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## CO<sub>2</sub>Sys Excel Version History

Previous versions (2007): CO<sub>2</sub>sys\_macro\_PC.xls and CO<sub>2</sub>sys\_macro\_MAC.xls

- . Two separate files for PC and MAC versions.

Version 1.0 (10 Octobre 2011): CO<sub>2</sub>Sys\_2011.xls

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

Version 2.0 (19 July 2012): CO<sub>2</sub>Sys\_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 K<sub>1</sub>, K<sub>2</sub>:
  - 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): CO<sub>2</sub>Sys\_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): CO<sub>2</sub>Sys\_v2.1 NH<sub>3</sub>-H<sub>2</sub>S

- . Added option to include NH<sub>3</sub> and H<sub>2</sub>S 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 fromTAfC02) 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\_v2.2.xls - 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 fromTAfC02) 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): C02sys\_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)

Version 3.0 (15 June 2019): C02sys\_v3.0.xls – based on Special v2.3

- . Updated the info about the macro and the NH4-H2S constants (06/07/2019)

- . Suppressed screen updating when selecting cells on INFO and INPUT sheets (06/07/2019)

- . Bug fix: affected calculation of KF of 'Perez and Fraga, 1987' (lnKF was spelled InKF instead– first letter was an upper case "i" instead of an "L").(07/18/2019)

- . Added Peng's correction of TA for case of input TA, Carbonate.(07/18/2019)

- . pH Scale and Constants used (column R in DATA sheet) are refreshed when activating the DATA sheet. (02/05/2021)