISSOLVED OXYGEN (umol/kg) " ;  
    doxywoa:units = " umol/kg " ;  
double Psatwoa(time, Depth, lat, lon) ;  
    Psatwoa:long_name = "%saturation" ;  
    Psatwoa:units = "%" ;  
double PSAL_WOA(time, Depth, lat, lon) ;  
    PSAL_WOA:long_name = "PRACTICAL SALINITY " ;  
    PSAL_WOA:units = "psu" ;  
double TEMP_WOA(time, Depth, lat, lon) ;  
    TEMP_WOA:long_name = "SEA TEMPERATURE " ;  
    TEMP_WOA:units = "degree_Celsius" ;  
double density(time, Depth, lat, lon) ;  
    density:long_name = "density" ;  
    density:units = "kg/m3" ;  
double preswoa(time, Depth, lat, lon) ;
```

```
preswoa:long_name = "pressure " ;
preswoa:units = "dbar" ;
```

Monthly climatological fields on a 1°x1° horizontal grid can be used for correcting Argo oxygen data.

LOCODOX is currently provided with a file based on the World Ocean Atlas (hereafter WOA) climatology. The upper 1500m are extracted from the World Ocean Atlas monthly climatologies. Deeper values are extracted from the annual mean fields.

Once loaded in LOCODOX, the WOA data are interpolated on the argo time and position, and over the argo data levels.

2.2.2 NCEP data

NCEP atmospheric reanalysis data are required for the correction based on oxygen in air measurements. Those data are downloaded as netcdf files from <ftp.cdc.noaa.gov> .

The three following fields are required for the computation : the air temperature at the surface (air.sig995.yyyy.nc), the relative humidity at sigma level 995 (rhum.sig995.yyyy.nc) and sea level pressure (slp.yyyy.nc).

LOCODOX proposes to update the files in downloading the last available data (see configuration file).

The NCEP reference data have to be colocalized regarding to the argo float trajectory. NCEP data are available on a 1/3° grid and with a time frequency of 6h (4 values a day). The nearest NCEP data in time are taken. Then, the NCEP data are colocalized on the argo latitude and longitude.

2.2.3 In situ reference profile

The main gain (or slope/offset correction) can be calculated comparing one or more Argo profiles with corresponding calibrated ship-based reference casts. In general, one of the reference profile is the ship-based CTD cast realized at float deployment which is compared to the first or second ascending profile of the float. Notice that the first ascending profile might not be chosen because it could be biased due the time required by the sensing foil to be fully operational.

The in situ reference profiles are stored in an *in situ* database that has been generated by users. The « Package_create_bddO2ref » folder can be used to create the database. This database is provided to LOCODOX as a matlab file (.mat) with the following structure :

For a database containing 1202 reference profiles, we will have :

```
REF.id [1202x1 cell] : reference profile id (in the RefArgoFile, it corresponds to « campaign_station »)
REF.lon [1202x1 double] : longitude of reference profiles
REF.lat [1202x1 double] : latitude of reference profiles
REF.juld [1202x1 single] : julian day of profiles
REF.temp [1202x401 single] : temperature for each pressure level
REF.psal [1202x401 single] : salinity for each pressure level
REF.sig0 [1202x401 single] : potential density in kg/m3
REF.doxy [1202x401 single] : dissolved oxygen concentration in umol/kg
REF.pres [1202x401 double] : level of pressure of each profile
```

REF.psat [1202x401 single] : percentage of oxygen saturation

For a given float, the correspondence between the reference profile and the float cycle is provided in a file (see parameter *RefArgoFile* found in the configuration file). The RefArgoFile should be a text file with 4 columns and n rows (n=number of float to be corrected):

RefArgoFile =

- wmo : it indicates the name of the floats (wmo)
- cycle : it indicates which cycle of the float to use for the correction (usually cycle 1)
- campaign : it indicates the id of the campaign to use for the correction
- station : it indicates the station number to use for the correction

Example :

wmo	cycle	campaign	station
6901023	1	cat12	49
6901027	1	cat12	63
6901030	1	cat12	78
5904988	1	geov	39
5904989	1	geov	40

Notice that in Locodox 4.2 more than one reference profile could be used but this is actually limited to 7 for writing limitations in the Netcdf files. In that case, the database contains 1 to 7 lines with the same wmo number. Once loaded in LOCODOX, the *in situ* reference data are interpolated over the pressure level of the corresponding argo profile.

2.3 Adjusting Oxygen Content data:

Oxygen data in Locodox4 are adjusted with the following equations

$$[DOXY_{corrected}] = G_{pres} * [DOXY]$$

$$[PPOX_{corrected}] = G * G_{TD} * [PPOX]$$

Notice that the oxygen profiles are first corrected with a pressure dependant gain referred as G_{pres} . G_{TD} is the time drift gain . G is the main Gain computed after correcting the rawdata with respectively G_{pres} and G_{TD} . All these gains will be discuss below.

2.4 G_{pres} : Pressure dependent gain

In some cases, the comparison to a reference profile reveals the need of a pressure dependent correction for some sensors. LOCODOX offers the possibility to correct such offset as follows:

$$G_{pres} = 1 + coeff * PRES / 1000$$

Where PRES is the pressure (dbar) and coeff provided by the operator and is actually not estimated by LOCODOX. This coefficient is comprised between -0.01 and 0.01.

The choice of *coeff* is an iterative process. LOCODOX has to be run a few times to estimate *coeff* because the result of such correction can only be seen in comparing the reference profile to the corrected data, so after using LOCODOX.

All DOXY data are first pressure corrected (see equation in 2.3).

2.5 G_{TD} : Time drift Gain

LOCODOX computes the sensor time drift as a Gain in comparing the float data to reference data, that is between argo profiles and climatological data, or between in-air measurements and atmospheric data provided by NCEP reanalysis.

LOCODOX computes a regression of the reference data and / argo data ratio which could be seen as the time drift gain. The resulting estimation is proposed to the user, who decides to apply or not the time drift Gain. The Gain is calculated on partial pressure of O₂ (PPOX) values.

The regression is based on:

- ⇒ a polynomial equation (up to degree 2) or on an equation defined by the operator. The polynomial order or the user's equation are defined in the configuration file. For the polynomial case, the estimated offset is not used to correct the data as the main gain is estimated at the next step.
- ⇒ For other kind of regression, LOCODOX computes and applies the correction by taking into account every term of the equation (including possible offset). We rather used a **linear regression** although a second degree polynomial expression is possible and was occasionally used in a recent past.
- ⇒ Since version 4.4, we introduced a **piece wise linear regression**. The purpose is to avoid using a second degree polynomial expression. This option makes any use of second degree polynomial expression obsolete which will be removed in a near future version of LOCODOX.

The time drift gain based on WOA is computed on the ascending profiles only and is applied on both descending and ascending profiles. In the same way, the time drift gain based on NCEP is computed on the in-air measurements and is applied on both descending and ascending profiles.

When the main gain (previously referred as the slope/offset correction) is based on the comparison between in-air measurements and NCEP data, the user has automatically the choice to compute the time drift gain using WOA or using NCEP. Notice that loading NCEP data takes some time, there is a parameter in the configuration file to allow or not the computation of the sensor time drift from in-air

measurements when the slope/offset correction (main gain) is based on the comparison to *in situ* data (REF or WOA methods).

2.5.1 G_{TD} based on climatological data

The time drift gain is estimated from the ratio between climatological data and Argo data in deep or surface layers.

Argo profiles and climatological are interpolated with a vertical spacing of 100 dbar on levels between a minimum depth (typically 1500 dbar) and 2000 dbar or 6000 dbar for core or deep Argo, respectively. The minimum and maximum depth value for the interpolation are defined by the user in the configuration file. When the calculation is done near surface, the interpolation parameters are defined in `locodox_config.m` as:

```
CONFIG.min_drift_depth_surf= 0;  
CONFIG.max_drift_depth_surf=25;  
CONFIG.step_drift_depth_surf=5;
```

Here, the interpolation spacing is set to 5m between surface to a depth of 25m.

LOCODOX applies the time drift compensation only with user approbation. To help the user make his choice, the drift estimated after 1 year and over the lifetime of the float are indicated. Some cases are also brought to the user's attention: if there are less than 10 deep profiles to estimate the time drift, if there is less than one year of data, and if there are less than 10 deep levels for each profile. Moreover, the user can also choose to apply a constant time drift gain from a certain day.

The time drift gain is always computed using PPOX, and is applied to DOXY. The corrected data could then be converted to PSAT. The conversion uses the pressure, temperature and salinity from the profile.

2.5.2 G_{TD} based on NCEP atmospheric data

The time drift gain is estimated from PPOX values acquired in air during the float surfacing with atmospheric oxygen partial pressure deduced from NCEP data colocalized on argo positions.

LOCODOX applies the time drift compensation only with the user approbation. The time drift gain estimated at launch, after 1 year and over the float lifetime are indicated to help the operator making his choice. As previously, the user can also choose to apply a constant time drift gain from a certain day.

The time drift gain is always computed using PPOX. Then, the corrected PPOX values are converted to PSAT and DOXY using the pressure, temperature and salinity from the profile.

2.5.3 Piece Wise linear fitting

We occasionally observed that the optode measurements drift in a non-linear way over the first cycles. We have introduced a piece-wise linear fitting (hereafter PWLF). In the configuration file, the following line can be found:

```
CONFIG.drift_PWLF_N = 2;% Number of linear segments
```

The number of linear segments is set to 2. Locodox prompts the user for using or not the PWLF:

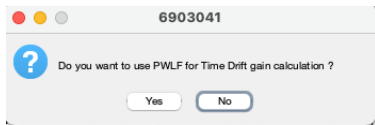


Figure 1: Locodox question

If the answer is no, Locodox doesn't use this function. If the answer is yes, the operator will choose on the figure the time separation for the 2 segments:

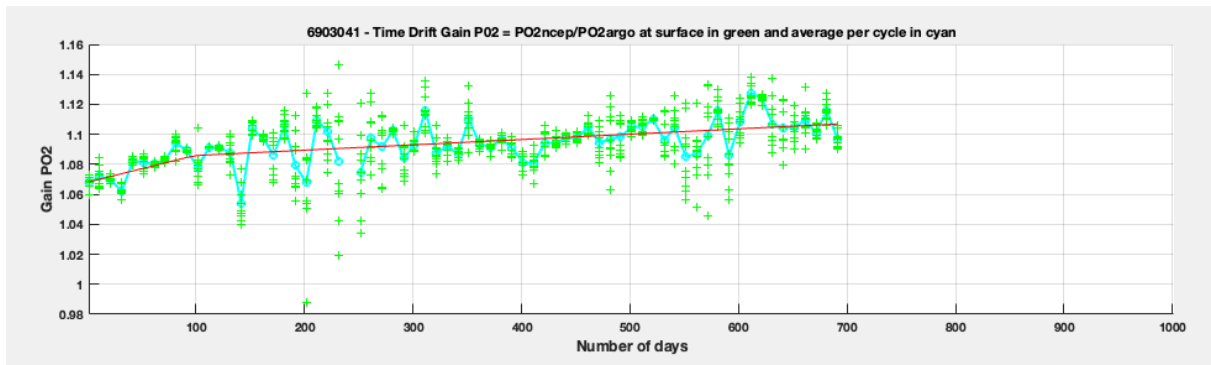


Figure 2: Time Drift correction

In Figure 2, the two linear segments are connected at 100 days roughly cycle number 10.

2.6 G: Main Gain or Slope/offset correction

The main gain or slope/offset correction of DOXY data can be computed following three methods (WOA, REF and INAIR). The general philosophy is to compute a regression between reference data and argo data. This computation is based on Takeshita et al. (2013).

For the WOA, REF or INAIR correction, LOCODOX compute the main gain using the PPOX data

2.6.1 G based on *in situ* data (WOA or REF methods)

The correction using the climatology (WOA) and the *in situ* Reference data (REF) computes a linear regression between the argo profile(s) and the reference profile(s). It relies on the method developed by Takeshita et al (2013²).

The correction can be written as follows:

$$O2_{adjusted} = slope \times O2_{argo} + offset$$

Where O2 can be either the concentration of dissolved oxygen (DOXY), the percentage of oxygen saturation (PSAT) or the partial pressure O2 content (PPOX). The *adjusted* and *argo* suffixes are used to describe the adjusted data (*adjusted*) and the initial data from the Argo float (*argo*).

The *slope* and *offset* coefficients are estimated between:

- **WOA method:** the whole interpolated WOA profiles and the whole argo float profiles to be corrected

- **REF method:** *in situ* reference profiles and the associated argo profile (see section 2.2.3). Notice than more than one reference profile could be used. This is currently technically limited to 7 REF profiles.

LOCODOX can force to origin the linear regression (offset = 0), with the underlying idea that in anoxic water, the optode indeed measures DOXY = 0. The choice is left to the operator.

If the correction is of poor quality (R^2 below a threshold value defined in the configuration file), it means that the vertical structure of the argo profile significantly differs from that of the reference profile, leading to an important deformation of the vertical structure of the corrected argo profile compared to the raw argo profile. LOCODOX therefore suggests computing a constant correction, applied equally at every depth :

$$O2_{adjusted} = O2_{argo} + offset$$

where the offset is the average of the differences over the whole water column between:

- WOA method: the mean WOA profile and the mean argo profile
- REF method: the reference CTD profile and the associated argo profile

The user can then chose to apply the constant correction or the linear correction.

2.6.2 G based on in air measurements (INAIR method)

This method is described in Bittig and Kortzinger (2015) and Bittig et al. (2018) and Johnson et al. (2015). This method only applies on an argo float that acquired oxygen, measurements in air during surfacing. It relies on a regression between three partial pressure values of oxygen (PPOX or PO_2):

- A reference atmospheric PO_2 estimated from NCEP reanalysis data;
- In-air PPOX measurement from the float (PPOX_DOXY). Those data are acquired by the floats during surfacing.
- In-water PPOX measurement of the float. Those data are acquired by the float before surfacing. Depending on the float and float software, those data are :
 - either the “in-water” part of the surface measurements (argo float NS/IA, specifically programmed to do a series of measurement just under the surface (NS) and just above the surface (IA)),
 - either the shallowest good data in the profile (main or primary), and DOXY is converted to PO_2

The regression correction is written as follows:

$$pO_{2(air,argo)} = c \times pO_{2(water,argo)} + \left(\frac{1-c}{m}\right)pO_{2(air,ncep)}$$

Where pO_2 is the partial pressure of oxygen (PPOX), the suffix (where,what) corresponding to in air measurements (air) or in water measurements (water), from NCEP data (ncep) or from Argo data (argo).

This equation takes into account the occasional submersion of the optode, and so the contamination of the in-air measurement by the in-water measurement (coefficient c). The user can choose to set the coefficient c to 0 in the configuration file (parameter 'isokC') and thus consider that there is no contamination of the in-air measurement by the in-water measurement. The m coefficient is then used to correct raw data, as follows:

$$pO_{2(argo)corrected} = m \times pO_{2(argo)}$$

2.7 Application of the correction and writing of the output netcdf files

Note that, except for Gpres, our first equation (see section 2.3) is consistent with that of Thierry et al. (2021) considering OFFSET=0 , INCLINE_T=0 and DRIFT2=0:

$$PPOX_{corrected} = \left(\text{SLOPE} \cdot \left(1 + \frac{\text{DRIFT}}{100} \cdot \frac{\text{profile}_{date_juld} - \text{launch}_{date_juld}}{365} + \frac{\text{DRIFT2}}{100} \cdot \left(\frac{\text{profile}_{date_juld} - \text{launch}_{date_juld}}{365} \right)^2 \right) + \text{INCLINE_T} \cdot \text{TEMP} \right) \cdot [\text{PPOX} + \text{OFFSET}]$$

The corresponding SLOPE , DRIFT and DRIFT2 values are calculated by LOCODOX and applied to both ascending and descending profiles, and to all vertical sampling schemes profiles.

If the PWLF option is activated, DRIFT2=0, SLOPE and DRIFT are calculated for each linear segment.

For the WOA, REF and INAIR method, the calculated gain is based on the PPOX parameter. To apply the correction to the profiles, LOCODOX first converts the DOXY profiles into PPOX profiles and then applies the correction to them. These PPOX profiles are then converted back to DOXY corrected profiles.

The DOXY_ADJUSTED field is then filled with the corrected values.

The DOXY_ADJUSTED_ERROR can be absolute or relative, and is specified by the user in the configuration file. It can also be modified when LOCODOX is running.

DOXY_ADJUSTED_QC is set from the DOXY_QC value according to the rules described in Table 1.

DOXY_QC	DOXY_ADJUSTED_QC	DOXY_ADJUSTED
1,2,3	1	Corrected value
4	4	Fillvalue
All other QC	4	Fillvalue

Table 1 : Changing QC rules for DOXY_ADJUSTED_QC

The following metadata fields are filled by LOCODOX as follow:

- **date_update:** It is set to the date of the creation of the netcdf file with the corrected data. The same value is attributed to the history_date and to the scientific_calibration_date
- **data_mode:** it is set to "D"
- **data_state_indicator:** it is filled with "2C"
- **parameter_data_mode:** it is set to "D"
- **history fields:** history_institution, history_action, history_software, history_software_release, history_parameter, history_date, history_start_pres, history_stop_pres
- **scientific calibration fields:** scientific_calibration_date, scientific_calibration_coefficient, scientific_calibration_comment, scientific_calibration_equation. The scientific calibration fields are filled following Thierry and Bittig, 2016.

These metadata fields are updated for all the DOXY parameter, the PRES parameter, and all the intermediate DOXY parameter (as MOLAR_DOXY, TPHASE_DOXY, etc) if the latter are available in the corrected profile.

LOCODOX write NetCDF argo 3.1 files, completed with corrected data and updated metadata fields. The vertical sampling scheme and the direction are taking into account to fill correctly the files.

3 How to install and run LOCODOX

3.1 LOCODOX package

3.1.1 Matlab Release and toolboxes

LOCODOX works with MATLAB v2021b and its Statistic Toolbox.

Note that the statistic Toolbox is necessary for IN AIR correction and also to compute a non linear drift. For other corrections, LOCODOX can work without the statistics toolbox but it will remove some correction options.

The cartography is based either on Google Map (which required an internet access) or on the M_MAP toolbox (<https://www.eoas.ubc.ca/~rich/map.html>, external and free). LOCODOX has been tested with the m_map release that uses GSHHS Geography data base.

3.1.2 LOCODOX files structure

LOCODOX is a suite of matlab programs. In the main directory, we can found the main program **locodox.m** and the configuration file **locodox_config.m**, which has to be adapted with the user needs. Three sub-directories are found in the main directory. They contain the necessary matlab routines required to run LOCODOX, some of the input data and results files.

Some Input data are retrieved from external directories specified in the configuration file. The organization is summarized in Table 2:

Name	Description	File or directory	Where
LOCODOX_User_Manual	User manual of LOCODOX	document	LOCODOX main directory
locodox.m	Main program	file	LOCODOX main directory
locodox_config.m	The configuration file	file	LOCODOX main directory
doxy_corr	all the LOCODOX matlab functions	directory	LOCODOX main directory
share	all other matlab based libraries or functions used by LOCODOX	directory	LOCODOX main directory
data_input	input data for LOCODOX : - Reference data, (reference in-situ data base) - The land mask file	directory	LOCODOX main directory

CONFIG.resultsDir	Contains the adjusted data, plots and log files	directory	LOCODOX main output directory. Path to be specified in the configuration file
Additional_Packages	<p>Package_create_bddO2ref: Function needed to create the reference database in the format used by LOCODOX.</p> <p>Package_create_woa: Functions read and rewrite the WOA climatologies for LOCODOX</p>	directory	LOCODOX main directory
CONFIG.DataDir	Contains the float data	directory	Path to be specified in the configuration file
CONFIG.BathyDataDir	contains etopo2 bottom topography	directory	Path to be specified in the configuration file
CONFIG.WOADataDir	contains World Ocean Atlas temperature, salinity and oxygen monthly climatology files rewritten for LOCODOX	directory	Path to be specified in the configuration file
CONFIG.NCEPDataDir	contains the National Center for Atmospheric Prediction (NCEP) annual daily netcdf files (relative humidity, sea level pressure, relative humidity)	directory	Path to be specified in the configuration file

Table 2 : Files and directories to run LOCODOX

The user can choose where to save the results, he has to specify the output directory in the locodox_config file (see later). Then, LOCODOX will create 3 sub-directories in the output directory.

Sub-directory « plots »

This directory contains the different figures appearing while correcting a float. Note that the figures are saved only if the parameter 'savePlot' is set to 1 in the configuration file (see part 3.2).

For each correction method, a folder will be created, which means that 3 subfolders could be found in the plot directory : INAIR, REF and WOA. Inside these correction method folders, the plot will be organized by WMO.

Exemple : For IN-AIR correction of the float 6902808, the figures will be found in the directory : .../plots/INAIR/6902808/.

Notice that runs using different pressure coefficient yield figures that overwrite older ones.

Sub-directory « data »

This directory contains the corrected data. There are two sub-folders, 'MAT' where data are saved in matlab format .mat and 'NC' where data are saved in NETCDF format, with one file per cycle of the float. For each type of correction, a specific folder will be created in the 'MAT' and 'NC' folders.

Exemple : for IN AIR correction, with the pressure effect not taken into account for conversion of DOXY/PSAT/PPOX and a drift computed on NCEP data, the netcdf files will be found in the directory :

« data/NC/INAIR_nopreseff_drift_onNCEP_nooffset_PPOX/ »

- « okpreseff » or « nopreseff » refers to the pressure effect parameter (see pressEff in the configuration file) for conversion of DOXY/PSAT/PPOX ;

- « koffset » or « nooffset » refers to the equation chosen by the user to compute the regression between the reference data (WOA or REF method) and the argo data.

For a constant correction (only possible with the REF correction or the WOA correction) the name of the folder will begin by « WOAconstant_ » or « REFconstant_ ».

Note that there isn't different names of folder if the pressure effect correction was applied or if a constant drift is applied, then new files can overwrite the last one.

[VT1][TR2] Sub-directory « logs »

This directory contains the log file resuming the configuration file and the choices made by the user. It is organized by correction and by WMO : for IN AIR correction of the float 6902808, log files will be found in the directory "logs/INAIR/6902808/". Several log file are saved in the folder :

- 'Summary_correction_options_6902808_[date]_[hour].txt' : This file contains all the parameters of the configuration file used for the correction, and all the user choices during the correction. A different file is created for each run of LOCODOX (the name of the file contains the time at which the correction was made). **Note that a correction was made correctly if the mention "CORRECTION COMPLETED" appears at the end of the log file.**[VT3]

- 'DOXY_VSS_choice_6902808' : it contains the files used for correction, the number of vertical sampling schemes of each cycle and the index of the vertical sampling schemes;

- 'DOXY_PTS_data_used_for_doxycorr_6902808' : (for REF and WOA method only) it contains the distribution of raw data and _adjusted data of pressure, temperature and salinity used for the correction;

- 'DOXY_get_primary_PTS_for_traj_PSAI_6902808' : (for INAIR method, or if the user choose to compute drift on NCEP data) : salinity taken in the primary profile in order to convert near-surface data. This file allows to know at which level of pressure the salinity was selected, and it's value.
- 'DOXY_get_nearsurf_PTS_for_traj_TEMP_6902808' : (for INAIR method, or if the user choose to compute drift on NCEP data) : temperature taken in the near-surface profile in order to convert near-surface data. This file allows to know at which level of pressure the salinity was selected, and it's value. If more than 30% of TEMP value are not valid, TEMP will be taken in the primary profile.
- 'DOXY_get_primary_PTS_for_traj_TEMP_6902808' : (for INAIR method, or if the user choose to compute drift on NCEP data) : temperature taken in the primary profile in order to convert near-surface data. This file allows to know at which level of pressure the temperature was selected, and it's value.

3.1.3 Install and run LOCODOX

Step	Comments	Section
Get LOCODOX	<p>The LOCODOX (matlab code only) can be downloaded from:</p> <p>https://github.com/euroargodev/LOCODOX</p> <p>In order to download code+external data, contact virginie.thierry@ifremer.fr</p>	
Updates the configuration file locodox_config.m	Update the directories path, filenames and parameters	
Update the RefArgoFile (optional)	The RefArgoFile is only necessary for a correction based on the REF method	
Open MATLAB	Be careful to be in the main LOCODOX directory	
LOCODOX is ready to be used!	<p>Run the following command in the command window of MATLAB :</p> <p>locodox('/your/full/path/for/config/file/<u>locodox_config</u>')</p> <p style="text-align: center;">Or</p> <p>Modify the default locodox_config.m path in locodox function, then launch directly :</p> <p>locodox</p>	

Table 5 : Steps to be done before running LOCODOX

3.2 Configuration file

The configuration file manages the different useful directories, files, parameters for correction, plots and NetCDF writing. It has been introduced previously and will be detailed here.

The users have to update and check all of them before running LOCODOX. The configuration file is a matlab program (extension in '.m'), which directly reads the information wrote inside. After each section, an example of the configuration file is presented.

3.2.1 Directories

Four kinds of directories are defined in the configuration files that must be defined:

- **CONFIG.LocodoxMainDir** : The main directory, where LOCODOX package is (this directory contains the configuration file "DOXY_config.m", the sub-directories "doxy_corr", "data_input" and "share");
- **CONFIG.DataDir** : The data directory, where argo data to be corrected are. In the 'DataDir', data must be organized by float number (WMO);
- **CONFIG.resultsDir** : The saving directory, where the LOCODOX output will be saved.
- **CONFIG.ExtDataDir**: Directories where are read external data used by LOCODOX: climatology, bottom topography and NCEP atmospheric fields.

Then, LOCODOX automatically creates the paths for the necessary sub-folders (section 'Add the useful paths' in the configuration file).

```
% Main directory of LOCODOX
CONFIG.LocodoxMainDir = '/Users/thierry_reynaud/IFREMER/MATLAB/LOCODOX/LOCODOX3-4/';

% Directory of the Argo NetCDF data
CONFIG.DataDir = '/Users/thierry_reynaud/IFREMER/MATLAB/LOCODOX/LOCODOX_EXTERNAL_FLOAT_DATA/';

% Directories for reading data
CONFIG.ExtDataDir = '/Users/thierry_reynaud/IFREMER/MATLAB/LOCODOX/LOCODOX_EXTERNAL_DATA/';

% Directory for saving results
CONFIG.resultsDir=
'/Users/thierry_reynaud/IFREMER/MATLAB/LOCODOX/LOCODOX3-4/results/';
```

3.2.2 Complementary Data access

LOCODOX needs access a set of data files located in the **data_input** and in **CONFIG.ExtDataDir** directories. The user could change this organization if needed. The users have to update or check the following files :

- **CONFIG.WOAfile** : The WOA climatology file is constructed from

```
WOA_YEAR='2018';% Release Year
WOA_DECAD='_DECAV';% Only for woa2018 : period choice DECAV versus A5B7

% WOA_YEAR='2009';% Release Year
% WOA_DECAD='';% % Leave empty for 2009

CONFIG.WOAfile = ['WOA',WOA_YEAR,WOA_DECAD,'_monthly_5500_1deg.nc'];
```

- **CONFIG.bddFile** : The reference In-Situ database. The user has to create his own database using the “Package_create_bddO2ref”. By default, the in-situ LOPS database “bddO2ref.mat” file is provided in the LOCODOX package.

```
% Reference In-Situ DataBase
CONFIG.bddFile='bddo2ref.mat';
```

- **CONFIG.RefArgoFile** : The “.txt” file that couples the in-situ database to the associated argo WMO (Note that this file is not necessary with correction method based on IN AIR or WOA);

```
% Reference data associated to a wmo
CONFIG.RefArgoFile='bdd REF ARGO.txt';%
```

- **CONFIG.maskFile** and **CONFIG.varMask** : The land mask file and the variable of the land mask to read;

```
% Mask file and the variable to be read in the mask file
CONFIG.maskFile = 'landsea_masks.cdf';
CONFIG.varMask = 'landsea';
```

- **CONFIG.logo** : The LOCODOX logo file ;

NCEP file and FTP address : NCEP data are located into the directory CONFIG.ExtDataDir/ncep (see 3.1.3 above). This directory is also used to save the NCEP data updated. The configuration file manages the setting for the automatic updating of the NCEP reference database :

- **CONFIG.ncepDoUpdate** : If the parameter is set to 1, then LOCODOX will updates the directory content.
- **CONFIG.ncepFtp** : the ftp website of NCEP where the new NCEP data are loaded.
- **CONFIG.ncepFtpDir** : The path where to find the NCEP data in the ftp website
- **CONFIG.ncepFiles** : the NCEP files to be read
- **CONFIG.ncepYears** : the parameter ncepYears manages the years of NCEP you want to read for IN-AIR correction.
- **CONFIG.ncepGetYears** : the parameter ncepGetYears manages the years of NCEP you want to download.

```

CONFIG.ncepDoUpdate = 1;
CONFIG.ncepFtp = 'ftp.cdc.noaa.gov';
CONFIG.ncepFtpDir = 'Datasets/ncep.reanalysis/';
CONFIG.ncepFtpSubDir = {'surface', 'surface', 'surface'};
CONFIG.ncepFiles = {'slp', 'air.sig995', 'rhum.sig995'};
CONFIG.ncepYears = [2014:2020]; % To be used
CONFIG.ncepGetYears = str2double(datestr(now, 'YYYY')); % To be downloaded

```

3.2.3 Parameters for correction

The user can choose between different options for correcting the vertical profiles of DOXY measured by Argo floats. Some options should be defined initially in the configuration file and some other will be asked when running LOCODOX. In the configuration file the parameters to set are the following :

- **CONFIG.refUnit:** The conversion of DOXY to PSAT or to PPOX, and the contrary, is usually effectuated when running LOCODOX. Therefore, the user should indicate the units of DOXY in the variable *refUnit*. [VT4][TR5]

```

% Possible options:
%     mL/L, milliliter per liter, milliliter/L
%     mumol/m3, micromole per m3, mmol/m3, micromole/m3
%     mumol/L, micromole per liter, mmol/L, micromole/L
%     mg/L, milligram per liter, milligram/L
%     mumol/kg, micromole per kilo, mmol/kg, micromole per kilogram, mi-
cromole/kg
CONFIG.refUnit = 'mumol/kg';

```

CONFIG.presEff: The conversions between DOXY-PSAT and PPOX is always done applying the equations proposed by Garcia and Gordon (1992). The user will decided whether to take the effect of the pressure into account when converting DOXY-PSAT-PPOX in the variable *presEff*.

```

% Conversion DOXY/PSAT/PPOX : take into account pressure effect or not
CONFIG.presEff = 0; % 0/1 option unactivated/activated

```

- [VT6][TR7] **CONFIG.isokC:** Carry over parameter for calculation with the IN AIR method. If isokC is set to 0, we suppose that in air oxygen measurements are not biased by splash of water; isokC is set to 1 otherwise (See Bittig et al, 2018).

```

% Carry over parameter. If isokC is set to 0, we suppose that in air oxygen
measurements are not biased by splash of water; C is set to 1 otherwise
% See "Oxygen Optode Sensors : Principle Characterization, Calibration, and
% Application in the Ocean", Henry Bittig and al (2018)
CONFIG.isokC=1;

```

- **CONFIG.DM_[pres/temp/psal]** : datamode selection, if equal to 0, LOCODOX will use the real time mode. If set to 1 and if the delayed_mode is available and non-filled with NaN, LOCODOX will take the delayed mode (“_adjusted” fields).

If the main profile is the Near-Surface profile, LOCODOX always choose the real-time profile for PSAL, because the unpumped adjusted PSAL profile gets artificially QC=4 (and so will lead to a PSAT filled with NaN).

- **CONFIG.QC_[O/P/T/S]** : Data Quality Code selection, it sets the quality codes considered as good enough to be used for the correction computation.
- **Time drift correction** :it sets the type of fitting equation to estimate the temporal drift correction. LOCODOX proposes
 - **CONFIG.drift_fitPolynomialDegree** : order of the polynomial fitting (= one, two or three).
 - **CONFIG.drift_spec** : if set to 0, the polynomial fitting will be used; if set to 1 the fitting equation defined in CONFIG.drift_fittype will be used.
 - **CONFIG.drift_fittype** : fitting equation
 - **[VT8][TR9]CONFIG.ok_inair_drift** : if set to 1, LOCODOX will search for PPOX data when the user choose REF or WOA correction, to compute time drift on NCEP database
 - **CONFIG.min_drift_depth** : Minimum depth for calculating drift

```
%Compute inair drift if possible for WOA and REF correction
CONFIG.ok_inair_drift=1;
```

```
% Time Drift correction
% .....
% By default, the data drift is computed using the polynomial fitting
% (order 1, y ~ ax+b). The polynomial degree can be increased up to 3.
% A new equation could be used if the parameter CONFIG.drift_spec is
% activated and if the parameter CONFIG.drift_fittype is filled.
CONFIG.drift_fitPolynomialDegree = 1;
CONFIG.drift_spec = 0;
if CONFIG.drift_spec == 1
    % If the fitting equation is a classical one (ex : a*exp(b*x)), enter
    % the name. If it is not a classical one, create the new equation using
    % the matlab "fittype" fonction defining way (see the matlab help).
    % Example : g = fittype('a*u+b*exp(n*u)', 'problem', 'n', 'independent', 'u')
    CONFIG.drift_fittype = fittype('exp1');
end
```

- **CONFIG.R2threshold** : The vertical correction of DOXY data is based on a linear regression between the DOXY data measured by the float and the reference. LOCODOX computes the regression coefficients and R². It indicates the quality of the fit. If the linear regression is not reliable (R²<CONFIG.R2threshold), LOCODOX offers the possibility to apply a constant correction, independent of the depth. It is calculated as the vertical average of the differences

```
% WOA or REF correction
% .....
% Linear correction R2 coefficient : treshold under which LOCODOX suggests
% to apply Constant correction
CONFIG.R2threshold = 0.80;
```

between the reference profile and the data measured by Argo float.

- **Specific to the InAir correction:**

- **CONFIG.inWaterMC and CONFIG.inAirMC** : The measurement code corresponding to the in-air and the in-water samples of the surface sequence has to be set. Currently, these measurements codes are [690 710] for inWater and [699 711 799] for inAir (see “Near_surface_&_in_air_data_processing_at_coriolis_V2.020180920-1.docx”)
- **CONFIG.inAirMaxPresForTS** : maximum depth allowed in which to look for TEMP and PSAL, to be used as “surface” samples.
- **Error on adjusted fields**: The user will be able to choose which kind of error to apply to the data at the end of LOCODOX. He will still be able to change the values before writing the files at the end of the program.
 - **CONFIG.adjusted_error_abs** : value of the absolute error (a constant error will be applied independently of the depth).
 - **CONFIG.adjusted_error_rel** : % of the relative error (the error will be equal to a % of the adjusted DOXY at each depth).

3.2.4 Writing NetCDF

The NetCDF argo 3.1 files output by LOCODOX need three information given in the configuration file:

- **CONFIG.history_software** : The software name, by default, it is set to LOCODOX.
- **CONFIG.history_software_release** : The software version. As example, for 2019, the software version could be set to “3,1”, as “version 3,1” (March 2019).
- **CONFIG.history_reference** : The reference database used. As example, for 2018, the reference database was 'LOPS2018_WOA09'.
- **CONFIG.prefix** : the prefix of the NetCDF file has to be set as recommended by the argo data management: **BD** for Bio files and **Delayed** mode.

```

% -----
% FOR NetCDF writing and FOR HISTORY
% -----
CONFIG.history_software = 'LOCODOX';
CONFIG.history_reference = ['LOPS2020_WOA',WOA_YEAR];
CONFIG.history_software_release = '3.4';
CONFIG.prefix = 'BD';

```

3.2.5 Graphical information

This part of the configuration file is dedicated to the graphical part of the software.

- **CONFIG.savePlot**: could be set to 0/1. If savePlot is set to 1, the plots are saved in the savePlotDir.
- **CONFIG.fontSize**: manage the size of the font for all plots (title, labels, ...)[VT10][TR11]
- **CONFIG.resolution** : resolution: manage the resolution of the saved plot.
- **CONFIG.formattype**: manage the output format of the saved plot. It can be multiple.

```
CONFIG.savePlot = 1;
CONFIG.fontsize = 12;
CONFIG.resolution = 100;
CONFIG.formattype = {'-dpng'};
```

3.2.6 mapping

The Google mapping toolbox is used by default in LOCODOX. It requires an internet access.

```
CONFIG.M_MAP_ACTIVE=1; % set to 0 ==> google_map plots
```

The M_MAP Toolbox could be used instead, no internet access is required once the toolbox installed. The following changes are needed in DOXY_config.m:

```
% -----
% M_MAP INFORMATION
% -----
% Added by Thierry Reynaud 06/02/2020
% The M_MAP Library is introduced to replace Google Plot Maps which requered inter-
net.
% The M_MAP path is defined here:
CONFIG.M_MAP_ACTIVE=1; % set to 0 ==> google_map plots
mmp = fullfile(CONFIG.LocodoxMainDir, 'share', 'm_map1.4m', filesep);
CONFIG.M_MAP_PATH=mmp;
CONFIG.M_MAP_PLOT_BATHY=1;% PLOTTING ==> Reading ETOPO2 File
```

3.3 The LOCODOX - User interactions

When running LOCODOX, the user has to make choices on the correction to apply, figures are displayed to facilitate the user's choice in the oxygen correction. The user interaction with LOCODOX is common for the three methods defined for the oxygen correction, however some differences can be presented.

3.3.1 Step of LOCODOX and user action

Step	Step and user action
Initialization	<p>Read the configuration file</p> <p>Read the WOA reference data</p> <p>User action : Enter the WMO to be corrected</p> <p>User action : Choose the Gain correction Method type : WOA, REF or INAIR</p> <p>Read the in-situ reference data if the REF method chosen by the user or if the WMO of the float is mentioned in the RefArgoFile</p> <p>Read profile data</p> <p>Read the NCEP data if IN AIR method had been selected or if parameter ok_inair_drift is set to 1 in the configuration file</p> <p>User action : choose to apply a pressure effect correction or not</p> <p>Read trajectory data for INAIR correction or if parameter ok_inair_drift is set to 1 in the configuration file</p>
Presentation of data	<p>Plot data QC and main profiles</p> <p>Read trajectory data</p> <p>Plot the argo float trajectory</p> <p>Plot vertical profiles of oxygen</p>
Time drift Correction	<p>User action : choose on which reference data the Time Drift should be computed (WOA or NCEP)</p> <p>Compute and plot the temporal drift</p> <p>User action : choose to use a constant drift from a certain day</p> <p>User action : choose to apply the drift correction or not</p>
Gain Correction (Slope/offset correction)	<p>User action for [WOA or REF method] : choose the parameter, PSAT or DOXY, on which the correction will be based.</p> <p>Compute correction</p> <p>User action for [WOA or REF method] : choose the equation for the oxygen correction.</p> <p>Apply the correction</p>
Prepare data to be written	<p>Update the metadata fields</p> <p>User action : Choose the kind of error of the corrected DOXY (absolute, relative)</p> <p>Prepare data to be written in the NetCDF argo 3,1 file</p> <p>Write the data in the NetCDF argo 3.1 file</p>
End	<p>Stop LOCODOX or continue to manage a new WMO;</p>

Table 6 : User action

3.3.2 Initialization

Dialogue box waiting for input : WMO name.

First, the WMO of the float to be corrected should be introduced. After introducing the float, the user should press “OK” or “Cancel”.

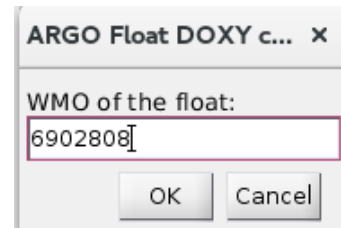


Figure 1. First dialogue box showed by LOCODOX, it asks for the float to be corrected.

Dialogue box waiting for input : Method for the oxygen correction.

Second, the user should choose the Gain method to apply for the slope/offset calculation of the oxygen data (see section 3.3.1). After selecting the method, the user should press “OK” or “Cancel”.

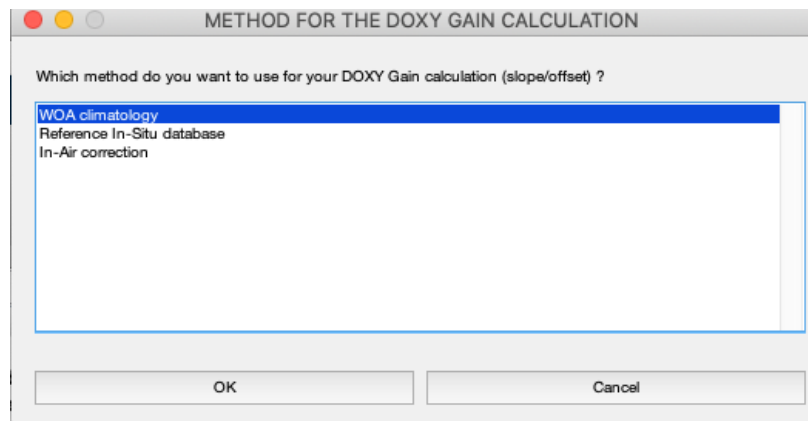


Figure 2. Dialogue box waiting for the user choice of the Gain method for correcting the oxygen data.

Dialogue box waiting for answer : Pressure effect correction^[VT12]^[TR13].

The user must choose if a pressure effect correction is applied or not.

If the user answered 'Yes' to the dialogue box (Fig. 3a), another one asks to introduce the value of the coefficient to correct the data (Fig. 3b). Note that the value is usually positive and comprised between 0.0 and 0.01.

Then the results of the pressure effect correction will be displayed in a new figure (Fig. 3c), raw data is displayed in blue and corrected data in red.

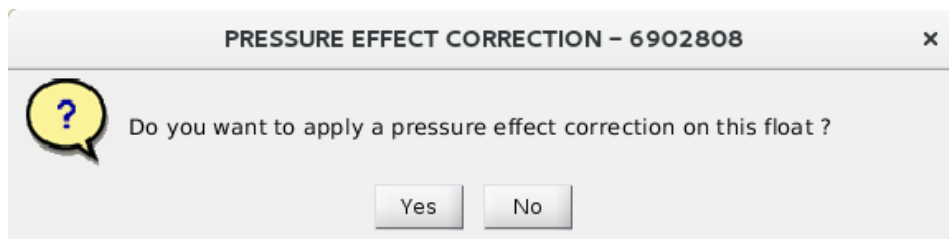


Figure 3a. Dialogue box : The user must choose if a pressure effect correction should be applied.

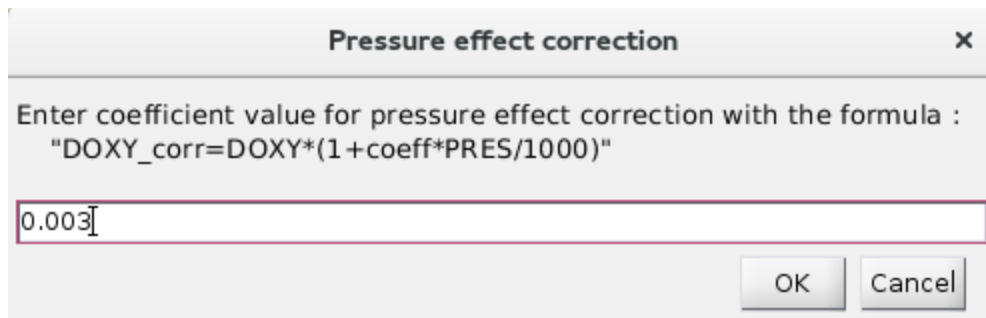


Figure 3b. Dialogue box waiting for the coefficient value for pressure effect correction. [VT14][TR15]

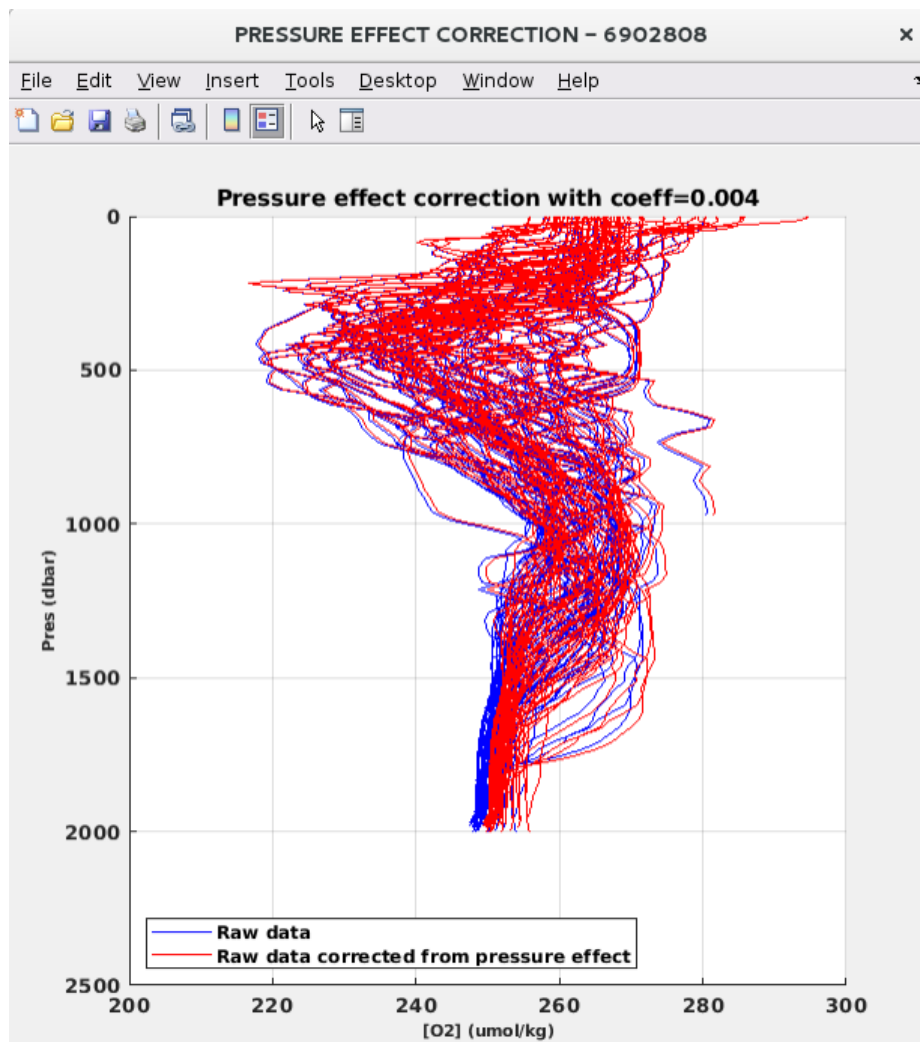


Figure 3c. Figure showing the data before/after the pressure effect correction.

3.3.3 Presentation of data

Figure showing the time evolution of QC

LOCODOX shows a figure representing the QC of the Argo data (pressure, temperature and salinity, see Fig. 5).



Figure 4. (saved as “DOXY_PLOT_PTS_QC...”) Time evolution as function of the float cycle number, of the vertical profiles of quality control (QC) of pressure (upper plot), temperature (central plot) and salinity (lower plot). QC range from 1 (green) to 9 (blue).

Figure showing primary sampling (and near surface sampling for IN AIR correction)

Next, LOCODOX displays the primary or secondary sampling (Fig. 5a) and the near surface sampling if the IN AIR correction method had been choose (Fig. 5b).

On the left, the surface referenced potential density versus the pressure is displayed. In the middle, the oxygen data is displayed with a color corresponding to the QC of each point (Example : here data in red have a QC=4). Finally, the data considered for the oxygen correction are represented on the right in cyan.

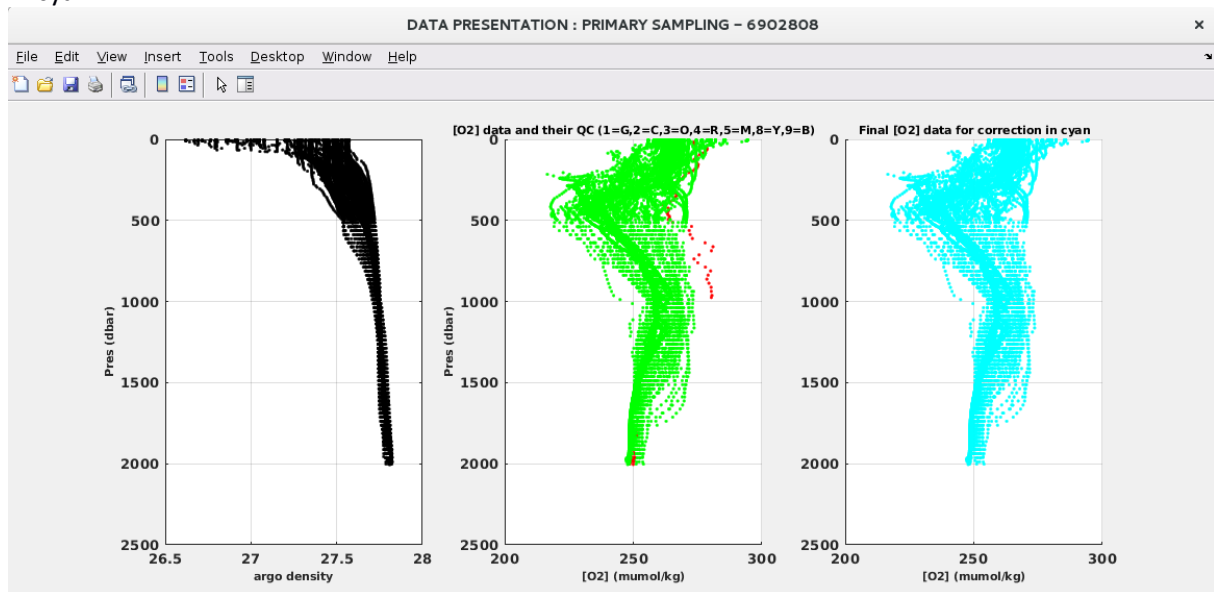


Figure 5a: Oxygen and density data measured by the float before the oxygen correction for primary sampling (saved as “DATA_PRESENTATION...”)

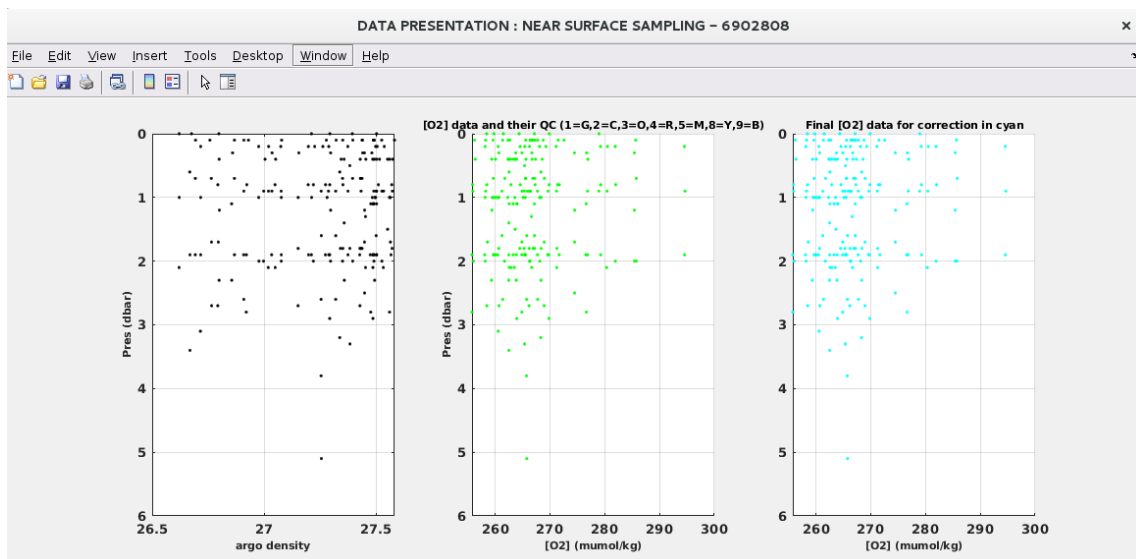


Figure 5b. Oxygen and density data measured by the float before the oxygen correction for near surface sampling.

Trajectory of the float

Fig. 6 displays the float trajectory (Gain correction based on the WOA method). If the method applied is REF, the positions of profiles in the in-situ database are shown in yellow circle; the red square highlights the position of the reference profile used for the correction of a specific float.

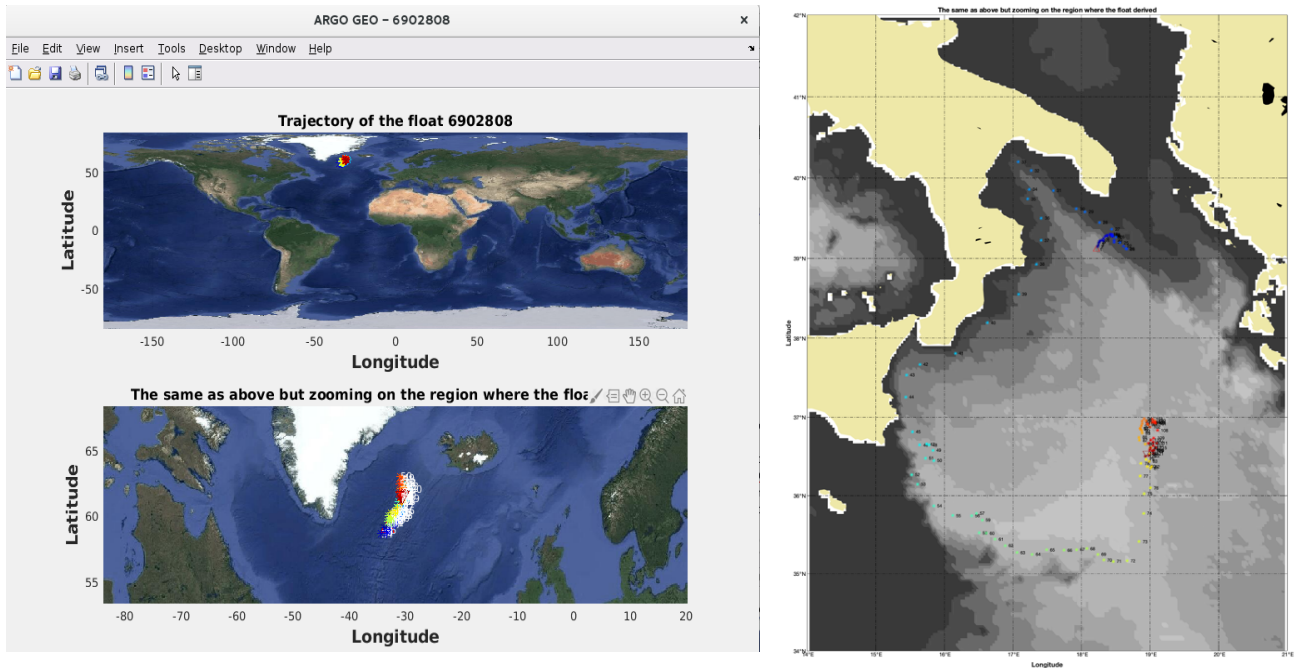


Figure 6. Trajectory of the float Google map (left) and M_MAP (right). The lower plot (left) is a zoom of the region where the float drifted. The color points represented the date of the position of the float, from the oldest position (blue) to most recent position (red). The numbers indicate the cycle done by the float. (saved as "DOXY_MAP...") [VT16] [TR17]

Vertical profile of oxygen used for the correction.

LOCODOX displays the vertical profiles of oxygen in colors, from the oldest (blue) to the most recent (red). Only data used to estimate the correction are displayed. The color scale provides clues indicating whether a time drift by the oxygen-sensor happened.

The WOA data coupled to each Argo float, interpolated to the position and the pressure levels given by the Argo float, are represented in black.

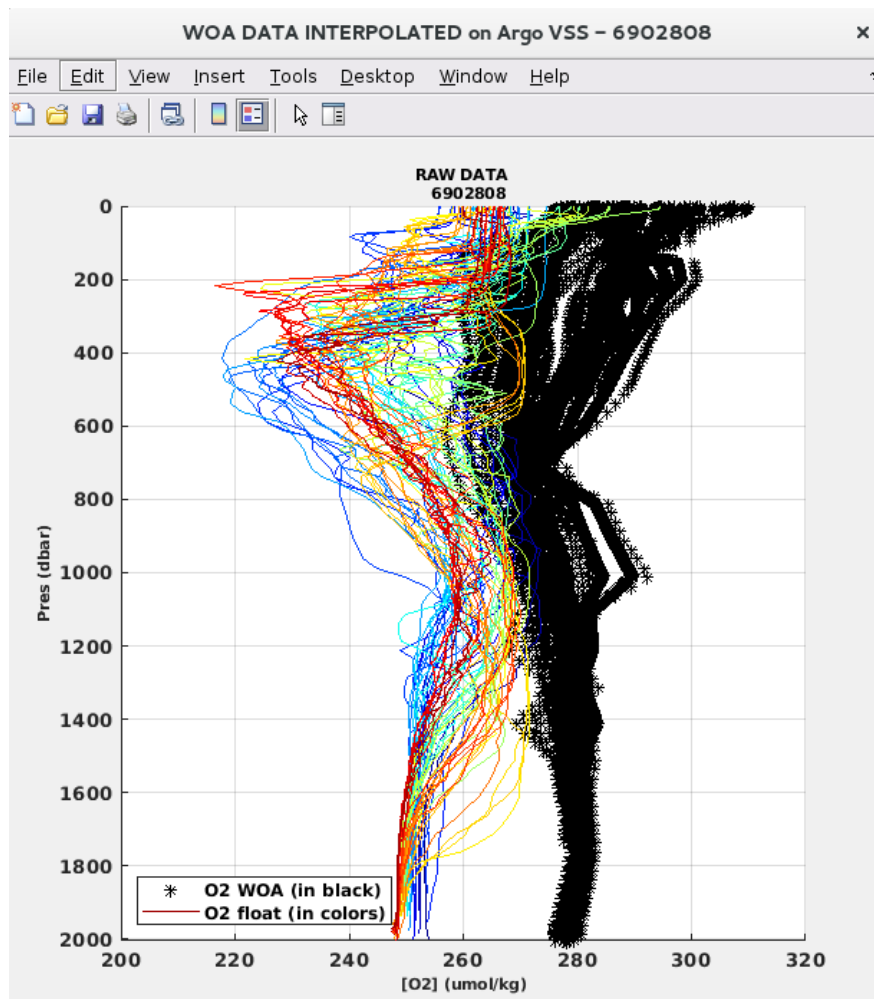


Figure 7. Vertical profiles of oxygen used to compute the oxygen correction from the oldest (blue) to the most recent (red). The WOA data coupled to each Argo float, interpolated to the position and the pressure levels given by the Argo float, are represented in black (saved as "DOXY_PLOT_interpolation...").

When the user choose the REF method for the correction, Fig. 8b is displayed, which shows all the oxygen profiles of the float, the vertical profile of oxygen used for the correction (here cycle 1) and the reference profile used to compute the correction.

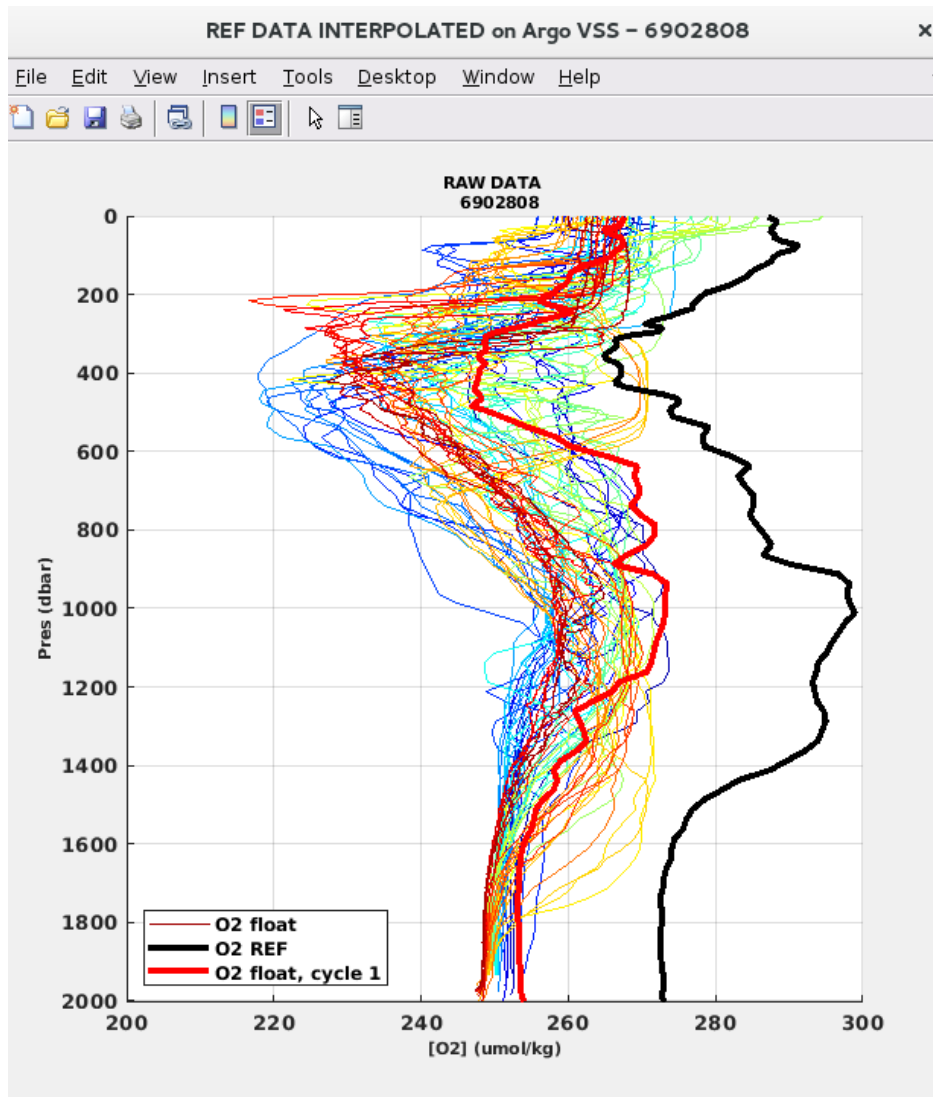


Figure 8. Vertical profiles of oxygen used to compute the oxygen correction from the oldest (blue) to the most recent (red). The cycle measured by the float and used for the correction is represented in red. The reference profile used compute the oxygen correction is represented in black (saved as "DOXY_PLOT_interpolation...").^{[VT18][TR19]}

3.3.4 Time drift gain estimation

Dialogue box asking on with reference data the drift should be computed

The user can choose (Fig. 9a) to compute the time drift gain on WOA or on NCEP data using in air measurements. If the user choose to compute the drift on NCEP, instead of the Fig 9b, the figure 9d will be displayed.

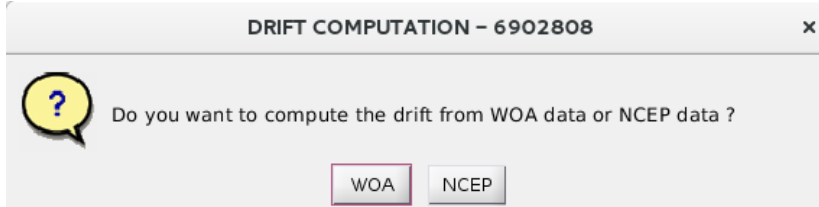


Figure 9a. Dialogue box asking the user to chose to compute the time drift gain from WOA data or NCEP data.

3.3.4.1 Time drift gain estimation from WOA data

Time evolution of oxygen concentration at deeper levels than “min_drift_depth” parameter (see the configuration file).

The figure 9b (top) shows the time evolution of WOA and Argo float PPOX data.. The ratio of WOA and Argo float PPOX data is shown in the lower figure. The best equation fitted is proposed as a gain to compensate the time drift (here a polynomial of degree 1). This time drift gain is shown in Figure 9b (bottom).

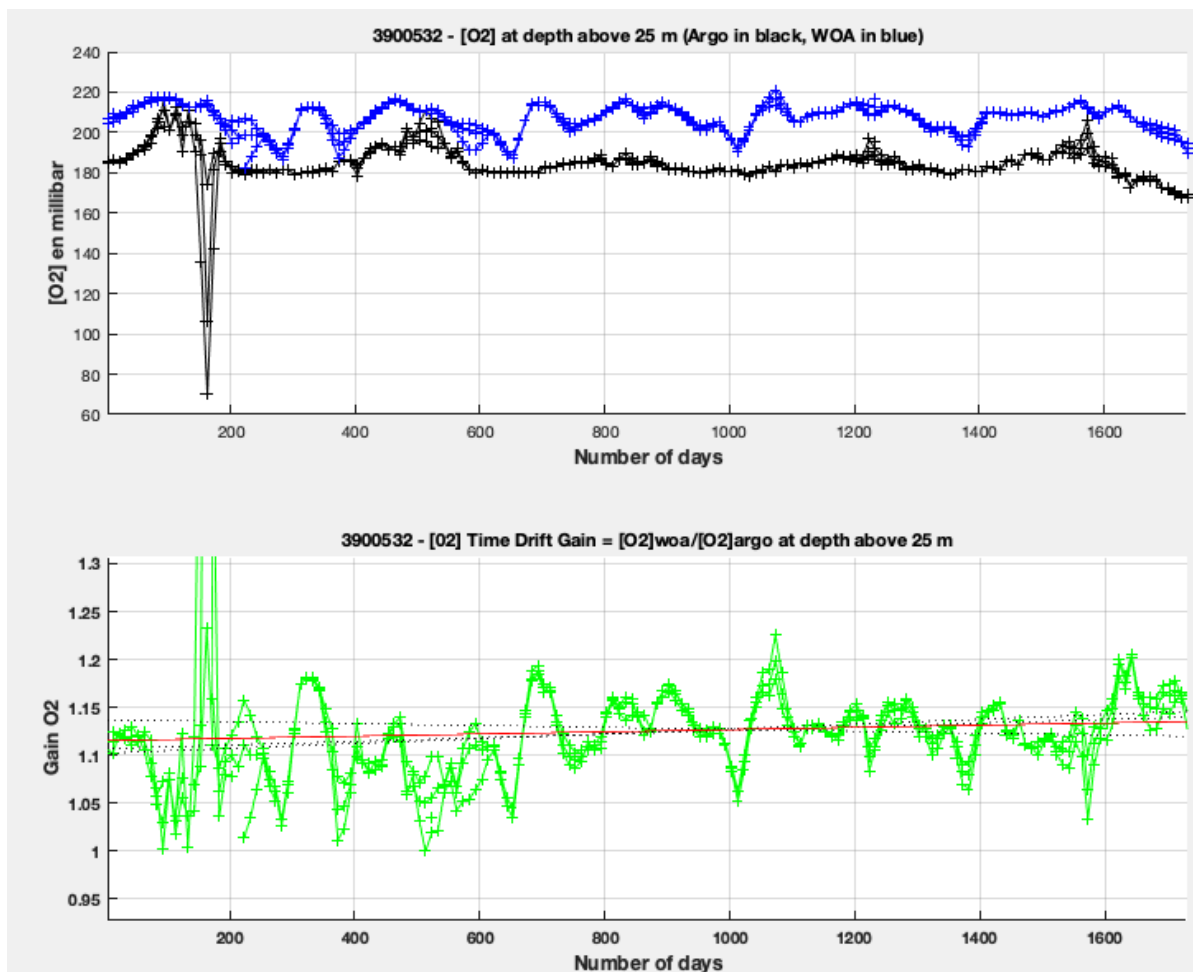


Figure 9b : Time Drift Gain calculation from float and WOA PPOX data (top) and ratio (bottom)

The variables `min_drift_depth_surf`, `max_drift_depth_surf`, `min_drift_depth_deep`, and `max_drift_depth_deep` are defined in the Locodox configuration file. These define the upper and lower bounds of the layer used for calculating the Time Drift Gain based on surface data (`min_drift_depth_surf`, `max_drift_depth_surf`) or in deep layers (`min_drift_depth_deep` and `max_drift_depth_deep`).

The operator will then decide if LOCODOX will apply a constant drift from a given date. If not, the time drift gain will be computed as shown in Figure 9b. If yes, another dialogue box waiting for input appears. It asks to chose the day J from which the time drift gain applied will be constant.

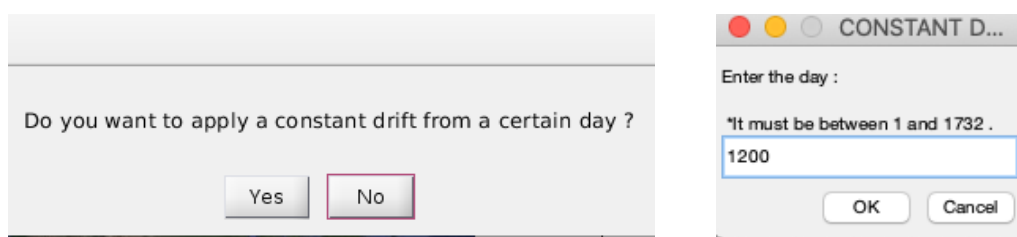


Figure 9c. On the left, dialogue box asking whether the user wants to apply a constant time drift gain from a certain day and on the right the box asking from which day the drift should be constant.

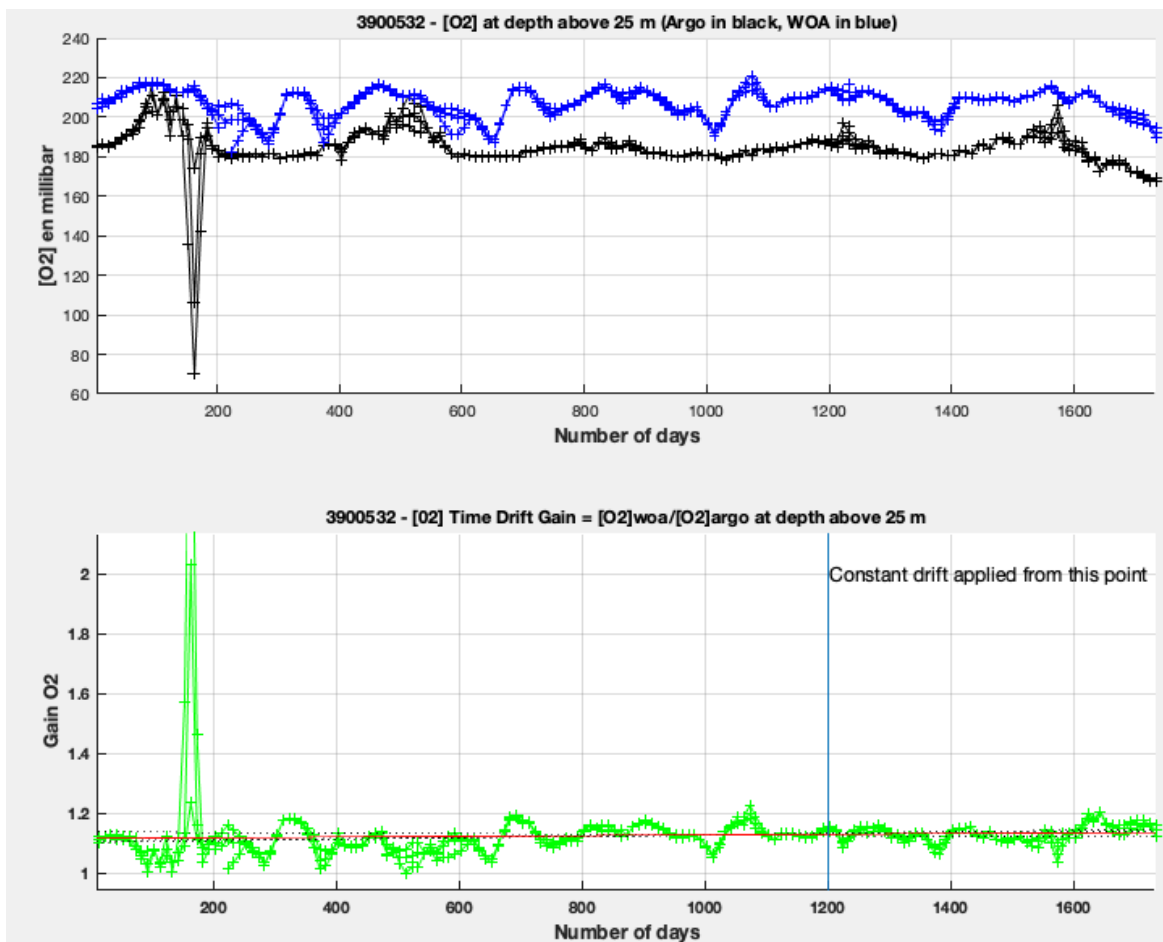


Figure 9d. Same as the Fig. 9b updated if the user choose to apply a constant drift from a certain day (here J=1200).

3.3.4.2 Time drift estimation from NCEP data

For Time drift computed on NCEP data, the time evolution of oxygen near the surface will be presented as in the fig 9 e.

Note that the user can also choose to apply a constant drift from a certain day when the drift is computed on NCEP data.

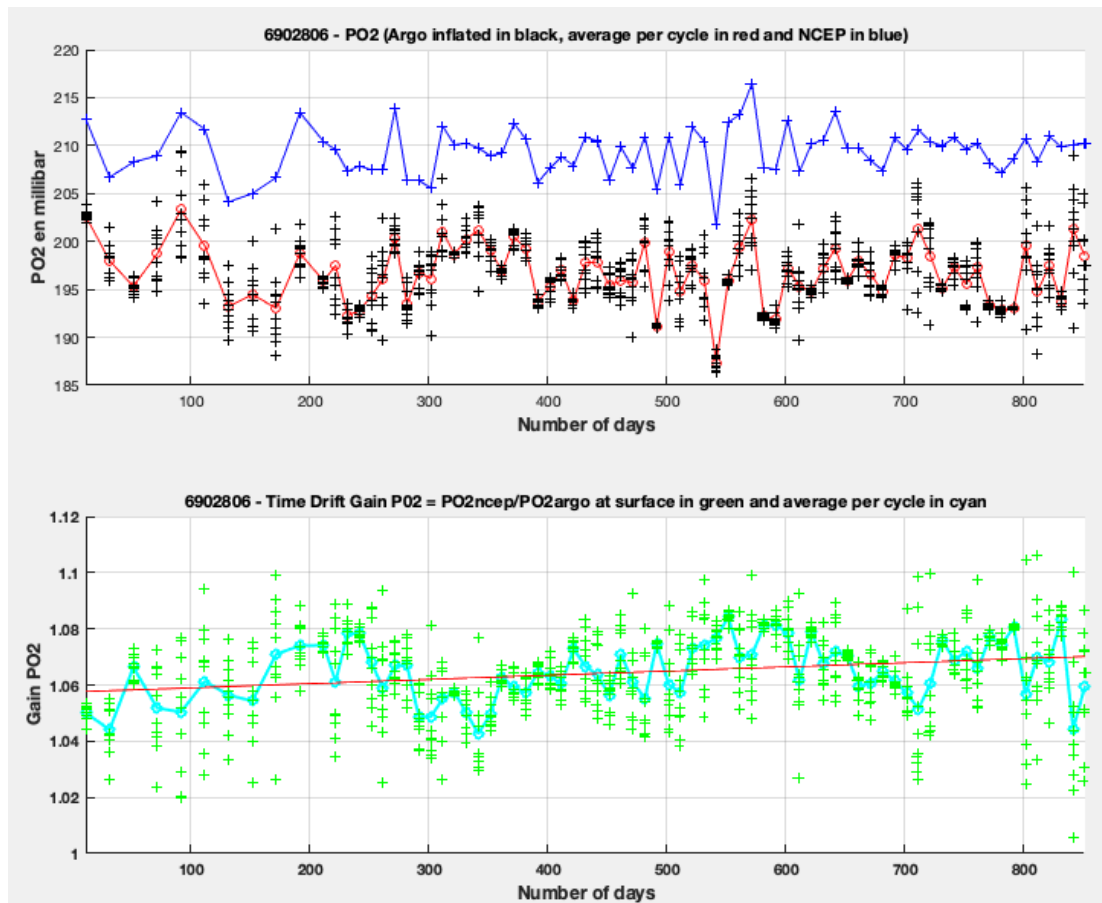


Figure 9e. Time evolution of partial pressure of oxygen (mBar) measured at the surface by the float (in black), the average per cycle is represented in red and the coupled NCEP data in blue. The difference between the data measured by Argo float and its coupled NCEP data is in green. The average per cycle is represented in cyan. The best adjust equation is represented in red (saved as « DOXY_drift_onNCEP... »)

3.3.4.3 Apply time drift

Then, LOCODOX shows a dialogue box (see Fig. 10) summarizing the statistical result of the best fitting equation proposed for the correction. The user should decide whether to apply the temporal drift correction clicking YES or NO.

The relevance of the time drift correction application could be double checked in the LOCODOX correction control plot (see Fig. 11.1d, 11.1e, 11.1g). The surface time series of the raw data, the corrected data and the WOA data are shown on it. If time drift correction is wrongly applied, then the

corrected data diverge significantly from the WOA data, which indicates that the time drift correction has no sense. An additional information is added if the user choose to apply a constant drift.

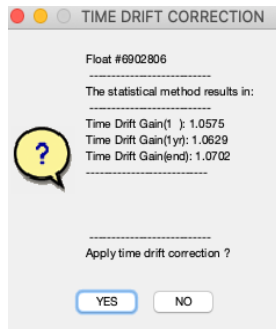


Figure 10. Dialogue box that summaries the statistical results obtained by LOCODOX for the best fitting equation proposed to correct the oxygen data. The user should decide whether to apply the temporal drift correction clicking on YES or NO.

3.3.5 Main Gain correction (Slope/offset computation)

This section is divided in two part. The first one explains the figures and the dialogue box appearing when the user chooses a correction based on the REF method or on the WOA method. Then in the second part, the figure and interactions for the IN AIR method will be detailed.

3.3.5.1 For REF or WOA methods

Figure 11: “Main Gain CORRECTION on PPOX”.

The oxygen main gain, after the time drift correction, is always calculated as a linear regression of data measured by the float, and the reference (WOA or REF) data. LOCODOX displays Figure 11, where both variable are represented and the coefficients of the best fitting equation are shown.

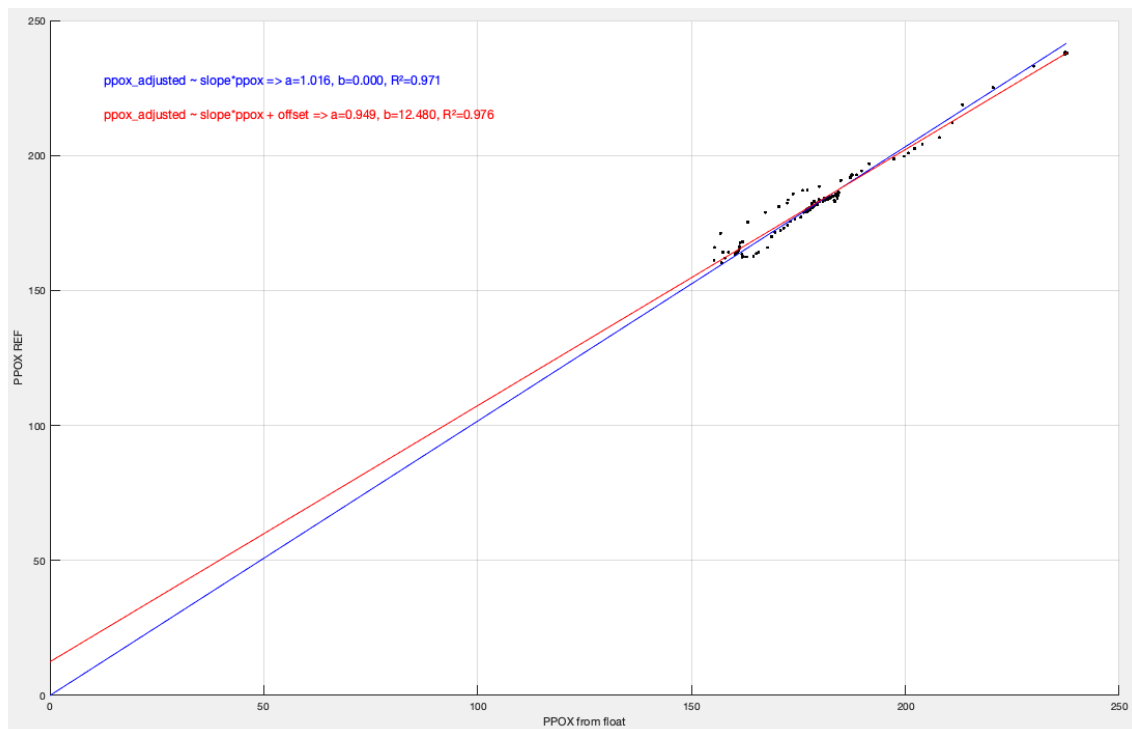


Figure 11: PPOX measured by the float (x axis) and the reference data (y axis). Two equations are shown: the equation forcing the line to cross the origin point (in blue), and the not forced equation (in red). Both equations present the regression coefficient indicating the robustness of the fitting.

Box waiting for input : “DOXY CORRECTION”

The following step is to choose the equation to correct the oxygen data between the equation forced to pass by the origin and the whole fitting equation. Note that LOCODOX suggests to apply the first option because, if the optode is well calibrated, it should read 0 when there is no oxygen in the water. The choice is left to the user (Fig. 11.1a).

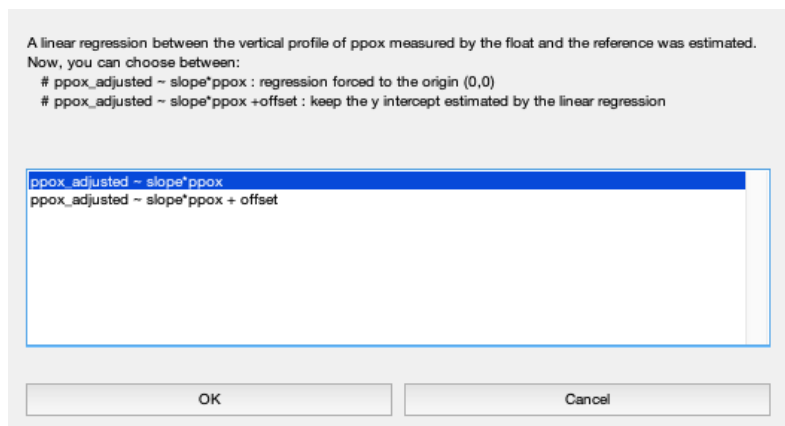


Figure 11.1a: Dialogue box that allows choosing the equation type for the oxygen correction. Choose the equation and click on OK or Cancel

Figure : “CORRECTION DOXY and PSAT “

The next emergent figure visualizes the different actions implemented by LOCODOX. Depending of the choice done up to now the figure can be different :

- Figure 11.1b is an example of the emergent figure when the WOA method was chosen for the correction. The first line summarizes the different steps of data selection. It shows the linear regression equation and the R^2 . The second line presents the results comparing the time series at the surface (the three shallowest levels) of the variable measured by the float, the corrected data and the WOA data. The comparisons of the raw, corrected and WOA data for the profiles of PSAT (central) and DOXY (right) are also shown. The third line is dedicated to the constant correction in this first example no constant correction need to be applied because the estimated R^2 is above the defined threshold (see configuration file).

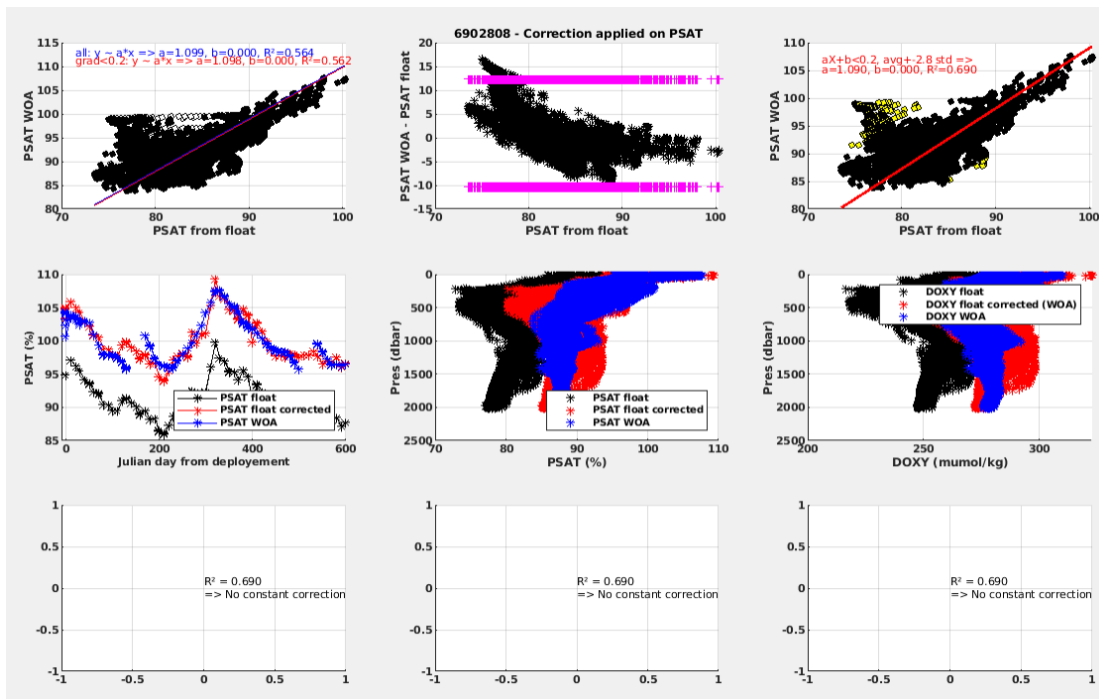


Figure 11.1b. Figure of control of the different steps implemented when WOA method was selected. The first line controls the data selection and the regression calculation. The second line controls the results respect to the WOA data (blue). The raw data are in black, and the corrected data are in red. The third line shows here that no constant correction has been applied, because the R^2 is above the indicated threshold in the configuration file (saved as "DOXY_PLOT_corr...").

- Figure 11.1c is an example of the figure displayed when the REF method was chosen for the correction. The plot is organized exactly the same way as in the plots of the WOA correction. The difference is that the first line is less dense because the correction has been computed with a single in-situ reference profile, instead of a set of WOA profiles. Another difference is in the time-series on the left of the second line; even if the selected method is the REF one, the time evolution is shown in respect to the WOA data, since the REF profile provide a single point.

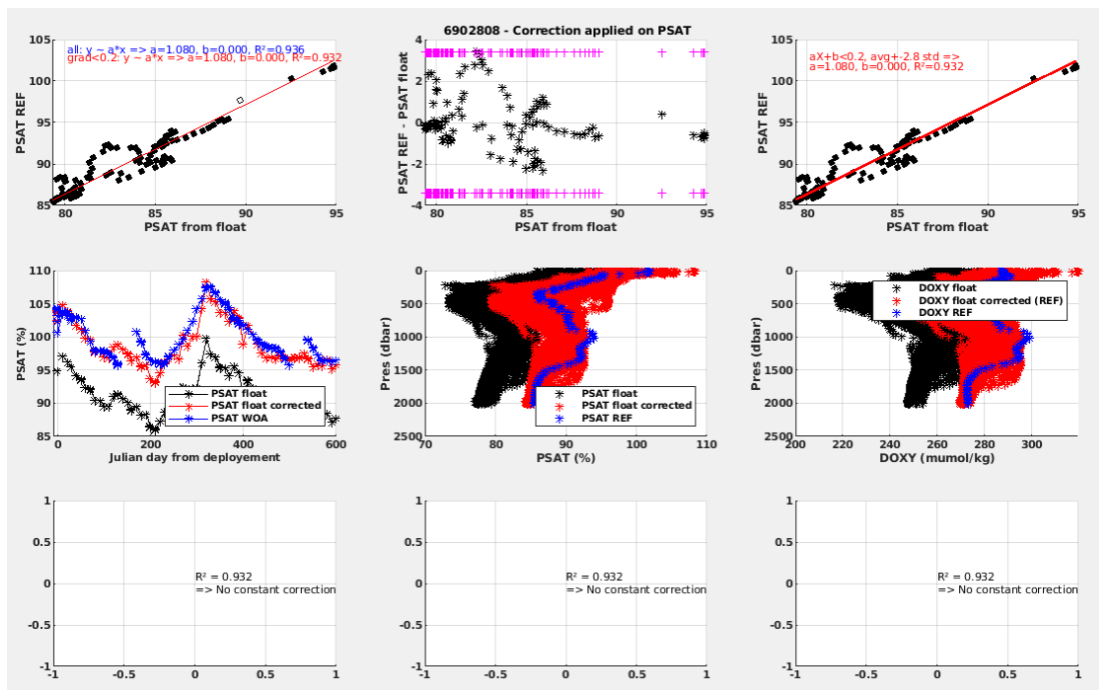


Figure 11.1c. The same as Fig. 11,1b but when the REF method was selected (saved as “DOXY_PLOT_corr...”).

Box waiting for input : “APPLY CONSTANT CORRECTION ?” (it appears only when R2< than the threshold indicated in the configuration file)

In the examples of Fig. 11.1b and Fig. 11.1c the estimated R2 was above the threshold indicated in the configuration file, so, no constant correction should be applied. However, when the R2 is below the threshold indicated in the configuration file, a constant correction is proposed to apply instead of the linear regression correction (see 3.2.3). When R2 is below the threshold indicated in the configuration file another question dialogue box emerges (Fig. 11.1d).

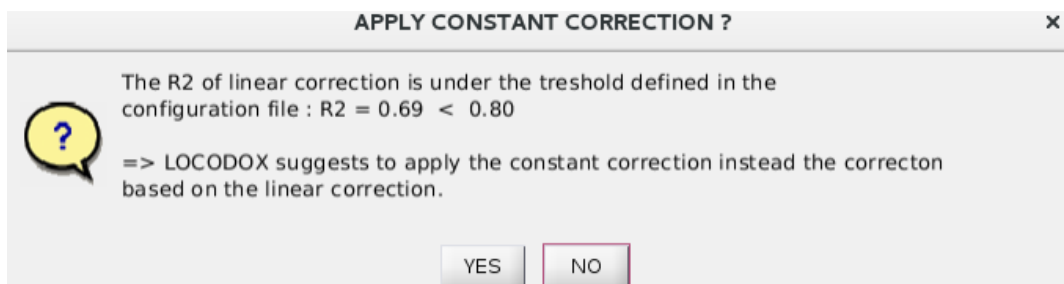


Figure 11.1d. When the estimated R2 corresponding to the linear regression is below the threshold indicated in the configuration file a constant correction is suggested. The user should chose YES or NO.

If the user choose YES, a constant correction is applied, which can be checked in the third line of Fig. 11.1e.

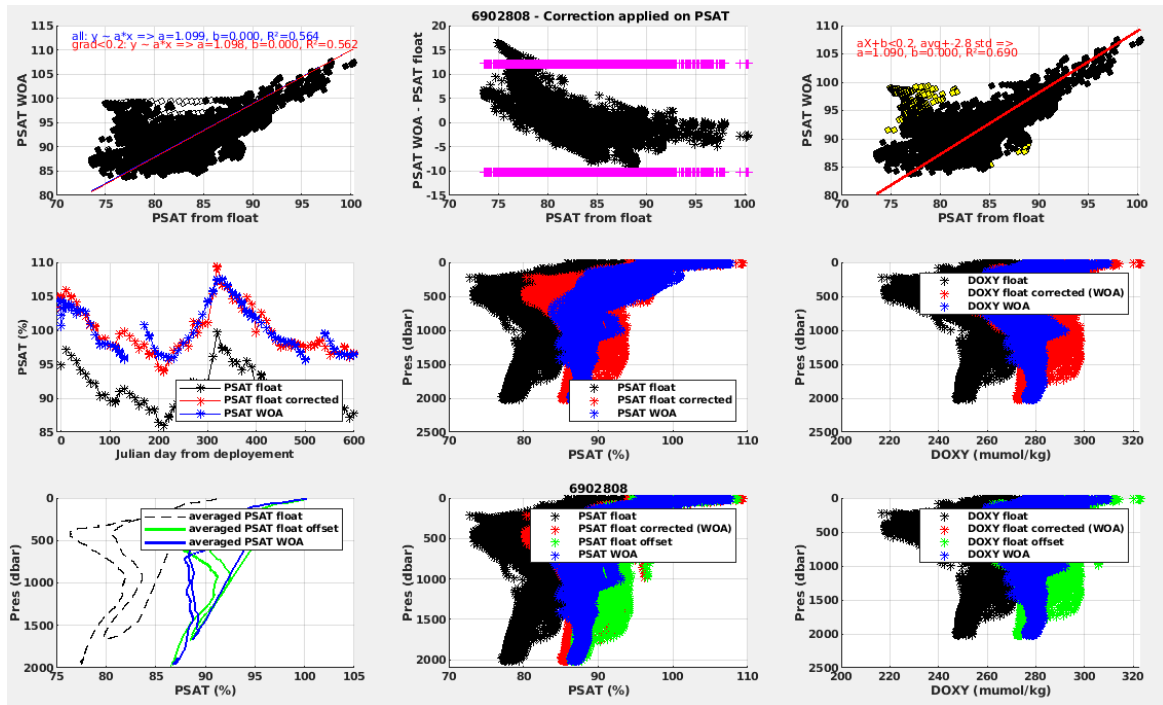


Figure 11.1e. The two first lines are as in Fig. 11.1b, the third line compared the raw data, the reference data and the corrected data obtained by applying the constant correction (saved as “DOXY_PLOT_corr...”).

Figure : “CORRECTED DATA AND REFERENCE PROFILE”

If the correction is based on REF method, a figure representing the corrected data with the reference profile and the cycle used to compute the correction will be displayed (see Fig 11.1f).

Note that if LOCODOX finds the wmo of the float and a reference profile in the RegArgoFile, while using the IN AIR or the WOA correction method, this figure will also be displayed. It can help to detect the need to apply a pressure effect correction.

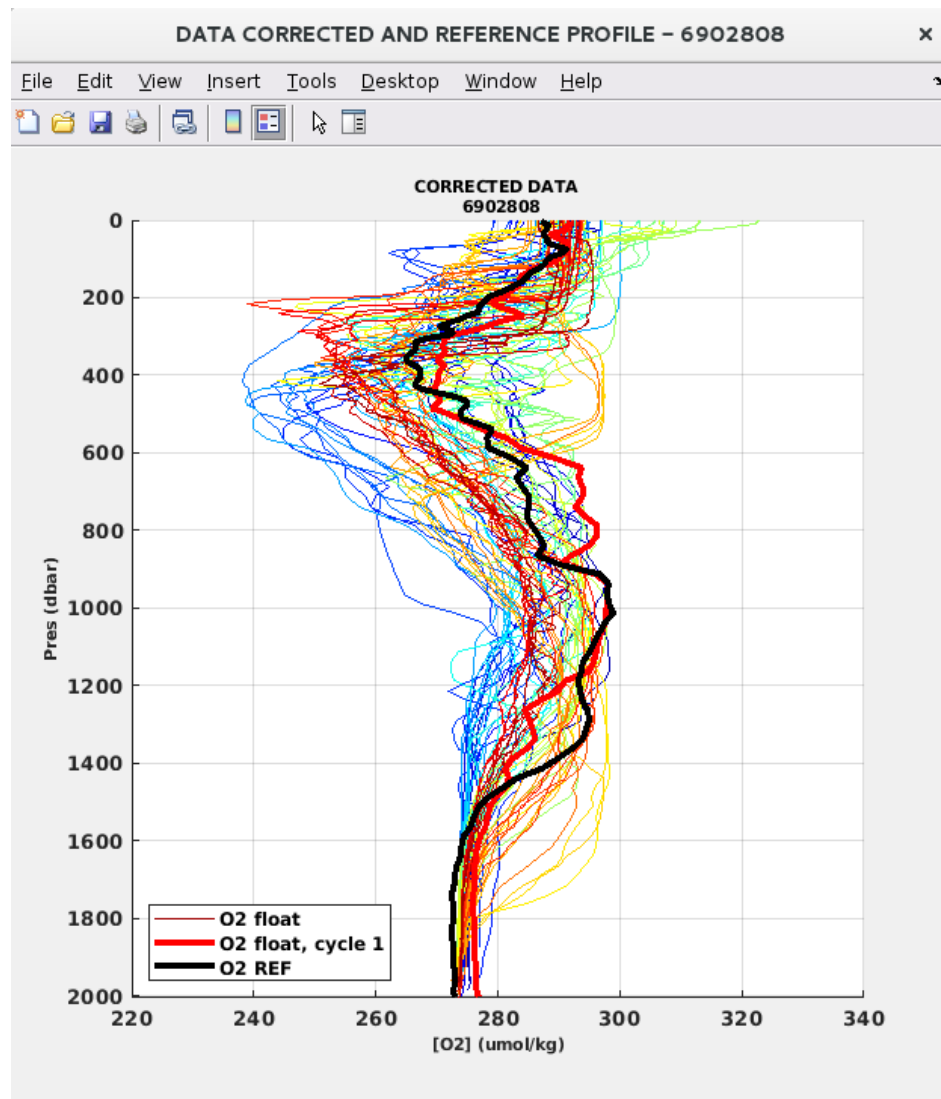


Figure 11.1f. Figure showing the corrected data if the correction is based on a reference profile or if the reference profile is given in the RefArgoFile (saved as “DOXY_PLOT_data_corr...”).

3.3.5.2 For INAIR method

With IN AIR correction there is only one emergent figure which visualizes the different actions implemented by LOCODOX and the data corrected (see Fig 12).

The first plot on the left (In-Air measurement time series) represents different partial pressure of oxygen :

- In black, the atmospheric reference NCEP;

- The red symbols represent the PO₂ in-air measurement of the float before correction (the values have been averaged over each cycle and the standard deviation is represented by a vertical line)

- The blue symbols represent the PO₂ in-water measurement of the float before correction (the values have been averaged over each cycle and the standard deviation is represented by a vertical line)

The results of the regression (see eq 1) are displayed on the right of the figure. The equation, the value(s) of the coefficient(s) (m and c or only m) and the statistics of the regression are presented.

$$pO_{2(air,argo)} = c \times pO_{2(water,argo)} + \left(\frac{1-c}{m}\right)pO_{2(air,ncep)}$$

The m coefficient is then used to correct raw data, as follows:

$$pO_{2(argo)corrected} = m \times pO_{2(argo)}$$

Where pO₂ is the partial pressure of oxygen, the suffix (where,what) corresponding to in air measurements (air) or in water measurements (water), for NCEP data (ncep) or for Argo data (argo).

This equation takes into account the occasional submersion of the optode, and so the contamination of the in-air measurement by the in-water measurement (coefficient c). The user can chose to set the coefficient c to 0 in the configuration file (parameter 'isokC') and thus consider that there is no contamination of the in-air measurement by the in-water measurement.

The second plot on the left represent the corrected PO₂ in-air measurement in pink and the corrected in-water measurement in cyan. We aim to have PO₂ in-air measurement as close as possible to NCEP (in black).

The last line of plots corresponds to what we can find with others corrections. It presents the results comparing the time series at the surface (the three shallowest levels) of the variable measured by the float, the corrected data and the WOA data. The comparisons of the raw, corrected and WOA data for the profiles of PSAT (central) and DOXY (right) are also shown.

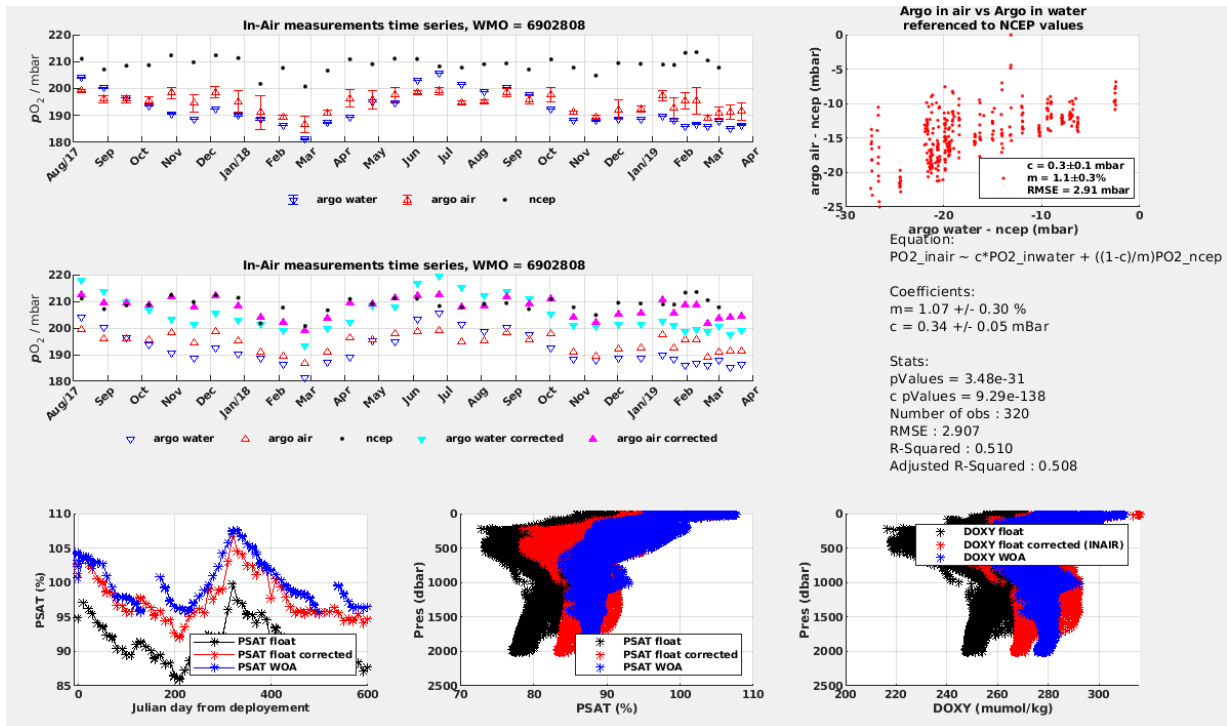


Figure 12. Figure of control of the different steps implemented when IN AIR method was selected. The first two lines shows the regression calculation, the data before and after correction. The last line controls the results respect to the WOA data (blue). The raw data are in black, and the corrected data are in red.

3.3.6 Prepare data to be written and end of program

Dialogue box : "ERROR ON DOXY ADJUSTED"

Finally, once the correction was applied, the user should defined the error for the corrected oxygen (DOXY ADJUSTED) between raw and relative, which were previously defined in the configuration file. Otherwise, the user can change these error by clicking Change in the dialogue box showed in Fig. 13.

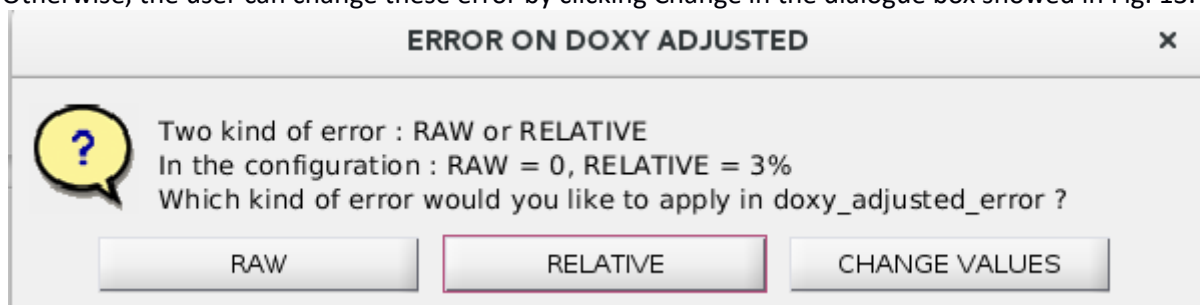


Figure 13. Dialogue box that allow choosing the type of error to apply to the corrected oxygen (DOXY ADJUSTED).

Box waiting for answer : LOCODOX : continue the correction.

Once the oxygen correction was implemented the final step is to answer to the dialogue box displayed in Fig. 14.

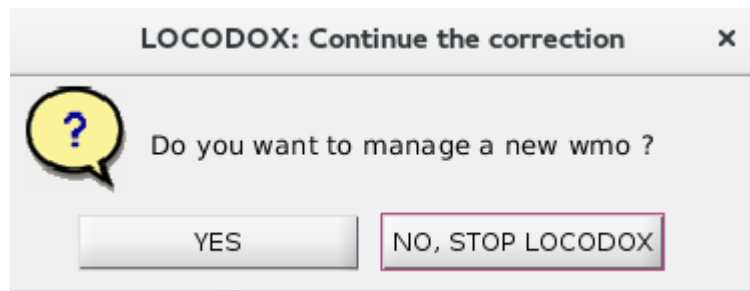


Figure 14. Last dialogue box showed by LOCODOX after correcting oxygen data measured by a float.

4 References

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Appendix A : Program descriptions

4.1 Data organization

LOCODOX works with MATLAB structures array, which gather data, metadata and some intermediate parameters. The structures arrays concern both reference data (WOA, In-situ reference data, NCEP data) and Argo data.

Argo data are available in the argo structure array. These data are never modified during the correction process by LOCODOX if a pressure effect correction haven't been applied.

The structure array named Work carries all the computation information, the interpolated reference data, and some metadata.

The argoWork structure array is an evolving array that contains either data to which intermediate corrections were applied or the final corrected data.

The different structures arrays are used as inputs for the sub-functions and carry information along the whole correction process.

4.2 LOCODOX specific programs

The dedicated programs are found in the *doxy_corr* directory. The Table 4 lists and describes the programs.

Program name	Description
DOXY_argo_prepare.m	Prepare argp data to be ready for correction computation
DOXY_argo_prepare_main.m	Preparing argo data main program
DOXY_argo_read.m	Read the argo data
DOXY_argo_write.m	Write the argo adjusted data
DOXY_argoTraj_read.m	Read the argo trajectory data
DOXY_convert.m	Convert oxygen to one unit to another
DOXY_corr_apply.m	Apply the correction to data
DOXY_corr_apply_main.m	Applying correction main program
DOXY_corr_compute.m	Compute the correction
DOXY_corr_compute_main.m	Computing correction main program
DOXY_corr_cst.m	Compute the constant correction
DOXY_corr_linreg.m	Calculation of a linear correction between argo and reference oxygen
DOXY_corr_main.m	MAIN PROGRAM

Locodox.m	Symbolic link toward de main program
DOXY_corr_prepare.m	Prepare the data to be corrected
DOXY_drift.m	Compute the temporal sensor drift (using the pressure)
DOXY_get_ppox.m	Get the spatio-temporal information for PPOX
DOXY_get_primary_PTS_for_traj.m	Get PTS from the primary profile. Use for INAIR correction.
DOXY_get_profile_temp_for_traj.m	Get Temp and Pres from the main profile. Use for INAIR correction.
DOXY_get_PTS.m	Get the correct Pressure, Temperature and Salinity
DOXY_inair_corr.m	Main program for the correction with in-air measurements
DOXY_inair_prepare_for_drift.m	Prepare PPOX data to compute the drift on NCEP with WOA or REF correction
DOXY_interp_REF_2_argo.m	Interpolate the in-situ reference data to the argo data levels
DOXY_interp_REF_main.m	Interpolate the in-situ reference data to the argo data levels main program
DOXY_interp_WOA_2_argo.m	Interpolate the WOA data to the argo data levels
DOXY_interp_WOA_main.m	Interpolate the WOA data to the argo data levels main program
DOXY_MAP.m	Map the argo trajectory (and the in-situ database if possible)
DOXY_MAP2.m	Map the argo trajectory (and the in-situ database if possible) using M_MAP
DOXY_mono_to_multi.m	Compute a multiprofile from the monoprofiles
DOXY_NCEP_colocalize.m	Colocalize the NCEP data on the argo trajectory
DOXY_NCEP_read.m	Read the NCEP data
DOXY_PLOT_corr.m	Make the plots for the correction step
DOXY_PLOT_drift.m	Make the plots for the sensor drift estimation step
DOXY_PLOT_interpolation.m	Make the plots for the reference data interpolation step
DOXY_PLOT_PTS_QC.m	Make the plots for the QC respect to the pressure and the cycle
DOXY_PLOT_QC.m	Make the plots for the QC step
DOXY_PLOT_settingsToPrint.m	Prepare and print the plots
DOXY_print_config_in_logfile.m	Print the parameters defined in the config file and the user choices in the log file
DOXY_QC.m	Quality control the data
DOXY_ref_corr.m	Main program for the correction with In-Situ reference data
DOXY_update_fields.m	Update the adjusted and metadata fields in the argo structure
DOXY_woa_corr.m	Main program for the correction with WOA climatology
DOXY_WOA_read.m	Read the WOA data
DOXY_write_prepare.m	Prepare the data to be written

Table 5 : LOCODOX dedicated programs name and description

4.3 LOCODOX useful programs

LOCODOX uses a set of program not specifically dedicated to the oxygen correction programs. These useful programs could be found in the *share* directory, and are listed and described in the Table 6.

Program name	Description
api_key.mat	API key for plot_google_map.m
cat_profile_dim.m	Concatenate structure along one dimension
check_FirstDimArray.m	Check the first dimension of data
check_isfillval_prof.m	Determine if all the data in Co is equal to the FillValue
check_LastDimArray.m	Check the last dimension of data
check_profile_qc.m	Update the profile_param_qc respect to the param_adjusted_qc.
construct_best_param.m	Replace param by adjusted parameter if exist
cprintf	directory. Function that displays styled formatted text in the command window.
dist.m	Computes distance and bearing between points on the earth
dynamicDateTicks.m	Create dynamic date tick labels for plots with dates on the X-axis
extract_profile_dim.m	Extract one or more profiles or one or more levels, along one dimension
fillValue_2_nan.m	Replace fillvalue by NaN
findstr_tab.m	Find string in a cell array or a string array
fitnlm.m	Create nonlinear regression model by fitting to data
format_flags_char2num.m	Change flag char strings to numerical vectors
gravit.m	Compute the gravity respect to the latitude
hydcsl	directory. Module with useful function dedicated to hydrography.
listdlg.m	List selection dialog box (Matlab native modified)
lsqfitma.m	Calculate a "2-way" least squares fit
nan_2_fillValue.m	Replace NaN by fillValue
nanmax.m	Find maximum, ignoring NaNs
nanmean.m	Compute mean, ignoring NaNs
nanmedian.m	Compute median, ignoring NaNs
nanmin.m	Find minimum, ignoring NaNs
nanstd.m	Compute standard deviation, ignoring NaNs, if NaN fraction is not too big
nansum.m	Compute sum, ignoring NaNs
NCR_file.m	Read NetCDF argo file (parameter and attributes), organised it in a structure
NCW_file.m	Write NetCDF argo file (parameter and attributes), from a structure
nlinfitsci.m	Call fitnlm and get the confidence interval and the non linear model
nlparci.m	Compute confidence intervals for parameters in nonlinear regression
O2ctoO2p.m	Convert oxygen concentration ($\mu\text{mol/L}$) to oxygen partial pressure (dBar)
O2ctoO2s.m	Convert oxygen concentration ($\mu\text{mol/L}$) to oxygen saturation (%)
O2ptoO2c.m	Convert oxygen partial pressure (dBar) to oxygen saturation (%)
O2ptoO2s.m	Convert oxygen partial pressure (dBar) to oxygen saturation (%)
O2stoO2c.m	Convert oxygen saturation (%) to oxygen concentration ($\mu\text{mol/L}$)
O2stoO2p.m	Convert oxygen saturation (%) to oxygen partial pressure (dBar)
plot_google_map.m	Plot a google map on the current axes using the Google Static Maps API
questdlg.m	Question dialog box (Matlab native modified)
rsquare.m	Calculate r square evaluating a regression, using data y and estimates yhat
seawater	Seawater Library v3.3
statjacobian.m	Estimate the Jacobian of a function
str2numQC.m	Convert string to numbers, with NaN instead of blanks.
watervapor.m	Calculate pH ₂ O / atm after Weiss and Price 1980

Table 6 : LOCODOX useful programs name and description