

Works Cited
in CO2SYS code notes and QUODcarb code notes

(Compiled by M. Fennell, see 'CO2SYS_code_notes.pdf' taken from the notes in the
CO2SYSv3 code)

Broecker, W. S., Spencer, D. W., & Craig, H (1982). *Pacific expedition: hydrographic data 1973-1974*. International Decade of Ocean Exploration, National Science Foundation.

Cai, W. J., & Wang, Y. (1998). The chemistry, fluxes, and sources of carbon dioxide in the estuarine waters of the Satilla and Altamaha Rivers, Georgia. *Limnology and Oceanography*, 43(4), 657-668.

Clegg, S. L., & Whitfield, M. (1995). A chemical model of seawater including dissolved ammonia and the stoichiometric dissociation constant of ammonia in estuarine water and seawater from -2 to 40 °C. *Geochimica et Cosmochimica Acta*, 59(12), 2403-2421.

Culberson, C. H. & Pytkowicz, R. M. (1968). Effect of pressure on carbonic acid, boric acid, and the pH of seawater, *Limnology and Oceanography* 13:403-417.

Dickson, A. G., & Riley, J. P. (1979). The estimation of acid dissociation constants in seawater media from potentiometric titrations with strong base. I. The ionic product of water— K_w . *Marine Chemistry*, 7(2), 89-99.

Dickson, A. G., & Millero, F. J. (1987). A comparison of the equilibrium constants for the dissociation of carbonic acid in seawater media. *Deep Sea Research Part A. Oceanographic Research Papers*, 34(10), 1733-1743.

Dickson, A. G. (1990). Standard potential of the reaction: $\text{AgCl (s)} + 12\text{H}_2\text{(g)} = \text{Ag (s)} + \text{HCl (aq)}$, and the standard acidity constant of the ion HSO_4^- in synthetic sea water from 273.15 to 318.15 K. *The Journal of Chemical Thermodynamics*, 22(2), 113-127.

Dickson, A. G. (1990). Thermodynamics of the dissociation of boric acid in synthetic seawater from 273.15 to 318.15 K. *Deep Sea Research Part A. Oceanographic Research Papers*, 37(5), 755-766.

DOE (1994) Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water; version 2, A. G. Dickson & C. Goyet, eds. ORNL/CDIAC-74.

Edmond, J. M. & Gieskes, J. M. T. M. (1970). The calculation of the degree of seawater with respect to calcium carbonate under in situ conditions, *Geochemica et Cosmochemica Acta*, 34:1261-1291.

Goff, J. A., & Gratch, S. (1946). Transactions of the American Society of Heating and Ventilating Engineers, 52:95-122.

Goyet, C., & Poisson, A. (1989). New determination of carbonic acid dissociation constants in seawater as a function of temperature and salinity. *Deep Sea Research Part A. Oceanographic Research Papers*, 36(11), 1635-1654.

Hansson, I. (1973). The determination of dissociation constants of carbonic acid in synthetic sea water in the salinity range of 20–40‰ and temperature range of 5–30° C. *Acta Chemica Scandinavica*, 27, 931-944.

Hansson, I. (1973, May). A new set of acidity constants for carbonic acid and boric acid in sea water. In *Deep Sea Research and Oceanographic Abstracts* (Vol. 20, No. 5, pp. 461-478). Elsevier.

Harned, H. S., & Davis Jr, R. (1943). The ionization constant of carbonic acid in water and the solubility of carbon dioxide in water and aqueous salt solutions from 0 to 50. *Journal of the American Chemical Society*, 65(10), 2030-2037.

Harned, H. S., & Scholes Jr, S. R. (1941). The Ionization Constant of HCO_3^- from 0 to 50. *Journal of the American Chemical Society*, 63(6), 1706-1709.

Humphreys, M.P., Lewis, E.R., Sharp, J.D., & Pierrot, D. (2022). PyCO2SYS: marine carbonate system calculations in Python. *Geoscientific Model Development* 15, 15-43.

Kester, D. R., & Pytkowicz, R. M. (1967). Determination of the apparent dissociation constants of phosphoric acid in seawater 1. *Limnology and Oceanography*, 12(2), 243-252.

Khoo, K. H., Ramette, R. W., Culberson, C. H., & Bates, R. G. (1977). Determination of hydrogen ion concentrations in seawater from 5 to 40. degree. C: standard potentials at salinities from 20 to 45‰. *Analytical Chemistry*, 49(1), 29-34.

Pierrot, D., Lewis, E., & Wallace, D. W. R. (2006). CO2SYS DOS Program developed for CO2 system calculations. *ORNL/CDIAC-105. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, US Department of Energy, Oak Ridge, TN.*

Prieto, F. J. M., & Millero, F. J. (2002). The values of $pK_1 + pK_2$ for the dissociation of carbonic acid in seawater. *Geochimica et Cosmochimica Acta*, 66(14), 2529-2540.

Lueker, T. J., Dickson, A. G., & Keeling, C. D. (2000). Ocean pCO_2 calculated from dissolved inorganic carbon, alkalinity, and equations for K_1 and K_2 : validation based on laboratory measurements of CO_2 in gas and seawater at equilibrium. *Marine chemistry*, 70(1-3), 105-119.

Lee, K., Kim, T. W., Byrne, R. H., Millero, F. J., Feely, R. A., & Liu, Y. M. (2010). The universal ratio of boron to chlorinity for the North Pacific and North Atlantic oceans. *Geochimica et Cosmochimica Acta*, 74(6), 1801-1811.

Lewis, E., & Wallace, D. W. R. (1998). Program Developed for CO_2 System Calculations. ORNL/CDIAC-105. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, TN.

Li, Y. H., Takahashi, T., & Broecker, W. S. (1969). Degree of saturation of $CaCO_3$ in the oceans. *Journal of Geophysical Research*, 74(23), 5507-5525.

Lyman, J. (1957). Buffer mechanism of seawater. Ph.D Thesis, University of California, Los Angeles 196 pp.

Mehrbach, C., Culberson, C. H., Hawley, J. E., & Pytkowicz, R. M. (1973). Measurement of the apparent dissociation constants of carbonic acid in seawater at atmospheric pressure 1. *Limnology and oceanography*, 18(6), 897-907.

Millero, F. J. (1979). The thermodynamics of the carbon dioxide system in seawater, *Geochemica et Cosmochemica Acta* 43:1651-1661.

Millero, Frank J. (1983) Influence of pressure on chemical processes in the sea. Chapter 43 in *Chemical Oceanography*, eds. Riley, J. P. and Chester, R., Academic Press.

Millero, F. J., Plese, T., & Fernandez, M. (1988). The dissociation of hydrogen sulfide in seawater 1. *Limnology and Oceanography*, 33(2), 269-274.

Millero, Frank J., & Sohn, Mary L., *Chemical Oceanography*, CRC Press (1992). See chapter 6.

Millero, F. J. (1995). Thermodynamics of the carbon dioxide system in the oceans, *Geochemica et Cosmochemica Acta* 59:661-677.

Millero, F. J., Pierrot, D., Lee, K., Wanninkhof, R., Feely, R., Sabine, C. L., Key, R. M., & Takahashi, T. (2002). Dissociation constants for carbonic acid determined from field measurements. *Deep Sea Research Part I: Oceanographic Research Papers*, 49(10), 1705-1723.

Millero, F. J., Graham, T. B., Huang, F., Bustos-Serrano, H., & Pierrot, D. (2006). Dissociation constants of carbonic acid in seawater as a function of salinity and temperature. *Marine Chemistry*, 100(1-2), 80-94.

Millero, F. J. (2010). Carbonate constants for estuarine waters. *Marine and Freshwater Research*, 61(2), 139-142.

Mojica Prieto, F. J., & Millero, F. J. (2002). The values of $pK_1 + pK_2$ for the dissociation of carbonic acid in seawater. *Geochimica et Cosmochimica Acta*, 66(14), 2529-2540.

Mook, W. G., & Koene, B. K. S. (1975). Chemistry of dissolved inorganic carbon in estuarine and coastal brackish waters. *Estuar. Coastal Mar. Sci.*, 3: 325-336.

Morris, A. W., & Riley, J. P. (1966, August). The bromide/chlorinity and sulphate/chlorinity ratio in sea water. In *Deep sea research and oceanographic Abstracts* (Vol. 13, No. 4, pp. 699-705). Elsevier.

Munhoven, G. (2013). Mathematics of the total alkalinity–pH equation – pathway to robust and universal solution algorithms: the SolveSAPHE package v1.0.1. *Geoscientific Model Development* 6, 1367–1388.

Orr, J. C., Epitalon, J. M., & Gattuso, J. P. (2015). Comparison of ten packages that compute ocean carbonate chemistry. *Biogeosciences*, 12(5), 1483-1510.

Orr, J.C., Epitalon, J.-M., Dickson, A. G., & Gattuso, J.-P. (2018). Routine uncertainty propagation for the marine carbon dioxide system. *Marine Chemistry* 207, 84-107.

Peng, T. H., Takahashi, T., Broecker, W. S., & Olafsson, J. O. N. (1987). Seasonal variability of carbon dioxide, nutrients and oxygen in the northern North Atlantic surface water: observations and a model. *Tellus B: Chemical and Physical Meteorology*, 39(5), 439-458.

Perez, F. F., & Fraga, F. (1987). Association constant of fluoride and hydrogen ions in seawater. *Marine Chemistry*, 21(2), 161-168.

Riley, J. P. (1965). The occurrence of anomalously high fluoride concentrations in the North Atlantic. *Deep Sea Research A*, 12(2), 219-220.

Robinson, R. A. (1954). The vapour pressure and osmotic equivalence of sea water. *Journal of the Marine Biological Association of the United Kingdom*, 33(2), 449-455.

Roy, R. N., Roy, L. N., Vogel, K. M., Porter-Moore, C., Pearson, T., Good, C. E., Millero, F. J., & Campbell, D. M. (1993). The dissociation constants of carbonic acid in seawater at salinities 5 to 45 and temperatures 0 to 45 C. *Marine Chemistry*, 44(2-4), 249-267.

Schockman, K. M., & Byrne, R. H. (2021). Spectrophotometric determination of the bicarbonate dissociation constant in seawater. *Geochimica et Cosmochimica Acta*, 300, 231-245.

Sharp, J.D., Pierrot, D., Humphreys, M.P., Epitalon, J.-M., Orr, J.C., Lewis, E.R., & Wallace, D.W.R. (2023, Jan. 19). CO2SYSv3 for MATLAB (Version v3.2.1). Zenodo. <http://doi.org/10.5281/zenodo.3950562>

Skirrow, G., & Riley, J. P. (Eds.). (1965). *Chemical oceanography*. Academic Press.

Sulpis, O., Lauvset, S. K., & Hagens, M. (2020). Current estimates of K1* and K2* appear inconsistent with measured CO2 system parameters in cold oceanic regions. *Ocean Science Discussions*, 1-27.

Takahashi, T., Williams, R., & Bos, D. (1982) Chapter 3: Carbonate Chemistry. In W. S. Broecker, D. W. Spencer, H. Craig (Eds.), *Pacific Expedition: Hydrographic Data 1973-1974*, 77-82. International Decade of Ocean Exploration, National Science Foundation.

Uppström, L. R. (1974). The boron/chlorinity ratio of deep-sea water from the Pacific Ocean. *Deep Sea Research A*, 21(2), 161-162.

van Heuven, S., Pierrot, D., Rae, J.W.B., Lewis, E., & Wallace, D.W.R. (2011). MATLAB Program Developed for CO2 System Calculations. ORNL/CDIAC-105b. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, TN.

Waters, J. F., & Millero, F. J. (2013). The free proton concentration scale for seawater pH. *Marine Chemistry*, 149, 8-22.

Waters, J., Millero, F. J., & Woosley, R. J. (2014). Corrigendum to “The free proton concentration scale for seawater pH”,[MARCHE: 149 (2013) 8–22]. *Mar. Chem*, 165, 66-67.

Weiss, R. (1974). Carbon dioxide in water and seawater: the solubility of a non-ideal gas. *Marine chemistry*, 2(3), 203-215.

Yao, W., & Millero, F. J. (1995). The chemistry of the anoxic waters in the Framvaren Fjord, Norway. *Aquatic Geochemistry*, 1, 53-88.