Package ‘seacarb’

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Description

The variables are:

- volume: Volume of acid added to the sample in ml
- E: Potential measured during the titration in mV
- temperature: Temperature in degrees Celsius
- weight: Weight of the sample in g
- S: Salinity
- normality: Normality of the acid
- ETris: Potential used for the calibration of the electrode in mV
- pHTris: pH used for the calibration of the electrode with the TRIS buffer

Usage

alkalinity

Format

A data frame with 29 rows and 8 variables
amp

Source
Data come from a potentiometric titration performed by Steeve Comeau.

Description
pH value of the AMP buffer (on the total scale in mol/kg)

Usage
amp(S=35,T=25)

Arguments
S Salinity, default is 35
T Temperature in degrees Celsius, default is 25°C

Details
Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value
AMP pH value of the AMP buffer (on the total scale in mol/kg)

Author(s)
Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

See Also
tris, phslope, pH.

Examples

# Example from Dickson et al. (2007)
amp(S=35,T=25)
Calculates total alkalinity from potentiometric titration data

Description
Calculates total alkalinity from potentiometric titration data

Usage
\[ \texttt{at}(S=35, \ T=25, \ C=0.1, \ d=1, \ \texttt{pHTris}=\texttt{NULL}, \ \texttt{ETris}=\texttt{NULL}, \ \texttt{weight}, \ E, \ \texttt{volume}) \]

Arguments
- **S**: Salinity, default is 35. S must be a single value, not a vector.
- **T**: Temperature in degrees Celsius, default is 25°C, can be given as a vector or as a single value.
- **C**: Normality of the acid, default is 0.1. C must be a single value, not a vector.
- **d**: Density of the acid, default is 1. d must be a single value, not a vector.
- **pHTris**: pH used for the calibration of the electrode with the TRIS buffer. pHTris must be a single value, not a vector.
- **ETris**: Potential used for the calibration of the electrode in mV. ETris must be a single value, not a vector.
- **weight**: Weight of the sample in g. weight must be a single value, not a vector.
- **E**: Potential measured during the titration in mV. E must be a vector.
- **volume**: Volume of acid added to the sample in ml. volume must be a vector.

Details
Total alkalinity is estimated using the non-linear least-square procedure described by Dickson et al. (2007).

Value
\[ \text{AT} \quad \text{Total alkalinity in mol/kg} \]

Author(s)
Steeve Comeau, Heloise Lavigne and Jean-Pierre Gattuso

References
Bjerrum plot

Description
Plot the concentration of the various ionic forms of a molecule as a function of pH

Usage
bjerrum(K1=k1, K2=NULL, K3=NULL, phmin=2, phmax=12, by=0.1, conc=1, type="l", col="black", ylab="Relative concentration (%)", add=FALSE, ...)

Arguments
- K1: First dissociation constant
- K2: Second dissociation constant, default is NULL
- K3: Third dissociation constant, default is NULL
- phmin: Minimum pH value, default is 2
- phmax: Maximum pH value, default is 12
- by: Increment on the pH axis, default is 0.1
- conc: Concentration of molecule, default is 1
- type: Type of plot, default is line
- col: Color of plot, default is black
- ylab: Label of Y axis, default is (mol/kg)
- add: false: start new, true: add to current, default is false
- ...: Graphical parameters (see \texttt{par}) and any further arguments of \texttt{plot}, typically \texttt{plot.default}, may also be supplied as arguments to this function. Hence, the high-level graphics control arguments described under \texttt{par} and the arguments to \texttt{title} may be supplied to this function.

Details
Note that the concentration is plotted in mol/kg only if \texttt{conc} is given in mol/kg

See Also
alkalinity

Examples
data(alkalinity)
data \leftarrow alkalinity
AT \leftarrow \text{at}(S=\text{data}\$[1], T=\text{data}\$temperature, C=\text{data}\$normality[1], pHTris=\text{data}\$pHTris[1],
ETris=\text{data}\$ETris[1], E=\text{data}\$E, weight=\text{data}\$weight[1], volume=\text{data}\$volume)
bjerrum

Author(s)

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References


See Also

matplot, par, speciation.

Examples

## Plot the bjerrum plot for the carbonate system using the default values
bjerrum(K1(),K2(),main="DIC speciation",lwd=2)
abline(v=-log10(K1()),col="grey")
mtext(side=3,at=-log10(K1()),"pK1")
abline(v=-log10(K2()),col="grey")
mtext(side=3,at=-log10(K2()),"pK2")

## Plot the bjerrum plot for the carbonate system using the values other than the default ones, showing the effect of temperature
bjerrum(K1(T=25,S=35),K2(T=25,S=35),conc=1.3,main="effect of temperature")
bjerrum(K1(T=0,S=35),K2(T=0,S=35),conc=1.3,add=TRUE,col="red")
legend("left",lty=1,col=c("black","red"),legend=c("T=25 °C","T=0 °C"))

## Plot the bjerrum plot for the carbonate system using the values other than the default ones, showing the effect of salinity
bjerrum(K1(T=25,S=35),K2(T=25,S=35),conc=1.3,main="effect of salinity")
bjerrum(K1(T=25,S=5),K2(T=25,S=5),conc=1.3,add=TRUE,col="blue")
legend("left",lty=1,col=c("black","blue"),legend=c("S=35","S=5"))

## Plot the bjerrum plot for the carbonate system using the values other than the default ones, showing the effect of pressure
bjerrum(K1(P=0),K2(P=0),conc=1.3,main="effect of pressure")
bjerrum(K1(P=300),K2(P=300),conc=1.3,add=TRUE,col="green")
legend("left",lty=1,col=c("black","green"),legend=c("P=0","P=300"),title="atm")
**Total boron concentration (mol/kg)**

**Description**

Total boron concentration \((\text{mol kg}^{-1})\)

**Usage**

\(\text{bor}(S, b)\)

**Arguments**

- \(S\) : Salinity, default is 35
- \(b\) : "l10" for using the formulation of Lee et al. (2010), "u74" for using the Uppstrom (1974), or "k18" for using the Kulinski et al. (2018), default is "u74"

**Details**

Note that the formulation of Kulinski et al. (2018) is specifically designed for the Baltic Sea. Three formulations are described in their paper:

- based on their measurements: \(\text{TB} = [\text{umol/kg}] = 10.838 \times S + 13.821\)
- based on Kremling (1970 and 1972): \(\text{TB} [\text{umol/kg}] = 11.44 \times S + 12.6; \text{R}^2 = 0.95\)
- consensus regression (Kremling + their data): \(\text{TB} [\text{umol/kg}] = 11.405 \times S + 11.869; \text{R}^2 = 0.97\)

The latter formulation is used here.

**Value**

\(\text{bor}\) : total boron concentration \((\text{mol kg}^{-1})\)

**Author(s)**

Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

**References**


Examples

```
bor(35, "110")
```

---

**buffer**

*Buffer parameters of the seawater carbonate system*

---

**Description**

Returns buffer parameters of the seawater carbonate system.

**Usage**

```
buffer(flag, var1, var2, S = 35, T = 25, Patm = 1, P = 0, Pt = 0, Sit = 0,
k1k2 = "x", kf = "x", ks = "d", pHscale = "T", b = "u74", warn = "y",
eos = "eos80", long = 1e+20, lat = 1e+20)
```

**Arguments**

- **flag**: select the couple of variables available. The flags which can be used are:
  - flag = 1 pH and CO2 given
  - flag = 2 CO2 and HCO3 given
  - flag = 3 CO2 and CO3 given
  - flag = 4 CO2 and ALK given
  - flag = 5 CO2 and DIC given
  - flag = 6 pH and HCO3 given
  - flag = 7 pH and CO3 given
  - flag = 8 pH and ALK given
  - flag = 9 pH and DIC given
  - flag = 10 HCO3 and CO3 given
  - flag = 11 HCO3 and ALK given
  - flag = 12 HCO3 and DIC given
  - flag = 13 CO3 and ALK given
  - flag = 14 CO3 and DIC given
  - flag = 15 ALK and DIC given
  - flag = 21 pCO2 and pH given
  - flag = 22 pCO2 and HCO3 given
  - flag = 23 pCO2 and CO3 given
  - flag = 24 pCO2 and ALK given
  - flag = 25 pCO2 and DIC given
var1  enter value of the first variable in mol/kg, except for pH and for pCO2 in µatm
var2  enter value of the second variable in mol/kg, except for pH
S  Salinity
T  Temperature in degrees Celsius
Patm  Surface atmospheric pressure in atm
P  Hydrostatic pressure in bar (surface = 0)
Pt  Concentration of total phosphate in mol/kg; set to 0 if NA
Sit  Concentration of total silicate in mol/kg; set to 0 if NA
k1k2  "l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "w14".
kf  "pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks  "d" for using Ks from Dickson (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
phscale  choice of pH scale: "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b  Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"
warn  "y" to show warnings when T or S go beyond the valid range for constants; "n" to supress warnings. The default is "y".
eos  "teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.
long  longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.
lat  latitude of data point, used when eos parameter is "teos10".

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

• Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
• Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
• Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
• Millero (2010): $S$ ranging between 1 and 50 and $T$ ranging between 0 and 50°C. Millero (2010) provides a $K_1$ and $K_2$ formulation for the seawater, total and free pH scales. Therefore, when this method is used and if $P>0$, $K_1$ and $K_2$ are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For $K_f$:

• Perez and Fraga (1987): $S$ ranging between 10 and 40 and $T$ ranging between 9 and 33°C.
• Dickson and Riley (1979 in Dickson and Goyet, 1994): $S$ ranging between 0 and 45 and $T$ ranging between 0 and 45°C.

For $K_s$:

• Dickson (1990): $S$ ranging between 5 and 45 and $T$ ranging between 0 and 45°C.
• Khoo et al. (1977): $S$ ranging between 20 and 45 and $T$ ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

• For $K_0$, the pressure correction term of Weiss (1974) is used.
• For $K_1$, $K_2$, $pK_1$, $pK_2$, $pK_3$, $K_w$, $K_b$, $K_{hs}$ and $K_{si}$, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For $K_f$, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides $K_f$ on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, $K_f$ was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For $K_s$, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For $K_n$, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.
Value

The function returns a data frame containing the following columns:

- **PhiD**: PhiD, chemical buffer factor \( (d\text{pH}/d[\text{DIC}]) \); input/output of dissolved CO2 (unit pH per mol/kg)
- **BetaD**: BetaD, homogeneous or Revelle buffer factor \( (d\ln(p\text{CO}_2)/d\ln[\text{DIC}]) \); input/output of dissolved CO2
- **PiD**: PiD, chemical buffer factor \( (d\text{pCO}_2/d[\text{DIC}]) \); input/output of dissolved CO2 (\( \mu \text{atm} \) per mol/kg)
- **PhiB**: PhiB, chemical buffer factor \( (d\text{pH}/d[\text{DIC}]) \); from input/output of bicarbonate (unit pH per mol/kg)
- **BetaB**: BetaB, homogeneous buffer factor \( (d\ln(p\text{CO}_2)/d\ln[\text{DIC}]) \); input/output of bicarbonate
- **PiB**: PiB, chemical buffer factor \( (d\text{pCO}_2/d[\text{DIC}]) \); input/output of dissolved CO2 (\( \mu \text{atm} \) per mol/kg)
- **PhiC**: PhiC, chemical buffer factor \( (d\text{pH}/d[\text{DIC}]) \); input/output of carbonate (unit pH per mol/kg)
- **BetaC**: BetaC, homogeneous buffer factor \( (d\ln(p\text{CO}_2)/d\ln[\text{DIC}]) \); input/output of carbonate
- **PiC**: PiC, chemical buffer factor \( (d\text{pCO}_2/d[\text{DIC}]) \); input/output of carbonate (\( \mu \text{atm} \) per mol/kg)
- **PhiH**: PhiH, chemical buffer factor \( (d\text{pH}/d[\text{ALK}]) \); input/output of strong acid (unit pH per mol/kg)
- **PiH**: PiH, chemical buffer factor \( (d\text{pCO}_2/d[\text{ALK}]) \); input/output of strong acid (\( \mu \text{atm} \) per mol/kg)

Author(s)

Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-v1fr.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: \( \text{AgCl(s) + 1/2H}_2\text{(g)} = \text{Ag(s) + HCl(aq)} \), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* **22**, 113-127.


**Examples**

```r
# Computation with a couple of variables
buffer(flag=8, var1=8.2, var2=0.00234, S=35, T=25, Patm=1, P=0, Pt=0,
Sit=0, pHscale="T", kf="pf", k1k2="1", b="u74")

# Using vectors as arguments
flag <- c(8, 2, 8)
var1 <- c(8.2, 7.477544e-06, 8.2)
var2 <- c(0.002343955, 0.001649882, 2400e-6)
S <- c(35, 35, 30)
T <- c(25, 25, 30)
P <- c(0, 0, 0)
Pt <- c(0, 0, 0)
Sit <- c(0, 0, 0)
kf <- c("pf", "pf", "pf")
k1k2 <- c("1", "1", "1")
pHscale <- c("T", "T", "T")
b <- c("110", "110", "110")
buffer(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P, Pt=Pt,
Sit=Sit, kf=kf, k1k2=k1k2, pHscale=pHscale, b=b)

# Test for all flags
flag <- c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 21, 22, 23, 24, 25)
var1 <- c(8.200000, 7.477544e-06, 7.477544e-06, 7.477544e-06, 7.477544e-06, 8.2,
8.2, 8.2, 0.001685024, 0.001685024, 0.001685024, 0.0002888382, 0.0002888382,
var2 <- c(7.477544e-06, 0.001685024, 0.0002888382, 0.002391252, 0.001981340,
0.001685024, 0.0002888382, 0.002391252, 0.001981340, 0.0002888382, 0.002391252,
```
Buffer factors of the seawater carbonate system as defined by Hagens and Middelburg (2016)

Description

Returns the suite of buffer factors presented in Table 3 of Hagens and Middelburg (2016), as well as the proton concentration buffer factor (beta.H of Hofmann et al, 2010) and the classic Revelle factor. For practical purposes, this function excludes the nitrate and nitrite acid-base systems presented in this paper, as well as the fully protonated form of sulfate (H2SO4) and fully deprotonated form of sulfide (S2-), as their contributions to total alkalinity under natural seawater conditions are negligible. Its input arguments are identical to those in the carbfull function of seacarb.

Usage

`buffergen(flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0, k1k2="x", kf="x", ks="d", phscale="T", b="u74", gas="potential", NH4t=0, HSt=0)`

Arguments

- `flag`: select the couple of variables available. The flags which can be used are:
  - `flag = 1` pH and CO2 given
  - `flag = 2` CO2 and HCO3 given
  - `flag = 3` CO2 and CO3 given
  - `flag = 4` CO2 and ALK given
  - `flag = 5` CO2 and DIC given
  - `flag = 6` pH and HCO3 given
  - `flag = 7` pH and CO3 given
  - `flag = 8` pH and ALK given
  - `flag = 9` pH and DIC given
  - `flag = 10` HCO3 and CO3 given
  - `flag = 11` HCO3 and ALK given
  - `flag = 12` HCO3 and DIC given
  - `flag = 13` CO3 and ALK given
  - `flag = 14` CO3 and DIC given
  - `flag = 15` ALK and DIC given
  - `flag = 21` pCO2 and pH given
  - `flag = 22` pCO2 and HCO3 given
  - `flag = 23` pCO2 and CO3 given
flag = 24 pCO2 and ALK given
flag = 25 pCO2 and DIC given

var1
Value of the first variable in mol/kg, except for pH and for pCO2 in µatm

var2
Value of the second variable in mol/kg, except for pH

S
Salinity

T
Temperature in degrees Celsius

Patm
Surface atmospheric pressure in atm, default is 1 atm

P
Hydrostatic pressure in bar (surface = 0)

Pt
Concentration of total phosphate in mol/kg; set to 0 if NA

Sit
Concentration of total silicate in mol/kg; set to 0 if NA

k1k2
"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".

kf
"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".

ks
"d" for using Ks from Dickson (1990) and "k" for using Ks from Khoo et al. (1977), default is "d"

pHscale
"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)

b
Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

gas
used to indicate the convention for INPUT pCO2, i.e., when it is an input variable (flags 21 to 25): "insitu" indicates it is referenced to in situ pressure and in situ temperature; "potential" indicates it is referenced to 1 atm pressure and potential temperature; and "standard" indicates it is referenced to 1 atm pressure and in situ temperature. All three options should give identical results at surface pressure. This option is not used when pCO2 is not an input variable (flags 1 to 15). The default is "potential" and should be a unique value..

NH4t
Concentration of total ammonium in mol/kg; set to 0 if NA

HSt
Concentration of total hydrogen sulfide in mol/kg; set to 0 if NA

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
• Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
• Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50°C.
• Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:
• Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
• Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.

For Ks:
• Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45°C.
• Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:
• For K0, the pressure correction term of Weiss (1974) is used.
• For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs, Ksi and K2si, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Kn, the pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value
The function returns a list containing the following matrices:
Carbful1 Output of the carbfull function that is used within buffergen
buffergen

\[ d\text{ALK} \cdot dH \]
Sensitivity of ALK to a change in proton concentration (dimensionless). Species-specific.

\[ dtotX \cdot dH \]
Sensitivity of an acid-base species to a change in proton concentration (dimensionless). Species-specific.

\[ d\text{ALK} \cdot dX \]
Sensitivity of ALK to a change in an acid-base species (dimensionless). Species-specific.

\[ dtotX \cdot dX \]
Sensitivity of an acid-base species to a change in its total concentration (dimensionless). Species-specific.

\[ d\text{ALK} \cdot dpH \]
Sensitivity of ALK to a change in pH (mol/kg-soln). Species-specific.

\[ dtotX \cdot dpH \]
Sensitivity of an acid-species to a change in pH (mol/kg-soln). Species-specific.

\[ dH \cdot d\text{ALK} \]
Sensitivity of proton concentration to a change in ALK (dimensionless). Values are the same for all species and all acid-base systems, except for the fluoride and sulfate acid-base systems, which slightly deviate due to pH scale conversion effects.

\[ dH \cdot dtotX \]
Sensitivity of an acid-species to a change in its total concentration (dimensionless). Values are the same for all species of a specific acid-base system.

\[ dX \cdot d\text{ALK} \]
Sensitivity of an acid-species to a change in its total concentration (dimensionless). Species-specific.

\[ dX \cdot dtotX \]
Sensitivity of an acid-species to a change in its total concentration (dimensionless). Species-specific.

\[ dpH \cdot d\text{ALK} \]
Sensitivity of pH due to a change in ALK ((mol/kg-soln)-1). Values are the same for all species and all acid-base systems, except for the fluoride and sulfate acid-base systems, which slightly deviate due to pH scale conversion effects.

\[ dpH \cdot dtotX \]
Sensitivity of pH due to a change in the total concentration of an acid-base system ((mol/kg-soln)-1). Values are the same for all species of a specific acid-base system.

\[ \text{beta.H} \]
proton concentration buffer factor (Eq.4 of Hagens and Middelburg (2016), dimensionless)

\[ RF \]
Revelle factor (dimensionless)

If the total concentration of an acid-base system is 0, the values of the buffer factors corresponding to all species of that acid-base system return NA.

Author(s)
Mathilde Hagens <m.hagens@uu.nl>

References
Examples

```r
# With a couple of variables
buffergen(flag=8, var1=8.2, var2=0.00234, S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0, phscale="T", kfs="pf", klk2="1", ks="d", b="u74", gas="potential", NH4t=0, HSt=0)

# With a couple of variables and non-zero nutrient concentrations
buffergen(flag=8, var1=8.2, var2=0.00234, S=35, T=25, P=0, Patm=1.0, Pt=5e-6, Sit=2e-6, phscale="T", kfs="pf", klk2="1", ks="d", b="u74", gas="potential", NH4t=10e-6, HSt=0.1e-6)

# Using vectors as arguments
flag <- c(8, 2, 8)
var1 <- c(8.2, 7.477544e-06, 8.2)
var2 <- c(0.002343955, 0.001649802, 2400e-6)
S <- c(35, 35, 30)
T <- c(25, 25, 30)
P <- c(0, 0, 0)
Pt <- c(0, 0, 0)
Sit <- c(0, 0, 0)
kf <- c("pf", "pf", "pf")
klk2 <- c("1", "1", "1")
phscale <- c("T", "T", "T")
b <- c("110", "110", "110")
gas <- c("potential")
NH4t <- c(0, 0, 0)
HSt <- c(0, 0, 0)
buffergen(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P, Pt=Pt, Sit=Sit, kf=kf, klk2=klk2, phscale=phscale, b=b, gas=gas, NH4t=NH4t, HSt=HSt)

# Test with all flags
flag <- c((1:15), (21:25))
var1 <- c(8.2000000, 7.308171e-06, 7.308171e-06, 7.308171e-06, 7.308171e-06, 8.2, 8.2, 8.2, 8.2, 0.001646857, 0.001646857, 0.001646857, 0.0002822957, 0.0002822957, 0.00234, 258.2164, 258.2164, 258.2164, 258.2164, 258.2164)
var2 <- c(7.308171e-06, 0.001646857, 0.0002822957, 0.00234, 0.01936461, 0.00234, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461, 0.001936461)
buffergen(flag=flag, var1=var1, var2=var2)
```

**buffesm**

*Buffer capacities of the seawater carbonate system from Egleston et al. (2010), corrected and enhanced*

**Description**

Returns the six buffer factors of the seawater carbonate system as defined by Egleston, Sabine and Morel (2010), denoted here as ESM. Also returns the classic Revelle factor (relative change in pCO2 over that for DIC). In ESM, there are errors in the equations in Table 1 for $S$, $\Omega_{DIC}$,
and $\Omega_{\text{ALK}}$. These errors have been corrected here. The results of this routine have been validated: when input concentrations of Pt and Sit are set to zero, they produce results that are identical to those shown in ESM’s Fig. 2. But when Pt and Sit are nonzero, contributions from phosphoric and silicic acid systems are taken into account, an improvement to the Egleston et al. (2010) approach. This routine was inspired and adapted from seacarb’s “buffer” function. Its input arguments are identical to those in the “buffer” and “carb” functions of seacarb.

**Usage**

```plaintext
buffesm(flag, var1, var2, S = 35, T = 25, Patm = 1, P = 0, Pt = 0, Sit = 0, k1k2 = "x", kf = "x", ks = "d", phscale = "T", b = "u74", warn = "y", eos = "eos80", long = 1e+20, lat = 1e+20)
```

**Arguments**

- **flag**: select the couple of variables available. The flags which can be used are:
  - `flag = 1` pH and CO2 given
  - `flag = 2` CO2 and HCO3 given
  - `flag = 3` CO2 and CO3 given
  - `flag = 4` CO2 and ALK given
  - `flag = 5` CO2 and DIC given
  - `flag = 6` pH and HCO3 given
  - `flag = 7` pH and CO3 given
  - `flag = 8` pH and ALK given
  - `flag = 9` pH and DIC given
  - `flag = 10` HCO3 and CO3 given
  - `flag = 11` HCO3 and ALK given
  - `flag = 12` HCO3 and DIC given
  - `flag = 13` CO3 and ALK given
  - `flag = 14` CO3 and DIC given
  - `flag = 15` ALK and DIC given
  - `flag = 21` pCO2 and pH given
  - `flag = 22` pCO2 and HCO3 given
  - `flag = 23` pCO2 and CO3 given
  - `flag = 24` pCO2 and ALK given
  - `flag = 25` pCO2 and DIC given

- **var1**: enter value of the first variable in mol/kg, except for pH and for pCO2 in µatm

- **var2**: enter value of the second variable in mol/kg, except for pH

- **S**: Salinity

- **T**: Temperature in degrees Celsius

- **Patm**: Surface atmospheric pressure in atm, default 1 atm

- **P**: Hydrostatic pressure in bar (surface = 0)

- **Pt**: Concentration of total phosphate in mol/kg; set to 0 if NA; when nonzero, account for phosphoric acid system, unlike in Egleston et al. (2010).
**Sit**  Concentration of total silicate in mol/kg; set to 0 if NA; when nonzero, account for silicic acid system, unlike in Egleston et al. (2010).

**k1k2**  "l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

**kf**  "pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is "dg".

**ks**  "d" for using Ks from Dickson (1990), "k" for using Ks from Khoo et al. (1977), default is "d"

**pHscale**  choice of pH scale: "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)

**b**  Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

**warn**  "y" to show warnings when T or S go beyond the valid range for constants; "n" to suppress warnings. The default is "y".

**eos**  "teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.

**long**  longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

**lat**  latitude of data point, used when eos parameter is "teos10".

**Details**

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50°C.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag? "pHscale".

For K0:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.
For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, the pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

Value

The function returns a data frame containing the following columns:

- **gammaDIC**: $\gamma_{DIC}$, ocean’s capacity to buffer changes in [CO2] due to accumulation of CO2 from the atmosphere $(\partial \ln [CO_2]/\partial DIC)^{-1}$ (units = mol/kg; multiply by 1000 to get mmol/kg, i.e., the units presented in Egleston et al., 2010)
- **betaDIC**: $\beta_{DIC}$, ocean’s capacity to buffer changes in [H+] due to accumulation of CO2 from the atmosphere $(\partial \ln [H^+]/\partial DIC)^{-1}$ (units = mol/kg)
- **omegaDIC**: $\Omega_{DIC}$, ocean’s capacity to buffer changes in $[CO_3^{2-}]$ due to accumulation of CO2 from the atmosphere $(\partial \ln [CO_3^{2-}]/\partial DIC)^{-1}$; same as $(\partial \ln \Omega_A/\partial DIC)^{-1}$ and $(\partial \ln \Omega_C/\partial DIC)^{-1}$ (units= mol/kg)
gammaALK \( \gamma_{Alk} \), ocean’s capacity to buffer changes in [CO2] due to changes in alkalinity \((\partial \ln [CO_2] / \partial ALK) \) (units = mol/kg)

betaALK \( \beta_{Alk} \), ocean’s capacity to buffer changes in [H+] due to changes in alkalinity \((\partial \ln [H^+] / \partial ALK) \) (units = mol/kg)

omegaALK \( \Omega_{Alk} \), ocean’s capacity to buffer changes in \([CO_2^2^-]\) due to changes in alkalinity \((\partial \ln [CO_2^2^-] / \partial ALK) \) (units = mol/kg)

R \( R \), Revelle factor, relative change in \([CO_2]\) or \(pCO_2\) over the relative change in DIC \((\partial \ln [CO_2] / \partial \ln DIC) \) (unitless)

Author(s)

James Orr <James.Orr@lsce.ipsl.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* **22**, 113-127.


**Examples**

```r
## Computation with a couple of variables
buffersm(flag=8, var1=8.2, var2=0.002343955, S=35, T=25, P=0, Pt=0, Sit=0, pHscale="T", kT="pf", k1k2="1", b="u74")

## Using vectors as arguments
flag <- c(8, 2, 8)
var1 <- c(8.2, 7.477544e-06, 8.2)
var2 <- c(0.002343955, 0.001649802, 2400e-6)
S <- c(35, 35, 30)
T <- c(25, 25, 30)
P <- c(0, 0, 0)
Pt <- c(0, 0, 0)
Sit <- c(0, 0, 0)
kf <- c("pf", "pf", "pf")
k1k2 <- c("1", "1", "1")
pHscale <- c("T", "T", "T")
b <- c("110", "110", "110")
buffersm(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P, Pt=Pt, Sit=Sit, kf=kf, k1k2=k1k2, pHscale=pHscale, b=b)

## Test for all flags
flag <- c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 21, 22, 23, 24, 25)

var1 <- c(8.200000, 7.477544e-06, 7.477544e-06, 7.477544e-06, 8.2, 8.2, 8.2, 8.2, 0.001685024, 0.001685024, 0.001685024, 0.0002888382, 0.0002888382, 0.002391252, 264.2008, 264.2008, 264.2008, 264.2008, 264.2008)
var2 <- c(7.477544e-06, 0.001685024, 0.0002888382, 0.002391252, 0.001981340, 0.001981340, 0.001981340, 0.001981340, 264.2008, 0.002391252, 0.0002888382, 0.002391252, 0.002391252, 0.002391252, 0.002391252, 0.002391252, 0.0002888382, 0.0002888382, 0.0002888382)

buffersm(flag=flag, var1=var1, var2=var2)

## Compute 2 additional factors of interest (ratios of relative changes)
be <- buffersm(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P, Pt=Pt, Sit=Sit, kf=kf, k1k2=k1k2, pHscale=pHscale, b=b)
# Ratio of gammaDIC/betaDIC = d ln [H+] / d ln pCO2
HFac <- (be$gammaDIC/be$betaDIC)  # H+ factor
# Ratio of gammaDIC/omegaDIC = d ln [CO32-] / d ln pCO2
SatFac <- (be$gammaDIC/be$omegaDIC)  # Saturation factor
```

Parameters of the seawater carbonate system
Description

Returns parameters of the seawater carbonate system.

Usage

```r
carb(flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0,
     k1k2="x", kf="x", ks="d", phscale="T", b="u74", gas="potential",
     warn="y", eos="eos80", long=1.e20, lat=1.e20)
```

Arguments

- **flag**: select the couple of variables available. The flags which can be used are:
  - `flag = 1` pH and CO2 given
  - `flag = 2` CO2 and HCO3 given
  - `flag = 3` CO2 and CO3 given
  - `flag = 4` CO2 and ALK given
  - `flag = 5` CO2 and DIC given
  - `flag = 6` pH and HCO3 given
  - `flag = 7` pH and CO3 given
  - `flag = 8` pH and ALK given
  - `flag = 9` pH and DIC given
  - `flag = 10` HCO3 and CO3 given
  - `flag = 11` HCO3 and ALK given
  - `flag = 12` HCO3 and DIC given
  - `flag = 13` CO3 and ALK given
  - `flag = 14` CO3 and DIC given
  - `flag = 15` ALK and DIC given
  - `flag = 21` pCO2 and pH given
  - `flag = 22` pCO2 and HCO3 given
  - `flag = 23` pCO2 and CO3 given
  - `flag = 24` pCO2 and ALK given
  - `flag = 25` pCO2 and DIC given

- **var1**: Value of the first variable in mol/kg, except for pH and for pCO2 in µatm
- **var2**: Value of the second variable in mol/kg, except for pH
- **S**: Salinity
- **T**: Temperature in degrees Celsius
- **Patm**: Surface atmospheric pressure in atm, default is 1 atm
- **P**: Hydrostatic pressure in bar (surface = 0)
- **Pt**: Concentration of total phosphate in mol/kg; set to 0 if NA
- **Sit**: Concentration of total silicate in mol/kg; set to 0 if NA
carb

k1k2
"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

kf
"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is "dg".

ks
"d" for using Ks from Dickson (1990) and "k" for using Ks from Khoo et al. (1977), default is "d"

pHScale
"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)

b
Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

gas
used to indicate the convention for INPUT pCO2, i.e., when it is an input variable (flags 21 to 25): "insitu" indicates it is referenced to in situ pressure and in situ temperature; "potential" indicates it is referenced to 1 atm pressure and potential temperature; and "standard" indicates it is referenced to 1 atm pressure and in situ temperature. All three options should give identical results at surface pressure. This option is not used when pCO2 is not an input variable (flags 1 to 15). The default is "potential".

warn
"y" to show warnings when T or S go beyond the valid range for constants; "n" to suppress warnings. The default is "y".

eos
"teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.

long
longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

lat
latitude of data point, used when eos parameter is "teos10".

Details
The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50°C.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHScale".

For Kf:
Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.

Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.

For Ks:

Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45°C.

Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

Value

The function returns a data frame containing the following columns:

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius</td>
</tr>
<tr>
<td>Patm</td>
<td>Surface atmospheric pressure in atm</td>
</tr>
</tbody>
</table>
P: Hydrostatic pressure in bar
pH: pH
CO2: CO2 concentration (mol/kg)
pCO2: "standard" pCO2, CO2 partial pressure computed at in situ temperature and atmospheric pressure (µatm)
fCO2: "standard" fCO2, CO2 fugacity computed at in situ temperature and atmospheric pressure (µatm)
pCO2pot: "potential" pCO2, CO2 partial pressure computed at potential temperature and atmospheric pressure (µatm)
fCO2pot: "potential" fCO2, CO2 fugacity computed at potential temperature and atmospheric pressure (µatm)
pCO2insitu: "in situ" pCO2, CO2 partial pressure computed at in situ temperature and total pressure (atm + hydrostatic) (µatm)
fCO2insitu: "in situ" fCO2, CO2 fugacity computed at in situ temperature and total pressure (atm + hydrostatic) (µatm)
HCO3: HCO3 concentration (mol/kg)
CO3: CO3 concentration (mol/kg)
DIC: DIC concentration (mol/kg)
ALK: ALK, total alkalinity (mol/kg)
OmegaAragonite: Omega aragonite, aragonite saturation state
OmegaCalcite: Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

Author(s)

Heloise Lavigne, James Orr and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. Journal of Chemical Thermodynamics 22, 113-127.


## Examples

```r
## With a couple of variables
carb(flag=8, var1=8.2, var2=0.000034, S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0, phscale="T", kf="pf", k1k2="1", ks="d", b="u74")
```

```r
## Using vectors as arguments
flag <- c(8, 2, 8)
var1 <- c(8.2, 7.477544e-06, 8.2)
var2 <- c(0.0000343955, 0.0001649882, 2400e-6)
S <- c(35, 35, 30)
T <- c(25, 25, 30)
P <- c(0, 0, 0)
Pt <- c(0, 0, 0)
```
carbb

Parameters of the seawater carbonate system with boron addition

Description

Returns parameters of the seawater carbonate system when boron is added.

Usage

```
carbb(flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0,
    k1k2="x", kf="x", ks="d", pHscale="T", b="u74", gas="potential", badd=0,
    warn="y", eos = "eos80", long = 1e+20, lat = 1e+20)
```

Arguments

- **flag**: select the couple of variables available. The flags which can be used are:
  - flag = 1 pH and CO2 given
flag = 2 CO2 and HCO3 given
flag = 3 CO2 and CO3 given
flag = 4 CO2 and ALK given
flag = 5 CO2 and DIC given
flag = 6 pH and HCO3 given
flag = 7 pH and CO3 given
flag = 8 pH and ALK given
flag = 9 pH and DIC given
flag = 10 HCO3 and CO3 given
flag = 11 HCO3 and ALK given
flag = 12 HCO3 and DIC given
flag = 13 CO3 and ALK given
flag = 14 CO3 and DIC given
flag = 15 ALK and DIC given
flag = 21 pCO2 and pH given
flag = 22 pCO2 and HCO3 given
flag = 23 pCO2 and CO3 given
flag = 24 pCO2 and ALK given
flag = 25 pCO2 and DIC given

var1 Value of the first variable in mol/kg, except for pH and for pCO2 in µatm

var2 Value of the second variable in mol/kg, except for pH

S Salinity

T Temperature in degrees Celsius

Patm Surface atmospheric pressure in atm, default is 1 atm

P Hydrostatic pressure in bar (surface = 0)

Pt Concentration of total phosphate in mol/kg; set to 0 if NA

Sit Concentration of total silicate in mol/kg; set to 0 if NA

k1k2 "l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010) and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

kf "pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is "dg".

ks "d" for using Ks from Dickson (1990) and "k" for using Ks from Khoo et al. (1977), default is "d"

pHscale "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)

b Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrøm (1974) formulation, default is "u74"
gas used to indicate the convention for INPUT pCO2, i.e., when it is an input variable (flags 21 to 25): "insitu" indicates it is referenced to in situ pressure and in situ temperature; "potential" indicates it is referenced to 1 atm pressure and potential temperature; and "standard" indicates it is referenced to 1 atm pressure and in situ temperature. All three options should give identical results at surface pressure. This option is not used when pCO2 is not an input variable (flags 1 to 15). The default is "potential".

badd Amount of boron added in mol/kg.

warn "y" to show warnings when T or S go beyond the valid range for constants; "n" to suppress warnings. The default is "y".

eos "teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.

long longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

lat latitude of data point, used when eos parameter is "teos10".

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:
For K0, the pressure correction term of Weiss (1974) is used.

For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

**Value**

The function returns a data frame containing the following columns:

- **S** Salinity
- **T** Temperature in degrees Celsius
- **Patm** Surface atmospheric pressure in atm
- **P** Hydrostatic pressure in bar
- **pH** pH
- **CO2** CO2 concentration (mol/kg)
- **pCO2** "standard" pCO2, CO2 partial pressure computed at in situ temperature and atmospheric pressure (µatm)
- **fCO2** "standard" fCO2, CO2 fugacity computed at in situ temperature and atmospheric pressure (µatm)
- **pCO2pot** "potential" pCO2, CO2 partial pressure computed at potential temperature and atmospheric pressure (µatm)
- **fCO2pot** "potential" fCO2, CO2 fugacity computed at potential temperature and atmospheric pressure (µatm)
- **pCO2insitu** "in situ" pCO2, CO2 partial pressure computed at in situ temperature and total pressure (atm + hydrostatic) (µatm)
in situ fCO2, CO2 fugacity computed at in situ temperature and total pressure (atm + hydrostatic) (µatm)

HCO3  HCO3 concentration (mol/kg)
CO3   CO3 concentration (mol/kg)
DIC   DIC concentration (mol/kg)
ALK   ALK, total alkalinity (mol/kg)
OmegaAragonite  Omega aragonite, aragonite saturation state
OmegaCalcite    Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

Author(s)

Heloise Lavigne, James Orr and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References


Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. Journal of Chemical Thermodynamics 22, 113-127.


Examples

```r
## With a couple of variables
carb(flag=8, var1=8.2, var2=0.00234, S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0,
phscale="T", kf="pf", k1k2="1", ks="d", b="u74", badd=0)
```

---

**carbfull**

*Parameters of the seawater carbonate system - extension of carb*

**Description**

Returns parameters of the seawater carbonate system, including the ammonium and sulfide acid-base systems, as well as full acid-base speciation

**Usage**

```r
carbfull(flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0,
k1k2="x", kf="x", ks="d", phscale="T", b="u74", gas="potential",
Nh4t=0, HSt=0)
```

**Arguments**

- `flag` select the couple of variables available. The flags which can be used are:
  - `flag = 1` pH and CO2 given
  - `flag = 2` CO2 and HCO3 given
  - `flag = 3` CO2 and CO3 given
  - `flag = 4` CO2 and ALK given
flag = 5 CO2 and DIC given
flag = 6 pH and HCO3 given
flag = 7 pH and CO3 given
flag = 8 pH and ALK given
flag = 9 pH and DIC given
flag = 10 HCO3 and CO3 given
flag = 11 HCO3 and ALK given
flag = 12 HCO3 and DIC given
flag = 13 CO3 and ALK given
flag = 14 CO3 and DIC given
flag = 21 pCO2 and pH given
flag = 22 pCO2 and HCO3 given
flag = 23 pCO2 and CO3 given
flag = 24 pCO2 and ALK given
flag = 25 pCO2 and DIC given

var1
Value of the first variable in mol/kg-soln, except for pH and for pCO2 in $\mu$atm

var2
Value of the second variable in mol/kg-soln, except for pH

S
Salinity

T
Temperature in degrees Celsius

Patm
Surface atmospheric pressure in atm, default is 1 atm

P
Hydrostatic pressure in bar (surface = 0)

Pt
Concentration of total phosphate in mol/kg-soln; set to 0 if NA

Sit
Concentration of total silicate in mol/kg-soln; set to 0 if NA

k1k2
"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35$^o$C and/or S is outside the range 19 to 43. In these cases, the default value is "m10".

kf
"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33$^o$C and/or S is outside the range 10 to 40. In these cases, the default is "dg".

ks
"d" for using Ks from Dickson (1990) and "k" for using Ks from Khoo et al. (1977), default is "d"

pHscale
"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)

b
Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

gas
used to indicate the convention for INPUT pCO2, i.e., when it is an input variable (flags 21 to 25); "insitu" indicates it is referenced to in situ pressure and in situ temperature; "potential" indicates it is referenced to 1 atm pressure and
potential temperature; and "standard" indicates it is referenced to 1 atm pressure and in situ temperature. All three options should give identical results at surface pressure. This option is not used when pCO2 is not an input variable (flags 1 to 15). The default is "potential".

**NH4t**
Concentration of total ammonium in mol/kg-soln; set to 0 if NA

**HSt**
Concentration of total hydrogen sulfide in mol/kg-soln; set to 0 if NA

**Details**

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

**For K1 and K2:**

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50°C.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

**For Kf:**

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.

**For Ks:**

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

**Pressure corrections and pH scale:**

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs, Ksi and K2si, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied
as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

- For $K_s$, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

- For $K_n$, the pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

### Value

The function returns a data frame containing the following columns:

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius</td>
</tr>
<tr>
<td>Patm</td>
<td>Surface atmospheric pressure in atm</td>
</tr>
<tr>
<td>P</td>
<td>Hydrostatic pressure in bar</td>
</tr>
<tr>
<td>pH</td>
<td>pH</td>
</tr>
<tr>
<td>CO2</td>
<td>CO2 concentration (mol/kg-soln)</td>
</tr>
<tr>
<td>pCO2</td>
<td>&quot;standard&quot; pCO2, CO2 partial pressure computed at in situ temperature and atmospheric pressure ($\mu$atm)</td>
</tr>
<tr>
<td>fCO2</td>
<td>&quot;standard&quot; fCO2, CO2 fugacity computed at in situ temperature and atmospheric pressure ($\mu$atm)</td>
</tr>
<tr>
<td>pCO2pot</td>
<td>&quot;potential&quot; pCO2, CO2 partial pressure computed at potential temperature and atmospheric pressure ($\mu$atm)</td>
</tr>
<tr>
<td>fCO2pot</td>
<td>&quot;potential&quot; fCO2, CO2 fugacity computed at potential temperature and atmospheric pressure ($\mu$atm)</td>
</tr>
<tr>
<td>pCO2insitu</td>
<td>&quot;in situ&quot; pCO2, CO2 partial pressure computed at in situ temperature and total pressure (atm + hydrostatic) ($\mu$atm)</td>
</tr>
<tr>
<td>fCO2insitu</td>
<td>&quot;in situ&quot; fCO2, CO2 fugacity computed at in situ temperature and total pressure (atm + hydrostatic) ($\mu$atm)</td>
</tr>
<tr>
<td>HCO3</td>
<td>HCO3 concentration (mol/kg-soln)</td>
</tr>
<tr>
<td>CO3</td>
<td>CO3 concentration (mol/kg-soln)</td>
</tr>
<tr>
<td>DIC</td>
<td>DIC concentration (mol/kg-soln)</td>
</tr>
<tr>
<td>ALK</td>
<td>ALK, total alkalinity (mol/kg-soln)</td>
</tr>
<tr>
<td>OmegaAragonite</td>
<td>Omega aragonite, aragonite saturation state</td>
</tr>
<tr>
<td>OmegaCalcite</td>
<td>Omega calcite, calcite saturation state</td>
</tr>
<tr>
<td>NH4</td>
<td>NH4 concentration (mol/kg-soln)</td>
</tr>
<tr>
<td>NH3</td>
<td>NH3 concentration (mol/kg-soln)</td>
</tr>
<tr>
<td>BOH3</td>
<td>B(OH)3 concentration (mol/kg-soln)</td>
</tr>
<tr>
<td>BOH4</td>
<td>B(OH)4 concentration (mol/kg-soln)</td>
</tr>
<tr>
<td>H3PO4</td>
<td>H3PO4 concentration (mol/kg-soln)</td>
</tr>
</tbody>
</table>
H2PO4 H2PO4 concentration (mol/kg-soln)
HP04 HPO4 concentration (mol/kg-soln)
P04 PO4 concentration (mol/kg-soln)
H2S H2S concentration (mol/kg-soln)
HS HS concentration (mol/kg-soln)
SiOH4 SiOH4 concentration (mol/kg-soln)
SiOOH3 SiOOH3 concentration (mol/kg-soln)
SiO2OH2 SiO2OH2 concentration (mol/kg-soln)
HF HF concentration (mol/kg-soln)
F F concentration (mol/kg-soln)
HSO4 HSO4 concentration (mol/kg-soln)
SO4 SO4 concentration (mol/kg-soln)
H H concentration at specified pH scale (mol/kg-soln)
OH OH concentration (mol/kg-soln)
NH4t Supplied NHt concentration (mol/kg-soln); values are recycled if necessary
BOR Calculated total borate concentration (mol/kg-soln)
Pt Supplied Pt concentration (mol/kg-soln); values are recycled if necessary
HSt Supplied HSt concentration (mol/kg-soln); values are recycled if necessary
Sit Supplied Sit concentration (mol/kg-soln); values are recycled if necessary
FLUO Calculated total fluoride concentration (mol/kg-soln)
ST Calculated total sulfate concentration (mol/kg-soln)

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

Heloise Lavigne, James Orr, Mathilde Hagens and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References


Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. Journal of Chemical Thermodynamics 22, 113-127.


**Examples**

```r
# With a couple of variables
f Carsonfull(f$flag=8, f$var1=8.2, f$var2=0.00234, f$S=35, f$T=25, f$P=0, f$Pmat=1.0, f$Pt=0, f$Sit=0, f$pHscale="T", f$kf="pf", f$k1k2="1", f$ks="d", b="u74", gas="potential", NH4t=0, HSt=0)

# With a couple of variables and non-zero nutrient concentrations
f Carsonfull(f$flag=8, f$var1=8.2, f$var2=0.00234, f$S=35, f$T=25, f$P=0, f$Pmat=1.0, f$Pt=5e-6, f$Sit=2e-6, f$pHscale="T", f$kf="pf", f$k1k2="1", f$ks="d", b="u74", gas="potential", NH4t=10e-6, HSt=0.1e-6)
```
### Using vectors as arguments

```r
flag <- c(8, 2, 8)
var1 <- c(8.2, 7.477544e-06, 8.2)
var2 <- c(0.002343955, 0.001649802, 2400e-6)
S <- c(35, 35, 30)
T <- c(25, 25, 30)
P <- c(0, 0, 0)
Pt <- c(0, 0, 0)
Sit <- c(0, 0, 0)
kf <- c("pf", "pf", "pf")
k1k2 <- c("1", "1", "1")
phscale <- c("T", "T", "T")
b <- c("110", "110", "110")
gas <- c("potential", "potential", "potential")
NH4t <- c(0, 0, 0)
HSt <- c(0, 0, 0)
carbfull(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P, Pt=Pt, Sit=Sit,
    kf=kf, k1k2=k1k2, phscale=phscale, b=b, gas=gas, NH4t=NH4t, HSt=HSt)
```

### Test with all flags

```r
flag <- c((1:15), (21:25))
var1 <- c(8.2000000, 7.308171e-06, 7.308171e-06, 7.308171e-06, 7.308171e-06, 8.2, 8.2, 8.2, 8.2, 0.001646857, 0.001646857, 0.001646857, 0.0002822957, 0.0002822957, 0.00234, 258.2164, 258.2164, 258.2164, 258.2164, 258.2164)
var2 <- c(7.308171e-06, 0.001646857, 0.0002822957, 0.00234, 0.001936461, 0.001936461, 0.001936461, 8.2, 0.001646857, 0.0002822957, 0.00234, 0.001936461)
carbfull(flag=flag, var1=var1, var2=var2)
```

---

**d2p**

*Converts depth in meters to pressure in dbar*

### Description

Converts depth in meters to pressure in dbar

### Usage

```r
d2p(depth, lat=40)
```

### Arguments

- `depth` Depth in meters
- `lat` Latitude in degrees, N and S is irrelevant, default is 40°

### Value

- `pressure` Pressure corresponding to the depth given, in dbar
**derivnum**

**Author(s)**
Heloise Lavigne and Jean-Pierre Gattuso <gattuso@obs-cnfr.fr>

**References**

**See Also**
p2d

**Examples**
d2p(depth=7500, lat=30)

---

**derivnum**

**Numerical derivatives of seawater carbonate system variables**

**Description**
Returns numerical derivatives of the seawater carbonate system output variables with respect to input variables.

**Usage**
```
derivnum(varid, flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0, k1k2="x", kf="x", ks="d", phscale="T", b="u74", gas="potential", warn="y", eos = "eos80", long = 1e+20, lat = 1e+20)
```

**Arguments**

- **varid**
  Variable length, case insensitive, character identifier of variable with respect to which derivatives are requested. Possible values are:
  - '1' or 'var1' : Variable 1 of the input pair (This is TAlk if flag is 15)
  - '2' or 'var2' : Variable 2 of the input pair (This is DIC if flag is 15)
  - 'sil', 'silt', 'silicate' : Total silicate concentration
  - 'phos', 'phost', 'tphos' or 'phosphate' : Total phosphate concentration
  - 't', 'temp' or 'temperature' : temperature
  - 's', 'sal' or 'salinity' : salinity
  - 'K0', 'K1', 'K2', 'Kb', 'Kw', 'Kspa' or 'Kspc' : one of the dissociation constants
  - 'bor' : total boron

- **flag**
  select the input pair of carbonate-system variables available by choosing the following flag:
  - flag = 1 pH and CO2 given
  - flag = 2 CO2 and HCO3 given
flag = 3 CO2 and CO3 given
flag = 4 CO2 and ALK given
flag = 5 CO2 and DIC given
flag = 6 pH and HCO3 given
flag = 7 pH and CO3 given
flag = 8 pH and ALK given
flag = 9 pH and DIC given
flag = 10 HCO3 and CO3 given
flag = 11 HCO3 and ALK given
flag = 12 HCO3 and DIC given
flag = 13 CO3 and ALK given
flag = 14 CO3 and DIC given
flag = 15 ALK and DIC given
flag = 21 pCO2 and pH given
flag = 22 pCO2 and HCO3 given
flag = 23 pCO2 and CO3 given
flag = 24 pCO2 and ALK given
flag = 25 pCO2 and DIC given

var1 Value of the first variable in mol/kg, except for pH and for pCO2 in \( \mu \) atm

var2 Value of the second variable in mol/kg, except for pH

S Salinity

T Temperature in degrees Celsius

Patm Surface atmospheric pressure in atm, default is 1 atm

P Hydrostatic pressure in bar (surface = 0)

Pt Concentration of total phosphate in mol/kg; set to 0 if NA

Sit Concentration of total silicate in mol/kg; set to 0 if NA

k1k2 "l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

kf "pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is "dg".

ks "d" for using Ks from Dickson (1990) and "k" for using Ks from Khoo et al. (1977), default is "d"

pHscale "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)

b Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"
gas

used to indicate the convention for INPUT \( pCO_2 \), i.e., when it is an input variable (flags 21 to 25): "insitu" indicates it is referenced to in situ pressure and in situ temperature; "potential" indicates it is referenced to 1 atm pressure and potential temperature; and "standard" indicates it is referenced to 1 atm pressure and in situ temperature. All three options should give identical results at surface pressure. This option is not used when \( pCO_2 \) is not an input variable (flags 1 to 15). The default is "potential".

warn

"y" to show warnings when T or S go beyond the valid range for constants; "n" to suppress warnings. The default is "y".

eos

"teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.

long

longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

lat

latitude of data point, used when eos parameter is "teos10".

Details

This subroutine has same input parameters as subroutine carb(). For details on these parameters, refer to documentation of 'carb'.

This subroutine computes partial derivatives of each output variable with respect to each of the input variable (including each of the two chosen carbonate system variables, each of the nutrients (total silicon and total phosphorus), temperature, and salinity.

It computes these derivatives \((dy/dx)\) using the method of central differences, i.e.,

• for \( dx \), it adds a positive and negative perturbation, same and equal in magnitude, to each input variable, one at a time, and

• for \( dy \), it then computes the corresponding induced change in output variables

All arguments but the first (\( \text{varid} \)), can be given as scalers or vectors. If the lengths of the vectors differs, only the longest vector is retained and the other arguments are set equal to the first value of the other vectors are used. Hence users should use either vectors with the same dimension or one vector for one argument and scalars for others; otherwise, results may not be as intended.

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

Value

The function returns a data frame containing the following columns:

- \( H \) derivative of \([H^+]\) concentration (mol/kg/...)
- \( pH \) derivative of pH
- \( CO_2 \) derivative of CO2 concentration (mol/kg/...)

pCO2  "standard" pCO2, CO2 partial pressure computed at in situ temperature and atmospheric pressure (µatm/...)
fCO2  "standard" fCO2, CO2 fugacity computed at in situ temperature and atmospheric pressure (µatm/...)
HCO3 derivative of HCO3 concentration (mol/kg/...)
CO3  derivative of CO3 concentration (mol/kg/...)
DIC  derivative of DIC concentration (mol/kg/...)
ALK  derivative of ALK, total alkalinity (mol/kg/...)
OmegaAragonite derivative of Omega aragonite, aragonite saturation state
OmegaCalcite derivative of Omega calcite, calcite saturation state

If all input data have the same 'flag' value, returned data frame does not show derivatives of input pair of carbonate system variables. For example, if all input flags are 15, the input pair is DIC and ALK; hence, derivatives of DIC and ALK are not returned.

Units of derivative dy/dx is unit(y)/unit(x) where unit(x) are as follows:

degree C when x is Temperature
psu when x is Salinity
µatm when x is pCO2
mol/kg for all other cases

Author(s)

Jean-Marie Epitalon, James Orr, and Jean-Pierre Gattuso@gattuso@obs-Mlfr.fr

References


Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* 22, 113-127.


Examples

```r
# 1) For the input pair ALK and DIC (var1 and var2 when flag=15)
# compute derivatives of all output varialbes
# with respect to DIC (i.e., var2)
derivnum(varid='var2', flag=15, var1=2300e-6, var2=2000e-6,
  S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0,
  phscale="T", kf="pf", k1k2="1", ks="d", b="u74")

# 2) For the input pair pH and ALK (var1 and var2 when flag=8)
# compute derivatives of all output variables
# with respect to [H+] concentration
derivnum(varid='var1', flag=8, var1=8.2, var2=0.00234,
  S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0,
  phscale="T", kf="pf", k1k2="1", ks="d", b="u74")

# 3) Using vectors as arguments and compute derivatives of all output
# variables with respect to temperature
flag <- c(8, 2, 8)
var1 <- c(8.2, 7.477544e-06, 8.2)
var2 <- c(0.002343955, 0.001649882, 2400e-6)
```
**Description**

Converts in situ temperature to conservative temperature and practical to absolute salinity (SA). Salinity conversion depends on total alkalinity as well as the concentrations of dissolved inorganic carbon, nitrate and silicate.

**Usage**

```r
eos2teosChem(SP, T, P=0, TA=2300e-6, DIC=2000e-6, NO3=0, SIOH4=0)
```

**Arguments**

- **SP** Practical salinity on the practical salinity scale
- **T** In situ temperature in deg. C
- **P** Sea water pressure in dbar
- **TA** Total alkalinity, in mol/kg, default is 2300 Âµmol/kg
- **DIC** Dissolved inorganic carbon concentration in mol/kg, default is 2000 Âµmol/kg
- **NO3** Total nitrate concentration in mol/kg, default is 0
- **SIOH4** Total silicate concentration in mol/kg, default is 0

**Details**

Conversion from practical to absolute salinity depends on carbonate system parameters and ion concentration which mostly affect water density anomalies.

**Value**

The function returns a data frame containing the following columns:

- **CT** Conservative temperature (deg C)
- **SA** Absolute salinity (g/kg)
Author(s)

Jean-Marie Epitalon

References


See Also

teos2eos Chem does the reverse, eos2teos geo, sp2sa Chem

package gsw

Examples

```r
# Calculate Conservative Temperature and Absolute Salinity of a sample with
# Practical salinity of 35 psu, in-situ temperature of 18 deg C,
# at 0 dbar and total alkalinity of 0.00234 mol/kg and DIC of 0.00202 mol/kg
f <- eos2teos Chem(SP=35, T=18, P=0, TA=0.00234, DIC=0.00202)
CT <- f$CT   # Conservative Temperature
SA <- f$SA   # Absolute Salinity
```

eos2teos geo

*Convert temperature and salinity from EOS-80 to TEOS-10*

Description

Converts in situ to conservative temperature and practical to absolute salinity (SA). Salinity conversion depends on depth and geographic location.

Usage

eos2teos geo(SP, T, P=0, long=1.1e20, lat=1.1e20)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SP</td>
<td>Practical salinity on the practical salinity scale</td>
</tr>
<tr>
<td>T</td>
<td>In situ temperature in deg. C</td>
</tr>
<tr>
<td>P</td>
<td>Sea water pressure in dbar</td>
</tr>
<tr>
<td>long</td>
<td>Longitude in decimal degrees [ 0...+360 ] or [ -180...+180 ]</td>
</tr>
<tr>
<td>lat</td>
<td>Latitude in decimal degrees [-90...90]</td>
</tr>
</tbody>
</table>
Details

Conversion from practical to absolute salinity depends on water density anomaly which is correlated with silicate concentration. This function relies on silicate concentration taken from WOA (World Ocean Atlas) to evaluate density anomaly.

Value

The function returns a data frame containing the following columns:

- CT: Conservative temperature (deg C)
- SA: Absolute salinity (g/kg)

Author(s)

Jean-Marie Epitalon

References


See Also

teos2eos_geo does the reverse, eos2teos_chem, sp2sa_geo, package gsw

Examples

```r
# Calculate conservative temperature and absolute salinity of a sample with
# Practical salinity of 35 psu, in situ temperature of 18 deg C,
# depth is 10 dbar and location is 188 degrees East and 4 degrees North.
f <- eos2teos_geo(SP=35, T=18, P=10, long=188, lat=4)
CT <- f$CT  # Conservative temperature
SA <- f$SA  # Absolute salinity
```

Description

Estimates combined standard uncertainties in computed carbonate system variables by propagating inout uncertainties (standard uncertainties) in six input variables, including (Orr et al., Mar. Chem., in press):

- the input pair of carbonate system variables,
- the 2 input nutrients (silicate and phosphate concentrations),
• temperature and salinity. It also accounts for
• the errors in the key dissociation constants pK0, pK1, pK2, pKb, pKw, pKspa and pKspc
• the error in total boron

Usage

```matlab
errors(flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0,
evar1=0, evar2=0, eS=0.01, eT=0.01, ePt=0, eSit=0,
epK=c(0.002, 0.0075, 0.015, 0.01, 0.01, 0.02, 0.02),
eBt=0.02, method = "ga", r=0.0, runs=10000,
k1k2='x', kf='x', ks="d", pHscale="T", b="u74", gas="potential",
warn="y", eos = "eos80", long = 1e+20, lat = 1e+20)
```

Arguments

**flag**
select the pair of carbonate system input variables. The flags to be used are as follows:
- flag = 1 pH and CO2 given
- flag = 2 CO2 and HCO3 given
- flag = 3 CO2 and CO3 given
- flag = 4 CO2 and ALK given
- flag = 5 CO2 and DIC given
- flag = 6 pH and HCO3 given
- flag = 7 pH and CO3 given
- flag = 8 pH and ALK given
- flag = 9 pH and DIC given
- flag = 10 HCO3 and CO3 given
- flag = 11 HCO3 and ALK given
- flag = 12 HCO3 and DIC given
- flag = 13 CO3 and ALK given
- flag = 14 CO3 and DIC given
- flag = 15 ALK and DIC given
- flag = 21 pCO2 and pH given
- flag = 22 pCO2 and HCO3 given
- flag = 23 pCO2 and CO3 given
- flag = 24 pCO2 and ALK given
- flag = 25 pCO2 and DIC given

**var1**
Value of the first variable (in mol/kg, except for pH and for pCO2 in µatm)

**var2**
Value of the second variable (in mol/kg, except for pH)

**S**
Salinity (practical salinity scale)

**T**
Temperature in degrees Celsius

**Patm**
Surface atmospheric pressure in atm, default is 1 atm

**P**
Hydrostatic pressure in bar (surface = 0)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt</td>
<td>Concentration of total dissolved inorganic phosphorus (mol/kg); set to 0 if NA</td>
</tr>
<tr>
<td>Sit</td>
<td>Concentration of total dissolved inorganic silicon (mol/kg); set to 0 if NA</td>
</tr>
<tr>
<td>evar1</td>
<td>Standard uncertainty in var1 of input pair of carbonate system variables</td>
</tr>
<tr>
<td>evar2</td>
<td>Standard uncertainty in var2 of input pair of carbonate system variables</td>
</tr>
<tr>
<td>eS</td>
<td>Standard uncertainty in salinity; default is 0.01</td>
</tr>
<tr>
<td>eT</td>
<td>Standard uncertainty in temperature (degree C); default is 0.01</td>
</tr>
<tr>
<td>ePT</td>
<td>Standard uncertainty in total dissolved inorganic phosphorus concentration (mol/kg)</td>
</tr>
<tr>
<td>eSIT</td>
<td>Standard uncertainty in total dissolved inorganic silicon concentration (mol/kg)</td>
</tr>
<tr>
<td>ePK</td>
<td>Standard uncertainty in 7 key dissociation constants: pK0, pK1, pK2, pKb, pKw, pKspa and pKspc. This is a vector. The default is c(0.002, 0.0075, 0.015, 0.01, 0.01, 0.02, 0.02).</td>
</tr>
<tr>
<td>eBT</td>
<td>Standard uncertainty in total boron, given as a relative fractional error. The default is 0.02, which equates to a 2% error</td>
</tr>
<tr>
<td>method</td>
<td>Case insensitive character string to choose the error-propagation method: 1) Gaussian, 2) Method of Moments, or 3) Monte Carlo. These methods are specified using the 2-letter codes &quot;ga&quot;, &quot;mo&quot;, or &quot;mc&quot;, respectively. The default is &quot;ga&quot; (Gaussian).</td>
</tr>
<tr>
<td>r</td>
<td>Correlation coefficient between standard uncertainties of var1 and var2 (only useful with method=&quot;mo&quot;, i.e., ignored for the 2 other methods, the default is r=0.0</td>
</tr>
<tr>
<td>runs</td>
<td>Number of random samples (ignored unless method=&quot;mc&quot;; the default is runs=10000</td>
</tr>
<tr>
<td>k1k2</td>
<td>&quot;l&quot; for using K1 and K2 from Lueker et al. (2000), &quot;m06&quot; from Millero et al. (2006), &quot;m10&quot; from Millero (2010), &quot;w14&quot; from Waters et al. (2014), and &quot;r&quot; from Roy et al. (1993). &quot;x&quot; is the default flag; the default value is then &quot;l&quot;, except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is &quot;w14&quot;.</td>
</tr>
<tr>
<td>kf</td>
<td>&quot;pf&quot; for using Kf from Perez and Fraga (1987) and &quot;dg&quot; for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). &quot;x&quot; is the default flag; the default value is then &quot;pf&quot;, except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is &quot;dg&quot;.</td>
</tr>
<tr>
<td>ks</td>
<td>&quot;d&quot; for using Ks from Dickson (1990) and &quot;k&quot; for using Ks from Khoo et al. (1977), default is &quot;d&quot;</td>
</tr>
<tr>
<td>pHscale</td>
<td>&quot;T&quot; for the total scale, &quot;F&quot; for the free scale and &quot;SWS&quot; for using the seawater scale, default is &quot;T&quot; (total scale)</td>
</tr>
<tr>
<td>b</td>
<td>Concentration of total boron. &quot;l10&quot; for the Lee et al. (2010) formulation or &quot;u74&quot; for the Uppstrom (1974) formulation, default is &quot;u74&quot;</td>
</tr>
<tr>
<td>gas</td>
<td>used to indicate the convention for INPUT pCO2, i.e., when it is an input variable (flags 21 to 25): &quot;insitu&quot; indicates it is referenced to in situ pressure and in situ temperature; &quot;potential&quot; indicates it is referenced to 1 atm pressure and potential temperature; and &quot;standard&quot; indicates it is referenced to 1 atm pressure and in situ temperature. All three options should give identical results at surface pressure. This option is not used when pCO2 is not an input variable (flags 1 to 15). The default is &quot;potential&quot;.</td>
</tr>
</tbody>
</table>
errors

warn
"y" to show warnings when T or S go beyond the valid range for constants; "n" to suppress warnings. The default is "y".

eos
"teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.

long
longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

lat
latitude of data point, used when eos parameter is "teos10".

Details

Complete information on routine uncertainty propagation for the marine carbon dioxide system can be found in Orr et al. (in press). This function requires users to specify each input standard uncertainty as either the standard deviation or the standard error of the mean. The latter implies much smaller propagated uncertainties, but is appropriate only when interested in the error in the mean, not the error of a given measurement. Beware that it is easy to fool oneself when using the standard error of the mean rather than the standard deviation.

This function requires different types of standard uncertainties:

- Standard uncertainties for evar1, evar2, eS, eT, ePt, eSit (same units as the input data, e.g., mol/kg);
- Standard uncertainties in pK units for epK; and
- Standard uncertainties in relative fractional units (between 0.0 and 1.0) for eBt.

This function propagates standard uncertainty from input to output variables using one of three methods:

- Gaussian: The Gaussian method is the standard technique for estimating a computed variable’s (z) second moment (its variance or standard deviation) based on a first-order approximation to z. More precisely, we use here the basic 1st order, 2nd moment uncertainty analysis (a type of Taylor expansion), assuming no covariance between input variables. This is the approach used by Dickson and Riley (1978). It is the default method.

- Method of moments: The method of moments is a more general form of the Gaussian method. But in addition, it also accounts for covariance between input variables. In this case, the 'errors' routine allows the user to specify a value of the correlation coefficient ‘r’, having a value between -1.0 and 1.0, to indicate the correlation between standard uncertainties of the input pair of carbonate system variables. That correlation is used to compute the covariance. But by default, it is assumed that there is no covariance (r=0.0).

- Monte Carlo: The Monte Carlo method is a brute-force approach relying on repeated random sampling of input errors, adding those to each input variables, calculating the corresponding output variables for each sample, and finally assessing the standard deviation in each output variables.

This function has many input parameters that are identical to those in the carb function. For their details, refer to the 'carb' documentation.

All parameters may be scalars or vectors except epK, eBt, method, runs, and gas.

- runs and eBt must be scalars
- method and gas must each consist of a character string
- epK may be a vector of 7 values. In that case, it must list errors for pK0, pK1, pK2, pKb, pKw, pKspa and pKspc, respectively. That set of errors is identical for all input data. Alternatively, users may specify ‘epK=NULL’ or ‘epK=0’ to set all 7 values to zero and thus neglect errors in the equilibrium constants.

In constrast, for evar1, evar2, r, eS, eT, ePt and eSit:

- if they are vectors, they represent standard uncertainties associated with each data point
- if they are scalars (single real numbers), they represent one standard uncertainty value each associated to all data points

The same remark applies to parameter r (correlation coefficient).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

Value

The function returns a 2-dimensional dataframe, with the following columns:

- H combined standard uncertainty in [H+] concentration (mol/kg)
- pH combined standard uncertainty in pH
- CO2 combined standard uncertainty in CO2 concentration (mol/kg)
- pCO2 combined standard uncertainty in "standard" pCO2, CO2 partial pressure computed at in situ temperature and atmospheric pressure (µatm)
- fCO2 combined standard uncertainty in "standard" fCO2, CO2 fugacity computed at in situ temperature and atmospheric pressure (µatm)
- HCO3 combined standard uncertainty in HCO3 concentration (mol/kg)
- CO3 combined standard uncertainty in CO3 concentration (mol/kg)
- DIC combined standard uncertainty in DIC concentration (mol/kg)
- ALK combined standard uncertainty in ALK, total alkalinity (mol/kg)
- OmegaAragonite combined standard uncertainty in Omega aragonite (aragonite saturation state)
- OmegaCalcite combined standard uncertainty in Omega calcite (calcite saturation state)

If all input data have the same 'flag' value, the returned data frame does not show combined standard uncertainties on input pair of carbonate system variables. For example, if all input flags are 15, the input pair is DIC and ALK; hence, errors on DIC and ALK are not returned.
Correlation coefficient

By default, 'r' is zero. However, for some pairs the user may want to specify a different value. For example, measurements of pCO2 and pH are often anti-correlated. The same goes for two other pairs: 'CO2 and CO3' and 'pCO2 and CO3'. But even for these cases, care is needed before using non-zero values of 'r'.

When the user wishes to propagate standard uncertainties for an individual measurement, 'r' should ALWAYS be zero if each member of the input pair is measured independently. In this case, we are interested in the correlation between the uncertainties in those measurements, not in the correlation between the measurements themselves. Uncertainties from those measurements are probably not correlated if they come from different instruments. Conversely, if users are interested in the error in the mean of a distribution of measurements (i.e., if they are propagating standard errors instead of standard deviations), one should then also account for the correlation between the measurements of the two variables of the input pair.

For input pairs where one member is pH (flags 1, 6, 7, 8, 9, and 21), this 'errors' function automatically inverses the sign of 'r'. The reason for that is that the associated derivatives are computed in terms of the hydrogen ion concentration (H+), not pH. Therefore for each of these 6 flags, if the user wants to compute their own 'r' that should be done by (1) using the H+ concentration instead of pH, and (2) inversing the sign of that computed 'r' before passing it as an argument to this routine. Usually though (when not calculating r for pH), the user may just use the 'r' in the expected way. For example, to include the covariance term when there is a perfect anticorrelation of pH with pCO2, one would use 'r=1.0'.

Computation time

Computation time depends on the method chosen; the Monte Carlo method takes much longer to execute. The computational time required for the Monte Carlo method is proportional to the number of runs. More runs, implies improved accuracy: runs = 10000 appears a minimum to obtain an accuracy of less than 1%. Accuracy is inversely proportional to the number of runs.

Computation time also depends on the chosen pair of input variables. For example, with the input pair DIC and Total alkalinity (flag=15), it is much longer than for input pair pH and Total alkalinity (flag=8)

Author(s)

Jean-Marie Epitalon, James Orr, and Jean-Pierre Gattuso<gattuso@obs-vlfr.fr>

References


Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. Journal of Chemical Thermodynamics 22, 113-127.


### Examples

```r
## 1) For the input pair ALK and DIC (var1 and var2 when flag=15),
## compute resulting uncertainty from given uncertainty on ALK and DIC (5 umol/kg)
## and default uncertainties in dissociation constants and total boron
```
## Using the default method (Gaussian)

```r
errors(flag=15, var=2300e-6, var2=2000e-6, S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0,
  evar=5e-6, evar2=5e-6, eS=0, eT=0, ePt=0, eSit=0,
  pHscale="T", kf="pf", k1k2="1", ks="d", b="u74")
```

## Typical output:

```r
typical.output =
  pH CO2 fCO2 pCO2 HC03 ...
  3.721614e-10 0.01796767 5.441869e-07 19.25338 19.31504 9.170116e-06 ...
```

## 2) Do the same as in one, but assign a 4% uncertainty to total boron

This uncertainty is the amount by which estimates from Lee et al. (2010) and Uppstrom (1974) differ. The default for the latter is `eBt`:

```r
errors(flag=15, var=2300e-6, var2=2000e-6, S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0,
  evar=5e-6, evar2=5e-6, eS=0, eT=0, ePt=0, eSit=0, eBt=0.04,
  pHscale="T", kf="pf", k1k2="1", ks="d", b="u74")
```

## 3) For the input pair pH and ALK (var1 and var2 when flag=8)

Compute standard errors in output variables from errors in input variables, i.e., for pH (0.005 pH units) and in ALK (5 umol/kg), along with errors in total dissolved inorganic phosphorus (0.1 umol/kg) and total dissolved inorganic silicon (2 umol/kg) concentrations, while assuming no uncertainty in dissociation constants & boron, using the Gaussian method:

```r
errors(flag=8, var=8.25, var2=2300e-6, S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0,
  evar=0.005, evar2=5e-6, eS=0, eT=0, ePt=0.1, eSit=2, eBt=0, eBt=0,
  method="ga", pHscale="T", kf="pf", k1k2="1", ks="d", b="u74")
```

## 4) For the input pair pCO2 and pH (var1 and var2 when flag=21)

Compute standard errors in output variables from errors in input variables, i.e., for pCO2 (2 uatm) and pH (0.005 pH units), with no uncertainties in Pt and Sit nor in the dissociation constants BUT a perfect anticorrelation between pCO2 and pH, (the input pair) using the Method of Moments:

```r
errors(flag=21, var=400, var2=8.1, S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0,
  evar=2, evar2=0.005, eS=0, eT=0, ePt=0.0, eSit=0, eBt=0, eBt=0,
  method="mo", r=-1.0, pHscale="T", kf="pf", k1k2="1", ks="d", b="u74")
```

## 5) Use vectors as arguments and compute errors on all output variables

Using Monte Carlo method taking into account input errors on pH, ALK, DIC and dissociation constants (pKx):

```r
flag <- c(8, 15, 8)
var1 <- c(8.2, 0.000394, 8.25)
var2 <- c(0.000343955, 0.0002017, 24000e-6)
S <- c(35, 35, 30)
T <- c(25, 25, 22)
P <- 0
Pt <- 0
Sit <- 0
evar1 <- c(0.005, 2e-6, 0.005)
evar2 <- c(2e-6, 2e-6, 2e-6)
epKx <- c(0.002, 0.01, 0.02, 0.01, 0.01, 0.01)
eBtx <- 0.01
method <- "mc"
kf <- "pf"
k1k2 <- "1"
pHscale <- "T"
```
Description

Converts fCO2 (fugacity of CO2) into pCO2 (partial pressure in CO2)

Usage

f2pCO2(T = 25, Patm=1, P=0, fCO2)

Arguments

T 
Temperature in degrees Celsius, default is 25°C

Patm 
Surface atmospheric pressure in atm, default 1 atm

P 
Hydrostatic pressure in bar, default is 0 bar (surface)

fCO2 
Fugacity of CO2 in µatm, the same units as that for the pCO2 output

Value

pCO2 
Partial pressure of CO2 in µatm, the same units as that for the fCO2 input

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

Author(s)

Heloise Lavigne, Jean-Pierre Gattuso, and James Orr <gattuso@obs-vlfr.fr>

References


See Also

p2fCO2.

Examples

```r
f2pCO2(T=25, Patm=1.0, P=0, fCO2=380)
```

<table>
<thead>
<tr>
<th>( K0 )</th>
<th>Henry's constant mol/(kg/atm)</th>
</tr>
</thead>
</table>

Description

Henry’s constant mol/(kg/atm)

Usage

```r
K0(S=35, T=25, P=0, Patm=1, warn="y")
```

Arguments

- **S**: Salinity, default is 35
- **T**: Temperature in degrees Celsius, default is 25°C
- **P**: Hydrostatic pressure in bar (surface = 0), default is 0
- **Patm**: Surface atmospheric pressure in atm, default is 1 atm
- **warn**: "y" to show warnings when T or S go beyond the valid range for \( K0 \); "n" to suppress warnings. The default is "y".

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between -1 and 45°C.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

For pressure corrections: the pressure correction term of Weiss (1974) is used.

Value

\( K0 \)  
Henry’s constant mol/(kg/atm)
Author(s)
Jean-Marie Epitalon, Aurelien Proye, and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Examples
K0(S=35, T=25, P=0)

---

**K1**
First dissociation constant of carbonic acid (mol/kg)

---

Description
First dissociation constant of carbonic acid (mol/kg)

Usage
K1(S=35, T=25, P=0, k1k2="x", pHscale="T", kSWS2scale=0, ktotal2SWS_P0=0, warn="y")

Arguments
- **S** Salinity, default is 35
- **T** Temperature in degrees Celsius, default is 25°C
- **P** Hydrostatic pressure in bar (surface = 0), default is 0
- **k1k2** "l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is "w14".
- **pHscale** choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
- **kSWS2scale** Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. It is not required when k1k2 is "m10" or "w14" and the hydrostatic pressure is 0. If it is required and not given, it is computed, which slows down computations.
- **ktotal2SWS_P0** Conversion factor from the total scale to the SWS at an hydrostatic pressure of 0. It is only required when k1k2 is "l" or "r". If it is required and not given, it is computed, which slows down computations.
- **warn** "y" to show warnings when T or S go beyond the valid range for K1; "n" to suppress warnings. The default is "y".
Details

The Lueker et al. (2000) constant is recommended by Guide to Best Practices for Ocean CO2 Measurements (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".
- Waters et al.(2014): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

The pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

K1

First dissociation constant of carbonic acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References


**See Also**

*K2.*

**Examples**

```r
K1(S=35,T=25,P=0,k1k2="l",pHscale="T")
```

---

**K1p**

*First dissociation constant of phosphoric acid (mol/kg)*

**Description**

First dissociation constant of phosphoric acid (mol/kg)

**Usage**

```
K1p(S=35, T=25, P=0, pHscale="T", kSWS2scale=0, warn="y")
```

**Arguments**

- **S** Salinity, default is 35
- **T** Temperature in degrees Celsius, default is 25°C
- **P** Hydrostatic pressure in bar (surface = 0), default is 0
- **pHscale** Choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
- **kSWS2scale** Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.
- **warn** "y" to show warnings when T or S go beyond the valid range for K1p; "n" to supress warnings. The default is "y".
Details
This formulation is only valid for specific ranges of temperature and salinity:

- $S$ ranging between 0 and 45 and $T$ ranging between 0 and 45°C.

The pressure correction was applied on the seawater scale. Hence, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value
$k_1p$  
First dissociation constant of phosphoric acid (mol/kg)

Author(s)
Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

See Also
$k_2p$, $K_3p$.

Examples
$k_1p(35, 25, 0)$

---

$k_2$  
Second dissociation constant of carbonic acid (mol/kg)

Description
Second dissociation constant of carbonic acid (mol/kg)

Usage
$k_2(S=35, T=25, P=0, k1k2="x", pHscale="T", kSWS2scale=0, ktotal2SWS_P0=0, warn="y")$
Arguments

- **S**  
  Salinity, default is 35

- **T**  
  Temperature in degrees Celsius, default is 25°C

- **P**  
  Hydrostatic pressure in bar (surface = 0), default is 0

- **k1k2**  
  "l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

- **pHscale**  
  Choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale

- **kSW2scale**  
  Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. It is not required when k1k2 is "m10" or "w14" and the hydrostatic pressure is 0. If it is required and not given, it is computed, which slows down computations.

- **ktotal2SWS_P0**  
  Conversion factor from the total scale to the SWS at an hydrostatic pressure of 0. It is only required when k1k2 is "l" or "r". If it is required and not given, it is computed, which slows down computations.

- **warn**  
  "y" to show warnings when T or S go beyond the valid range for K2; "n" to suppress warnings. The default is "y".

Details

The Lueker et al. (2000) constant is recommended by Guide to Best Practices for Ocean CO2 Measurements (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50°C.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".
- Waters et al.(2014): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

The pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
K2

Value

\[ K_2 \]  
Second dissociation constant of carbonic acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vfr.fr>

References


DOE 1994 Handboook of methods for the analysis of the various parameters of the carbon dioxide system in sea water. ORNL/CDIAC-74. Oak Ridge,Tenn.: Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory.


See Also

k1.

Examples

\[ K_2(35, 25, 0) \]
Description

Second dissociation constant of phosphoric acid (mol/kg)

Usage

\[ K_2p(S=35, T=25, P=0, \text{pHscale}="T", k\text{SWS2scale}=0, \text{warn}="y") \]

Arguments

- **S** Salinity, default is 35
- **T** Temperature in degrees Celsius, default is 25°C
- **p** Hydrostatic pressure in bar (surface = 0), default is 0
- **phscale** choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
- **kSWS2scale** Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.
- **warn** "y" to show warnings when T or S go beyond the valid range for \( K_2p \); "n" to suppress warnings. The default is "y".

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45°C.

The pressure correction was applied on the seawater scale. Hence, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

- \( K_2p \) Second dissociation constant of phosphoric acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>
References


See Also

*K1p, K3p.*

Examples

\(K2p(35, 25, 0)\)

---

**K2si**

*Second dissociation constant of Si(OH)4*

Description

Second dissociation constant of Si(OH)4 (mol/kg)

Usage

\(K2si(S=35, T=25, P=0, pHscale="T", kSWS2scale=0, ktotal2SWS_P0=0)\)

Arguments

- **S** Salinity, default is 35
- **T** Temperature in degrees Celsius, default is 25°C
- **P** Hydrostatic pressure in bar (surface = 0), default is 0
- **pHscale** choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
- **kSWS2scale** Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.
- **ktotal2SWS_P0** Conversion factor from the total scale to the SWS at an hydrostatic pressure of 0. If it is not given, it is computed, which slows down computations.
Details

This equation is modified from Wischmeyer et al. (2003), who fitted the temperature-dependent $K_{2si}$ from Nordstrom et al. (1990) for freshwater to a value of 12.56 for $T=25$ and an ionic strength of 0.5 mol/kg. The temperature and salinity ranges in which it is valid are not well constrained.

The pressure correction is applied on the seawater scale. Hence, values are first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value is transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

$K_{2si}$  
Second dissociation constant of $\text{Si(OH)}_4$ (mol/kg)

Author(s)

Mathilde Hagens (<m.hagens@uu.nl>)

References


Examples

$K_{2si}(S=35, T=25, P=0, \text{pHscale}="T")$

---

$K_{3p}$  
*Third dissociation constant of phosphoric acid (mol/kg)*

Description

Third dissociation constant of phosphoric acid (mol/kg)

Usage

$K_{3p}(S=35, T=25, P=0, \text{pHscale}="T", kSWS2scale=0, \text{warn}="y")$
Arguments

S  Salinity, default is 35
T  Temperature in degrees Celsius, default is 25°C
P  Hydrostatic pressure in bar (surface = 0), default is 0
phscale  choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
kSWS2scale  Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.
warn  "y" to show warnings when T or S go beyond the valid range for K3p; "n" to supress warnings. The default is "y".

Details

This formulation is only valid for specific ranges of temperature and salinity:

• S ranging between 0 and 45 and T ranging between 0 and 45°C.

The pressure correction was applied on the seawater scale. Hence, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

K3p  Third dissociation constant of phosphoric acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References


See Also

K1p, K2p.

Examples

K3p(35, 25, 0)
Description

Dissociation constant of boric acid (mol/kg)

Usage

\[ \text{Kb}(S=35, \, T=25, \, P=0, \, \text{pHscale}="T", \, k\text{SWS2scale}=0, \, k\text{total2SWS}_P=0, \, \text{warn}="y") \]

Arguments

- **S**: Salinity, default is 35
- **T**: Temperature in degrees Celsius, default is 25°C
- **P**: Hydrostatic pressure in bar (surface = 0), default is 0
- **pHscale**: choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
- **kSWS2scale**: Conversion factor from SWS pH scale to chosen scale at chosen pressure; if needed and not given, it is computed; if given, computation speed is increased
- **ktotal2SWS_P0**: Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. It is not required when the selected pH scale is SWS and the hydrostatic pressure is 0. If it is required and not given, it is computed, which slows down computations.
- **warn**: "y" to show warnings when T or S go beyond the valid range for Kb; "n" to supress warnings. The default is "y".

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 5 and 45 and T ranging between 0 and 45°C.

The pressure correction is applied on the seawater scale. Hence, values are first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

\[ \text{Kb} \] Dissociation constant of boric acid (mol/kg)
Author(s)
Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References
DOE 1994 Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water. ORNL/CDIAC-74. Oak Ridge,Tenn.: Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory.

Examples
Kb(S=35,T=25,P=0,pHscale="T")

<table>
<thead>
<tr>
<th>kconv</th>
<th>Conversion factors to change the pH scale of dissociation constants</th>
</tr>
</thead>
</table>

Description
Conversion factors from the total scale to the free and seawater scales

Usage
kconv(S=35, T=25, P=0, kf, Ks, Kff, warn="y")

Arguments
S  Salinity, default is 35
T  Temperature in degrees Celsius, default is 25oC
P  Hydrostatic pressure in bar (surface = 0), default is 0
kf  "pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994); if the fonction Kf was used previously, the default value is the value given for the argument kf in the fonction Kf. If the Kf function was not used previously, the default value is "pf", except if T is outside the range 9 to 33oC or of S is outside the range 10 to 40. In these cases, the default is "dg".
Ks  Stability constant of hydrogen sulfate (mol/kg) at given S, T and P, optional; if not given, it will be computed, if given, it allows for speed optimisation
**Kff**  
Stability constant of hydrogen fluoride (mol/kg) on free pH scale at given S, T and P; optional; if not given, it will be computed, if given, it allows for speed optimisation and kf parameter is then ignored.

**warn**  
"y" to show warnings when T or S go beyond the valid range for constants; "n" to supress warnings. The default is "y".

**Details**

It is critical to consider that each formulation is valid in specific ranges of temperature and salinity:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.

Note that kconv may be called in many functions (i.e. K1, K2, K1p, K2p, K3p, Kw, Ksi, K2si, etc...) without user controls it. To force a particular formulation for Kf, it is recommended to call kconv() first then pass the resulting conversion factors to these functions.

**Value**

The function returns a list with 6 conversion factors:

- ktotal2SWs: to convert from the total scale to seawater scale
- ktotal2free: to convert from the total scale to the free scale
- kfree2SWs: to convert from the free scale to the seawater scale
- kfree2total: to convert from the free scale to total scale
- kSWs2total: to convert from the seawater scale to the total scale
- kSWs2free: to convert from the seawater scale to the free scale

**Author(s)**

Karline Soetaert <k.soetaert@nioo.knaw.nl>

**References**


**See Also**

phconv.

**Examples**

```r
# To convert dissociation constants from the total scale to the free scale
# (at salinity=35, temperature=25°C and atmospheric pressure):
kconv(35, 25, 0)
conv <- kconv()
c(K1_total=K1(), K1_SWS=K1() * conv$ktotal2SWs, K1_free=K1() * conv$ktotal2free)
```
**Kf**

*Equilibrium constant of hydrogen fluoride (mol/kg)*

**Description**

Stability constant of hydrogen fluoride (mol/kg)

**Usage**

\[ Kf(S=35, \ T=25, \ P=0, \ kf="x", \ pHscale="T", \ Ks_p0=0, \ Ks_p=0, \ warn="y") \]

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>Salinity, default is 35</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius, default is 25°C</td>
</tr>
<tr>
<td>P</td>
<td>Hydrostatic pressure in bar (surface = 0), default is 0</td>
</tr>
<tr>
<td>kf</td>
<td>&quot;pf&quot; for using Kf from Perez and Fraga (1987) &quot;dg&quot; for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994), default is &quot;pf&quot;. Attention do not use a vector for this argument.</td>
</tr>
<tr>
<td>pHscale</td>
<td>choice of pH scale: &quot;T&quot; for the total scale, &quot;F&quot; for the free scale and &quot;SWS&quot; for using the seawater scale, default is &quot;T&quot; (total scale)</td>
</tr>
<tr>
<td>Ks_p0</td>
<td>Stability constant of hydrogen sulfate (mol/kg) at pressure zero; needed if kf = &quot;pf&quot; ; if needed and not given, it is computed; if given, computation speed is increased</td>
</tr>
<tr>
<td>Ks_p</td>
<td>Stability constant of hydrogen sulfate (mol/kg) at chosen pressure if not given, it is computed; if given, computation speed is increased</td>
</tr>
<tr>
<td>warn</td>
<td>&quot;y&quot; to show warnings when T or S go beyond the valid range for Kf, &quot;n&quot; to supress warnings. The default is &quot;y&quot;.</td>
</tr>
</tbody>
</table>

**Details**


It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.
The pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

**Value**

Kf

Stability constant of hydrogen fluoride (mol/kg)

**Author(s)**

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-mlo.fr>

**References**


**Examples**

\[ \text{Kf}(S=35, T=25, P=0, \text{pf"}, \text{pHscale="T"}) \]

---

**kfg**

variable for internal use

**Description**

nothing
**Khs**

*Description*

Dissociation constant of hydrogen sulfide (mol/kg)

*Usage*

\[ \text{Khs}(S=35, \ T=25, \ P=0, \ \text{pHscale}="T", \ \text{warn}="y") \]

*Arguments*

- **S**  
  Salinity, default is 35

- **T**  
  Temperature in degrees Celsius, default is 25°C

- **P**  
  Hydrostatic pressure in bar (surface = 0), default is 0

- **pHscale**  
  choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale

- **warn**  
  "y" to show warnings when T or S go beyond the valid range for Khs; "n" to suppress warnings. The default is "y".

*Details*

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45°C.

The pressure correction is applied on the seawater scale. Hence, the values are first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value is transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

*Value*

\[ \text{Khs} \]

Dissociation constant of hydrogen sulfide

*Author(s)*

Karline Soetaert <K.Soetaert@nioo.knaw.nl> and Heloise Lavigne

*References*

Examples

\[ K_{hs}(S=35, T=25, P=0, \text{pHscale}="T") \]

\[ K_n \quad \text{Dissociation constant of ammonium (mol/kg)} \]

Description

Dissociation constant of ammonium on the total scale (mol/kg)

Usage

\[ K_n(S=35, \, T=25, \, P=0, \, \text{pHscale}="T", \, \text{warn}="y") \]

Arguments

- **S**: Salinity, default is 35
- **T**: Temperature in degrees Celsius, default is 25°C
- **P**: Hydrostatic pressure in bar (surface = 0), default is 0
- **pHscale**: choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
- **warn**: "y" to show warnings when T or S go beyond the valid range for Kn; "n" to supress warnings. The default is "y".

Details

This formulation is only valid for specific ranges of temperature and salinity:

- **S** ranging between 0 and 45 and **T** ranging between 0 and 45°C.

The pressure correction is applied on the seawater scale. Hence, values are first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value is transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

\[ K_n \quad \text{Dissociation constant of ammonium (mol/kg)} \]

Author(s)

Karline Soetaert <K.Soetaert@nioo.knaw.nl> and Heloise Lavigne
References

Examples
\[ K_n(S=35, T=25, P=0, \text{pHscale}="T") \]

\[ \begin{array}{ll}
\text{Ks} & \text{Stability constant of hydrogen sulfate (mol/kg)} \\
\end{array} \]

Description
Stability constant of hydrogen sulfate (mol/kg)

Usage
\[ \text{Ks}(S=35, \ T=25, \ P=0, \ \text{ks}="d", \ \text{warn}="y") \]

Arguments
\begin{itemize}
  \item \textbf{S} Salinity, default is 35
  \item \textbf{T} Temperature in degrees Celsius, default is 25°C
  \item \textbf{P} Hydrostatic pressure in bar (surface = 0), default is 0
  \item \textbf{ks} "d" for using Ks from Dickson (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
  \item \textbf{warn} "y" to show warnings when T or S go beyond the valid range for Ks; "n" to supress warnings. The default is "y".
\end{itemize}

Details
The Dickson (1990) constant is recommended by Guide to Best Practices for Ocean CO2 Measurements (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

The pressure correction is applied on the free scale as described by Millero (1995), and the value transformed back to the required scale (T, F or SWS).
Value

ks

Stability constant of hydrogen sulfate (mol/kg), pHscale = free scale

Author(s)

Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-mfr.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. Journal of Chemical Thermodynamics 22, 113-127.


Examples

ks(S=35, T=25, P=0, ks="d")

Ksi

Dissociation constant of Si(OH)4

Description

Dissociation constant of Si(OH)4 on total scale (mol/kg)

Usage

Ksi(S=35, T=25, P=0, pHscale="T", kSWS2scale=0, warn="y")

Arguments

S  Salinity, default is 35
T  Temperature in degrees Celsius, default is 25oC
P  Hydrostatic pressure in bar (surface = 0), default is 0
pHscale  choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
kSWS2scale  Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.
warn  "y" to show warnings when T or S go beyond the valid range for Ksi; "n" to suppress warnings. The default is "y".
Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45°C.

The pressure correction is applied on the seawater scale. Hence, values are first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value is transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

ksi Dissociation constant of Si(OH)₄ (mol/kg)

Author(s)

Karline Soetaert <K.Soetaert@nioo.knaw.nl> and Heloise Lavigne

References

DOE 1994 Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water. ORNL/CDIAC-74. Oak Ridge, Tenn.: Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory.


Examples

ksi(S=35, T=25, P=0, pHscale="T")

| Ks pa | Solubility product of aragonite (mol/kg) |

Description

Solubility product of aragonite (mol/kg)

Usage

Kspa(S=35, T=25, P=0, warn="y")
Arguments

- **S**: Salinity, default is 35
- **T**: Temperature in degrees Celsius, default is 25°C
- **P**: Hydrostatic pressure in bar (surface = 0), default is 0
- **warn**: "y" to show warnings when T or S go beyond the valid range for Kspa; "n" to suppress warnings. The default is "y".

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 5 and 44 and T ranging between 5 and 40°C.

Pressure correction was performed as described by Millero (1995).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

- **Kspa**: Solubility product of aragonite (mol²/kg)

Author(s)

Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References


See Also

- **Kspc**.

Examples

- `Kspa(S=35,T=25,P=0)`
**Kspc**

**Solubility product of calcite (mol/kg)**

---

**Description**

Solubility product of calcite (mol/kg)

**Usage**

\[ \text{kspc}(S=35, \ T=25, \ P=0, \ \text{warn}="y") \]

**Arguments**

- **S**: Salinity, default is 35
- **T**: Temperature in degrees Celsius, default is 25°C
- **P**: Hydrostatic pressure in bar (surface = 0), default is 0
- **warn**: "y" to show warnings when T or S go beyond the valid range for Kspc; "n" to suppress warnings. The default is "y".

**Details**

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 5 and 44 and T ranging between 5 and 40°C.

The pressure correction was performed as described by Millero (1995).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

**Value**

\[ \text{Kspc} \]

Solubility product of calcite (mol/kg)

**Author(s)**

Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

**References**


See Also

Kspa.

Examples

Kspc(S=35, T=25, P=0)

---

**Kw**

*Ion product of water (mol2/kg2)*

**Description**

Ion product of water (mol2/kg2)

**Usage**

Kw(S=35, T=25, P=0, pHscale="T", kSWS2scale=0, warn="y")

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>Salinity, default is 35</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius, default is 25°C</td>
</tr>
<tr>
<td>P</td>
<td>Hydrostatic pressure in bar (surface = 0), default is 0</td>
</tr>
<tr>
<td>pHscale</td>
<td>choice of pH scale: &quot;T&quot; for using the total scale, &quot;F&quot; for using the free scale and &quot;SWS&quot; for using the seawater scale, default is total scale</td>
</tr>
<tr>
<td>kSWS2scale</td>
<td>Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.</td>
</tr>
<tr>
<td>warn</td>
<td>&quot;y&quot; to show warnings when T or S go beyond the valid range for Kw; &quot;n&quot; to supress warnings. The default is &quot;y&quot;.</td>
</tr>
</tbody>
</table>

**Details**

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45°C.

The pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.
**Value**

\[ K_w \]

Ion product of water (mol2/kg2)

**Author(s)**

Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

**References**


**Examples**

\[ K_w(S=35,T=25,P=0,\text{pHscale}="T") \]

**Description**

Describes the various approaches that can be used to alter the seawater carbonate system. Its main purpose is to assist the design of ocean acidification perturbation experiments.

**Usage**

\[ \text{oa}(\text{flag}, \text{var1}, \text{var2}, \text{pCO}_2\text{f}, \text{pCO}_2s=1e6, \text{S}=35, \text{T}=25, \text{P}=0, \text{Pt}=0, \text{Sit}=0, k1k2='x', \text{kf}='x', \text{ks}="d", \text{pHscale}="T", \text{plot}={\text{FALSE}}, \text{b}="u74", \text{eos} = "eos80", \text{long} = 1e+20, \text{lat} = 1e+20) \]

**Arguments**

- **flag**: select the couple of variables available to describe the initial seawater. The flags which can be used are:
  - flag = 1 pH and CO2 given
  - flag = 2 CO2 and HCO3 given
  - flag = 3 CO2 and CO3 given
  - flag = 4 CO2 and ALK given
  - flag = 5 CO2 and DIC given
  - flag = 6 pH and HCO3 given
  - flag = 7 pH and CO3 given
  - flag = 8 pH and ALK given
  - flag = 9 pH and DIC given
flag = 10 HCO3 and CO3 given
flag = 11 HCO3 and ALK given
flag = 12 HCO3 and DIC given
flag = 13 CO3 and ALK given
flag = 14 CO3 and DIC given
flag = 15 ALK and DIC given
flag = 21 pCO2 and pH given
flag = 22 pCO2 and HCO3 given
flag = 23 pCO2 and CO3 given
flag = 24 pCO2 and ALK given
flag = 25 pCO2 and DIC given

var1
Value of the first variable available to describe the initial seawater, in mol/kg except for pH and for pCO2 in uatm

var2
Value of the second variable available to describe the initial seawater, in mol/kg except for pH

pCO2f
pCO2 target value, in uatm

pCO2s
pCO2s is the pCO2, in uatm, of the “high-CO2” seawater that will be mixed with “normal seawater”. The default value is 10^6 uatm, that is seawater bubbled with pure CO2 gas and saturated with CO2.

S
Salinity, default is 35

T
Temperature in degrees Celsius, default is 25

P
Hydrostatic pressure in bar (surface = 0), default is 0

Pt
Concentration of total phosphate in mol/kg, default is 0

Sit
Concentration of total silicate in mol/kg, default is 0

k1k2
"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

kf
"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is "dg".

ks
"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"

pHscale
"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)

plot
A plot of the different perturbation methods can be plotted in a DIC vs ALK field with pCO2 isoclines are drawn in the back. Default is false.

b
Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74".

eos
"teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.
longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

latitude of data point, used when eos parameter is "teos10".

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): T ranging between 5 and 45 and S ranging between 0 and 45°C.
- Lueker et al. (2000): T ranging between 19 and 43 and S ranging between 2 and 35°C.
- Millero et al. (2006): T ranging between 0.1 and 50 and S ranging between 1 and 50°C.
- Millero (2010): T ranging between 1 and 50 and S ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if $P=0$, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): T ranging between 10 and 40 and S ranging between 9 and 33°C.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): T ranging between 0 and 45 and S ranging between 0 and 45°C.

For Ks:

- Dickson (1990): T ranging between 5 and 45 and S ranging between 0 and 45°C.
- Khoo et al. (1977): T ranging between 20 and 45 and S ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

• For Kn, the pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a list built as follows:

| description | A table describing in plain English the various ways to reach the target pCO2. Note that if a vector is given in argument only the first value is used. |
| perturbation | Table providing key parameters for the following methods: CO2 bubbling: high-CO2 air is bubbled in seawater. The first parameter is the value of the pCO2 in the air required to bubble the seawater (in uatm). SW mixing: mixing of “normal” and “high-CO2” seawater. The first parameter, “Weight fraction high-CO2 SW” or wf, is the weight fraction of the high-CO2 seawater per kg seawater. Addition of acid: strong acid is added to seawater. Note that this method is not recommended because it does not closely mimic natural ocean acidification (Gattuso and Lavigne, 2009). The first parameter, H+ (mol/kg), is the amount of H+ that must be added (mol/kg). The acid must be fortified with NaCl in order to have the same salinity than seawater. Addition of HCO3 and acid: bicarbonate (HCO3) and a strong acid are added. The first parameter, HCO3, is the amount of HCO3 that must be added (mol/kg). The second parameter, H+, is the quantity of H+ that must be added (mol/kg). The acid must be fortified with NaCl in order to have the same salinity than seawater. Addition of CO3 and acid: carbonate, CO3, and a strong acid are added. The first parameter, HCO3, is the quantity of CO3 that must be added (mol/kg). The second parameter, H+, is the quantity of H+ that must be added (mol/kg). |
| summary | Table summarizing the carbonate chemistry before and after applying each perturbation: pCO2 bubbling, mixing with high-CO2 seawater, addition of strong acid, and addition of bicarbonate/carbonate and strong acid. |

Warnings

• It is recommended to use concentrated solutions of acid or base in order to add small volumes.

• The addition of strong acid does not simulate well natural ocean acidification (higher concentration of dissolved inorganic carbon at constant total alkalinity) since it generates a decrease in total alkalinity while dissolved inorganic carbon is kept constant.

• Other important advice is provided in Gattuso and Lavigne (2009), Schulz et al. (2009) and in the “Guide for Best Practices on Ocean Acidification Research and Data Reporting” (https://www.iaea.org/sites/default/files/18/06/oa-guide-to-best-practices.pdf)

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity.
and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

Author(s)

Heloise Lavigne and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: $\text{AgCl}(s) + \frac{1}{2}\text{H}_2(\text{g}) = \text{Ag}(s) + \text{HCl}(\text{aq})$, and the standard acidity constant of the ion $\text{HSO}_4^-$ in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* 22, 113-127.


See Also
carb, pgas, pmix, ppH, pTA.

Examples
```
oa(flag=24, var1=384, var2=2325e-6, pCO2s=1e6, pCO2f=793, S=34.3, T=16,
P=0, pHscale="T", kf="pf", k1k2="1", ks="d", plot=TRUE, b="u74")
```

---

**Om**

*Carbonate saturation state for magnesian calcites*

**Description**

Calculates the calcium carbonate saturation state for magnesian calcite

**Usage**

```
Om(x, flag, var1, var2, k1k2='x', kf='x', ks='d', pHscale="T", b="u74")
```

**Arguments**

- **x**: mole fraction of magnesium ions, note that the function is only valid for x ranging between 0 and 0.25
- **flag**: select the couple of variables available. The flags which can be used are:
  - flag = 1 pH and CO2 given
  - flag = 2 CO2 and HCO3 given
  - flag = 3 CO2 and CO3 given
  - flag = 4 CO2 and ALK given
  - flag = 5 CO2 and DIC given
  - flag = 6 pH and HCO3 given
  - flag = 7 pH and CO3 given
  - flag = 8 pH and ALK given
  - flag = 9 pH and DIC given
  - flag = 10 HCO3 and CO3 given
  - flag = 11 HCO3 and ALK given
  - flag = 12 HCO3 and DIC given
  - flag = 13 CO3 and ALK given
  - flag = 14 CO3 and DIC given
  - flag = 15 ALK and DIC given
  - flag = 21 pCO2 and pH given
  - flag = 22 pCO2 and HCO3 given
  - flag = 23 pCO2 and CO3 given
  - flag = 24 pCO2 and ALK given
  - flag = 25 pCO2 and DIC given
\textbf{Details}

It is important to note that this function is \textbf{only valid} for:

- Salinity = 35
- Temperature = 25 degrees Celsius
- Hydrostatic pressure = 0 bar (surface)
- Concentration of total phosphate = 0 mol/kg
- Concentration of total silicate = 0 mol/kg

Note that the stoichiometric solubility products with respect to Mg-calcite minerals have not been determined experimentally. The saturation state with respect to Mg-calcite minerals is therefore calculated based on ion activities, i.e.,

$$\Omega_x = \frac{\{Ca^{2+}\}^{1-x}\{Mg^{2+}\}^x\{CO_3^{2-}\}^2}{K_x}$$

The ion activity \{a\} is calculated based on the observed ion concentrations [C] multiplied by the total ion activity coefficient, $\gamma_T$, which has been determined experimentally or from theory (e.g. Millero & Pierrot 1998): \{a\}=$\gamma_T$[C]. Because a true equilibrium cannot be achieved with respect to Mg-calcite minerals, $K_x$ represents a metastable equilibrium state obtained from what has been referred to as stoichiometric saturation (Thorstenson & Plummer 1977; a term not equivalent to the definition of the stoichiometric solubility product, see for example Morse et al. (2006) and references therein). In the present calculation calcium and magnesium concentrations were calculated based on salinity. Total ion activity coefficients with respect to $Ca^{2+}$, $Mg^{2+}$, and $CO_3^{2-}$ were adopted from Millero & Pierrot (1998).

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

\textit{For K1 and K2:}
• Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45°C.
• Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
• Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50°C.
• Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

• Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
• Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.

For Ks:

• Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45°C.
• Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

• For K0, the pressure correction term of Weiss (1974) is used.
• For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a list with

OmegaMgCa_biogenic

Mg-calcite saturation state for minimally prepared biogenic Mg-calcite.
OmegaMgCa_biogenic_cleaned

Mg-calcite saturation state for cleaned and annealed biogenic Mg-calcite.

Author(s)

Heloise Lavigne, Andreas J. Andersson and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Only the references related to the saturation state of magnesian calcite are listed below; the other references are listed under the carb function.


Examples

```
Om(x=seq(0.01, 0.252, 0.01), flag=8, var1=8.2, var2=0.00234,
   k1k2='x', kf='x', ks="d", pHscale="T", b='u74')
```

```
p2d

Converts pressure in dbar to depth in meters

Description

Converts pressure in dbar to depth in meters

Usage

p2d(pressure, lat=40)
```
Arguments

- pressure: Pressure in dbar
- lat: Latitude in degrees, N and S is irrelevant, default is 40°

Value

- depth: Depth corresponding to the pressure given, in meters

Author(s)

Heloise Lavigne and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References


See Also

d2p

Examples

```r
p2d(pressure=7686, lat=30)
```

---

**p2fCO2**

Converts pCO2 (partial pressure in CO2) into fCO2 (fugacity of CO2)

**Description**

Converts pCO2 (partial pressure in CO2) into fCO2 (fugacity of CO2)

**Usage**

```r
p2fCO2(T = 25, Patm=1, P=0, pCO2)
```

**Arguments**

- T: Temperature in degrees Celsius, default is 25°C
- Patm: Surface atmospheric pressure in atm, default is 1 atm
- P: Hydrostatic pressure in bar, default is 0 bar (surface)
- pCO2: Partial pressure in CO2 in µatm, the same units as that for the fugacity output

**Value**

- fCO2: Fugacity of CO2 in µatm, the same units as that for the pCO2 input.
Note

**Warning:** pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

Author(s)

Heloise Lavigne, Jean-Pierre Gattuso, and James Orr <gattuso@obs-v1fr.fr>

References


See Also

f2pCO2.

Examples

```r
p2fCO2(T=25, Patm=0.97, P=0, pCO2=380)
```

---

Converts partial pressure of CO2 to mole fraction of CO2

**Description**

Converts pCO2 (partial pressure of CO2) into xCO2 (mole fraction of CO2)

**Usage**

```r
p2xCO2(S=35, T=25, Patm=1, pCO2)
```

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>Salinity on the practical salinity scale, default is 35</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius, default is 25°C</td>
</tr>
<tr>
<td>Patm</td>
<td>Atmospheric pressure in atmospheres, default is 1.0 (this is not the hydrostatic pressure)</td>
</tr>
<tr>
<td>pCO2</td>
<td>Partial pressure of CO2 in µatm</td>
</tr>
</tbody>
</table>
Details

The $\text{xCO}_2$ (ppm) is computed from $\text{pCO}_2$ ($\mu\text{atm}$) using the following equation: $\text{xCO}_2 = \frac{\text{pCO}_2}{(\text{Patm} - \text{pH}_2\text{O})}$, where pH20 is the vapor pressure of seawater computed following best practices (Dickson et al., 2007). That computed pH20 is identical, when rounded to the 4th decimal place, with that computed by the equation from Weiss and Price (1980).

Value

$\text{xCO}_2$ Mole fraction of CO2 in ppm.

Note

Warning: $\text{pCO}_2$ estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

Author(s)

James Orr <james.orr@lsce.ipsl.fr>

References


See Also

$x2pCO2$ and $\text{vapress}$

Examples

```
## Convert atmospheric pressure from mbar to atm
Patm_mbar = 1052  # in millibar
Patm    = Patm_mbar / 1013.25  # in atm
## Compute xCO2 from pCO2
pCO2 = 380
xCO2 = p2xCO2(T=25, S=35, Patm=Patm, pCO2=pCO2)
print(xCO2)
## The result is 377.1546 ppm
```
Description

Calculates the changes in the saturation states of aragonite and calcite resulting from the manipulation of the calcium concentration

Usage

\texttt{pCa(flag, var1, var2, Ca, S=35, T=20, P=0, Pt=0, Sit=0, k1k2="x", kf="x", ks="d", pHscale="T", b="u74", eos = "eos80", long = 1e+20, lat = 1e+20)}

Arguments

\texttt{flag} select the couple of variables available. The flags which can be used are:
- \texttt{flag = 1 pH and CO2 given}
- \texttt{flag = 2 CO2 and HCO3 given}
- \texttt{flag = 3 CO2 and CO3 given}
- \texttt{flag = 4 CO2 and ALK given}
- \texttt{flag = 5 CO2 and DIC given}
- \texttt{flag = 6 pH and HCO3 given}
- \texttt{flag = 7 pH and CO3 given}
- \texttt{flag = 8 pH and ALK given}
- \texttt{flag = 9 pH and DIC given}
- \texttt{flag = 10 HCO3 and CO3 given}
- \texttt{flag = 11 HCO3 and ALK given}
- \texttt{flag = 12 HCO3 and DIC given}
- \texttt{flag = 13 CO3 and ALK given}
- \texttt{flag = 14 CO3 and DIC given}
- \texttt{flag = 15 ALK and DIC given}
- \texttt{flag = 21 pCO2 and pH given}
- \texttt{flag = 22 pCO2 and HCO3 given}
- \texttt{flag = 23 pCO2 and CO3 given}
- \texttt{flag = 24 pCO2 and ALK given}
- \texttt{flag = 25 pCO2 and DIC given}

\texttt{var1} Value of the first variable in mol/kg, except for pH and for pCO2 in \textmu atm

\texttt{var2} Value of the second variable in mol/kg, except for pH

\texttt{Ca} Calcium concentration in mol/kg

\texttt{S} Salinity

\texttt{T} Temperature in degrees Celsius

\texttt{P} Hydrostatic pressure in bar (surface = 0)
The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

**For K1 and K2:**

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

**For Kf:**

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

**For Ks:**

- Dickson (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
Dickson (1990): $S$ ranging between 5 and 45 and $T$ ranging between 0 and 45°C.
Khoo et al. (1977): $S$ ranging between 20 and 45 and $T$ ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

**Pressure corrections and pH scale:**

- For $K_0$, the pressure correction term of Weiss (1974) is used.
- For $K_1$, $K_2$, $pK_1$, $pK_2$, $K_w$, $K_b$, $K_{hs}$ and $K_{si}$, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For $K_f$, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides $K_f$ on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, $K_f$ was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For $K_s$, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For $K_n$, the pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

**Value**

The function returns a data frame containing the following columns:

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>comment</td>
<td>The initial or final state water</td>
</tr>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius</td>
</tr>
<tr>
<td>P</td>
<td>Pressure in bar</td>
</tr>
<tr>
<td>pH</td>
<td>pH</td>
</tr>
<tr>
<td>CO2</td>
<td>CO2 concentration (mol/kg)</td>
</tr>
<tr>
<td>pCO2</td>
<td>pCO2, CO2 partial pressure (µatm)</td>
</tr>
<tr>
<td>fCO2</td>
<td>fCO2, CO2 fugacity (µatm)</td>
</tr>
</tbody>
</table>
Note

**Warning:** pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

**Author(s)**

Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

**References**


Dickson A. G., 1990 Standard potential of the reaction: $\text{AgCl(s)} + 1/2\text{H}_2(g) = \text{Ag(s)} + \text{HCl(aq)}$, and the standard acidity constant of the ion $\text{HSO}_4^-$ in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* **22**, 113-127.


Examples

```r
pCa(flag=15, var1=2302e-6, var2=2050e-6, Ca=0.01028, S=35, T=20, P=0, Pt=0, Sit=0, pHScale="T", kf="pf", k1k2="1", ks="d", b="u74") # with normal Ca concentration
pCa(flag=15, var1=2302e-6, var2=2050e-6, Ca=0.01028/2, S=35, T=20, P=0, Pt=0, Sit=0, pHScale="T", kf="pf", k1k2="1", ks="d", b="u74") # with 0.5 * Ca concentration
```

<table>
<thead>
<tr>
<th>Pcoeffs</th>
<th>Coefficients used for pressure-correcting the equilibrium constants</th>
</tr>
</thead>
</table>

Description

Pressure corrections are based on the following equations:

\[
\ln \frac{K_i^P}{K_i^0} = -\frac{\Delta V_i}{RT}P + 0.5 \frac{\Delta K_i}{RT}P^2
\]

with

\[
\Delta V_i = a_0 + a_1 T + a_2 T^2
\]

and

\[
\Delta K_i = b_0 + b_1 T + b_2 T^2
\]

The variables are:

- \( K \) indicating the type of equilibrium constant
- coefficient \( a_0 \)
- coefficient \( a_1 \)
- coefficient \( a_2 \)
- coefficient \( b_0 \)
- coefficient \( b_1 \)
- coefficient \( b_2 \)

Usage

Pcoeffs

Format

A data frame with 15 rows and 7 variables

Details

For \( K_b \), to be consistent with Millero (1979) \( a_2 \) was changed to -2.608e-3 instead of 2.608e-3 (value given in Millero, 1995) For \( K_w \), coefficients are from Millero (1983).
Source


See Also

Pcorrect

---

**Pcorrect**

*Pressure correction of equilibrium constants*

**Description**

Computes the pressure correction of the equilibrium constants

**Usage**

```r
Pcorrect(Kvalue, Ktype, T=25, S=35, P=0, pHscale="T", kconv2ScaleP0=0, kconv2Scale=, warn="y")
```

**Arguments**

<table>
<thead>
<tr>
<th>Kvalue</th>
<th>Value of the constant at P=0 (hydrostatic pressure in bar, surface = 0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ktype</td>
<td>Name of the constant,</td>
</tr>
<tr>
<td></td>
<td>• K1 First dissociation constant of carbonic acid (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• K2 Second dissociation constant of carbonic acid (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• Kb Dissociation constant of boric acid (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• Kw Ion product of water (mol2/kg2)</td>
</tr>
<tr>
<td></td>
<td>• Ks Stability constant of hydrogen sulfate (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• Kf Stability constant of hydrogen fluoride (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• Kspc Solubility product of calcite (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• Kspa Solubility product of aragonite (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• K1p First dissociation constant of phosphoric acid (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• K2p Second dissociation constant of phosphoric acid (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• K3p Third dissociation constant of phosphoric acid (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• Khs Dissociation constant of hydrogen sulfide (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• Kn Dissociation constant of ammonium (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• Kspi Dissociation constant of Si(OH)4 (mol/kg)</td>
</tr>
<tr>
<td></td>
<td>• K2si Second dissociation constant of Si(OH)4 (mol/kg)</td>
</tr>
</tbody>
</table>
**T** Temperature in degrees Celsius, default is 25°C

**S** Salinity, default is 35

**P** Hydrostatic pressure in bar (surface = 0), default is 0

**pHscale** pH scale of the constant given in Kvalue

**kconv2ScaleP0** Conversion factor from the pH scale selected to the SWS (or free for Kf) scale at pressure zero. It is computed if it is not given, which significantly slows down the computation

**kconv2Scale** Conversion factor from the pH scale selected to the SWS (or free for Kf) scale at the hydrostatic pressure value indicated. It is computed if it is not given, which significantly slows down the computation

**warn** "y" to show warnings when T or S go beyond the valid range for constants; "n" to suppress warnings. The default is "y".

**Details**

- The pressure correction is applied on the seawater scale for K1, K2, K1p, K2p, K3p, Kb, Khs, Kn, Ksi, K2si and Kw. Hence the K value is first converted on the seawater scale if needed. After pressure correction, the constant is converted back to the initial pH scale.
- The pressure correction is applied on the free scale for Kf.
- There is no issue of pH scale for Ks, Kspa and Kspc.

**Value**

The equilibrium constant given in argument but after pressure correction

**Author(s)**

Heloise Lavigne and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

**References**


**See Also**

Pcoeffs

**Examples**

```r
k10 <- K1(T=25, P=0, S=35)
Pcorrect(Kvalue=k10, Ktype="K1", P=300, T=25, S=35, pHscale="T")
```
Description
Calculates the carbonate chemistry after changes in pCO2 generated by gas bubbling

Usage
pgas(flag, var1, var2, pCO2g, S=35, T=20, P=0, Pt=0, S1=0, k1k2=“x”,
kf=“x”, k2=“d”, pHscale=“T”, b=“u74”, eos = “eos80”, long = 1e+20, lat = 1e+20)

Arguments
flag
select the couple of variables available. The flags which can be used are:
  flag = 1 pH and CO2 given
  flag = 2 CO2 and HCO3 given
  flag = 3 CO2 and CO3 given
  flag = 4 CO2 and ALK given
  flag = 5 CO2 and DIC given
  flag = 6 pH and HCO3 given
  flag = 7 pH and CO3 given
  flag = 8 pH and ALK given
  flag = 9 pH and DIC given
  flag = 10 HCO3 and CO3 given
  flag = 11 HCO3 and ALK given
  flag = 12 HCO3 and DIC given
  flag = 13 CO3 and ALK given
  flag = 14 CO3 and DIC given
  flag = 15 ALK and DIC given
  flag = 21 pCO2 and pH given
  flag = 22 pCO2 and HCO3 given
  flag = 23 pCO2 and CO3 given
  flag = 24 pCO2 and ALK given
  flag = 25 pCO2 and DIC given

var1
Value of the first variable in mol/kg, except for pH and for pCO2 in µatm

var2
Value of the second variable in mol/kg, except for pH

pCO2g
CO2 partial pressure of the gas used for bubbling in µatm

S
Salinity

T
Temperature in degrees Celsius

P
Hydrostatic pressure in bar (surface = 0)

Pt
Concentration of total phosphate in mol/kg
Concentration of total silicate in mol/kg

"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".

"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"

"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)

Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74".

"teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.

longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

latitude of data point, used when eos parameter is "teos10".

**Details**

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

**For K1 and K2:**
- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 450C.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 350C.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 500C.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 500C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

**For Kf:**
- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 330C.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 450C.

**For Ks:**
- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 450C.
Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

**Pressure corrections and pH scale:**

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

**Value**

The function returns a data frame containing the following columns:

<table>
<thead>
<tr>
<th>column</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>comment</td>
<td>The initial or final state water</td>
</tr>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius</td>
</tr>
<tr>
<td>P</td>
<td>Pressure in bar</td>
</tr>
<tr>
<td>pH</td>
<td>pH</td>
</tr>
<tr>
<td>C02</td>
<td>CO2 concentration (mol/kg)</td>
</tr>
<tr>
<td>pC02</td>
<td>pCO2, CO2 partial pressure (µatm)</td>
</tr>
<tr>
<td>fC02</td>
<td>fCO2, CO2 fugacity (µatm)</td>
</tr>
<tr>
<td>HCO3</td>
<td>HCO3 concentration (mol/kg)</td>
</tr>
</tbody>
</table>
C03  CO3 concentration (mol/kg)
DIC  DIC concentration (mol/kg)
ALK  ALK, total alkalinity (mol/kg)
OmegaAragonite  Omega aragonite, aragonite saturation state
OmegaCalcite  Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

Author(s)

Jean-Pierre Gattuso and Heloise Lavigne <gattuso@obs-vlfr.fr>

References


Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. Journal of Chemical Thermodynamics 22, 113-127.


Examples

```r
gas(flag=15, var1=2302e-6, var2=2050e-6, pCO2g=750, S=35, T=20, P=0, Pt=0, Sit=0, ph scale=T", kf="pf", k1k2="l", ks="d", b="u74")
```

<table>
<thead>
<tr>
<th>pH</th>
<th>Potentiometric pH</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description

Calculation of potentiometric pH

Usage

```r
pH(Ex=-67,Etris=-72.4,S=35,T=25)
```

Arguments

- `Ex`: e.m.f. of the seawater sample in mV, default is 67
- `Etris`: e.m.f. of the TRIS buffer in mV, default is -72.4
- `S`: Salinity, default is 35
- `T`: Temperature in degrees Celsius, default is 25°C

Details

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

- `pH`: Potentiometric pH (in mol/kg on the total scale)

Author(s)

Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References


See Also

- `tris`, `amp`, `phslope`.
**Description**

Converts pH from one scale to another one chosen between the total scale, the free scale and the seawater scale

**Usage**

phconv(flag=1, pH=8.10, S=35, T=25, P=0, ks="d")

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>flag</td>
<td>choice of the type of conversion: flag=1: seawater scale to total scale, flag=2: free scale to total scale, flag=3: total scale to seawater scale, flag=4: total scale to free scale, flag=5: seawater scale to free scale, flag=6: free scale to seawater scale, default is flag=1</td>
</tr>
<tr>
<td>pH</td>
<td>Enter the value of pH which need to be converted, default is 8.100</td>
</tr>
<tr>
<td>S</td>
<td>Salinity, default is 35</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius, default is 25oC</td>
</tr>
<tr>
<td>P</td>
<td>Hydrostatic pressure in bar (surface = 0), default is 0</td>
</tr>
<tr>
<td>ks</td>
<td>&quot;d&quot; for using Ks from Dickson (1990), &quot;k&quot; for using Ks from Khoo et al. (1977), default is &quot;d&quot;</td>
</tr>
</tbody>
</table>

**Details**

The Dickson (1990) constant is recommended by the Guide to Best Practices for Ocean CO2 Measurements (2007). It is critical to consider that each formulation is valid in specific ranges of temperature and salinity:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

**Value**

The function returns the values of pH converted
Author(s)

Heloise Lavigne and Jean-PierreGattuso <gattuso@obs-vlfr.fr>

References


Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* 22, 113-127.


See Also

kconv.

Examples

```r
c # To convert pH=8.10 from the seawater scale to the total scale
# at salinity=35, temperature=25oC and atmospheric pressure:

phc <- phconv(flag=1, pH=8.10, S=35, T=25, P=0, ks="d")

# Note that phc is the value of the pH converted in total scale

# By using vectors
# to convert the pH values: 8, 8.05, 8.10, 8.15, 8.20
# from the free to the total scale

pH <- c(8, 8.05, 8.10, 8.15, 8.20)
phc <- phconv(flag=2, pH=pH, S=35, T=25, P=0, ks="d")

# Note that phc is a vector containing the value of the pH converted
# to the total scale
```

pHinsi

*pH at in situ temperature and pressure*

Description

pH at in situ temperature and pressure
Usage

\[ \text{pH}\text{insi}(\text{pH}=8.2, \text{ALK}=2.4e-3, \text{Tinsi}=20, \text{Tlab}=25, \text{Pinsi}=0, \text{S}=35, \text{Pt}=0, \text{Sit}=0, \]
\[ \text{k1k2} = "x", \text{ kf} = "x", \text{ ks}="d" , \text{pHscale} = "T", \text{ b}="u74", \text{ eos} = "eos00", \]
\[ \text{long} = 1e+20, \text{ lat} = 1e+20) \]

Arguments

<table>
<thead>
<tr>
<th>Arguments</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH</td>
<td>pH measured in the laboratory</td>
</tr>
<tr>
<td>ALK</td>
<td>ALK, total alkalinity (mol/kg)</td>
</tr>
<tr>
<td>Tinsi</td>
<td>In situ temperature in degrees Celsius</td>
</tr>
<tr>
<td>Tlab</td>
<td>Measurement temperature in degrees Celsius</td>
</tr>
<tr>
<td>Pinsi</td>
<td>In situ hydrostatic pressure in bar (surface = 0)</td>
</tr>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>Pt</td>
<td>value of the concentration of total phosphate in mol/kg</td>
</tr>
<tr>
<td>Sit</td>
<td>the value of the total silicate in mol/kg</td>
</tr>
<tr>
<td>k1k2</td>
<td>&quot;l&quot; for using K1 and K2 from Lueker et al. (2000), &quot;m06&quot; from Millero et al. (2006), &quot;m10&quot; from Millero (2010), &quot;w14&quot; from Waters et al. (2014), and &quot;r&quot; from Roy et al. (1993). &quot;x&quot; is the default flag; the default value is then &quot;l&quot;, except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is &quot;w14&quot;.</td>
</tr>
<tr>
<td>kf</td>
<td>&quot;pf&quot; for using Kf from Perez and Fraga (1987) and &quot;dg&quot; for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). &quot;x&quot; is the default flag; the default value is then &quot;pf&quot;, except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is &quot;dg&quot;.</td>
</tr>
<tr>
<td>ks</td>
<td>&quot;d&quot; for using Ks from Dickon (1990), &quot;k&quot; for using Ks from Khoo et al. (1977), default is &quot;d&quot;</td>
</tr>
<tr>
<td>pHscale</td>
<td>choice of pH scale: &quot;T&quot; for the total scale, &quot;F&quot; for the free scale and &quot;SWS&quot; for using the seawater scale, default is &quot;T&quot; (total scale)</td>
</tr>
<tr>
<td>b</td>
<td>&quot;110&quot; for computing boron total from the Lee et al. (2010) formulation or &quot;u74&quot; for using the Uppstrom (1974) formulation, default is &quot;u74&quot;</td>
</tr>
<tr>
<td>eos</td>
<td>&quot;teos10&quot; to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); &quot;eos80&quot; to specify T and S according to EOS-80.</td>
</tr>
<tr>
<td>long</td>
<td>longitude of data point, used when eos parameter is &quot;teos10&quot; as a conversion parameter from absolute to practical salinity.</td>
</tr>
<tr>
<td>lat</td>
<td>latitude of data point, used when eos parameter is &quot;teos10&quot;.</td>
</tr>
</tbody>
</table>

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45°C.
• Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
• Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
• Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:
• Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
• Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.

For Ks:
• Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45°C.
• Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:
• For K0, the pressure correction term of Weiss (1974) is used.
• For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.
**pHslope**

**Value**

pH

pH at in situ temperature and pressure

**Author(s)**

Jean-Pierre Gattuso, <gattuso@obs-vlfr.fr>

**References**


**Examples**

```
pHinsi(pH=8.2,ALK=2.4e-3,Tinsi=25,Tlab=25,Pinsi=200,S=35,Pt=0,Sit=0)
```

```
pHslope
Slope of the calibration curve of a pH electrode
```

**Description**

Slope of the calibration curve of a pH electrode (percent of theoretical slope)

**Usage**

```
pHslope(Etris=-72.4,Eamp=4.9,S=35,T=25)
```

**Arguments**

- **Etris**: e.m.f. of the TRIS buffer in mV, default is -72.4
- **Eamp**: e.m.f. of the AMP buffer in mV, default is 4.9
- **S**: Salinity, default is 35
- **T**: Temperature in degrees Celsius, default is 25oC
Details

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

**phslope**

Slope of the calibration curve (in percent of theoretical slope)

Author(s)

Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References


See Also

tris, amp, pH.

Examples

```r
# Example from Dickson et al. (2007)
phslope(Etris=-72.4, Eamp=4.9, S=35, T=25)
```

### phspec

_Calculates pH from results of spectrophotometric measurements_

Description

Calculates pH of a water sample from absorbance ratios R, obtained from spectrophotometric measurements with pH indicator dyes (on the total scale in mol/kg-soln)

Usage

```r
phspec(S=35, T=25, R=1, d="mCP", k="m18", warn="y")
```

Arguments

- **S** Salinity, default is 35
- **T** Temperature in degrees Celsius, default is 25°C
- **R** Absorbance ratio, default is 1
- **d** Dye used for spectrophotometric measurement, default is "mCP"
- **k** "m18" for using mCP characterization by Mueller and Rehder (2018)
- **warn** "y" to show warnings when S and/or T go beyond the valid range for the chosen d and k; "n" to suppress warnings. The default is "y".
Details

The model used to calculate the return value of this function is based on experimental data. It is critical to consider that the formulation refers to the conditions studied during the characterization experiment and is only valid for the studied ranges of temperature and salinity:

- Mueller and Rehder (2018): S ranging between 0 and 40, T ranging between 5 and 35°C, and the dye used being m-Cresol purple (mCP) with R referring to the ratio of absorbances at wavelengths 578 and 434 nm.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

\[ pH_{spec} \]

The function returns the pH value of a water sample from absorbance ratios R, obtained from spectrophotometric measurements with pH indicator dyes (on the total scale in mol/kg-soln)

Author(s)

Jens Daniel Mueller <jens.mueller@io-warnemuende.de> Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References


See Also

amp, phslope, ph.tris.

Examples

```r
# Example should give test value pH = 7.6713
pHspec(S=35, T=25, R=1, d="mCP", k="m18", warn="y")
```

pmix

Calculates the carbonate chemistry after mixing of two water samples with different pCO2

Usage

```r
pmix(flag, var1, var2, pCO2s, wf, S=35, T=20, P=0, Pt=0, Sit=0, k1k2="x", kf="x", ks="d", pHscale="T", b="u74", eos = "eos80", long = 1e+20, lat = 1e+20)
```
Arguments

**flag**

select the couple of variables available. The flags which can be used are:

- flag = 1 pH and CO₂ given
- flag = 2 CO₂ and HCO₃ given
- flag = 3 CO₂ and CO₃ given
- flag = 4 CO₂ and ALK given
- flag = 5 CO₂ and DIC given
- flag = 6 pH and HCO₃ given
- flag = 7 pH and CO₃ given
- flag = 8 pH and ALK given
- flag = 9 pH and DIC given
- flag = 10 HCO₃ and CO₃ given
- flag = 11 HCO₃ and ALK given
- flag = 12 HCO₃ and DIC given
- flag = 13 CO₃ and ALK given
- flag = 14 CO₃ and DIC given
- flag = 15 ALK and DIC given
- flag = 21 pCO₂ and pH given
- flag = 22 pCO₂ and HCO₃ given
- flag = 23 pCO₂ and CO₃ given
- flag = 24 pCO₂ and ALK given
- flag = 25 pCO₂ and DIC given

**var1**

Value of the first variable in mol/kg except for pH and for pCO₂ in µatm

**var2**

Value of the second variable in mol/kg except for pH

**pCO₂s**

Partial pressure of the high CO₂ component in µatm

**wf**

Weight fraction of the high CO₂ seawater per kg seawater

**S**

Salinity

**T**

Temperature in degrees Celsius

**P**

Hydrostatic pressure in bar (surface = 0)

**Pt**

Concentration of total phosphate in mol/kg

**Sit**

Concentration of total silicate in mol/kg

**k1k2**

"l" for using K₁ and K₂ from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

**kf**

"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is "dg".

**ks**

"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pmix

choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWs" for using the seawater scale, default is total scale.

Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74".

"teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.

longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

latitude of data point, used when eos parameter is "teos10".

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50°C.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

• For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

• For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

Value

The function returns a data frame containing the following columns:

<table>
<thead>
<tr>
<th>comment</th>
<th>The initial or final state water</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius</td>
</tr>
<tr>
<td>P</td>
<td>Pressure in bar</td>
</tr>
<tr>
<td>pH</td>
<td>pH</td>
</tr>
<tr>
<td>CO2</td>
<td>CO2 concentration (mol/kg)</td>
</tr>
<tr>
<td>pCO2</td>
<td>pCO2, CO2 partial pressure (µatm)</td>
</tr>
<tr>
<td>fCO2</td>
<td>fCO2, CO2 fugacity (µatm)</td>
</tr>
<tr>
<td>HCO3</td>
<td>HCO3 concentration (mol/kg)</td>
</tr>
<tr>
<td>CO3</td>
<td>CO3 concentration (mol/kg)</td>
</tr>
<tr>
<td>DIC</td>
<td>DIC concentration (mol/kg)</td>
</tr>
<tr>
<td>ALK</td>
<td>ALK, total alkalinity (mol/kg)</td>
</tr>
<tr>
<td>OmegaAragonite</td>
<td>Omega aragonite, aragonite saturation state</td>
</tr>
<tr>
<td>OmegaCalcite</td>
<td>Omega calcite, calcite saturation state</td>
</tr>
</tbody>
</table>

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)
Author(s)

Jean-Pierre Gattuso and Heloise Lavigne<hattuso@obs-v1f.fr>

References


Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. Journal of Chemical Thermodynamics 22, 113-127.


Examples

pmix(flag=24, var1=384, var2=2302e-6, pcO2s=1e6, wf=0.003, S=34.3, T=16, P=0, pHscale="T", kf="pf", k1k2="1", ks="d", b="u74")
Description

Calculates the carbonate chemistry after pH manipulations through addition of acid or base

Usage

```python
ppH(flag, sys, var1, var2, pCO2a, vol, N, S=35, T=20, P=0, Pt=0,
Sit=0, pHscale="T", k1k2="x", kf="x", ks="d", eos = "eos88",
long = 1e+20, lat = 1e+20)
```

Arguments

- **flag**: Select the couple of variables available. The flags which can be used are:
  - `flag = 1 pH and CO2 given`
  - `flag = 2 CO2 and HCO3 given`
  - `flag = 3 CO2 and CO3 given`
  - `flag = 4 CO2 and ALK given`
  - `flag = 5 CO2 and DIC given`
  - `flag = 6 pH and HCO3 given`
  - `flag = 7 pH and CO3 given`
  - `flag = 8 pH and ALK given`
  - `flag = 9 pH and DIC given`
  - `flag = 10 HCO3 and CO3 given`
  - `flag = 11 HCO3 and ALK given`
  - `flag = 12 HCO3 and DIC given`
  - `flag = 13 CO3 and ALK given`
  - `flag = 14 CO3 and DIC given`
  - `flag = 15 ALK and DIC given`
  - `flag = 21 pCO2 and pH given`
  - `flag = 22 pCO2 and HCO3 given`
  - `flag = 23 pCO2 and CO3 given`
  - `flag = 24 pCO2 and ALK given`
  - `flag = 25 pCO2 and DIC given`

- **sys**: 0 if the manipulation is carried out in a system closed to the atmosphere or 1 if it is carried out in a system open to the atmosphere

- **var1**: Value of the first variable in mol/kg, except for pH and for pCO2 in µatm

- **var2**: Value of the second variable in mol/kg, except for pH

- **pCO2a**: CO2 partial pressure in the atmosphere pCO2 in µatm. It is only used in systems open to the atmosphere (i.e. when sys=1)
Volume of acid or base added in liter. By convention, it is given a negative sign for acid additions and a positive sign for base additions. The acid must be fortified with NaCl in order to have the same salinity than seawater.

Normality of the acid or base in mol/kg

Salinity

Temperature in degrees Celsius

Hydrostatic pressure in bar (surface = 0)

Concentration of total phosphate in mol/kg

Concentration of total silicate in mol/kg

"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".

"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"

choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale

"teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.

longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

latitude of data point, used when eos parameter is "teos10".

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:


• Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
• Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 450°C.

For Ks:
• Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 450°C.
• Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:
• For K0, the pressure correction term of Weiss (1974) is used.
• For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
• For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

<table>
<thead>
<tr>
<th>Comment</th>
<th>The initial or final state water</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius</td>
</tr>
</tbody>
</table>
ppH

P Pressure in bar
pH pH
CO2 CO2 concentration (mol/kg)
pCO2 pCO2, CO2 partial pressure (µatm)
fCO2 fCO2, CO2 fugacity (µatm)
HCO3 HCO3 concentration (mol/kg)
CO3 CO3 concentration (mol/kg)
DIC DIC concentration (mol/kg)
ALK ALK, total alkalinity (mol/kg)
OmegaAragonite Omega aragonite, aragonite saturation state
OmegaCalcite Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

Author(s)

Jean-Pierre Gattuso and Heloise Lavigne<gattuso@obs-vlfr.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. Journal of Chemical Thermodynamics 22, 113-127.
See Also

buffer.

Examples

```
ppH(flag=24, sys=0, var1=384, var2=2302e-6, pCO2a=384, vol=-12e-3, N=0.01, S=34.3, T=16, P=0, pHscale="T", kf="pf", k1k2="1", ks="d")

ppH(flag=24, sys=1, var1=384, var2=2302e-6, pCO2a=384, vol=-12e-3, N=0.01, S=34.3, T=16, P=0, pHscale="T", kf="pf", k1k2="1", ks="d")
```

psi

*Molar ratio of CO2 released vs CaCO3 precipitated*

Description

Returns the molar ratio of CO2 released vs CaCO3 precipitated described by Frankignoulle et al. (1994).

Usage

```
psi(flag, var1, var2, S=35, T=20, Patm, P=0, Pt=0, Sit=0, pHscale="T", kf="x", k1k2="x", ks="d", eos = "eos80", long = 1e+20, lat = 1e+20)
```

Arguments

- **flag**: select the couple of variables available. The flags which can be used are:
  - flag = 1 pH and CO2 given
  - flag = 2 CO2 and HCO3 given
  - flag = 3 CO2 and CO3 given
  - flag = 4 CO2 and ALK given
  - flag = 5 CO2 and DIC given
  - flag = 6 pH and HCO3 given
  - flag = 7 pH and CO3 given
  - flag = 8 pH and ALK given
  - flag = 9 pH and DIC given
  - flag = 10 HCO3 and CO3 given
  - flag = 11 HCO3 and ALK given
  - flag = 12 HCO3 and DIC given
  - flag = 13 CO3 and ALK given
  - flag = 14 CO3 and DIC given
  - flag = 15 ALK and DIC given
  - flag = 21 pCO2 and pH given
  - flag = 22 pCO2 and HCO3 given
flag = 23 pCO₂ and CO₃ given
flag = 24 pCO₂ and ALK given
flag = 25 pCO₂ and DIC given

<table>
<thead>
<tr>
<th>var1</th>
<th>enter value of the first variable in mol/kg, except for pH and for pCO₂ in µatm</th>
</tr>
</thead>
<tbody>
<tr>
<td>var2</td>
<td>enter value of the second variable in mol/kg, except for pH</td>
</tr>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius</td>
</tr>
<tr>
<td>Patm</td>
<td>Surface atmospheric pressure in atm, default is 1 atm</td>
</tr>
<tr>
<td>P</td>
<td>Hydrostatic pressure in bar (surface = 0)</td>
</tr>
<tr>
<td>Pt</td>
<td>Concentration of total phosphate in mol/kg; set to 0 if NA</td>
</tr>
<tr>
<td>Sit</td>
<td>Concentration of total silicate in mol/kg; set to 0 if NA</td>
</tr>
<tr>
<td>pHscale</td>
<td>choice of pH scale: &quot;T&quot; for the total scale, &quot;F&quot; for the free scale and &quot;SWS&quot; for using the seawater scale, default is &quot;T&quot; (total scale)</td>
</tr>
<tr>
<td>k1k2</td>
<td>&quot;I&quot; for using K1 and K2 from Lueker et al. (2000), &quot;m06&quot; from Millero et al. (2006), &quot;m10&quot; from Millero (2010), &quot;w14&quot; from Waters et al. (2014), and &quot;r&quot; from Roy et al. (1993). &quot;x&quot; is the default flag; the default value is then &quot;I&quot;, except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is &quot;w14&quot;.</td>
</tr>
<tr>
<td>kf</td>
<td>&quot;pf&quot; for using Kf from Perez and Fraga (1987) and &quot;dg&quot; for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). &quot;x&quot; is the default flag; the default value is then &quot;pf&quot;, except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is &quot;dg&quot;.</td>
</tr>
<tr>
<td>ks</td>
<td>&quot;d&quot; for using Ks from Dickon (1990), &quot;k&quot; for using Ks from Khoo et al. (1977), default is &quot;d&quot;</td>
</tr>
<tr>
<td>eos</td>
<td>&quot;teos10&quot; to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); &quot;eos80&quot; to specify T and S according to EOS-80.</td>
</tr>
<tr>
<td>long</td>
<td>longitude of data point, used when eos parameter is &quot;teos10&quot; as a conversion parameter from absolute to practical salinity.</td>
</tr>
<tr>
<td>lat</td>
<td>latitude of data point, used when eos parameter is &quot;teos10&quot;.</td>
</tr>
</tbody>
</table>

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K₁ and K₂:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50°C.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K₁ and K₂ formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K₁ and K₂ are computed with the formulation corresponding to the pH scale given in the flag "pHscale".
For $K_f$:

- Perez and Fraga (1987): $S$ ranging between 10 and 40 and $T$ ranging between 9 and 33°C.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): $S$ ranging between 0 and 45 and $T$ ranging between 0 and 45°C.

For $K_s$:

- Dickson (1990): $S$ ranging between 5 and 45 and $T$ ranging between 0 and 45°C.
- Khoo et al. (1977): $S$ ranging between 20 and 45 and $T$ ranging between 5 and 40°C.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For $K_0$, the pressure correction term of Weiss (1974) is used.
- For $K_1$, $K_2$, $pK_1$, $pK_2$, $pK_3$, $K_w$, $K_b$, $K_{hs}$ and $K_{si}$, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For $K_f$, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides $K_f$ on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, $K_f$ was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For $K_s$, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For $K_n$, the pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

Value

The function returns a data frame containing the following columns:

| psi | ratio of CO2 released vs CaCO3 precipitated (mol/mol) |
Author(s)

Jean-Pierre Gattuso and Heloise Lavigne <gattuso@obs-vlfr.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: AgCl(s) + 1/2H2(g) = Ag(s) + HCl(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* 22, 113-127.


See Also

speciation.

Examples

```r
## Calculation using the numerical example given in Frankignoulle et al. (1994)
psi(flag=24, var1=350, var2=2400e-6, S=35, T=25, P=0, Pt=0,
Sit=0, pHscale="T", kf="pf", k1k2="l", ks="d")
```

<table>
<thead>
<tr>
<th>pTA</th>
<th>pTA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description

Calculates the carbonate chemistry following addition of $CO_3^{2-}$ or $HCO_3^-$
Usage

\texttt{pTA(flag, sys=0, var1, var2, pCO2a, co3, hco3, S=35, T=20, P=0,}
\texttt{Pt=0, Sit=0, k1k2="x", kf="x", ks="d", pHscale="T", b="u74",}
\texttt{eos = "eos80", long = 1e+20, lat = 1e+20)}

Arguments

- **flag** select the couple of variables available. The flags which can be used are:
  - flag = 1 pH and CO2 given
  - flag = 2 CO2 and HCO3 given
  - flag = 3 CO2 and CO3 given
  - flag = 4 CO2 and ALK given
  - flag = 5 CO2 and DIC given
  - flag = 6 pH and HCO3 given
  - flag = 7 pH and CO3 given
  - flag = 8 pH and ALK given
  - flag = 9 pH and DIC given
  - flag = 10 HCO3 and CO3 given
  - flag = 11 HCO3 and ALK given
  - flag = 12 HCO3 and DIC given
  - flag = 13 CO3 and ALK given
  - flag = 14 CO3 and DIC given
  - flag = 15 ALK and DIC given
  - flag = 21 pCO2 and pH given
  - flag = 22 pCO2 and HCO3 given
  - flag = 23 pCO2 and CO3 given
  - flag = 24 pCO2 and ALK given
  - flag = 25 pCO2 and DIC given

- **sys** 0 if the manipulation is carried out in a system closed to the atmosphere or 1 if its is carried out in a system open to the atmosphere

- **var1** Value of the first variable in mol/kg, except for pH and for pCO2 in \(\mu\text{atm}\)

- **var2** Value of the second variable in mol/kg, except for pH

- **pCO2a** CO2 partial pressure in the atmosphere pCO2 in \(\mu\text{atm}\). It is only used in systems open to the atmosphere (i.e. when sys=1)

- **co3** Amount of \(CO_3^{2-}\) added in \(\text{mol kg}^{-1}\)

- **hco3** Amount of \(HCO_3^{2-}\) added in \(\text{mol kg}^{-1}\)

- **S** Salinity

- **T** Temperature in degrees Celsius

- **P** Hydrostatic pressure in bar (surface = 0)

- **Pt** Concentration of total phosphate in mol/kg

- **Sit** Concentration of total silicate in mol/kg
"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35°C and/or S is outside the range 19 to 43. In these cases, the default value is "w14".

"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33°C and/or S is outside the range 10 to 40. In these cases, the default is "dg".

"d" for using Ks from Dickson (1990), "k" for using Ks from Khoo et al. (1977), default is "d"

"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)

Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74".

"teos10" to specify T and S according to Thermodynamic Equation Of Seawater - 2010 (TEOS-10); "eos80" to specify T and S according to EOS-80.

longitude of data point, used when eos parameter is "teos10" as a conversion parameter from absolute to practical salinity.

latitude of data point, used when eos parameter is "teos10".

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35°C.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50°C.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50°C. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For K0:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33°C.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45°C.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45°C.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40°C.
The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

**Pressure corrections and pH scale:**

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

long and lat are used as conversion parameters from absolute to practical salinity: when seawater is not of standard composition, practical salinity alone is not sufficient to compute absolute salinity and vice-versa. One needs to know the density. When long and lat are given, density is inferred from WOA silicate concentration at given location. When they are not, an arbitrary geographic point is chosen: mid equatorial Atlantic. Note that this implies an error on computed salinity up to 0.02 g/kg.

**Value**

The function returns a data frame containing the following columns:

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>comment</td>
<td>The initial or final state water</td>
</tr>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius</td>
</tr>
<tr>
<td>P</td>
<td>Pressure in bar</td>
</tr>
<tr>
<td>pH</td>
<td>pH</td>
</tr>
<tr>
<td>CO2</td>
<td>CO2 concentration (mol/kg)</td>
</tr>
<tr>
<td>pCO2</td>
<td>pCO2, CO2 partial pressure (µatm)</td>
</tr>
<tr>
<td>fCO2</td>
<td>fCO2, CO2 fugacity (µatm)</td>
</tr>
<tr>
<td>HCO3</td>
<td>HCO3 concentration (mol/kg)</td>
</tr>
<tr>
<td>C03</td>
<td>CO3 concentration (mol/kg)</td>
</tr>
</tbody>
</table>
DIC \quad \text{DIC concentration (mol/kg)}

ALK \quad \text{ALK, total alkalinity (mol/kg)}

OmegaAragonite \quad \text{Omega aragonite, aragonite saturation state}

OmegaCalcite \quad \text{Omega calcite, calcite saturation state}

**Note**

**Warning:** pCO₂ estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

**Author(s)**

Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

**References**


Dickson A. G., 1990 Standard potential of the reaction: \( \text{AgCl(s)} + \frac{1}{2}\text{H}_2(g) = \text{Ag(s)} + \text{HCl(aq)} \), and the standard acidity constant of the ion HSO₄ in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* 22, 113-127.


**Examples**

\[
\text{rhoHs} \]  
**S**  
**T**  
**P**  
\[
\text{rho}(S = 35, \ T = 25, \ P = 0)
\]

**Arguments**

- **S**: Practical Salinity (PSS-78), default is 35
- **T**: Temperature in degrees Celsius (ITS-90), default is 25°C
- **P**: Hydrostatic pressure in bar (surface = 0), default is 0

**Value**

\[
\text{rho} \quad \text{Density of seawater (kg/m3)}
\]

**Author(s)**

Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

**References**


**Examples**

\[
\text{rho}(35, 25, 0)
\]
Description

Converts from absolute to practical salinity (SP). Salinity conversion depends on total alkalinity as well as the concentrations of dissolved inorganic carbon, nitrate and silicate.

Usage

```r
sa2sp_chem(SA, TA=2300e-6, DIC=2000e-6, NO3=0, SiOH4=0)
```

Arguments

- **SA**: Absolute salinity in g/kg
- **TA**: Total alkalinity, in mol/kg, default is 2300 Âµmol/kg
- **DIC**: Dissolved inorganic carbon concentration in mol/kg, default is 2000 Âµmol/kg
- **NO3**: Total nitrate concentration in mol/kg, default is 0
- **SiOH4**: Total silicate concentration in mol/kg, default is 0

Details

Convert from absolute to practical salinity from carbon system parameters and ion concentration which most affect water density anomalies.

Value

- **SP**: Practical salinity (in psu)

Author(s)

Jean-Marie Epitalon

References


See Also

- `sp2sa_chem` does the reverse, `sa2sp_geo`
Examples

# Calculate the practical salinity of a sample with Absolute Salinity of 35 g/kg, # Total Alkalinity of 0.00234 mol/kg and DIC of 0.00202 mol/kg
SP <- sa2sp_chem(SA=35, TA=0.00234, DIC=0.00202)

Description

Converts from absolute to practical salinity based on depth and geographic location.

Usage

sa2sp_geo(SA, P=0, long=1.2, lat=1.2)

Arguments

SA  Absolute salinity in g/kg
P   Sea water pressure in dbar
long Longitude in decimal degrees [ 0 ... +360 ] or [ -180 ... +180 ]
lat  Latitude in decimal degrees [-90 ... 90]

Details

This function is almost an alias of subroutine gsw_SP_from_SA from gsw package on which it relies. The only difference is in that depth and location are optional. If location is not given, or incomplete (either longitude or latitude missing), an arbitrary location is chosen: the mid equatorial atlantic ocean. Note that this implies an error on computed SA ranging from 0 up to 0.02 g/kg.

Value

SP  Practical salinity (psu)

Author(s)

Jean-Marie Epitalon

References


See Also

sp2sa_geo does the reverse, sa2sp_chem

Examples

# Calculate the practical salinity of a sample whose absolute Salinity is 35,
# depth is 10 dbar and location is 188 degrees East and 4 degrees North.
SP <- sa2sp_geo(35, 10, 188, 4)

Description

The variables are:

- Flag indicating which couple of variables is used
- Value of the first variable in mol/kg, except for pH and for pCO2 in µatm
- Value of the second variable in mol/kg, except for pH
- Salinity
- Temperature in degrees Celsius
- Hydrostatic pressure in bar (surface = 0)
- Value of the concentration of total phosphate in mol/kg
- Value of the total silicate in mol/kg

Usage

seacarb_test_P0

Format

A data frame with 20 rows and 8 variables

Source

None, these data were invented for this purpose. The input variables were chosen in order to check that the carbonate chemistry is identical for all flags.
### seacarb_test_P300

**Test data file (at P=300) to test the use of the carb function**

#### Description

The variables are:

- Flag indicating which couple of variables is used
- Value of the first variable in mol/kg, except for pH and for pCO2 in µatm
- Value of the second variable in mol/kg, except for pH
- Salinity
- Temperature in degrees Celsius
- Hydrostatic pressure in bar (P=300)
- Value of the concentration of total phosphate in mol/kg
- Value of the total silicate in mol/kg

#### Usage

```r
seacarb_test_P300
```

#### Format

A data frame with 20 rows and 8 variables

#### Source

None, these data were invented for this purpose. The input variables were chosen in order to check that the carbonate chemistry is identical for all flags.

### seaFET

**Test seaFET data file**

#### Description

Short test file for using with functions sf_calc and sf_calib. It is an excerpt of a file produced by a SeaFET pH sensor.

#### Usage

```r
seaFET
```

#### Format

A data frame with 8 variables (datetime, Eint, Eext, Salinity, Temperature, pHspectro, E0int25, E0ext25) and 10 rows
**sf_calc**

**Calculation of calibrated pH for seaFET sensor**

**Description**

The function `sf_calc()` calculates pH time series (pHint_tot and pHext_tot) for SeaFET pH sensors, using calibration coefficients E0int25 and E0ext25 from the function `sf_calib()`. Both functions are R-adaptations from MATLAB scripts published by Bresnahan et al. (2014).

**Usage**

```
sf_calc(calEint=0.0865, calEext= -0.93, E0int25 =-0.39, E0ext25=-1.46, calT=16.2, calSal=35.6)
```

**Arguments**

- `calEint`: EINT (V), default is 0.0865
- `calEext`: EEXT (V), default is -0.93
- `E0int25`: Coefficient of calibration related to the internal sensor and obtained via `sf_calib` function, default is -0.39. If time-serie, we use the mean per period of deployment
- `E0ext25`: Coefficient of calibration related to the external sensor and obtained via `sf_calib` function, default is -1.46. If time-serie, we use the mean per period of deployment
- `calT`: Temperature in degrees Celsius, default is 16.2
- `calSal`: Salinity, default is 35.6

**Details**

Input values should be vectors of equal length. E0int25 and E0ext25 should be constant throughout the time series. When multiple reference samples are available for one SeaFET deployment, mean E0int25 and mean E0ext25 should be calculated and used in `sf_calc()`. Each unique SeaFET deployment requires a new calculation of mean E0int25 and mean E0ext25 based on reference pH samples (total hydrogen ion scale). For detailed SeaFET calibration instructions and recommendations see Bresnahan et al. (2014) and Rivest et al. (2016).

**Value**

This function returns a dataframe comprising 2 variables:

- `pHint_tot`: Calibrated pH of the internal sensor at in situ temperature.
- `pHext_tot`: Calibrated pH of the external sensor at in situ temperature.

**Author(s)**

Samir Alliouane, Lydia Kapsenberg, Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>
References


See Also

sf_calib.

Examples

```r
sf_calc(calcEint=0.0865, calcExt= -0.93, E0int25 =-0.39, E0ext25=-1.46, calT=16.2, calSal=35.6)
```

```r
## Using the test file seaFET
sf_calc(calcEint=seaFET$Eint, calcExt=seaFET$Ext,
        E0int25=seaFET$E0int25, E0ext25=seaFET$E0ext25,
        calT=seaFET$Temperature, calSal=seaFET$Salinity)
```

---

**sf_calib**

*Calibration coefficients for seaFET sensor*

Description

Calibration coefficients E0INT,25, E0EXT,25

Usage

```r
sf_calib(calcEint=0.0865, calcExt=-0.93, calpH=8.132, calT=16.2, calSal=35.6)
```

Arguments

- `calcEint` EINT (V), default is 0.0865
- `calcExt` EEXT (V), default is -0.93
- `calpH` spectrophotometric pH in Total scale, default is 8.132
- `calT` Temperature in degrees Celsius, default is 16.2
- `calSal` Salinity, default is 35.6
Details

Outputs E0INT25 and E0EXT25 must be calculated for each reference sample collected during a SeaFET deployment. Multiple E0INT25 and E0EXT25 may be calculated if there is more than one reference sample for a given deployment. As such, arguments can be given as unique numbers or as vectors (vectors should be of the same length).

It is critical that Eint (calEint) and Eext (calEext) recorded by the SeaFET match reference sample measurements of temperature (calT), salinity (calSal), and spectrophotometric pH (calpH, total hydrogen ion scale) taken at the same time. Note that SeaFET temperature measurements may require calibration via an applied offset. When possible, calibrated CTD temperature and salinity measurements may be used, while spectrophotometric pH measurements always require discrete ‘reference’ water samples (unless in situ, certified, seawater-based, Tris pH buffer is used). The accepted time offset between collection of reference samples and SeaFET measurements depends on the hydrology and pH variability of the location. For detailed SeaFET calibration instructions and recommendations see Bresnahan et al. (2014) and Rivest et al. (2016).

Value

This function returns a dataframe comprising 2 variables:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>E0INT25</td>
<td>Calibration coefficients of the internal sensor at 25oC.</td>
</tr>
<tr>
<td>E0EXT25</td>
<td>Calibration coefficients of the external sensor at 25oC.</td>
</tr>
</tbody>
</table>

Author(s)

Samir Alliouane, Lydia Kapsenberg, Jean-Pierre Gattuso <gattuso@obs-v1fr.fr>

References


See Also

sf_calc.

Examples

```r
sf_calib(calEint=0.0865, calEext=-0.93, calpH=8.132, calT=16.2, calSal=35.6)
```

```
## Using the test file seaFET
sf_calib(calEint=seaFET$Eint, calEext=seaFET$Eext,
```
From Practical to absolute salinity

Description

Converts from practical to absolute salinity based on total alkalinity as well as on the concentrations of dissolved inorganic carbon, nitrate and silicate.

Usage

\[
\text{sp2sa\_chem}(\text{SP, TA}=2300\text{e-6}, \text{DIC}=2000\text{e-6, NO3}=0, \text{SIOH4}=0)
\]

Arguments

- \text{SP} \hspace{1cm} \text{Practical salinity on the practical salinity scale}
- \text{TA} \hspace{1cm} \text{Total alkalinity, in mol/kg, default is 2300 \text{\AA}mol/kg}
- \text{DIC} \hspace{1cm} \text{Dissolved inorganic carbon concentration in mol/kg, default is 2000 \text{\AA}mol/kg}
- \text{NO3} \hspace{1cm} \text{Total nitrate concentration in mol/kg, default is 0}
- \text{SIOH4} \hspace{1cm} \text{Total silicate concentration in mol/kg, default is 0}

Details

Converts from practical to absolute salinity from carbonate system parameters and ion concentration which mostly affect water density anomalies.

Value

\[
\text{SA} \hspace{1cm} \text{Absolute salinity (g/kg)}
\]

Author(s)

Jean-Marie Epitalon

References


sp2sa_geo

See Also

sa2sp_chem does the reverse, sp2sa_geo

Examples

```
# Calculate the absolute salinity of a sample with practical Salinity of 35,
# Total Alkalinity of 0.00234 mol/kg and DIC of 0.00202 mol/kg
SA <- sp2sachem(SP=35, TA=0.00234, DIC=0.00202)
```

Description

Converts from practical to absolute salinity based on depth and geographic location.

Usage

```
sp2sa_geo(SP, P=0, long=1.2e0, lat=1.2e0)
```

Arguments

- **SP**: Practical salinity on the practical salinity scale
- **P**: Sea water pressure in dbar
- **long**: Longitude in decimal degrees [0 ... +360] or [-180 ... +180]
- **lat**: Latitude in decimal degrees [-90 ... 90]

Details

This function is almost an alias of function gsw_SA_from_SP of the gsw package on which it relies. The only difference is in that depth and location are optional. If location is not given, or incomplete (either longitude or latitude missing), an arbitrary location is chosen: the mid equatorial atlantic ocean. Note that this implies an error on computed SA ranging from 0 up to 0.02 g/kg.

Value

- **SA**: Absolute salinity (g/kg)

Author(s)

Jean-Marie Epitalon

References

speciation

See Also

sa2sp_geo does the reverse, sp2sa_chem

Examples

# Calculate the absolute salinity of a sample whose practical salinity is 35,
# depth is 10 dbar and location is 188 degrees East and 4 degrees North.
SA <- sp2sa_geo(35, 10, 188, 4)  # 34.711778348814114

Description

Estimates the concentration of the various ionic forms of a molecule as a function of pH

Usage

speciation(K1=K1(), K2=NULL, K3=NULL, pH, conc=1)

Arguments

K1  First dissociation constant
K2  Second dissociation constant, default is NULL
K3  Third dissociation constant, default is NULL
pH  pH value, default is 8
conc concentration of molecule in mol/kg, default is 1 mol/kg

Value

The function returns a data frame containing the following concentrations (in mol/kg if conc is given in mol/kg):

C1  ionic form 1, univalent, bivalent and trivalent molecules
C2  ionic form 2, univalent, bivalent and trivalent molecules
C3  ionic form 3, bivalent and trivalent molecules
C4  ionic form 4, trivalent molecules

Author(s)

Karline Soetaert <K.Soetaert@nioo.knaw.nl>

References

See Also

bjerrum.

Examples

## Speciation of divalent species; example to estimate the various ionic forms
## of dissolved inorganic carbon (DIC = 0.0021 mol/kg) at a salinity of 35,
## a temperature of 25°C and an hydrostatic pressure of 0:
spec <- speciation(K1(35, 25, 0), K2(35, 25, 0), pH=8, conc=0.0021)
## where (spec$C1=[CO2], spec$C2=[HCO3-], spec$C3=[CO3--])

## Speciation of trivalent species (e.g., H3PO4, H2PO4-, HPO4-- , PO4--):
speciation(K1p(), K2p(), K3p(), conc=0.001)

## Effect of temperature on pCO2 - Figure 1.4.18 of Zeebe and Wolf-Gladrow (2001)
Tseq <- seq(0, 30, by=0.5)
pHseq <- carb(flag=15, var1=2300e-6, var2=1900e-6, S=35, T=Tseq, P=0)$pH
CO2 <- speciation(K1(T=Tseq), K2(T=Tseq), conc=1900, pH=pHseq)$C1
pCO2 <- CO2/K0(T=Tseq)
plot(Tseq, pCO2, xlab="Temperature (°C)", ylab="pCO2 (uatm)", type="l",
main="Effect of temperature on pCO2")
legend("topleft", c(expression(sum(CO[2]))==1900-umol-kg^-"-1"),
expression(TA==2300-umol-kg^-"-1"))

Description

Converts conservative temperature to in situ temperature and absolute salinity to practical salinity (SP). Salinity conversion depends on total alkalinity as well as on the concentrations of dissolved inorganic carbon, nitrate and silicate.

Usage

teos2eos_chem(SA, CT, P=0, TA=2300e-6, DIC=2000e-6, NO3=0, SIO4=0)

Arguments

SA Absolute salinity in g/kg
CT Conservative temperature in degrees C
P Sea water pressure in dbar
TA Total alkalinity, in mol/kg, default is 2300 Âµmol/kg
DIC Dissolved inorganic carbon concentration in mol/kg, default is 2000 Âµmol/kg
NO3 Total nitrate concentration in mol/kg, default is 0
SIO4 Total silicate concentration in mol/kg, default is 0
Details

Conversion from absolute to practical salinity depends on carbonate system parameters and ion concentration which mostly affect water density anomalies.

Value

The function returns a data frame containing the following columns:

- T: In situ temperature (deg C)
- SP: Practical salinity (psu)

Author(s)

Jean-Marie Epitalon

References


See Also
eos2teos Chem, teos2eos Geo, sa2sp cham, package gsw

Examples

```r
# Calculate in situ temperature and practical salinity of a sample with
# Absolute salinity of 35 g/kg, Conservative temperature of 18 deg C,
# at 0 dbar and Total alkalinity of 0.00234 mol/kg and DIC of 0.00202 mol/kg
f <- teos2eos_chem(SA=35, CT=18, P=0, TA=0.00234, DIC=0.00202)
T <- f$T      # insitu temperature
SP <- f$SP    # Practical salinity
```

---

**teos2eos_geo**  
*Convert temperature and salinity from TEOS-10 to EOS-80*

---

Description

Converts conservative temperature to in situ temperature and absolute salinity to practical salinity (SP). Salinity conversion depends on depth and geographic location.
teos2eos_geo

Usage

teos2eos_geo(SA, CT, p=0, long=1.e20, lat=1.e20)

Arguments

SA    Absolute salinity in g/kg
CT    Conservative temperature in degrees C
p     Sea water pressure in dbar
long  Longitude in decimal degrees [ 0 ... +360 ] or [ -180 ... +180 ]
lat   Latitude in decimal degrees [-90 ... 90]

Details

Conversion from absolute to practical salinity depends on water density anomaly which is correlated with silicate concentration. This function relies on silicate concentration taken from WOA (World Ocean Atlas) to evaluate the density anomaly.

Value

The function returns a data frame containing the following columns:

T   In situ temperature (deg C)
SP  Practical salinity (psu)

Author(s)

Jean-Marie Epitalon

References


See Also

eos2teos_geo does the reverse, teos2eos_chem, sa2sp_geo, package gsw
Examples

# Calculate in situ temperature and practical salinity of a sample with
# Absolute salinity of 35 g/kg, conservative temperature of 18 deg C,
# depth is 10 dbar and location is 188 degrees East and 4 degrees North.
f <- teos2osgeo(SA=35, CT=18, P=10, long=188, lat=4)
T <- f$T       # in situ temperature
SP <- f$SP     # Practical salinity

theta             Potential temperature of seawater

Description

Computes theta, the potential temperature of seawater given original temperature, salinity, pressure, and reference pressure.

Usage

theta(S=35, T=25, P=0, Pref=0)

Arguments

S       Salinity on the practical salinity scale, default is 35
T       Temperature in degrees Celsius, default is 25oC
P       Hydrostatic pressure in bar (surface = 0; 1000 db = 100 bar), default is 0
Pref    Reference hydrostatic pressure in bar, default is 0

Details

Computes the potential temperature of seawater relative to a chosen reference pressure following Fofonoff and Millard (1983). The potential temperature \( \theta \) is the temperature that a water parcel would have if were moved adiabatically to another pressure level \( Pref \). Typically, the potential temperature is referenced to the surface \( (Pref = 0) \). The potential temperature depends on the original salinity \( S \), in-situ temperature \( T \) and pressure \( P \).

This routine is essentially a wrapper for the \texttt{swTheta} routine of the 'oce' package. Unlike the latter, pressure units here are given in bars and method="unesco" is prescribed.

Value

theta             potential temperature of seawater (C)

Author(s)

James Orr <james.orr@lsce.ipsl.fr>
References


See Also

swTheta.

Examples

#Calculate the potential temperature for a sample at 1000 db referenced to the surface theta <- theta(S=35, T=25, P=100, Pref=0)

Tris

pH of TRIS buffer

Description

Calculates the pH value of TRIS buffered artificial seawater solutions (on the total scale in mol/kg-soln)

Usage

tris(S=35,T=25,b=0.04,k="d98",warn="y")

Arguments

S   Salinity, default is 35
T   Temperature in degrees Celsius, default is 25oC
b   Molality if TRIS/TRISH+ in moles per kg of water, default is 0.04 mol/kg-H2O
k   "d98" for DelValls and Dickson 1998, "m18" for using tris characterization by Mueller et al (2018), default is "d98"
warn "y" to show warnings when S,T and/or b go beyond the valid range for the chosen k; "n" to suppress warnings. The default is "y".

Details

The models used to calculate the return value of this function are based on experimental data. It is critical to consider that each formulation refers to the artificial seawater solution applied during the characterization experiment and is only valid for the studied ranges of temperature and salinity:

- DelValls and Dickson (1998): S ranging between 20 and 40, T ranging between 0 and 45oC, and b being 0.04 mol/kg-H2O.
- Mueller et al. (2018): S ranging between 5 and 40, T ranging between 5 and 45oC, and b ranging between 0.01 and 0.04 mol/kg-H2O.
Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

tris The function returns the pH value of TRIS buffered artificial seawater solutions (on the total scale in mol/kg-soln)

Author(s)

Jean-Pierre Gattuso <gattuso@obs-vlfr.fr> and Jens Daniel Mueller <jens.mueller@io-warnemuende.de>

References


See Also

amp, phslope, ph.

Examples

```r
# Example from Mueller et al. (2018), should give test value pH = 8.0703
tris(S=20, T=25, b=0.04, k="m18")
```

vapress Computes vapor pressure of seawater

Description

Computes vapor pressure of seawater (atm) from temperature and salinity

Usage

```r
vapress(S=35, T=25, form="d2007")
```
Arguments

S  Salinity on the practical salinity scale, default is 35
T  Temperature in degrees Celsius, default is 25°C
form  choose either "d2007" for the best-practices formulation to compute vapor pressure of seawater from Dickson et al. (2007) or "wp1980" for the formulation from Weiss and Price (1980).

Details

Computes the vapor pressure of seawater pH20 following best practices (Dickson et al., 2007). That computed pH20 is identical, when rounded to the 4th decimal place, with that computed by the equation from Weiss and Price (1980).

Value

vapress  Vapor pressure of seawater in atm

Author(s)

James Orr <james.orr@lsce.ipsl.fr>

References


See Also

x2pCO2, and p2xCO2.

Examples

pH20 <- vapress(S=35, T=25, form="d2007")
**Description**

Converts xCO₂ (mole fraction of CO₂) into pCO₂ (partial pressure of CO₂)

**Usage**

\[ x_{2pCO2}(S=35, T=25, Patm=1.0, xCO2=400) \]

**Arguments**

- \( S \): Salinity on the practical salinity scale, default is 35
- \( T \): Temperature in degrees Celsius, default is 25°C
- \( Patm \): Atmospheric pressure in atmospheres, default is 1.0
- \( xCO2 \): Mole fraction of CO₂ in ppm, default is 400

**Details**

The mole fraction \( xCO2 \) (ppm) is computed from \( pCO2 \) (\( \mu \)atm) using the following equation:

\[ xCO2 = \frac{pCO2(Patm - pH2O)}{\text{Where \( pH2O \) is the vapor pressure of seawater computed following best practices (Dickson et al., 2007). That computed \( pH2O \) is identical, when rounded to the 4th decimal place, with that computed by the equation from Weiss and Price (1980).}}\]

**Value**

\( pCO2 \): Partial pressure of CO₂ in \( \mu \)atm.

**Note**

**Warning:** pCO₂ estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

**Author(s)**

James Orr <james.orr@lsce.ipsl.fr>

**References**


See Also

p2xC02 and vapress

Examples

```r
## Atmospheric pressure is rarely equal to 1 atm exactly
## Over the Southern Ocean Patm=0.97 is more realistic
pCO2_socn <- x2pCO2(S=35, T=0, Patm=0.97, xCO2=400.0)
print(pCO2_socn)
## The result (385.6322 uatm) is 12 uatm less than if it was wrongly assumed that Patm=1.0

## Show effect of temperature on pCO2 computed from xCO2, and on resulting variables from "carb"
S <- 35
ALK <- 2300e-6
T <- seq(0,30,5)
xCO2 <- 400
pCO2 <- x2pCO2(S=35, T=T, Patm=1, xCO2=400)
results <- carb(flag=24, var1=pCO2, var2=ALK, S=S, T=T, P=0, Pt=0, S1t=0,
               pHscale="T", kf="pf", k1k2="1", ks="d", b="u74")
print(results)
```
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