O$_2$ quantity conversions

SCOR WG 142:
Quality Control Procedures for Oxygen and Other Biogeochemical Sensors on Floats and Gliders

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

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$_{STP}$ 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.

\[ c_{O_2} \text{ (µmol L$^{-1}$)} = 44.6596 \cdot c_{O_2} \text{ (mL$_{STP}$ L$^{-1}$)} \]

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

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.
O₂ quantities

There are three (equivalent) ways to state the O₂ content of seawater:

- **O₂ concentration:** amount of O₂ in a given volume (molarity, μmol L⁻¹) or mass of seawater (molinity, μmol kg⁻¹, DOXY)

- **O₂ partial pressure \( pO₂ \):** (hypothetical) gas pressure in equilibrium with the seawater if O₂ were the only gas in the gas mixture (at the same conditions, i.e., temperature T, hydrostatic pressure P, ...); units of mbar

- **O₂ saturation:** ratio of the O₂ amount present in a given sample and its equilibrium O₂ concentration (or ratio of \( pO₂ \) to the equilibrium air \( pO₂ \)); dimensionless / %
Conversion between $O_2$ quantities

Currently, $O_2$ sensor manufacturers use different temperature & salinity dependencies (solubility equation). This affects the conversion of the sensor output (MLPL_DOXY / MOLAR_DOXY) to the final $O_2$ concentration (DOXY). However, the conversion should not depend on the manufacturer but only on physical principles and be uniform for all $O_2$ sensors → SCOR WG142 recommendations for $O_2$ quantity conversions to be used instead of (varying) manufacturer equations.
A. Conversion from mL L$^{-1}$ (MLPL_DOXY) to μmol L$^{-1}$ (MOLAR_DOXY)

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

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

D. Conversion from salinity-uncorrected MOLAR_DOXY optode data to partial pressure $pO_2$

E. Conversion from molar oxygen concentration $c_{O_2}(T,S)$ to oxygen partial pressure $pO_2$

F. Conversion from molar oxygen concentration $c_{O_2}(T,S)$ to oxygen concentration 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., μmol kg$^{-1}$ seawater (DOXY).

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

where

$\rho$ = potential density of seawater (kg L$^{-1}$) 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).
Summary

- Provides a reference set of equations for O₂ conversions
- Uniform for all O₂ sensors, independent of manufacturers
- Should use the best available temperature (TEMP?)
- Includes calculation of partial pressure $pO_2$ required for in air measurements, because it is not possible to state a DOXY in air (= amount of O₂ in a given mass of seawater, μmol kg⁻¹)