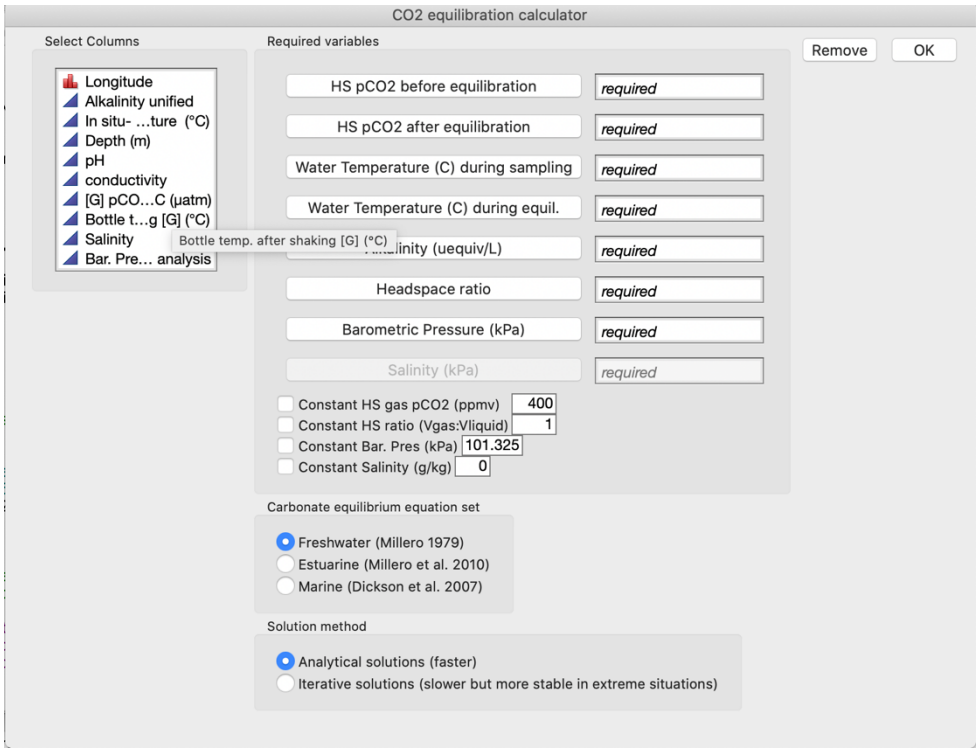
Usage notes for JSL code for the CO_2 equilibration calculator script

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) CO_2 of headspace before equilibration (ppmv). This value is 0 when N_2 or CO_2-free gas is used as headspace. If ambient air is used, its CO_2 should be measured or assumed to be close to atmospheric average (currently about 402 ppmv).
2) CO_2 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



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 CO_2 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 (Alk> 4000 (µequiv/L and $pCO_{2(after\ equil.)}$<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 [CO2]) Partial pressures are in µatm and concentrations in µmole/L. The code is available as a JSL script and as a JMP add-in.

References:

Dickson, A. G. & Riley, J. P. (1979).The estimation of acid dissociation constants in seawater media from potentionmetric titrations with strong base. I. The ionic product of water — Kw. *Mar Chem* **7**, 89–99.

Dickson, A. G., Sabine, C. L., and Christian, J. R. (2007): Guide to best practices for ocean CO2 measurements, PICES Special Publication 3, 191 pp.

Millero, F. (1979). **The thermodynamics of the carbonate system in seawater** Geochimica et Cosmochimica Acta 43(10), 1651 1661. https://dx.doi.org/10.1016/0016-7037(79)90184-4.

Millero, F. (2010). **Carbonate constants for estuarine waters** Marine and Freshwater Research 61(2), 139. https://dx.doi.org/10.1071/mf09254

Orr, J. C., Epitalon, J.-M. & Gattuso, J.-P. Comparison of ten packages that compute ocean carbonate chemistry. *Biogeosciences* **12**, 1483–1510 (2015).

Weiss, R. F. Carbon dioxide in water and seawater: the solubility of a non-ideal gas. *Mar Chem* **2**, 203–215 (1974).