

Package ‘AquaEnv’

January 15, 2012

Version 1.0-2

Date 2011-04-04

Title AquaEnv - an integrated development toolbox for aquatic chemical model generation

Author Andreas F. Hofmann, Karline Soetaert, Filip J.R. Meysman

Maintainer Andreas F. Hofmann <ahofmann@mbari.org> and <a.hofmann@nioo.knaw.nl>

Depends minpack.lm, deSolve

Description AquaEnv is an integrated development toolbox for aquatic chemical model generation focused on (ocean) acidification and CO₂ air-water exchange. It contains all elements necessary to model the pH, the related CO₂ air-water exchange, as well as aquatic acid-base chemistry in general for an arbitrary marine, estuarine or freshwater system. Also chemical batches can be modelled. Next to the routines necessary to calculate desired information, AquaEnv also contains a suite of tools to visualize this information. Furthermore, AquaEnv can not only be used to build dynamic models of aquatic systems, but it can also serve as a simple desktop tool for the experimental aquatic chemist to generate and visualize all possible derived information from a set of measurements with one single easy to use R function. Additionally, the sensitivity of the system to variations in the input variables can be visualized. The corresponding publication in Aquatic Geochemistry can be found at <http://www.springerlink.com/content/14747417w0k50463/>

License GPL (>= 2)

LazyData yes

Repository CRAN

Repository/R-Forge/Project aquaenv

Repository/R-Forge/Revision 88

Date/Publication 2011-04-06 16:32:39

R topics documented:

aquaenv	3
AquaEnv_package	8
as.data.frame.aquaenv	10
c.aquaenv	10
ConcRelCl	11
convert	11
DeltaPcoeffs	13
gauge_p	13
K0_CO2	14
K0_O2	15
Ksp_aragonite	15
Ksp_calcite	16
K_BOH3	17
K_CO2	18
K_H2PO4	19
K_H2S	20
K_H3PO4	21
K_HCO3	22
K_HF	23
K_HPO4	24
K_HSO4	25
K_NH4	26
K_SiOH4	27
K_SiOOH3	28
K_W	29
length.aquaenv	30
MeanMolecularMass	30
merge.aquaenv	31
PhysChemConst	31
plot.aquaenv	32
sample_dickson1981	37
sample_dickson2007	38
TAfit	38
Technicals	45
titration	46
watdepth	48

aquaenv	<i>aquaenv</i>
---------	----------------

Description

PUBLIC function: the main function of the package AquaEnv: creates an object of class aquaenv

Usage

```
aquaenv(S, t, p=pmax((P-Pa), gauge_p(d, lat, Pa)),
        P=Pa, Pa=1.01325, d=0, lat=0,
        SumCO2=0, SumNH4=0, SumH2S=0, SumH3PO4=0,
        SumSiOH4=0, SumHNO3=0, SumHNO2=0, SumBOH3=NULL,
        SumH2SO4=NULL, SumHF=NULL, TA=NULL, pH=NULL, fCO2=NULL, CO2=NULL,
        speciation=TRUE, dsa=FALSE, ae=NULL, from.data.frame=FALSE,
        SumH2SO4_Koffset=0, SumHF_Koffset=0, reveille=FALSE, skeleton=FALSE,
        k_w=NULL, k_co2=NULL, k_hco3=NULL, k_boh3=NULL, k_hso4=NULL,
        k_hf=NULL, k1k2="roy", khf="dickson", k_hso4="dickson", fCO2atm=0.000390, fO2atm=0.20946)
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars, standard is calculated either from the given P, or the given d, lat, and Pa
P	total pressure in bars, standard: Pa (at the surface)
Pa	atmospheric pressure in bars, standard: 1 atm (at sea-level)
d	depth below the surface in meters, standard: 0 (at the surface)
lat	latitude in degrees (-90 to +90) to calculate the gravitational constant g for calculating the water depth from the pressure and vice versa, standard: 0
SumCO2	total carbonate concentration in mol/kg-solution, if NULL is supplied it is calculated
SumNH4	total ammonium concentration in mol/kg-solution, optional
SumH2S	total sulfide concentration in mol/kg-solution, optional
SumH3PO4	total phosphate concentration in mol/kg-solution, optional
SumSiOH4	total silicate concentration in mol/kg-solution, optional
SumHNO3	total nitrate concentration in mol/kg-solution, optional
SumHNO2	total nitrite concentration in mol/kg-solution, optional
SumBOH3	total borate concentration in mol/kg-solution, calculated from S if not supplied
SumH2SO4	total sulfate concentration in mol/kg-solution, calculated from S if not supplied
SumHF	total fluoride concentration in mol/kg-solution, calculated from S if not supplied
TA	total alkalinity in mol/kg-solution, if supplied, pH will be calculated

pH	pH on the free proton concentration scale, if supplied, total alkalinity will be calculated
fCO2	fugacity of CO2 in the water in atm (i.e. the fugacity of CO2 in a small volume of air fully equilibrated with a sufficiently large sample of water), can be used with either [TA], pH, or [CO2] to define the system
CO2	concentration of CO2, can be used with either [TA], pH, or fCO2 to define the system
speciation	flag: TRUE = full speciation is calculated
dsa	flag: TRUE = all information necessary to build a pH model with the direct substitution approach (DSA, Hofmann2008) is calculated
ae	either an object of class aquaenv used for the cloning functionality or a dataframe used for the from.data.frame functionality. Note that for cloning the desired k1k2 and khf values need to be specified! (otherwise the default values are used for the cloned object)
from.data.frame	flag: TRUE = the object of class aquaenv is built from the data frame supplied in ae
SumH2SO4_Koffset	only used internally to calculate dTAdKdKdSumH2SO4
SumHF_Koffset	only used internally to calculate dTAdKdKdSumHF
revelle	flag: TRUE = the revelle factor is calculated
skeleton	flag: TRUE = a reduced amount of information is calculated yielding a smaller object of type aquaenv
k_w	a fixed K_W can be specified
k_co2	a fixed K_CO2 can be specified; used for TA fitting: give a K_CO2 and NOT calculate it from T and S: i.e. K_CO2 can be fitted in the routine as well
k_hco3	a fixed K_HCO3 can be specified
k_boh3	a fixed K_BOH3 can be specified
k_hso4	a fixed K_HSO4 can be specified
k_hf	a fixed K_HF can be specified
k1k2	either "roy" (default, Roy1993a), "lueker" (Lueker2000), or "millero" (Millero2006) for K_CO2 and K_HCO3.
khf	either "dickson" (default, Dickson1979a) or "perez" (Perez1987a) for K_HF
khso4	either "dickson" (default, Dickson1990) or "khoo" (Khoo1977) for K_HSO4
fCO2atm	atmospheric fugacity of CO2 in atm, default = 0.000390 atm
fO2atm	atmospheric fugacity of O2 in atm, default = 0.20946 atm

Value

a list containing: "S" "t" "p" "T" "Cl" "I" "P" "Pa" "d" "density" "SumCO2" "SumNH4" "SumH2S" "SumHNO3" "SumHNO2" "SumH3PO4" "SumSiOH4" "SumBOH3" "SumH2SO4" "SumHF" "Br" "ClConc" "Na" "Mg" "Ca" "K" "Sr" "molal2molin" "free2tot" "free2sws" "tot2free" "tot2sws" "sws2free" "sws2tot" "K0_CO2" "K0_O2" "fCO2atm" "fO2atm" "CO2_sat" "O2_sat" "K_W"

"K\ _HSO4" "K\ _HF" "K\ _CO2" "K\ _HCO3" "K\ _BOH3" "K\ _NH4" "K\ _H2S" "K\ _H3PO4" "K\ _H2PO4"
 "K\ _HPO4" "K\ _SiOH4" "K\ _SiOOH3" "K\ _HNO2" "K\ _HNO3" "K\ _H2SO4" "K\ _HS" "Ksp_calcite"
 "Ksp_aragonite" "TA" "pH" "fCO2" "CO2" "HCO3" "CO3" "BOH3" "BOH4" "OH" "H3PO4"
 "H2PO4" "HPO4" "PO4" "SiOH4" "SiOOH3" "SiO2OH2" "H2S" "HS" "S2min" "NH4" "NH3"
 "H2SO4" "HSO4" "SO4" "HF" "F" "HNO3" "NO3" "HNO2" "NO2" "omega_calcite" "omega_aragonite"
 "revelle" "c1" "c2" "c3" "dTAdSumCO2" "b1" "b2" "dTAdSumBOH3" "so1" "so2" "so3" "dTAdSumH2SO4"
 "f1" "f2" "dTAdSumHF" "dTAdH" "dTAdKdKdS" "dTAdKdKdT" "dTAdKdKdd" "dTAdKdKd-
 SumH2SO4" "dTAdKdKdSumHF" or a subset of this set. Please consult the vignette of AquaEnv
 for more details

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

Examples

```
## Not run:
#####
# Minimal aquaenv definition
#####
ae <- aquaenv(S=30, t=15)
ae$K_CO2

ae$Ksp_calcite
ae$Ksp_aragonite

ae <- aquaenv(S=30, t=15, p=10)
ae <- aquaenv(S=30, t=15, P=11)
ae <- aquaenv(S=30, t=15, d=100)
ae <- aquaenv(S=30, t=15, d=100, Pa=0.5)
ae$K_CO2

ae$Ksp_calcite
ae$Ksp_aragonite

ae

#####
# Defining the complete aquaenv system in different ways
#####
S <- 30
t <- 15
p <- gauge_p(d=10) # ~ p <- 0.1*10*1.01325
SumCO2 <- 0.0020
pH <- 8
TA <- 0.002140798
fCO2 <- 0.0005326744
CO2 <- 2.051946e-05

ae <- aquaenv(S, t, p, SumCO2=SumCO2, pH=pH)
ae$TA
```

```

ae <- aquaenv(S, t, p, SumCO2=SumCO2, TA=TA)
ae$pH

ae <- aquaenv(S, t, p, SumCO2=SumCO2, CO2=CO2)
ae$pH

ae <- aquaenv(S, t, p, SumCO2=SumCO2, fCO2=fCO2)
ae$pH

ae <- aquaenv(S, t, p, SumCO2=SumCO2, CO2=CO2, fCO2=fCO2)
ae <- aquaenv(S, t, p, SumCO2=SumCO2, pH=pH, TA=TA)
ae <- aquaenv(S, t, p, SumCO2=SumCO2, pH=pH, CO2=CO2)
ae <- aquaenv(S, t, p, SumCO2=SumCO2, pH=pH, fCO2=fCO2)
ae <- aquaenv(S, t, p, SumCO2=SumCO2, TA=TA, CO2=CO2)
ae <- aquaenv(S, t, p, SumCO2=SumCO2, TA=TA, fCO2=fCO2)

#####
# Cloning the aquaenv system: 1 to 1 and with different pH or TA
#####
S      <- 30
t      <- 15
SumCO2 <- 0.0020
TA     <- 0.00214

ae <- aquaenv(S, t, SumCO2=SumCO2, TA=TA)

aeclone1 <- aquaenv(ae=ae)

pH <- 9

aeclone2 <- aquaenv(ae=ae, pH=pH)

TA <- 0.002

aeclone3 <- aquaenv(ae=ae, TA=TA)

ae$pH
aeclone1$pH
aeclone2$TA
aeclone3$pH

#####
# Vectors as input variables (only ONE input variable may be a vector)
# (with full output: including the Revelle factor and the DSA properties)
#####
SumCO2 <- 0.0020
pH     <- 8

```

```

S      <- 30
t      <- 1:15
p      <- gauge_p(10)
ae <- aquaenv(S, t, p, SumCO2=SumCO2, pH=pH, revelle=TRUE, dsa=TRUE)
plot(ae, xval=t, xlab="T/(deg C)", newdevice=FALSE)

S <- 1:30
t <- 15
ae <- aquaenv(S, t, p, SumCO2=SumCO2, pH=pH, revelle=TRUE, dsa=TRUE)
plot(ae, xval=S, xlab="S", newdevice=FALSE)

S <- 30
p <- gauge_p(seq(1,1000, 100))
ae <- aquaenv(S, t, p, SumCO2=SumCO2, pH=pH, revelle=TRUE, dsa=TRUE)
plot(ae, xval=p, xlab="gauge pressure/bar", newdevice=FALSE)

TA <- 0.0023

S <- 30
t <- 1:15
d <- gauge_p(10)
ae <- aquaenv(S, t, p, SumCO2=SumCO2, TA=TA, revelle=TRUE, dsa=TRUE)
plot(ae, xval=t, xlab="T/(deg C)", newdevice=FALSE)

S <- 1:30
t <- 15
ae <- aquaenv(S, t, p, SumCO2=SumCO2, TA=TA, revelle=TRUE, dsa=TRUE)
plot(ae, xval=S, xlab="S", newdevice=FALSE)

S <- 30
p <- gauge_p(seq(1,1000, 100))
ae <- aquaenv(S, t, p, SumCO2=SumCO2, TA=TA, revelle=TRUE, dsa=TRUE)
plot(ae, xval=p, xlab="gauge pressure/bar", newdevice=FALSE)

#####
# Calculating SumCO2 by giving a constant pH&CO2, pH&fCO2, pH&TA,
# TA&CO2, or TA&fCO2
#####
fCO2 <- 0.0006952296
CO2 <- 2.678137e-05
pH <- 7.888573
TA <- 0.0021

S <- 30
t <- 15
p <- gauge_p(10)

ae <- aquaenv(S, t, p, SumCO2=NULL, pH=pH, CO2=CO2, dsa=TRUE, revelle=TRUE)
ae$SumCO2

```

```

ae$revelle
ae$dTAdH

ae <- aquaenv(S, t, p, SumCO2=NULL, pH=pH, fCO2=fCO2)
ae$SumCO2

ae <- aquaenv(S, t, p, SumCO2=NULL, pH=pH, TA=TA)
ae$SumCO2

ae <- aquaenv(S, t, p, SumCO2=NULL, TA=TA, CO2=CO2)
ae$SumCO2

ae <- aquaenv(S, t, p, SumCO2=NULL, TA=TA, fCO2=fCO2)
ae$SumCO2

t <- 1:15
ae <- aquaenv(S, t, p, SumCO2=NULL, pH=pH, CO2=CO2)
plot(ae, xval=t, xlab="T/(deg C)", mfrow=c(9,10), newdevice=FALSE)

ae <- aquaenv(S, t, p, SumCO2=NULL, pH=pH, CO2=CO2, revelle=TRUE, dsa=TRUE)
plot(ae, xval=t, xlab="T/(deg C)", newdevice=FALSE)

S <- 1:30
t <- 15
ae <- aquaenv(S, t, p, SumCO2=NULL, pH=pH, fCO2=fCO2, revelle=TRUE, dsa=TRUE)
plot(ae, xval=S, xlab="S", newdevice=FALSE)

S <- 30
p <- gauge_p(seq(1,1000, 100))
ae <- aquaenv(S, t, p, SumCO2=NULL, pH=pH, TA=TA, revelle=TRUE, dsa=TRUE)
plot(ae, xval=p, xlab="gauge pressure/bar", newdevice=FALSE)

## End(Not run)

```

AquaEnv_package

AquaEnv - an integrated development toolbox for aquatic chemical model generation

Description

AquaEnv is an integrated development toolbox for aquatic chemical model generation focused on (ocean) acidification and CO₂ air-water exchange.

It contains all elements necessary to model the pH, the related CO₂ air-water exchange, as well as aquatic acid-base chemistry in general for an arbitrary marine, estuarine or freshwater system. Also chemical batches can be modelled.

Next to the routines necessary to calculate desired information, AquaEnv also contains a suite of tools to visualize this information. Furthermore, AquaEnv can not only be used to build dynamic

models of aquatic systems, but it can also serve as a simple desktop tool for the experimental aquatic chemist to generate and visualize all possible derived information from a set of measurements with one single easy to use R function.

Additionally, the sensitivity of the system to variations in the input variables can be visualized.

Details

Package: AquaEnv
Type: Package
Version: 0.7
Date: 2009-01-21
License: GNU Public License 2 or above

Author(s)

Andreas Hofmann (Maintainer)

Examples

```
## Not run:
## show examples (see respective help pages for details)
example(aquaenv)

## open the directory with source code of demos
browseURL(paste(system.file(package="AquaEnv"), "/demo", sep=""))

## run demos
demo(basicfeatures )

## show package vignette with tutorial about how to use aquaenv
vignette("AquaEnv")
edit(vignette("AquaEnv"))
browseURL(paste(system.file(package="AquaEnv"), "/doc", sep=""))

## show index file of package vignettes and documentation files
browseURL(paste(system.file(package="AquaEnv"), "/doc/index.html", sep=""))

## show documentation about private functions in the packet
browseURL(paste(system.file(package="AquaEnv"), "/doc/AquaEnv-PrivateFunctions.pdf", sep=""))

## show documentation about physical-chemical constants and formulae used in the packet
browseURL(paste(system.file(package="AquaEnv"), "/doc/AquaEnv-ConstantsAndFormulae.pdf", sep=""))

## End(Not run)
```

as.data.frame.aquaenv *as.data.frame.aquaenv*

Description

PUBLIC function: converts an object of class aquaenv to a standard R data frame

Usage

```
as.data.frame.aquaenv(x, ...)
```

Arguments

x object of type aquaenv
... further arguments are passed on

Value

data frame containing all elements of aquaenv

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

c.aquaenv *c.aquaenv*

Description

PRIVATE function: adds an element to an object of class aquaenv

Usage

```
c.aquaenv(aquaenv, x, ...)
```

Arguments

aquaenv object of class aquaenv
x a vector of the form c(value, name) representing the element to be inserted into
 the object of class aquaenv
... further arguments will be passed

Value

object of class aquaenv with the added element

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

ConcRelCl

ConcRelCl

Description

PUBLIC data frame: a collection of concentrations of key chemical species in seawater, relative with respect to chlorinity (DOE1994))

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

convert

convert

Description

PUBLIC function: converts either a single value (the pH scale of a pH value, the pH scale of a dissociation constant (K^*), the unit of a concentration value), or all elements of a special unit or pH scale in an object of class aquaenv

Arguments

x	object to be converted: either a single value (pH value, K^* value, or concentration value) or an object of class aquaenv
vartype	only valid if x is a single value: the type of x, either "pHscale", "KHscale", or "conc"
what	only valid if x is a single value: the type of conversion to be done, for pH scales one of "free2tot", "free2sws", "free2nbs", ... (any combination of "free", "tot", "sws", and "nbs"); for concentrations one of "molar2molal", "molar2molin", ... (any combination of "molar" (mol/l), "molal" (mol/kg-H ₂ O), and "molin" (mol/kg-solution))
S	only valid if x is a single value: salinity (in practical salinity units: no unit)
t	only valid if x is a single value: temperature in degrees centigrade
p	only valid if x is a single value: gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	only valid if x is a single value: total sulfate concentration in mol/kg-solution; if not supplied this is calculated from S
SumHF	only valid if x is a single value: total fluoride concentration in mol/kg-solution; if not supplied this is calculated from S

khf	only valid if x is a single value: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a) for K_HF
khso4	only valid if x is a single value: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977) for K_HSO4
from	only valid if x is an object of class aquaenv: the unit which needs to be converted (as a string; must be a perfect match)
to	only valid if x is an object of class aquaenv: the unit to which the conversion should go
factor	only valid if x is an object of class aquaenv: the conversion factor to be applied: can either be a number (e.g. 1000 to convert from mol to mmol), or any of the conversion factors given in an object of class aquaenv
convattr	only valid if x is an object of class aquaenv: which attribute should be converted? can either be "unit" or "pH scale"

Details

Possible usages are

```
convert(x, vartype, what, S, t, p, SumH2SO4, SumHF, khf)
convert(x, from, to, factor, convattr)
```

Value

converted single value or object of class aquaenv with converted elements

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

Examples

```
## Not run:
### 1
#####

t <- 15
S <- 10

pH_NBS <- 8.142777
SumCO2molar <- 0.002016803

pH_free <- convert(pH_NBS, "pHscale", "nbs2free", S=S, t=t)
SumCO2molin <- convert(SumCO2molar, "conc", "molar2molin", S=S, t=t)

ae <- aquaenv(S, t, SumCO2=SumCO2molin, pH=pH_free)
ae$pH
ae$SumCO2
```

```
### 2
#####
ae <- aquaenv(30,10)
ae$SumBOH3
ae <- convert(ae, "mol/kg-soln", "umol/kg-H2O", 1e6/ae$molal2molin, "unit")
ae$SumBOH3

## End(Not run)
```

DeltaPcoeffs	<i>DeltaPcoeffs</i>
--------------	---------------------

Description

PUBLIC data frame: a collection of coefficients for the pressure correction of dissociation constants and solubility products (Millero1995 WITH CORRECTIONS BY Lewis1998 (CO2Sys!))

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

gauge_p	<i>gauge_p</i>
---------	-----------------

Description

PUBLIC function: calculates the gauge pressure (total pressure minus atmospheric pressure) from the depth (in m) and the latitude (in degrees: -90 to 90) and the atmospheric pressure (in bar)

Usage

```
gauge_p(d, lat=0, Pa=1.01325)
```

Arguments

d	water depth in meters
lat	latitude in degrees: -90 to 90, standard: 0
Pa	atmospheric pressure in bar, standard: 1 atm (at sea level)

Value

gauge pressure (total pressure minus atmospheric pressure) p in bars

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Fofonoff1983

Examples

```
gauge_p(100)
plot(gauge_p(1:100))
```

K0_CO2

K0_CO2

Description

PUBLIC function: calculates the Henry's constant (solubility) for CO2

Usage

```
K0_CO2(S, t)
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade

Value

the Henry's constant for CO2 in mol/(kg-solution*atm)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Weiss1974, DOE1994, Millero1995, Zeebe2001

Examples

```
K0_CO2(35, 15)
plot(K0_CO2(35, 1:25), xlab="temperature / degC")
```

`K0_O2``K0\O2`

Description

PUBLIC function: calculates the Henry's constant (solubility) for O2

Usage

```
K0_O2(S, t)
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade

Value

the Henry's constant for CO2 in mol/(kg-solution*atm)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

derived from a formulation for [O2]sat given in Weiss1970

Examples

```
K0_O2(35, 15)
plot(K0_O2(35, 1:25), xlab="temperature / degC")
```

`Ksp_aragonite``Ksp\aragonite`

Description

PUBLIC function: calculates the solubility product for aragonite

Usage

```
Ksp_aragonite(S, t, p=0)
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars

Value

the solubility product for aragonite in (mol/kg-solution)²

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Mucci1983, Boudreau1996

Examples

```
Ksp_aragonite(35, 15)
Ksp_aragonite(35, 15, 10)
plot(Ksp_aragonite(35, 1:25), xlab="temperature / degC")
```

Ksp_calcite

Ksp_calcite

Description

PUBLIC function: calculates the solubility product for aragonite

Usage

```
Ksp_calcite(S, t, p=0)
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars

Value

the solubility product for calcite in (mol/kg-solution)²

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Mucci1983, Boudreau1996

Examples

```
Ksp_calcite(35, 15)
Ksp_calcite(35, 15, 10)
plot(Ksp_aragonite(35, 1:25), xlab="temperature / degC")
```

K_BOH3

K_BOH3

Description

PUBLIC function: calculates the dissociation constant of B(OH)₃

Usage

```
K_BOH3(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	S, t relation for K_{HF} needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for K_{HSO4} needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of B(OH)₃ in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Dickson1990, DOE1994, Millero1995 (molality version given), Zeebe2001

Examples

```

K_BOH3(35, 15)
K_BOH3(35, 15, 10)
K_BOH3(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_BOH3(35, 1:25), xlab="temperature / degC")

```

K_CO2

K_CO2

Description

PUBLIC function: calculates the dissociation constant of CO2

Usage

```
K_CO2(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, k1k2="roy", khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
k1k2	"roy", "lueker", or "millero": specifies the S, t, dependency to be used. Default is "roy". (see section below for references)
khf	S, t relation for K_HF needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for K_HSO4 needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of CO2 in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

k1k2 = "roy": Roy1993b, DOE1994, Millero1995, Zeebe2001; k1k2 = "lueker": Lueker2000; k1k2 = "millero": Millero2006

Examples

```
K_CO2(35, 15)
K_CO2(35, 15, 10)
K_CO2(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_CO2(35, 1:25), xlab="temperature / degC")
```

K_H2PO4

*K_H2PO4***Description**

PUBLIC function: calculates the dissociation constant of H2PO4

Usage

```
K_H2PO4(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	S, t relation for <i>K_HF</i> needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for <i>K_HSO4</i> needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of H2PO4 in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Millero1995 (original, SWS pH version), DOE1994 (in a later revision cites Millero1995)

Examples

```
K_H2PO4(35, 15)
K_H2PO4(35, 15, 10)
K_H2PO4(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_H2PO4(35, 1:25), xlab="temperature / degC")
```

K_H2S

*K_H2S***Description**

PUBLIC function: calculates the dissociation constant of H2S

Usage

```
K_H2S(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	S, t relation for K_{HF} needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for K_{HSO4} needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of H2S in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Millero1988, Millero1995

Examples

```
K_H2S(35, 15)
K_H2S(35, 15, 10)
K_H2S(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_H2S(35, 1:25), xlab="temperature / degC")
```

`K_H3PO4``K\H3PO4`

Description

PUBLIC function: calculates the dissociation constant of H3PO4

Usage

```
K_H3PO4(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	S, t relation for K\HF needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for K\HSO4 needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of H3PO4 in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Millero1995 (original, SWS pH version), DOE1994 (in a later revision cites Millero1995)

Examples

```
K_H3PO4(35, 15)
K_H3PO4(35, 15, 10)
K_H3PO4(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_H3PO4(35, 1:25), xlab="temperature / degC")
```

K_HCO3

*K_HCO3***Description**

PUBLIC function: calculates the dissociation constant of HCO3

Usage

K_HCO3(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, k1k2="roy", khf="dickson", khso4="dickson")

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
k1k2	"roy", "lueker", or "millero": specifies the S, t, dependency to be used. Default is "roy". (see section below for references)
khf	S, t relation for K_HF needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for K_HSO4 needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of HCO3 in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

k1k2 = "roy": Roy1993b, DOE1994, Millero1995, Zeebe2001; k1k2 = "lueker": Lueker2000; k1k2 = "millero": Millero2006

Examples

```
K_HCO3(35, 15)
K_HCO3(35, 15, 10)
K_HCO3(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_HCO3(35, 1:25), xlab="temperature / degC")
```

K_HF

 K_{HF}

Description

PUBLIC function: calculates the dissociation constant of HF

Usage

```
K_HF(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	"dickson" or "perez": specifies the S, t, dependency to be used. Default is "dickson". (see section below for references)
khso4	S, t relation for K_{HSO4} needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of HF in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

khf = "dickson": Dickson1979a, Dickson1987, Roy1993b, DOE1994, Millero1995, Zeebe2001;
khf = "perez": Perez1987

Examples

```
K_HF(35, 15)
K_HF(35, 15, 10)
plot(K_HF(35, 1:25), xlab="temperature / degC")
```

K_HPO4

*K_HPO4***Description**

PUBLIC function: calculates the dissociation constant of HPO4

Usage

```
K_HPO4(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	S, t relation for K_HF needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for K_HSO4 needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of HPO4 in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Millero1995 (original, SWS pH version), DOE1994 (in a later revision cites Millero1995)

Examples

```
K_HPO4(35, 15)
K_HPO4(35, 15, 10)
K_HPO4(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_HPO4(35, 1:25), xlab="temperature / degC")
```

`K_HSO4`*K_HSO4*

Description

PUBLIC function: calculates the dissociation constant of HSO4

Usage

```
K_HSO4(S, t, p=0, khs04="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
khs04	"dickson" or "khoo": specifies the S, t, dependency to be used. Default is "dickson". (see section below for references)

Value

the dissociation constant of HSO4 in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

"dickson": Dickson1990, DOE1994, Zeebe2001; "khoo": Khoo1977, Roy1993, Millero1995

Examples

```
K_HSO4(35, 15)
K_HSO4(35, 15, 10)
plot(K_HSO4(35, 1:25), xlab="temperature / degC")
```

K_NH4

*K_NH4***Description**

PUBLIC function: calculates the dissociation constant of NH4

Usage

```
K_NH4(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	S, t relation for K_{HF} needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for K_{HSO4} needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of NH4 in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Millero1995a, Millero1995, corrected by Lewis1998

Examples

```
K_NH4(35, 15)
K_NH4(35, 15, 10)
K_NH4(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_NH4(35, 1:25), xlab="temperature / degC")
```

K_SiOH4

K_SiOH4

Description

PUBLIC function: calculates the dissociation constant of SiOH4

Usage

```
K_SiOH4(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	S, t relation for <i>K_HF</i> needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for <i>K_HSO4</i> needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of SiOH4 in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Millero1988, DOE1994, Millero1995

Examples

```
K_SiOH4(35, 15)
K_SiOH4(35, 15, 10)
K_SiOH4(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_SiOH4(35, 1:25), xlab="temperature / degC")
```

K_SiOOH3

*K_SiOOH3***Description**

PUBLIC function: calculates the dissociation constant of SiOOH3

Usage

```
K_SiOOH3(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")
```

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	S, t relation for K_HF needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for K_HSO4 needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the dissociation constant of SiOOH3 in mol/kg-solution on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Wischmeyer2003 (incl. corrections)

Examples

```
K_SiOOH3(35, 15)
K_SiOOH3(35, 15, 10)
K_SiOOH3(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_SiOOH3(35, 1:25), xlab="temperature / degC")
```

K_W

 K_W

Description

PUBLIC function: calculates the ion product of H₂O

Usage

K_W(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson", khso4="dickson")

Arguments

S	salinity in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution (calculated from S if not supplied)
SumHF	total fluoride concentration in mol/kg-solution (calculated from S if not supplied)
khf	S, t relation for K_HF needed for scale conversion: either "dickson" (default, Dickson1979a) or "perez" (Perez1987a)
khso4	S, t relation for K_HSO4 needed for scale conversion: either "dickson" (default, Dickson1990) or "khoo" (Khoo1977)

Value

the ion product of H₂O in (mol/kg-solution)² on the free proton pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Millero1995 (SWS pH version), DOE1994 (cites Millero1995), Zeebe2001

Examples

```
K_W(35, 15)
K_W(35, 15, 10)
K_W(S=35, t=15, p=10, SumH2SO4=0.03)
plot(K_W(35, 1:25), xlab="temperature / degC")
```

length.aquaenv	<i>length.aquaenv</i>
----------------	-----------------------

Description

PRIVATE function: returns the (maximal) length of the elements in an object of class aquaenv (i.e. > 1 if one of the input variables was a vector)

Usage

```
length.aquaenv(x, ...)
```

Arguments

x	object of class aquaenv
...	further arguments will be passed

Value

the maximal length of the elements in the object of class aquaenv

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

MeanMolecularMass	<i>MeanMolecularMass</i>
-------------------	--------------------------

Description

PUBLIC data frame: a collection of mean molecular masses of key chemical species in seawater in g/mol (DOE1994))

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

merge.aquaenv	<i>merge.aquaenv</i>
---------------	----------------------

Description

PRIVATE function: merges the elements of two objects of class aquaenv: element names are taken from the first argument, the elements of which are also first in the merged object

Usage

```
merge.aquaenv(x, y, ...)
```

Arguments

x	object of class aquaenv: this is where the element names are taken from
y	object of class aquaenv: must contain at least all the element (names) as aquaenv1, extra elements are ignored
...	further arguments will be passed

Value

object of class aquaenv with merged elements

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

PhysChemConst	<i>PhysChemConst</i>
---------------	----------------------

Description

PUBLIC list: a collection of physical and chemical constants

Value

A list containing:

R	(bar*cm ³)/(mol*K) the gas constant (corrected after Lewis1998, in Millero1995: R = 83.131); digits extended after Dickson2007)
F	C/mol the Faraday constant (charge per mol of electrons) (N _A *e ⁻): Dickson2007
uMolToMol	conversion factor from umol to mol
absZero	absolute zero in degrees centigrade

e	relative dielectric constant of seawater (Zeebe2001)
K_HNO2	dissociation constant of HNO ₂ : mol/l, NBS pH scale, hybrid constant (Riordan2005)
K_HNO3	dissociation constant of HNO ₃ : assumed on mol/kg-soln and free pH scale, stoichiometric constant (Soetaert pers. comm.)
K_H2SO4	dissociation constant of H ₂ SO ₄ : assumed on mol/kg-soln and free pH scale, stoichiometric constant (Atkins1996)
K_HS	dissociation constant of H ₂ S: assumed on mol/kg-soln and free pH scale, stoichiometric constant (Atkins1996)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

plot.aquaenv

plot.aquaenv

Description

PUBLIC function: high level plot function for objects of class aquaenv

Arguments

x	object of class aquaenv
xval	only valid if bjerrum=FALSE: a vector of the (maximal) length of the elements of aquaenv against which they are to be plotted
what	a list of names of the elements of aquaenv that are to be plotted, if not supplied and bjerrum=FALSE and cumulative=FALSE: all elements are plotted, if not supplied and bjerrum=TRUE then what is set to be c("CO ₂ ", "HCO ₃ ", "CO ₃ ", "BOH ₃ ", "BOH ₄ ", "OH", "H ₃ PO ₄ ", "H ₂ PO ₄ ", "HPO ₄ ", "PO ₄ ", "SiOH ₄ ", "SiOOH ₃ ", "SiO ₂ OH ₂ ", "H ₂ S", "HS", "S ₂ min", "NH ₄ ", "NH ₃ ", "H ₂ SO ₄ ", "HSO ₄ ", "SO ₄ ", "HF", "F", "HNO ₃ ", "NO ₃ ", "HNO ₂ ", "NO ₂ "), needs to be supplied for cumulative=TRUE
bjerrum	flag: TRUE = a bjerrum plot is done (by calling bjerrumplot)
cumulative	flag: TRUE = a cumulative plot is done (by calling cumulativeplot)
newdevice	flag: if TRUE, new plot device is opened
setpar	flag: if TRUE parameters are set with the function par
xlab	x axis label
log	only valid if bjerrum=TRUE: should the plot be on a logarithmic y axis?
total	only valid if cumulative=TRUE: should the sum of all elements specified in what be plotted as well?
device	the device to plot on; default: "x11" (can also be "eps" or "pdf")
filename	filename to be used if "eps" or "pdf" is selected for device

size	the size of the plot device; default: 12 (width) by 10 (height) inches
ylim	standard plot parameter; if not supplied it will be calculated by range() of the elements to plot
lwd	standard plot parameter; width of the lines in the plot
mgp	standard plot parameter; default: axis title on line 1.8, axis labels on line 0.5, axis on line 0
mar	standard plot parameter; default: margin of 3 lines bottom and left and 0.5 lines top and right
oma	standard plot parameter; default: no outer margin
palette	only valid if bjerrum=TRUE or cumulative=TRUE: a vector of colors to use in the plot (either numbers or names given in colors())
legendposition	only valid if bjerrum=TRUE or cumulative=TRUE: position of the legend
legendinset	only valid if bjerrum=TRUE or cumulative=TRUE: standard legend parameter inset
legendlwd	only valid if bjerrum=TRUE or cumulative=TRUE: standard legend parameter lwd: line width of lines in legend
bg	only valid if bjerrum=TRUE or cumulative=TRUE: standard legend parameter: default background color: white
y.intersp	standard legend parameter; if cumulative=TRUE then default: 1.2 lines space between the lines in the legend
...	further arguments are passed on to the plot function

Details

Top level generic usage is

```
plot.aquaenv(x, xval, what=NULL, bjerrum=FALSE,
             cumulative=FALSE, newdevice=TRUE, setpar=TRUE,
             device="x11", ...)
```

Generic usages for standard plotting are

```
plot.aquaenv(x, xval, ...)
```

```
plot.aquaenv(x, xval, what, mfrow=c(1,1), size=c(7,7), ...)
```

Generic usage for creating a bjerrum plot is

```
plot.aquaenv(x, what, log=FALSE, palette=NULL,
             device="x11", filename="aquaenv",
             size=c(12,10), ylim=NULL, lwd=2, xlab="free scale pH",
             mgp=c(1.8, 0.5, 0), mar=c(3,3,0.5,0.5), oma=c(0,0,0,0),
             legendposition="bottomleft", legendinset=0.05,
             legendlwd=4, bg="white", newdevice=TRUE, setpar=TRUE,
             device="x11",...)
```

Generic usage for creating a cumulative plot is

```
plot.aquaenv(x, xval, what, total=TRUE, palette=NULL,
             device="x11", filename="aquaenv", size=c(12,10), ylim=NULL,
             lwd=2, mgp=c(1.8, 0.5, 0), mar=c(3,3,0.5,0.5), oma=c(0,0,0,0),
             legendposition="bottomleft", legendinset=0.05, legendlwd=4,
             bg="white", y.intersp=1.2, newdevice=TRUE, setpar=TRUE,
             device="x11",...)
```

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

Examples

```
## Not run:
### 0
#####
A <- aquaenv(35, 15, SumCO2=0.003, TA=seq(0.001,0.004, 0.0001))
plot(A, xval=A$TA, xlab="[TA]/(mol/kg-soln)")
plot(A, what=c("CO2", "HCO3", "CO3"), bjerrum=TRUE, log=TRUE)
plot(A, xval=A$TA, xlab="[TA]/(mol/kg-soln)", what=c("CO2", "HCO3", "CO3"),
     cumulative=TRUE, ylab="mol/kg-soln", ylim=c(0,0.0031))

### 1
#####
SumCO2 <- 0.0020
pH <- 8

S <- 30
t <- 1:15
p <- 10
ae <- aquaenv(S, t, p, SumCO2=SumCO2, pH=pH, revelle=TRUE, dsa=TRUE)
plot(ae, xval=t, xlab="T/(deg C)", newdevice=FALSE)

### 2
#####
S <- 35
t <- 15

SumCO2 <- 0.003500
SumNH4 <- 0.000020

mass_sample <- 0.01 # the mass of the sample solution in kg
mass_titrant <- 0.02 # the total mass of the added titrant solution in
# kg
conc_titrant <- 0.01 # the concentration of the titrant solution in
# mol/kg-soln
```

```

S_titrant <- 0.5 # the salinity of the titrant solution (the
                # salinity of a solution with a ionic strength of
                # 0.01 according to:  $I = (19.924 S) / (1000 - 1.005S)$ )
steps      <- 50 # the amount of steps the mass of titrant is added
                # in
type       <- "HCl"

pHstart <- 11.3

ae <- titration(aquaenv(S=S, t=t, SumCO2=SumCO2, SumNH4=SumNH4,
                    pH=pHstart), mass_sample, mass_titrant, conc_titrant,
                S_titrant, steps, type)

# plotting everything
plot(ae, xval=ae$delta_mass_titrant, xlab="HCl solution added [kg]",
     mfrow=c(10,10))

# plotting selectively
size <- c(12,8) #inches
mfrow <- c(4,4)
what <- c("TA", "pH", "CO2", "HCO3", "CO3", "BOH3", "BOH4", "OH",
         "NH4", "NH3", "H2SO4", "HSO4", "SO4", "HF", "F", "pCO2")

plot(ae, xval=ae$delta_mass_titrant, xlab="HCl solution added [kg]",
     what=what, size=size, mfrow=mfrow)

plot(ae, xval=ae$pH, xlab="free scale pH", what=what, size=size,
     mfrow=mfrow)

# different x values
plot(ae, xval=ae$delta_conc_titrant, xlab="[HCl] offset added
     [mol/kg-soln]", what=what, size=size, mfrow=mfrow)

plot(ae, xval=ae$delta_moles_titrant, xlab="HCl added [mol]", what=what,
     size=size, mfrow=mfrow, newdevice=FALSE)

# bjerrum plots
plot(ae, bjerrum=TRUE)

what <- c("CO2", "HCO3", "CO3")
plot(ae, what=what, bjerrum=TRUE)
plot(ae, what=what, bjerrum=TRUE, lwd=4, palette=c("cyan", "magenta",
         "yellow"), bg="gray", legendinset=0.1, legendposition="topleft")

what <- c("CO2", "HCO3", "CO3", "BOH3", "BOH4", "OH", "NH4", "NH3",

```

```

      "H2SO4", "HSO4", "SO4", "HF", "F")

plot(ae, what=what, bjerrum=TRUE, log=TRUE, newdevice=FALSE)
plot(ae, what=what, bjerrum=TRUE, log=TRUE, ylim=c(-6,-1),
      legendinset=0, lwd=3, palette=c(1,3,4,5,6,colors())[seq(100,250,6)]))

### 3
####
parameters <- list(
  t      = 15      , # degrees C
  S      = 35      , # psu

  SumCO2_t0 = 0.002 , # mol/kg-soln (comparable to Wang2005)
  TA_t0    = 0.0022 , # mol/kg-soln (comparable to Millero1998)

  kc      = 0.5    , # 1/d      proportionality factor
                        #          for air-water exchange
  kp      = 0.000001 , # mol/(kg-soln*d) max rate of calcium
                        #          carbonate precipitation
  n       = 2.0    , # -        exponent for kinetic
                        #          rate law of precipitation

  modeltime = 20   , # d        duration of the model
  outputsteps = 100 , #        number of outputsteps
)

boxmodel <- function(timestep, currentstate, parameters)
{
  with (
    as.list(c(currentstate,parameters)),
    {
      ae <- aquaenv(S=S, t=t, SumCO2=SumCO2, pH=-log10(H), SumSiOH4=0,
                    SumBOH3=0, SumH2SO4=0, SumHF=0, dsa=TRUE)

      Rc <- kc * ((ae$CO2_sat) - (ae$CO2))
      Rp <- kp * (1-ae$omega_calcite)^n

      dSumCO2 <- Rc - Rp

      dHRc <- (      -(ae$dTAdSumCO2*Rc      ))/ae$dTAdH
      dHRp <- (-2*Rp -(ae$dTAdSumCO2*(-Rp)))/ae$dTAdH
      dH <- dHRc + dHRp

      ratesofchanges <- c(dSumCO2, dH)

      processrates <- c(Rc=Rc, Rp=Rp)
      outputvars <- c(dHRc=dHRc, dHRp=dHRp)

      return(list(ratesofchanges, list(processrates, outputvars, ae)))
    }
  )
}

```

```

with (as.list(parameters),
      {
        aetmp <- aquaenv(S=S, t=t, SumCO2=SumCO2_t0,
                        TA=TA_t0, SumSiOH4=0, SumBOH3=0,
                        SumH2SO4=0, SumHF=0)
        H_t0 <- 10^(-aetmp$pH)

        initialstate <- c(SumCO2=SumCO2_t0, H=H_t0)
        times <- seq(0,modeltime,(modeltime/outputsteps))
        output <- as.data.frame(vode(initialstate,times,
                                     boxmodel,parameters, hmax=1))
      })

what <- c("SumCO2", "TA", "Rc", "Rp",
          "omega_calcite", "pH", "dHRc", "dHRp")
plot(aquaenv(ae=output, from.data.frame=TRUE), xval=output$time,
      xlab="time/d", mfrow=c(3,3), size=c(15,10), what=what)

what <- c("dHRc", "dHRp")
plot(aquaenv(ae=output, from.data.frame=TRUE), xval=output$time,
      xlab="time/d", what=what, ylab="mol-H/(kg-soln*d)",
      legendposition="topright", cumulative=TRUE)

## End(Not run)

```

sample_dickson1981 sample_dickson1981

Description

PUBLIC dataset: theoretical titration curve for TA determination as given in table 1 of Dickson1981

Meta-data:

x-value mass of titrant added (in g)
y-value pH measured on the free proton scale

<i>t</i>	25	degC
<i>S</i>	35	
<i>mass_sample</i>	200	g
<i>conc_titrant</i>	0.3000	mol/kg-soln
<i>TA</i>	0.00245	mol/kg-soln
<i>SumCO2</i>	0.00220	mol/kg-soln
<i>SumBOH3</i>	0.00042	mol/kg-soln
<i>SumH2SO4</i>	0.02824	mol/kg-soln

<i>SumHF</i>	0.00007	mol/kg-soln
<i>K_W</i>	4.32e-14	(mol/kg-soln)*(mol/kg-soln)
<i>K_CO2</i>	1.00e-6	mol/kg-soln
<i>K_HCO3</i>	8.20e-10	mol/kg-soln
<i>K_BOH3</i>	1.78e-9	mol/kg-soln
<i>K_HSO4</i>	1/1.23e1	mol/kg-soln
<i>K_HF</i>	1/4.08e2	mol/kg-soln

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

sample_dickson2007 *sample_dickson2007*

Description

PUBLIC dataset: titration curve for TA determination as given on p. 11 of SOP3b in Dickson2007

Metadata:

x-value mass of titrant added (in cubic centimeters)
y-value E in V

<i>t</i>	24.25	degC
<i>S</i>	33.923	
<i>mass_sample</i>	140.32	g
<i>conc_titrant</i>	0.10046	mol/kg-soln
<i>density titrant</i>	1.02393	g/cm3
<i>calculated TA</i>	2260.06	umol/kg-soln
<i>calculated E0</i>	0.394401	V

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

TAfit

TAfit

Description

PUBLIC function: calculates [TA] and [SumCO2] (and optionally K_{CO2} and E0) from a titration curve using an optimization procedure (nls.lm from R package minpack.lm)

Usage

```
TAfit(ae, titcurve, conc_titrant, mass_sample, S_titrant=NULL,
      TASumCO2guess=0.0025, E0guess=0.4, type="HCl", Evals=FALSE,
      electrode_polarity="pos", K_CO2fit=FALSE,
      equalspaced=TRUE, seawater_titrant=FALSE,
      pHscale="free", debug=FALSE, k_w=NULL, k_co2=NULL, k_hco3=NULL,
      k_boh3=NULL, k_hso4=NULL, k_hf=NULL,
      nlscontrol=nls.lm.control(), verbose=FALSE,
      k1k2="roy", khf="dickson", datxbegin=0, SumCO2Zero=FALSE)
```

Arguments

ae	an object of type aquaenv: minimal definition, contains all information about the system: T, S, d, total concentrations of nutrients etc (Note that it is possible to give values for SumBOH4, SumHSO4, and SumHF in the sample other than the ones calculated from salinity)
titcurve	a table containing the titration curve: basically a series of tuples of added titrant solution mass and pH values (pH on free proton scale) or E values in V
conc_titrant	concentration of the titrant solution in mol/kg-soln
mass_sample	the mass of the sample solution in kg
S_titrant	the salinity of the titrant solution, if not supplied it is assumed that the titrant solution has the same salinity as the sample solution
TASumCO2guess	a first guess for [TA] and [SumCO2] to be used as initial values for the optimization procedure
E0guess	first guess for E0 in V
type	the type of titrant: either "HCl" or "NaOH"
Evals	are the supplied datapoints pH or E (V) values?
electrode_polarity	either "pos" or "neg": how is the polarity of the Electrode: $E = E0 - (RT/F)\ln(H^+)$ ("pos") or $-E = E0 - (RT/F)\ln(H^+)$ ("neg")?
K_CO2fit	should K_{CO2} be fitted as well?
equalspaced	are the mass values of titcurve equally spaced?
seawater_titrant	is the titrant based on natural seawater? (does it contain SumBOH4, SumHSO4, and SumHF in the same proportions as seawater, i.e., correlated to S?); Note that you can only assume a seawater based titrant (i.e. SumBOH4, SumHSO4, and SumHF ~ S) or a water based titrant (i.e. SumBOH4, SumHSO4, and SumHF = 0). It is not possible to give values for SumBOH4, SumHSO4, and SumHF of the titrant.

pHscale	either "free", "total", "sws" or "nbs": if the titration curve contains pH data: on which scale is it measured?
debug	debug mode: the last simulated titration tit, the converted pH profile calc, and the nls.lm output out are made global variables for investigation and plotting
k_w	a fixed K_W can be specified
k_co2	a fixed K_{CO2} can be specified; used for TA fitting: give a K_{CO2} and NOT calculate it from T and S: i.e. K_{CO2} can be fitted in the routine as well
k_hco3	a fixed K_{HCO3} can be specified
k_boh3	a fixed K_{BOH3} can be specified
k_hso4	a fixed K_{HSO4} can be specified
k_hf	a fixed K_{HF} can be specified
nlscontrol	nls.lm.control() can be specified
verbose	verbose mode: show the traject of the fitting in a plot
k1k2	either "roy" (default, Roy1993a) or "lueker" (Lueker2000) for K_{CO2} and K_{HCO3} .
khf	either "dickson" (default, Dickson1979a) or "perez" (Perez1987a) for K_{HF}
datxbegin	at what x value (amount of titrant added) does the supplied curve start? (i.e. is the complete curve supplied or just a part?)
SumCO2Zero	should $SumCO2 == 0$?

Value

a list of up to five values ([TA] in mol/kg-solution, [SumCO2] in mol/kg-solution, E0 in V, K1 in mol/kg-solution and on free scale, sum of the squared residuals)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

Examples

```
## Not run:

#####
# Calculating TA from titration data
#####

#### 1.) proof of concept #####
#####
#####

# generate "data":
S <- 35
t <- 15

SumCO2 <- 0.002000
```

```

TA      <- 0.002200
initial_ae <- aquaenv(S=S, t=t, SumCO2=SumCO2, TA=TA)

mass_sample <- 0.01 # the mass of the sample solution in kg
mass_titrant <- 0.003 # the total mass of the added titrant solution
                  # in kg
conc_titrant <- 0.01 # the concentration of the titrant solution in
                  # mol/kg-soln
S_titrant   <- 0.5 # the salinity of the titrant solution (the
                  # salinity of a solution with a ionic strength
                  # of 0.01 according to:
                  # I = (19.924 S) / (1000 - 1.005 S)
steps       <- 20 # the amount of steps the mass of titrant is
                  # added in
type        <- "HCl"

ae <- titration(initial_ae, mass_sample, mass_titrant, conc_titrant,
                S_titrant, steps, type)

plot(ae, ae$delta_mass_titrant, what="pH", newdevice=FALSE)

# the input data for the TA fitting routine: a table with the added
# mass of the titrant and the resulting free scale pH
titcurve <- cbind(ae$delta_mass_titrant, ae$pH)

# for the TA fitting procedure all total quantities except SumCO2
# (SumNH4, SumH2S, SumH3PO4, SumSiOH4, SumHNO3, SumHNO2, SumBOH3,
# SumH2SO4, SumHF) need to be known. However, the latter three
# can be calculated from salinity as it is done in this example.

fit1 <- TAfit(initial_ae, titcurve, conc_titrant, mass_sample,
              S_titrant)
fit1

# E (V) values as input variables: generate E values using
# E0=0.4 V and the nernst equation
tottitcurve <- convert(titcurve[,2], "pHscale", "free2sws", S=S,
                      t=t)

# (Nernst equation relates E to TOTAL [H+] (DOE1994, p.7,
# ch.4, sop.3), BUT, if fluoride is present, its SWS, so
# we use SWS!
Etitcurve <- cbind(titcurve[,1], (0.4 - ((PhysChemConst$R/10)
    *initial_ae$T/PhysChemConst$F)
    *log(10^-tottitcurve))) # Nernst equation

fit2 <- TAfit(initial_ae, Etitcurve, conc_titrant, mass_sample,
              S_titrant, Evals=TRUE, verbose=TRUE)
fit2

# k_co2 fitting: one K_CO2 (k_co2) for the whole titration curve
# is fitted, i.e. there is NO correction for K_CO2 changes due to

```

```

# changing S due to mixing with the titrant
fit3 <- TAfit(initial_ae, titcurve, conc_titrant, mass_sample,
             S_titrant, K_CO2fit=TRUE)
fit3

# assume the titrant has the same salinity as the sample
# (and is made up of natural seawater, i.e. containing SumBOH4,
# SumH2SO4 and SumHF as functions of S), then the "right" K_CO2
# should be fitted i.e we do NOT give the argument S_titrant
# and set the flag seawater_titrant to TRUE
ae <- titration(initial_ae, mass_sample, mass_titrant,
                conc_titrant, steps=steps, type=type,
                seawater_titrant=TRUE)
titcurve <- cbind(ae$delta_mass_titrant, ae$pH)

fit4 <- TAfit(initial_ae, titcurve, conc_titrant, mass_sample,
             K_CO2fit=TRUE, seawater_titrant=TRUE)
fit4

# fitting of TA, SumCO2, K_CO2 and E0
Etitcurve <- cbind(titcurve[,1], (0.4 - ((PhysChemConst$R/10)
                                     *initial_ae$T/PhysChemConst$F)
                                     *log(10^-titcurve[,2])))
fit5 <- TAfit(initial_ae, Etitcurve, conc_titrant, mass_sample,
             K_CO2fit=TRUE, seawater_titrant=TRUE, Evals=TRUE)
fit5

# fitting of non equally spaced data:
neqsptitcurve <- rbind(titcurve[1:9,], titcurve[11:20,])
fit6 <- TAfit(initial_ae, neqsptitcurve, conc_titrant,
             mass_sample, seawater_titrant=TRUE,
             equalspaced=FALSE)
fit6

#add some "noise" on the generated data
noisetitcurve <- titcurve * rnorm(length(titcurve),
                                mean=1, sd=0.01) #one percent error possible
plot(ae, ae$delta_mass_titrant, what="pH", type="l", col="red",
     xlim=c(0,0.003), ylim=c(3,8.1), newdevice=FALSE)
par(new=TRUE)
plot(noisetitcurve[,1],noisetitcurve[,2], type="l",
     xlim=c(0,0.003), ylim=c(3,8.1))

fit7 <- TAfit(initial_ae, noisetitcurve, conc_titrant,
             mass_sample, seawater_titrant=TRUE)
fit7

# 2.) test with generated data from Dickson1981 #
#####
#####

```

```

conc_titrant = 0.3      # mol/kg-soln
mass_sample   = 0.2      # kg
S_titrant     = 14.835  # is aequivalent to the ionic strength
                    # of 0.3 mol/kg-soln

SumBOH3 = 0.00042 # mol/kg-soln
SumH2SO4 = 0.02824 # mol/kg-soln
SumHF    = 0.00007 # mol/kg-soln

# convert mass of titrant from g to kg
sam <- cbind(sample_dickson1981[,1]/1000, sample_dickson1981[,2])

dicksonfit <- TAfit(aquaenv(t=25, S=35, SumBOH3=SumBOH3,
                          SumH2SO4=SumH2SO4, SumHF=SumHF), sam,
                  conc_titrant, mass_sample,
                  S_titrant=S_titrant, debug=TRUE)

dicksonfit
#TA      Dickson1981: 0.00245
#SumCO2  Dickson1981: 0.00220

# => not exactly the same! why?

# a.) does salinity correction (S_titrant) matter or not?
#####

# without salinity correction
dickson1 <- titration(aquaenv(t=25, S=35, SumCO2=0.00220,
                             SumBOH3=SumBOH3, SumH2SO4=SumH2SO4,
                             SumHF=SumHF, TA=0.00245),
                    mass_sample=mass_sample,
                    mass_titrant=0.0025,
                    conc_titrant=conc_titrant,
                    steps=50, type="HCl")

# with salinity correction
dickson2 <- titration(aquaenv(t=25, S=35, SumCO2=0.00220,
                             SumBOH3=SumBOH3, SumH2SO4=SumH2SO4,
                             SumHF=SumHF, TA=0.00245),
                    mass_sample=mass_sample,
                    mass_titrant=0.0025,
                    conc_titrant=conc_titrant,
                    S_titrant=S_titrant,
                    steps=50, type="HCl")

plot(dickson1, xval=dickson1$delta_mass_titrant,
     what="pH", xlim=c(0,0.0025), ylim=c(3,8.2), newdevice=FALSE,
     col="red")
par(new=TRUE)
plot(dickson2, xval=dickson2$delta_mass_titrant,
     what="pH", xlim=c(0,0.0025), ylim=c(3,8.2), newdevice=FALSE,

```

```

    col="blue")
par(new=TRUE)
plot(sam[,1], sam[,2], type="l", xlim=c(0,0.0025), ylim=c(3,8.2))

# => salinity correction makes NO difference, because the relation
# between total sample and added titrant is very large:
# salinity only drops from 35 to 34.75105

#BUT: there is an offset between the "Dickson" curve and our curve:
plot(dicksontitration2$pH - sam[,2])

# b.) does it get better if we fit K_CO2 as well?
#####
dicksonfit2 <- TAfit(aquaenv(t=25, S=35, SumBOH3=SumBOH3,
                          SumH2SO4=SumH2SO4, SumHF=SumHF), sam,
                  conc_titrant, mass_sample,
                  S_titrant=S_titrant, debug=TRUE,
                  K_CO2fit=TRUE)
dicksonfit2
#TA    Dickson1981: 0.00245
#SumCO2 Dickson1981: 0.00220

# => yes it does, but it is not perfect yet!

# c.) differing K values
#####
# Dickson uses fixed K values that are slightly different than ours
dicksontitration3 <- titration(aquaenv(t=25, S=35, SumCO2=0.00220,
                                       SumBOH3=SumBOH3, SumH2SO4=SumH2SO4,
                                       SumHF=SumHF, TA=0.00245, k_w=4.32e-14,
                                       k_co2=1e-6, k_hco3=8.20e-10,
                                       k_boh3=1.78e-9, k_hso4=(1/1.23e1),
                                       k_hf=(1/4.08e2)),
                             mass_sample=mass_sample,
                             mass_titrant=0.0025,
                             conc_titrant=conc_titrant,
                             steps=50, type="HCl",
                             S_titrant=S_titrant, k_w=4.32e-14,
                             k_co2=1e-6, k_hco3=8.20e-10,
                             k_boh3=1.78e-9, k_hso4=(1/1.23e1),
                             k_hf=(1/4.08e2))
plot(dicksontitration3, xval=dicksontitration3$delta_mass_titrant,
     what="pH", xlim=c(0,0.0025), ylim=c(3,8.2), newdevice=FALSE,
     col="blue")
par(new=TRUE)
plot(sam[,1], sam[,2], type="l", xlim=c(0,0.0025), ylim=c(3,8.2))

plot(dicksontitration3$pH - sam[,2])
# => no offset between the pH curves

# => exactly the same curves!

```

```
dicksonfit3 <- TAFit(aquaenv(t=25, S=35, SumBOH3=SumBOH3,
                        SumH2SO4=SumH2SO4, SumHF=SumHF, k_w=4.32e-14,
                        k_co2=1e-6, k_hco3=8.20e-10, k_boh3=1.78e-9,
                        k_hso4=(1/1.23e1), k_hf=(1/4.08e2)),
                    sam, conc_titrant, mass_sample,
                    S_titrant=S_titrant, debug=TRUE,
                    k_w=4.32e-14, k_co2=1e-6, k_hco3=8.20e-10,
                    k_boh3=1.78e-9, k_hso4=(1/1.23e1),
                    k_hf=(1/4.08e2))
dicksonfit3

# PERFECT fit!

plot(sam[,1], sam[,2], xlim=c(0,0.0025), ylim=c(3,8.2), type="l")
par(new=TRUE)
plot(tit$delta_mass_titrant, calc, xlim=c(0,0.0025), ylim=c(3,8.2),
     type="l", col="red")

## End(Not run)
```

Technicals

Technicals

Description

PUBLIC list: a collection programming-technical constants

Value

A list with elements:

Haccur	accuracy for iterative (Follows2006) pH calculations (max. deviation in [H+])
Hstart	start [H+] for an iterative pH calculation
maxiter	maximum number of iterations for iterative (Follows2006) pH calculation method as well as for the application of the standard R function uniroot
unirootinterval	the interval (in terms of [H+]) for pH calculation using the standard R function uniroot
uniroottol	the interval (in terms of [H+]) for pH calculation using the standard R function uniroot
epsilon_fraction	fraction of disturbance for the numerical calculation of derivatives of TA with respect to changes in the dissociation constants
revelle_fraction	fraction of disturbance for the numerical calculation of the revelle factor
CO2	fugacity of CO2 in atm

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

titration

titration

Description

PUBLIC function: creates an object of class aquaenv which contains a titration simulation

Usage

```
titration(aquaenv, mass_sample, mass_titrant, conc_titrant,
          S_titrant=NULL, steps, type="HCl", seawater_titrant=FALSE,
          k_w=NULL, k_co2=NULL, k_hco3=NULL, k_boh3=NULL, k_hso4=NULL,
          k_hf=NULL, k1k2="roy", khf="dickson")
```

Arguments

aquaenv	an object of type aquaenv: minimal definition, contains all information about the system: T, S, d, total concentrations of nutrients etc (Note that it is possible to give values for SumBOH4, SumHSO4, and SumHF in the sample other than the ones calculated from salinity)
mass_sample	the mass of the sample solution in kg
mass_titrant	the total mass of the added titrant solution in kg
conc_titrant	the concentration of the titrant solution in mol/kg-soln
S_titrant	the salinity of the titrant solution, if not supplied it is assumed that the titrant solution has the same salinity as the sample solution
steps	the amount of steps the mass of titrant is added in
type	the type of titrant: either "HCl" or "NaOH", default: "HCl"
seawater_titrant	is the titrant based on natural seawater? (does it contain SumBOH4, SumHSO4, and SumHF in the same proportions as seawater, i.e., correlated to S?); Note that you can only assume a seawater based titrant (i.e. SumBOH4, SumHSO4, and SumHF ~ S) or a water based titrant (i.e. SumBOH4, SumHSO4, and SumHF = 0). It is not possible to give values for SumBOH4, SumHSO4, and SumHF of the titrant.
k_w	a fixed K _W can be specified
k_co2	a fixed K _{CO2} can be specified; used for TA fitting: give a K _{CO2} and NOT calculate it from T and S: i.e. K _{CO2} can be fitted in the routine as well
k_hco3	a fixed K _{HCO3} can be specified
k_boh3	a fixed K _{BOH3} can be specified
k_hso4	a fixed K _{HSO4} can be specified

k_hf a fixed K_{HF} can be specified
 k1k2 either "roy" (default, Roy1993a) or "lueker" (Lueker2000) for K_{CO_2} and K_{HCO_3} .
 khf either "dickson" (default, Dickson1979a) or "perez" (Perez1987a) for K_{HF}

Value

object of class aquaenv which contains a titration simulation

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

Examples

```
## Not run:
#####
# Titration with HCl
#####
S <- 35
t <- 15

SumCO2 <- 0.003500
SumNH4 <- 0.000020

mass_sample <- 0.01 # the mass of the sample solution in kg
mass_titrant <- 0.02 # the total mass of the added titrant solution in
# kg
conc_titrant <- 0.01 # the concentration of the titrant solution in
# mol/kg-soln
S_titrant <- 0.5 # the salinity of the titrant solution (the
# salinity of a solution with a ionic strength of
# 0.01 according to:  $I = (19.924 S) / (1000 - 1.005S)$ )
steps <- 50 # the amount of steps the mass of titrant is added
# in
type <- "HCl"

pHstart <- 11.3

ae <- titration(aquaenv(S=S, t=t, SumCO2=SumCO2, SumNH4=SumNH4,
pH=pHstart), mass_sample, mass_titrant, conc_titrant,
S_titrant, steps, type)

# plotting everything
plot(ae, xval=ae$delta_mass_titrant, xlab="HCl solution added [kg]",
mfrow=c(10,10))

# plotting selectively
size <- c(12,8) #inches
```

```

mfrow <- c(4,4)
what <- c("TA", "pH", "CO2", "HCO3", "CO3", "BOH3", "BOH4", "OH",
         "NH4", "NH3", "H2SO4", "HSO4", "SO4", "HF", "F", "pCO2")

plot(ae, xval=ae$delta_mass_titrant, xlab="HCl solution added [kg]",
      what=what, size=size, mfrow=mfrow)

plot(ae, xval=ae$pH, xlab="free scale pH", what=what, size=size,
      mfrow=mfrow)

# different x values
plot(ae, xval=ae$delta_conc_titrant, xlab="[HCl] offset added
      [mol/kg-soln]", what=what, size=size, mfrow=mfrow)

plot(ae, xval=ae$delta_moles_titrant, xlab="HCl added [mol]", what=what,
      size=size, mfrow=mfrow)

# bjerrum plots
par(mfrow=c(1,1))
plot(ae, bjerrum=TRUE)

what <- c("CO2", "HCO3", "CO3")
plot(ae, what=what, bjerrum=TRUE)
plot(ae, what=what, bjerrum=TRUE, lwd=4, palette=c("cyan", "magenta",
         "yellow"), bg="gray", legendinset=0.1, legendposition="topleft")

what <- c("CO2", "HCO3", "CO3", "BOH3", "BOH4", "OH", "NH4", "NH3",
         "H2SO4", "HSO4", "SO4", "HF", "F")

plot(ae, what=what, bjerrum=TRUE, log=TRUE)
plot(ae, what=what, bjerrum=TRUE, log=TRUE, ylim=c(-6,-1),
      legendinset=0, lwd=3, palette=c(1,3,4,5,6,colors())[seq(100,250,6)])

## End(Not run)

```

watdepth

watdepth

Description

PUBLIC function: calculates the depth (in m) from the gauge pressure p (or the total pressure P) and the latitude (in degrees: -90 to 90) and the atmospheric pressure P_a (in bar)

Usage

```
watdepth(P=Pa, p=pmax(0, P-Pa), lat=0, Pa=1.013253)
```

Arguments

P	total pressure in bar, standard: 1 atm (at the sea surface)
p	gauge pressure in bar (total pressure minus atmospheric pressure), standard: 0 (at the water surface)
lat	latitude in degrees: -90 to 90, standard: 0
Pa	atmospheric pressure in bar, standard: 1 atm (at sea level)

Value

water depth *d* in meters

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Fofonoff1983

Examples

```
watdepth(100)  
plot(watdepth(1:100))
```

Index

*Topic **misc**

- aquaenv, 3
- as.data.frame.aquaenv, 10
- c.aquaenv, 10
- ConcRelCl, 11
- convert, 11
- DeltaPcoeffs, 13
- gauge_p, 13
- K0_CO2, 14
- K0_O2, 15
- K_BOH3, 17
- K_CO2, 18
- K_H2PO4, 19
- K_H2S, 20
- K_H3PO4, 21
- K_HCO3, 22
- K_HF, 23
- K_HP04, 24
- K_HS04, 25
- K_NH4, 26
- K_SiOH4, 27
- K_SiOOH3, 28
- K_W, 29
- Ksp_aragonite, 15
- Ksp_calcite, 16
- length.aquaenv, 30
- MeanMolecularMass, 30
- merge.aquaenv, 31
- PhysChemConst, 31
- plot.aquaenv, 32
- sample_dickson1981, 37
- sample_dickson2007, 38
- TAfit, 38
- Technicals, 45
- titration, 46
- watdepth, 48

*Topic **package**

- AquaEnv_package, 8
- AquaEnv (AquaEnv_package), 8

- aquaenv, 3
- AquaEnv_package, 8
- as.data.frame.aquaenv, 10
- c.aquaenv, 10
- ConcRelCl, 11
- convert, 11
- DeltaPcoeffs, 13
- gauge_p, 13
- K0_CO2, 14
- K0_O2, 15
- K_BOH3, 17
- K_CO2, 18
- K_H2PO4, 19
- K_H2S, 20
- K_H3PO4, 21
- K_HCO3, 22
- K_HF, 23
- K_HP04, 24
- K_HS04, 25
- K_NH4, 26
- K_SiOH4, 27
- K_SiOOH3, 28
- K_W, 29
- Ksp_aragonite, 15
- Ksp_calcite, 16
- length.aquaenv, 30
- MeanMolecularMass, 30
- merge.aquaenv, 31
- PhysChemConst, 31
- plot.aquaenv, 32
- sample_dickson1981, 37
- sample_dickson2007, 38
- TAfit, 38

Technicals, [45](#)
titration, [46](#)
watdepth, [48](#)