

Usage notes for JSL code for the CO₂ equilibration calculator script

Usage of this code requires JMP version 14 or higher (not tested on earlier versions). The input data can be an Excel, .CSV or JMP data file containing the following input variables:

- 1) CO₂ of headspace before equilibration (ppmv). This value is 0 when N₂ or CO₂-free gas is used as headspace. If ambient air is used, its CO₂ should be measured or assumed to be close to atmospheric average (currently about 402 ppmv).
- 2) CO₂ of headspace after equilibration(ppmv).
- 3) Temperature of water during sampling (°C).
- 4) Temperature of vessel during equilibration process (°C).
- 5) Alkalinity (µequiv/L).
- 6) Headspace ratio (Vol_(gas):Vol_(water), i.e. 30mL:30mL=1).
- 7) Barometric pressure (kPa)

Values for variables 1, 6, 7 and 8 are not required in the data file if they are constant.

Load or import the input data file in JMP. Load and launch the script file. The following dialog box will appear

CO₂ equilibration calculator

Select Columns

- Longitude
- Alkalinity unified
- In situ-...ture (°C)
- Depth (m)
- pH
- conductivity
- [G] pCO...C (µatm)
- Bottle t...g [G] (°C)
- Salinity
- Bar. Pre... analysis

Required variables

HS pCO₂ before equilibration required

HS pCO₂ after equilibration required

Water Temperature (C) during sampling required

Water Temperature (C) during equil. required

Bottle temp. after shaking [G] (°C) required

Alkalinity (uequiv/L) required

Headspace ratio required

Barometric Pressure (kPa) required

Salinity (kPa) required

☐ Constant HS gas pCO₂ (ppmv) 400

☐ Constant HS ratio (Vgas:Vliquid) 1

☐ Constant Bar. Pres (kPa) 101.325

☐ Constant Salinity (g/kg) 0

Carbonate equilibrium equation set

☒ Freshwater (Millero 1979)

☐ Estuarine (Millero et al. 2010)

☐ Marine (Dickson et al. 2007)

Solution method

☒ Analytical solutions (faster)

☐ Iterative solutions (slower but more stable in extreme situations)

Select or drag the data columns into the appropriate variable selection box. A choice a carbonate equilibrium equation set is given corresponding to various field sample types (freshwater, estuarine or marine). The Millero (2010) coefficients as amended in Orr et al. (2015). Water dissociation is from Dickon and Riley (1979) and CO₂ solubility from

Weiss et al. (1974). A choice of numerical solution methods is also given. The “Analytical solutions” is nearly instantaneous but can suffer minor imprecisions in extreme situations ($\text{Alk} > 4000$ ($\mu\text{equiv/L}$ and $\text{pCO}_2(\text{after equil.}) < 100$ ppmv) inherent to double precision calculations. The “iterative solutions” is much slower but more stable in such situations. In all cases, results are added as three new columns to the data table (uncorrected pCO_2 , corrected pCO_2 , corrected $[\text{CO}_2]$) Partial pressures are in μatm and concentrations in $\mu\text{mole/L}$. The code is available as a JSL script and as a JMP add-in.

References:

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