

Dissolved Inorganic Carbon in ocean chemistry is a conventional term used to indicate the sum of the concentration of seawater-dissolved CO₂, carbonic acid, bicarbonate and carbonate anions. It is measured in millimol/kg-of-solution. This value depends on different factors, the main being temperature, salinity and CO₂ concentration in the atmosphere

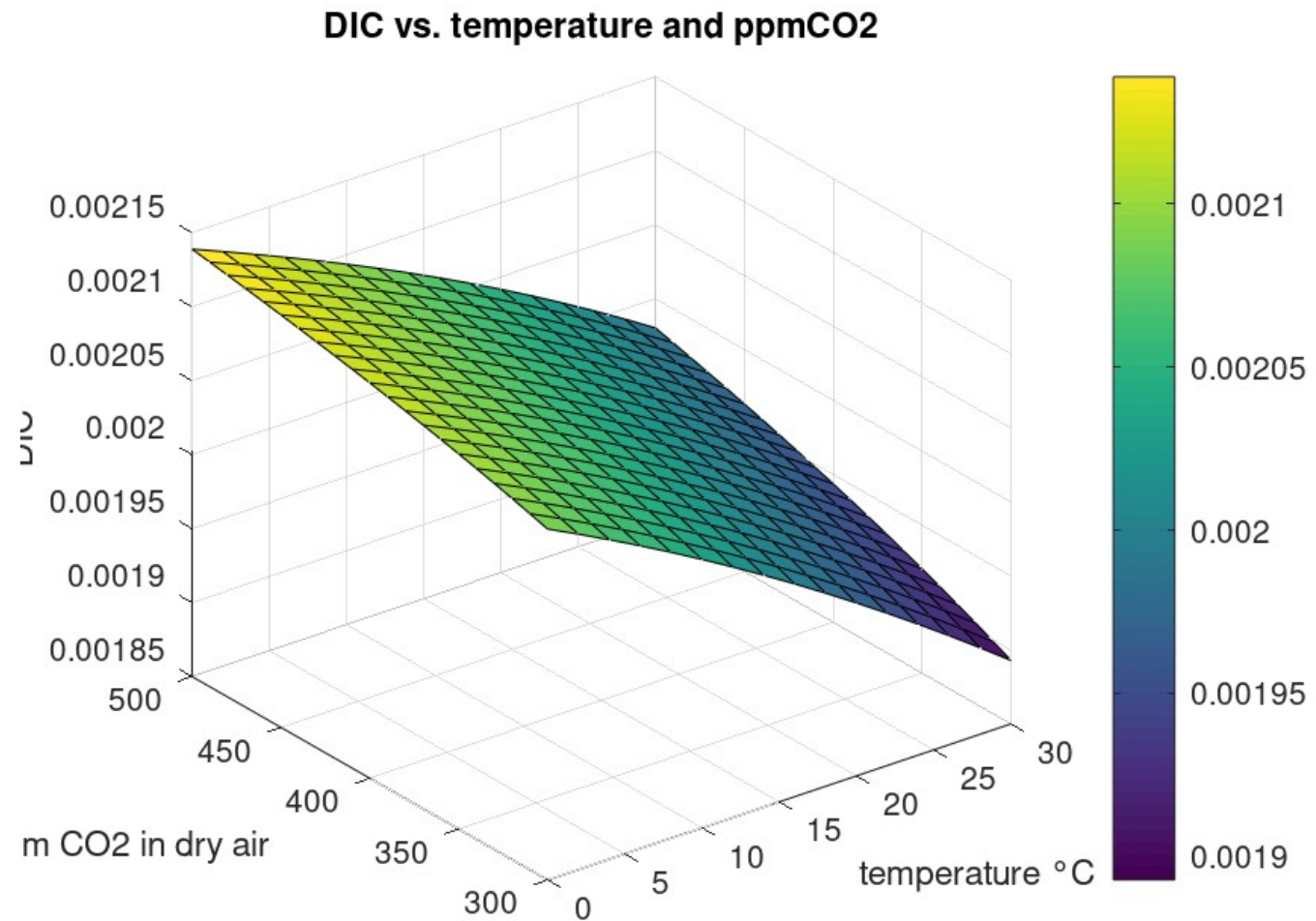
$$DIC[mmol/kg-soln] = [H_2CO_3]^* + [HCO_3^-] + [CO_3^{2-}] \quad \text{where} \quad [H_2CO_3]^* = [CO_2]_{aq} + [H_2CO_3]$$

The above graphs refer to a standard seawater salinity of 35 g/kg-soln and therefore to an imbalance of 0.00218 mol/kg-soln; This value can be varied according to a specific line in the script:

$$Imb = 0.00218 * 35 / S \quad (S = \text{salinity in g/kg-soln})$$

The program calculates the equilibrium values of DIC as a function of temperature and CO₂ concentration. However seawater reaches the thermodynamic equilibrium with a delay of some months.

Click here to learn more about seawater [chemical composition](#) ; [pH scales](#); [ionic strength](#) of seawater



Hydration of Carbon Dioxide (K_0) $\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{CO}_3$

$$K_0 = \frac{[H_2CO_3^*]}{f(CO_2)}$$

$$K_0 = \exp\left\{\frac{9345.17}{T} - 60.2409 + 23.3585 \cdot \log\left(\frac{T}{100}\right) + S \cdot [0.023517 - 0.00023656 \cdot T + 0.0047036 \cdot \left(\frac{T}{100}\right)^2]\right\} \quad T[K] \quad S[g/kg-soln], \quad \log = \log_e$$

$f(CO_2)$ is the fugacity of CO₂, which is numerically very similar to CO₂ partial pressure in μatm or ppmv (parts per million in volume), if total pressure is 1 atm. by the Dalton law. For sake of simplicity, here the CO₂ fugacity is approximated by its ppmv concentration, which in turn corresponds to its partial pressure in μatm for an total pressure of 1 atm..

H₂CO₃* is the sum of the true acid form H₂CO₃ and the hydrated CO₂, indicated by CO₂(aq). From now on asterisk is omitted, so that [H₂CO₃] indicates the sum of acid form and hydrated CO₂. The algorithm is taken from [Zeebe,2001](#)

Ionic Water Product due to 2 H₂O <==> H₃O⁺ + OH⁻ reaction

$$K_w = [H^+] \cdot [OH^-]$$

Water itself is a weak electrolyte whose dissociation must be carefully taken into account. In seawater the following expression is used to represent its dependence on temperature and salinity. As is the case for the following expressions, it should not be extrapolated to zero or near zero salinity, as it results from experiments with salinity from 25 to 45 (grams-of-salts/Kg-of-solution) (Zeebe,2001).

$$K_w = \exp\left\{148.96502 - \frac{13847.26}{T} - 23.6521 \cdot \log(T) + \left[\frac{118.67}{T} - 5.977 + 1.0495 \cdot \log(T)\right] \cdot S^{0.5} - 0.01615 \cdot S\right\}$$

$[H^+] = \text{Total scale}, \quad \log = \log_e, \quad pH = pH_{SWS}$

First Dissociation of Carbon Dioxide (K₁) H₂CO₃ <==> H⁺ + HCO₃⁻

$$K_1 = \frac{[HCO_3^-] \cdot [H^+]}{[H_2CO_3]}$$

$$K_1 = -10^{\wedge}\left\{\frac{6320.813}{T} + 19.568224 \cdot \log(T) - 126.34048 + 5.592953 \cdot S^{0.5} + 0.028845 \cdot S - (6.388 \cdot 10^{-5}) \cdot S^2 + \frac{(-225.7489 \cdot S^{0.5} - 4.761 \cdot S)}{T} - 0.8715109 \cdot S^{0.5} \cdot \log(T)\right\}$$

(Waters,2014) $T[K]$ $S[g/kg-soln]$ $\log = \log_e$, $pH = Free Scale$

Second Dissociation Constant of Carbon Dioxide (K_2) $HCO_3^- \rightleftharpoons H^+ + HCO_3^{2-}$

$$K_2 = \frac{[CO_3^{2-}] \cdot [H^+]}{[HCO_3^-]}$$

$$K_2 = -10^{\left\{ \frac{5143.692}{T} + 14.613358 \cdot \log(T) - 90.18333 + 13.396949 \cdot S^{0.5} + 0.12193009 \cdot S - (3.8362 \cdot 10^{-4}) \cdot S^2 + \frac{(-472.8633 \cdot S^{0.5} - 19.03634 \cdot S)}{T} - 2.1563270 \cdot S^{0.5} \cdot \log(T) \right\}}$$

(Waters,2014) $T[K]$, $\log = \log_e$, $pH = Free Scale$

```
clear;clc;format shortE;format compact;
global K1 K2 Kw H2CO3 HCO3 CO3 OH H Imb

function y = neut(pH) % ==> pH free scale, i.e. chemical true scale, always used if not otherwise stated !!
    global K1 K2 Kw H2CO3 HCO3 CO3 OH H Imb
    H = 10^(-pH);
    HCO3 = K1*H2CO3/H;
    CO3 = K2*HCO3/H;
    OH = Kw/H;
    y = Imb + H - OH - HCO3 - 2*CO3;
endfunction

R = 8.314;
i = 0;S = 35; % salinity, in grams of salts in 1 kg of solution , this can be varied
for Tc = 0:2:30 % temperature in Celsius (°C)
    ++i;j = 0;
    T = Tc + 273.15;Imb = 0.00218;
    Imb = Imb*35/S;
    % H2CO3 <==> H+ + HCO3- (Waters,2014)
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LnK1 = -log(10)*(6320.813/T + 19.568224*log(T) -126.34048 + 5.592953*S^0.5 + 0.028845*S - (6.388e-5)*S^2 + (-225.7489*S^0.5 -
4.761*S)/T -0.8715109*S^0.5*log(T));
% HCO3- <==> H+ + CO3-- (Waters,2014)
LnK2 = -log(10)*(5143.692/T + 14.613358*log(T) - 90.18333 + 13.396949*S^0.5 + 0.12193009*S - (3.8362e-4)*S^2 + (-472.8633*S^0.5 -
19.03634*S)/T - 2.1563270*S^0.5*log(T));
% CO2 + H2O <==> H2CO3 (Zeebe,2001)
LnK0 = 9345.17/T - 60.2409 + 23.3585*log(T/100) + S*(0.023517 - 0.00023656*T + 0.0047036*(T/100)^2);
% H2O <==> H+ + OH- (DOE 1994) (Zeebe,2001) pH = pH(SWS) considered = pH free !
LnKw = 148.9802 - 13847.26/T - 23.6521*log(T) + (118.67/T - 5.977 + 1.0495*log(T))*S^0.5 - 0.01615*S;
K1 = exp(LnK1);K2 = exp(LnK2);K0 = exp(LnK0);Kw = exp(LnKw);
for ppmCO2 = 300:10:500 % parts per million (in volume) of CO2 in the atmosphere
    H2CO3 = K0*ppmCO2*1e-6;++j;
    [pH,fval,info] = fzero(@neut,[0,14]); % call to fzero
    DIC(i,j) = H2CO3 + HCO3 + CO3;
    temp(i,j) = Tc;ppm(i,j) = ppmCO2;
endfor
endfor
plot(temp(:,11),DIC(:,11)*1000,'r','LineWidth',2);grid on;grid minor on;xlabel('temperature °C');ylabel('DIC [mmol/kg]')
title('DIC versus temperature @ 400 ppm CO2');
figure;
plot(ppm(11,:),DIC(11,:)*1000,'r','LineWidth',2);grid on;grid minor on;xlabel('ppm CO2 in dry air');ylabel('DIC [mmol/kg]')
title('DIC versus ppmCO2 @ 20 °C');
figure;
surf(temp,ppm,DIC);colorbar;title('DIC vs. temperature and ppmCO2');
xlabel('temperature °C');ylabel('ppm CO2 in dry air');zlabel('DIC');

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