## **CO2Sys Excel Version History**

**Previous versions** (2007): CO2sys\_macro\_PC.xls and CO2sys\_macro\_MAC.xls

. Two separate files for PC and MAC versions.

#### Version 1.0 (10 Octobre 2011): CO2Sys\_2011.xls

. Combined PC and MAC versions of previous macro into one file working on both platforms.

### Version 2.0 (19 July 2012): CO2Sys\_2011.xls

. New R formulation from NIST Physical Reference Data (http://physics.nist.gov/cgi-bin/cuu/Value?r)

Difference with old formulation is not numerically significant.

- . Matched formulation of Uppstrom's Total Boron with Matlab program (same numerical results).
  - . Added option of Total Boron from Lee et al., 2010
  - . Added a few formulations for K1, K2:
    - Cai and Wang, 1998
    - Lueker et al., 2000
    - Mojica Prieto et al., 2002
    - Millero et al., 2002
    - Millero et al., 2006
    - Millero, 2010
  - . Updated the INFO section
  - . Added the Macro Version History option in INFO Sheet.
- . Version number is displayed in cell B2 when the About this Macro option in INFO Sheet is selected.

#### Version 2.1 (18 September 2012): CO2Sys\_v2.1.xls

. Corrected an error in the code which affected the results when the constants of 'Millero et. al., 2002'

and 'Millero, 2010' were selected.

- . References to 'Cai and Wang, 2008' have been corrected to 'Cai and Wang, 1998'
- . Incorporated version number in the name of the file and removed it from the "INFO" sheet (see v.2.0)  $\,$

# Special Version 2.1 (03 May 2015): CO2Sys\_v2.1 NH3-H2S

- . Added option to include NH3 and H2S in the calculations of Alkalinity.
- NH3 constants were taken from the [Clegg Whitfield 1995 Geochimica et Cosmochimica Acta, Vol. 59, No. 12. pp. 2403-2421] paper referenced in the Bell et al (2007) article. Their values are valid from S=[0-40] and T=[-2-40 oC].
- H2S constants were taken from Millero et. al. (1988) Limnol. Oceanogr. 33,269-274 and are valid from S=[0-40] and T=[0-35 oC]

- Pressure correction taken from Millero (1983) "Influence of Pressure on Chemical Processes in the Sea" (the Millero 1995 had typos)
- . Bug fix: added code to prevent calculation of pH (fromTATC or fromTAfCO2) from getting stuck in infinite loop of alternatively negative and positive delta pHs.(taken from version 2.3 on 14 November 2016)
- . Bug fix: Corrected handling of -999 in data. would skip line at first encountered -999 in CO2 parameter. Would also not handle -999 in output conditions. (taken from version 2.3 on 11/18/2016)
- . Bug fix: KH2S from Yao Millero was actually given on Total Scale and not Seawater scale. Corrected in the code. Also cleaned up the code. (12/14/2016)
- . Issue fix: Added a check to stop iterations of pH estimation after 10,000 loops and flag data (pH did not converge). (12/14/2016)
- . Issue fix: data flag is now in proper column and text color is red when flagged (12/14/2016)
- **Version 2.2** (27 October 2015): CO2sys\_v2.2xls based on regular v2.1 (no H2S-NH3)
  - . Added the choice of 'Perez and Fraga, 1987' for KF
  - . Added the 'SubFlags' and 'Red data rows':
- If Pressure, Phosphate or Silica is '-999', calculations will be performed with 0 instead of -999
- and the resulting row of data will be colored in red. The 'SubFlag' column at the end will state the reason.
- **Version 2.3** (14 December 2016): **CO2sys\_v2.3.xls** based on regular v2.2 (no H2S-NH3)
  - . Corrected output format of results
- . Bug fix: added code to prevent calculation of pH (fromTATC or fromTAfCO2) from getting stuck in infinite loop of alternatively negative and positive delta pHs.
- . Bug fix: Corrected handling of -999 in data. would skip line at first encountered -999 in CO2 parameter. Would also not handle -999 in output conditions. (11/18/2016)
- . Bug fix: Corrected coloring of problematic line in red and expanded "results" range to clear to include flag in last column. (11/18/2016)
- . Issue fix: Added a check to stop iterations of pH estimation after 10,000 loops and flag data (pH did not converge). (12/14/2016)
- . Issue fix: data flag is now in proper column and text color is red when flagged (12/14/2016)
- . found numvar misspelled as "numbar". Doesn't seem to create issue. Fixed anyway (05/13/2019)

Special **Version 2.3** (14 December 2016): **CO2sys\_v2.3 NH3-H2S.xls** - based on regular v2.3 (no H2S-NH3) dated (12/14/2016)

- . See changes made to version 2.3 dated on 12/14/2016 and before, as well as those made to Special version 2.1 (12/14/2016) (called v2.4 on GitHub)
  . found numvar misspelled as "numbar". Doesn't seem to create issue. Fixed
- anyway (05/13/2019)