Inputs:

$Vrs := -1.0$ $k_0 := -1.2$ $k_2 := -9.9 \cdot 10^{-4}$ $T_{degC} := 2.1588$ $salinity_{psu} := 35$

$fp_0 := -1.2461$ $fp_1 := -9.8801 \cdot 10^{-6}$ $fp_2 := 9.6344 \cdot 10^{-9}$ $fp_3 := -7.7662 \cdot 10^{-12}$ $fp_4 := 2.3725 \cdot 10^{-15}$

$fp_5 := 2.831 \cdot 10^{-19}$ $fp_6 := -1.8339 \cdot 10^{-22}$

$$fp := fp_0 + \left(fp_1 \cdot 10^1\right) + \left(fp_2 \cdot 10^2\right) + \left(fp_3 \cdot 10^3\right) + \left(fp_4 \cdot 10^4\right) + \left(fp_5 \cdot 10^5\right) + \left(fp_6 \cdot 10^6\right) = -1.246$$

Constants

Gas constant: $R_{GC} := 8.3145$ $FaradayConst := 96485$

$T_{degK} := T_{degC} + 273.15 = 275.309$

$$S_{Nernst} := \frac{R_{GC} \cdot T_{degK}}{FaradayConst} \cdot \ln(10)$$

Bisulfate Equilibrium Constant Dickson et al. 2007 Chapter 5 page 12 Eq. 33

$$IonicStrength := \frac{19.924 \cdot salinity_{psu}}{1000 - 1.005 \cdot salinity_{psu}} = 0.723$$

$$Khs04 := \exp\left(\begin{array}{l} \frac{-4276.1}{T_{degK}} + 141.328 - \left(23.093 \cdot \ln\left(T_{degK}\right)\right) \\ + \left(\left(\frac{-13856}{T_{degK}}\right) + 324.57 - 47.986 \cdot \ln\left(T_{degK}\right)\right) \cdot IonicStrength^{0.5} \\ + \left(\left(\frac{35474}{T_{degK}}\right) - 771.54 + 114.723 \cdot \ln\left(T_{degK}\right)\right) \cdot IonicStrength \\ + \left(\left(\frac{2698}{T_{degK}}\right) \cdot IonicStrength^{1.5}\right) \\ \left(\frac{1776}{\right.} \end{array}\right) = 4.394 \cdot 10^4$$

$$\left(+\left(\frac{1776}{T_{degK}}\right)\cdot IonicStrength^{2}\right.$$
$$\left.+\ln\left(1-0.001005\cdot salinity_{psu}\right)\right)$$

Activity coefficient of HCl in seawater

$$A_{DH} := \left(3.4286\cdot 10^{-6}\cdot {T_{degC}}^{2}\right)+\left(6.7524\cdot 10^{-4}\cdot T_{degC}\right)+4.9172\cdot 10^{-1}=0.493$$ Martz 2010

$$exponent_{\gamma HCl} := \frac{A_{DH}\cdot IonicStrength^{0.5}}{\left(1+1.394\cdot IonicStrength^{0.5}\right)}+\left(0.08885-0.000111\cdot T_{degC}\right)\cdot IonicStrength=0.256$$ Khoo 1977

$$\gamma_H\gamma_{Cl} := 10^{exponent_{\gamma HCl}}=1.803$$

Total Sulfate

$$SO4_{total} := \frac{0.14}{96.062}\cdot\frac{salinity_{psu}}{1.80655}=0.028$$

seawater Chloride concentration (mol/kg solution

$$cCl := \frac{0.99889}{35.453}\cdot\frac{salinity_{psu}}{1.80655}=0.546$$

$$m_{Cl} := cCl\cdot\frac{1000}{1000-\left(salinity_{psu}\cdot\frac{35.165}{35}\right)}=0.566$$

$$k_{tp} := k_0 + k_2 \cdot T_{degC} + fp = -2.448$$

$$pH_{free} := \frac{\left(Vrs - k_{tp}\right)}{S_{Nernst}} \log\left(\gamma_H {\gamma_{Cl}}^2 \cdot m_{Cl}\right) = 7.012$$

$$pH := \frac{\left(Vrs - k_{tp}\right) + \left(S_{Nernst} \cdot 2 \cdot \log\left(\gamma_H \gamma_{Cl}\right)\right) + \left(S_{Nernst} \cdot \log\left(m_{Cl}\right)\right)}{S_{Nernst}} = 26.777$$

$$pH_{freeSW} := pH_{free} - \log\left(\frac{1000 - salinity_{psu} \cdot \frac{35.165}{35}}{1000}\right) = 7.028$$

$$pH_{total} := pH_{freeSW} - \log\left(1 + \frac{SO4_{total}}{Khs04}\right) = 7.028$$

Change in HCl Vrs as a function to temperature and pressure

$$P_{dBar} := 21$$

$$mean\gamma := -0.000113 \cdot T_{degC} + 0.9067 = 9.06456 \cdot 10^{-1}$$

$$\Delta V0 := 16.38 + 0.0896 \cdot T_{degC} - 0.001264 \cdot {T_{degC}}^2 = 16.5675$$

$$V_{ct} := \frac{-R_{GC} \cdot T_{degK}}{FaradayConst} \cdot \ln\left(\left(mean\gamma \cdot 0.01\right)^2\right) = 0.22317$$

$$V_{cp} := \frac{\Delta V0}{23061} \cdot 0.0242 \cdot \frac{\left(P_{dBar} - 10\right)}{10} \cdot \frac{1}{1.01} = 1.894 \cdot 10^{-5}$$

$$V_c := V_{ct} + V_{cp} = 0.223$$

$$-1.121740 - V_c = -1.34493$$

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