Recommendations on the conversion between oxygen quantities for Bio-Argo floats and other autonomous sensor platforms

Initial draft: Henry Bittig, Laboratoire océanographique de Villefranche-sur-Mer, October 2015
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Recommended implementation

A. Conversion from mL L$^{-1}$ (MLPL.DOXY) to µmol L$^{-1}$ (MOLAR.DOXY)

This conversion is required to convert Sea-Bird oxygen sensor data given in mL O$_2$ (gas at S.T.P) per L of seawater (i.e., MLPL.DOXY in mL$_{\text{STP}}$ L$^{-1}$) into µmol O$_2$ per L of seawater (i.e., MOLAR.DOXY in µmol L$^{-1}$). The conversion is valid both for salinity-corrected and salinity-uncorrected O$_2$ data.

$$c_{O_2} (\mu \text{mol L}^{-1}) = 44.6596 \cdot c_{O_2} (\text{mL} L_{\text{STP}}^{-1})$$

The molar volume of oxygen used here is 22.3916 L$_{\text{STP}}$ mol$^{-1}$ (Garcia and Gordon 1992). Its reciprocal gives the conversion factor of 44.6596 µmol mL$_{\text{STP}}^{-1}$.

B. Conversion from mg L$^{-1}$ to µmol L$^{-1}$ (MOLAR.DOXY)

For some applications, oxygen concentration is given as mass O$_2$ per L of seawater, e.g., mg L$^{-1}$. The molar weight of O$_2$ determines the conversion factor to µmol O$_2$ per L of seawater (i.e., MOLAR.DOXY in µmol L$^{-1}$). The conversion is valid both for salinity-corrected and salinity-uncorrected O$_2$ data.

$$c_{O_2} (\mu \text{mol L}^{-1}) = 31.2512 \cdot c_{O_2} (\text{mg} L^{-1})$$

The molar weight of O$_2$ used here is 31.9988 g mol$^{-1}$ (CIAAW 2015). Its reciprocal gives the conversion factor of 31.2512 µmol mg$^{-1}$.

C. Conversion from salinity-uncorrected MOLAR.DOXY optode data to salinity-corrected, molar oxygen concentration $c_{O_2}(T,S)$

Oxygen optodes are insensitive to the salinity $S$ of the ambient seawater, while the O$_2$ amount they measure follows the salinity dependence of the seawater O$_2$ solubility $c_{O_2}(T,S)$. Their initial O$_2$ concentration output $c_{O_2}(T,S_{\text{preset}})$ (e.g., MOLAR.DOXY; default $S_{\text{preset}} = 0$) thus needs to be salinity-compensated to yield the correct O$_2$ concentration $c_{O_2}(T,S)$. The correction relates the initial concentration output $c_{O_2}(T,S_{\text{preset}})$ to the seawater concentration (at $T$ and $S$) that has the same partial pressure. The correction term $S_{\text{corr}}$ is the salinity-dependent part of $c_{O_2}(T,S)$ according to Garcia and Gordon (1992), using the Benson and Krause refit coefficients. The Benson and Krause (1984) data is considered to be more accurate than the other datasets and recommended for general use (Garcia and Gordon 1992; Wong and Li...
2009). The Garcia and Gordon (1992) parameterization gives the O$_2$ concentration in equilibrium with an atmosphere of standard composition saturated with vapor pressure at a total pressure (including that of the water vapor) of 1 atm. The water vapor pressure changes with the salt content (colligative effect), i.e., the atmospheric composition (O$_2$ content) at a total pressure of 1 atm (including water vapor) is different at $S_{\text{preset}}$ and $S$. The water vapor terms account for that difference.

Note: The water vapor term is often not taken into account by optode manufacturer / optode on-board calculations. In that case, $S_{\text{preset}}$ only in the water vapor term needs to be replaced with 0.

\[
\text{salinity-corrected } c_{O_2}(T,S) = S_{\text{corr}} \cdot \frac{1013.25 - p_H H_2O(T,S_{\text{preset}})}{1013.25 - p_H H_2O(T,S)} \cdot \text{salinity-uncorrected } c_{O_2}(T,S_{\text{preset}})
\]

\[
S_{\text{corr}} = \exp\left( (S - S_{\text{preset}}) \cdot (B_0 + B_1 \cdot T_s + B_2 \cdot T_s^2 + B_3 \cdot T_s^3 + C_0 \cdot (S^2 - S_{\text{preset}}^2)) \right) \\
T_s = \ln \left( \frac{298.15 - T}{273.15 + T} \right)
\]

\[
B_0 = -6.24523 \times 10^{-3} \\
B_1 = -7.37614 \times 10^{-3} \\
B_2 = -1.03410 \times 10^{-3} \\
B_3 = -8.17083 \times 10^{-3}
\]

\[
C_0 = -4.88682 \times 10^{-7}
\]

(Garcia and Gordon 1992, Benson and Krause refit)

\[
p_H H_2O = 1013.25 \cdot \exp(D_0 + D_1 \cdot \frac{T_{abs}}{100} + D_2 \cdot \ln(T_{abs}) + D_3 \cdot S)
\]

\[
D_0 = 24.4543 \\
D_1 = -67.4509 \\
D_2 = -4.8489 \\
D_3 = -5.44 \times 10^{-4}
\]

\[
T_{abs} = T + 273.15
\]

where

- $T$ = temperature (°C)
- $S$ = salinity (dimensionless, Practical Salinity Scale 1978)
- $S_{\text{preset}}$ = salinity of the uncorrected oxygen concentration (dimensionless, PSS-78; default: 0)
- $p_H H_2O$ = water vapor pressure (mbar)
- $T_{abs}$ = absolute temperature (K)

**D. Conversion from salinity-uncorrected MOLAR_D oxy optode data to partial pressure $p_O_2$**

This conversion will be required for surface/air measurements by oxygen optodes reporting salinity-uncorrected MOLAR_D. It makes use of equation (4) of the background section (see below). The oxygen solubility $c^*_O_2(T,S)$ can be separated into a temperature-dependent part $T_{\text{corr}}$ and a salinity-dependent part $S_{\text{corr}}$.

\[
c^*_O_2(T,S) = T_{\text{corr}} \cdot S_{\text{corr}}
\]

Combining equations (4) and (5) with the conversion $C$ (with $S_{\text{preset}} = 0$) between salinity-corrected and uncorrected oxygen concentration, the $S_{\text{corr}}$ term drops out and the conversion below remains. It includes the effect of hydrostatic pressure on $p_O_2$, which is negligible near the surface.

Note: The water vapor term is often not taken into account by optode manufacturer / optode on-board calculations. In that case, $S_{\text{preset}}$ in the water vapor term needs to be replaced with 0.
\[ p_{O_2} = c_{O_2}(T,S_{\text{preset}}) \cdot \frac{x_{O_2} \cdot (1013.25 - p_{H_2}O(T,S_{\text{preset}}))}{T_{\text{corr}} \cdot S_{\text{corr}}} \cdot \exp \left( \frac{V_m \cdot P}{R \cdot T_{\text{abs}}} \right) \]

\[ x_{O_2} = 0.20946 \]  
\[ (\text{Glueckauf 1951}) \]

\[ T_{\text{corr}} = 44.6596 \cdot \exp( A_0 + A_1 \cdot T_s + A_2 \cdot T_s^2 + A_3 \cdot T_s^3 + A_4 \cdot T_s^4 + A_5 \cdot T_s^5 ) \]

\[ A_0 = 2.00907 \]
\[ A_1 = 3.22014 \]
\[ A_2 = 4.05010 \]
\[ A_3 = 4.94457 \]
\[ A_4 = -2.56847 e^{-1} \]
\[ A_5 = 3.88767 \]  
\[ (\text{Garcia and Gordon 1992, Benson and Krause refit}) \]

\[ V_m = 0.317 \]  
\[ (\text{Enns et al. 1965}) \]
\[ R = 8.314 \]  
\[ (\text{CODATA 2014}) \]

where

\[ p_{O_2} = \text{oxygen partial pressure (mbar)} \]
\[ c_{O_2}(T,S_{\text{preset}}) = \text{salinity-uncorrected oxygen concentration at } S=S_{\text{preset}} (\text{µmol L}^{-1}) \]
\[ T = \text{Temperature (°C)} \]
\[ S_{\text{preset}} = \text{salinity of the uncorrected oxygen concentration (dimensionless, PSS-78; default: 0)} \]
\[ x_{O_2} = \text{mixing ratio of oxygen in dry air (dimensionless)} \]
\[ V_m = \text{molar volume of oxygen (m}^3 \text{mol}^{-1} \text{Pa dbar}^{-1}) \]
\[ P = \text{hydrostatic pressure (dbar)} \]
\[ R = \text{universal gas constant (J mol}^{-1} \text{K}^{-1}) \]

**E. Conversion from molar oxygen concentration** \( c_{O_2}(T,S) \)** to oxygen partial pressure** \( p_{O_2} \)**

This conversion between salinity-corrected oxygen concentration \( c_{O_2}(T,S) \) and partial pressure \( p_{O_2} \) follows equations 4 and 5 of the background section, i.e.,

\[ p_{O_2} = c_{O_2}(T,S) \cdot \frac{x_{O_2} \cdot (1013.25 - p_{H_2}O(T,S))}{T_{\text{corr}} \cdot S_{\text{corr}}} \cdot \exp \left( \frac{V_m \cdot P}{R \cdot T_{\text{abs}}} \right) \]

where

\[ p_{O_2} = \text{oxygen partial pressure (mbar)} \]
\[ c_{O_2}(T,S) = \text{salinity-corrected oxygen concentration (µmol L}^{-1}) \]

All other terms required \( (x_{O_2}, p_{H_2}O, T_{\text{corr}}, S_{\text{corr}}, V_m, R, T_{\text{abs}}) \) are given above with references.

**F. Conversion from molar oxygen concentration** \( c_{O_2}(T,S) \)** to oxygen concentration** \( \text{DOXY} \)** on the molinity scale

This conversion is just added for completeness in an Argo framework, to give the final fully corrected \( O_2 \) concentration in units of molinity, i.e., \( \text{µmol kg}^{-1} \text{ seawater} \) (DOXY).

\[ c_{O_2} (\text{µmol kg}^{-1}) = c_{O_2} (\text{µmol L}^{-1}) / \rho , \]

where
\[ \rho = \text{potential density of seawater (kg L}^{-1}\text{) referenced to a hydrostatic pressure of 0 dbar and using practical salinity. We recommend using the equation of state based on Fofonoff and Millard (1983) and Millero et al. (1980).} \]

**Background**


Oxygen saturation can be expressed both in terms of oxygen concentration as the ratio of \( c_{O_2} \) to \( O_2 \) solubility \( c_{O_2}^* \), and in terms of partial pressure as the ratio of water \( pO_2 \) to the atmospheric equilibrium partial pressure \( pO_{2,atm} \),

\[
sat\,O_2 = \frac{c_{O_2}}{c_{O_2}^*} = \frac{pO_2}{pO_{2,atm}}. \tag{1}
\]

Equation 1 can thus be used to easily convert between concentrations and partial pressures.

At the sea surface, \( pO_{2,atm} \) follows

\[
pO_{2,atm} = \chi_{O_2} \cdot (p_{air} - pH_2O), \tag{2}
\]

where \( pH_2O \) is the saturation water vapor pressure after Weiss and Price (1980) and \( \chi_{O_2} = 0.20946 \) the mixing ratio of \( O_2 \) in dry air (Glueckauf 1951). \( pO_{2,atm} \) and thus \( O_2 \) saturation are therefore dependent on the ambient atmospheric pressure \( p_{air} \) as well as on saturation water vapor pressure which is a function of seawater temperature and salinity. The temperature \( (T) \) and salinity \( (S) \) dependent seawater \( O_2 \) solubility \( c_{O_2}^*(T,S) \) is given for a pressure of one atmosphere (Garcia and Gordon 1992) and needs to be scaled to ambient pressure for surface applications according to

\[
c_{O_2}(T,S,p_{air}) = c_{O_2}^*(T,S) \cdot \frac{p_{air} - pH_2O(T,S)}{1013.25 \text{ mbar} - pH_2O(T,S)} \tag{3}
\]

in order to yield the correct saturation (equ. 1). In the above equation, only components other than water vapor are scaled since \( pH_2O \) depends on temperature and salinity only but not on atmospheric pressure \( p_{air} \).

Inserting (2) and (3) into (1) yields

\[
c_{O_2} = \frac{c_{O_2}^*(T,S)}{\chi_{O_2} \cdot (1013.25 \text{ mbar} - pH_2O(T,S))} \cdot pO_2 \tag{4}
\]

i.e., the conversion of partial pressure \( pO_2 \) to \( O_2 \) concentration \( c_{O_2} \) is independent of \( p_{air} \) (since the change in \( O_2 \) saturation cancels out).

Below the surface, hydrostatic pressure \( P \) affects both the oxygen solubility and partial pressure. Enns et al. (1965) describe an exponential increase in \( pO_2 \) of about 14% per 1000 dbar and Taylor (1978) provides a theoretical relationship,

\[
pO_2(P) = pO_2 \cdot \exp \left( \frac{V_0(O_2) \cdot P}{R \cdot (T + 273.15 \text{ K})} \right) \tag{5}
\]

where \( V_0(O_2) = 31.7 \text{ mL mol}^{-1} \) is the molar volume of \( O_2 \) in seawater (Enns et al. 1965) and \( R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1} \) the universal gas constant. The \( pO_2 \) increase with hydrostatic pressure reflects a higher outgassing tendency with depth, i.e., a reduced solubility \( c_{O_2}^*(T,S,P) \). Consequently, equ. 5 and 4 need to be combined for the conversion between \( pO_2(P) \) and \( c_{O_2} \) for sub-surface applications. For the solubility follows
\[ c_{O_2}^*(T,S,P,p_{air}) = \frac{p_{O_2} - p_{H_2O(T,S)}}{1013.25 \text{ mbar} - p_{H_2O(T,S)}} \exp \left( \frac{V_L(O_2) \cdot P}{R \cdot (T + 273.15 \text{ K})} \right) . \]

As a consequence, the conversion from oxygen concentration or oxygen partial pressure to oxygen saturation depends on temperature \( T \), salinity \( S \), hydrostatic pressure \( P \), and the ambient air pressure \( p_{air} \).

Especially the last quantity poses a challenge for subsurface applications since \( p_{air} \) is no conservative tracer that easily tracks with the water mass from its formation region nor is it easily measurable. Commonly, one atmosphere (1013.25 mbar) as default is used as a workaround. However, a value of "100 % saturation at 1 atm" is incompatible with the interpretation of "being in equilibrium with the atmosphere" over most portions of the ocean. As an example, \( p_{air} \) over the Southern Ocean is typically (significantly) below one atmosphere. There, "100 % saturation at 1 atm" would consistently give supersaturated waters relative to equilibrium, i.e., "100 % saturation at local atmospheric pressure". When working with oxygen saturations, it is thus essential to state the reference state, 1 atm or ambient \( p_{air} \), together with the saturation value to indicate whether the scaling of equation 3 has been performed or not.

**Nomenclature**

Oxygen concentration, \( c_{O_2} \): amount of \( O_2 \) in a given volume (molarity, \( \mu \text{mol L}^{-1} \)) or mass of seawater (molinity, \( \mu \text{mol kg}^{-1} \))

Oxygen partial pressure, \( p_{O_2} \): gas pressure of \( O_2 \) in a gas mixture (mbar)

Oxygen solubility, \( c_{O_2}^* \): The saturation equilibrium concentration of \( O_2 \) with air at ambient conditions of temperature \( T \), salinity \( S \), air pressure \( p_{air} \), and hydrostatic pressure \( P \). Laboratory experimental values are tabulated at zero dbars hydrostatic pressure, \( P \), and an air pressure, \( p_{air} \), of one atmosphere (1013.25 mbar). Units are the same as for concentration.

Oxygen saturation, \( \text{sat } O_2 \): ratio of the \( O_2 \) amount present in a given sample and its equilibrium \( O_2 \) concentration (i.e., ratio of \( c_{O_2} \) and \( c_{O_2}^* \), or ratio of \( p_{O_2} \) to the equilibrium air \( p_{O_2}^* \); see equ. 1). This value is also frequently presented as the percent difference from saturation equilibrium, i.e., \( \Delta O_2 \text{ (\%)} = \frac{(c_{O_2} - c_{O_2}^*)}{c_{O_2}^*} \cdot 100 \text{ \%} \).

**References**


