

marelac : utilities for the MArine, Riverine, Estuarine, LAcustrine and Coastal sciences

Karline Soetaert
NIOO-CEME
The Netherlands

Thomas Petzoldt
Technische Universität Dresden
Germany

Filip Meysman
NIOO-CEME
The Netherlands

Abstract

Rpackage **marelac** (Soetaert, Petzoldt, and Meysman 2008) contains chemical and physical constants and functions, datasets, routines for unit conversion, and other utilities useful for MArine, Riverine, Estuarine, LAcustrine and Coastal sciences.

Keywords: marine, riverine, estuarine, lacustrine, coastal science, utilities, constants, R .

1. Introduction

R-package **marelac** has been designed as a tool for use by scientists working in the MArine, Riverine, Estuarine, LAcustrine and Coastal sciences.

It contains:

- chemical and physical constants, e.g. atomic weights, gas constants.
- conversion factors, e.g. gram to mol to liter conversions; conversions between different barometric units, temperature units, salinity units.
- physical functions, e.g. to estimate concentrations of conservative substances as a function of salinity, gas transfer coefficients, diffusion coefficients, estimating the coriolis force, gravity ...
- the thermophysical properties of the seawater, as from the UNESCO polynomial (Fofonoff and Millard 1983) or as from the more recent derivation based on a gibbs funtion (Feistel 2008), (McDougall, Feistel, Millero, Jackett, Wright, King, Marion, Chen, and Spitzer 2009).

2. Constants and datasets

2.1. Physical constants

Dataset **Constants** contains commonly used physical and chemical constants, as in (Mohr and Taylor 2005):

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```
> data.frame(cbind(acronym=names(Constants),
+                   matrix(ncol=3, byrow=TRUE, data=unlist(Constants),
+                   dimnames=list(NULL, c("value", "units", "description")))))

  acronym      value     units           description
1      g        9.8   m/s^2    gravity acceleration
2     SB  5.6697e-08 W/m^2/K^4 Stefan-Boltzmann constant
3  gasCt1  0.08205784 L*atm/K/mol   ideal gas constant
4  gasCt2    8.314472 m3*Pa/K/mol   ideal gas constant
5  gasCt3    83.1451 cm3*bar/K/mol   ideal gas constant
6      E  1.60217653e-19          C Elementary charge
7      F     96485.3   C/mol charge per mol of electrons
8      P0     101325          Pa one standard atmosphere
9      B1  1.3806505e-23          J/K Boltzmann constant
10     B2  8.617343e-05          eV/K Boltzmann constant
11     Na  6.0221415e+23          mol^-1 Avogadro constant
12      C     299792458          m s^-1 Vacuum light speed
```

2.2. Ocean characteristics

Dataset `Oceans` contains surfaces and volumes of the world ocean as in (Sarmiento and Gruber 2006):

```
> data.frame(cbind(acronym=names(Oceans),
+                   matrix(ncol=3, byrow=TRUE, data=unlist(Oceans),
+                   dimnames=list(NULL, c("value", "units", "description"))))

  acronym      value     units           description
1      Mass  1.35e+25      kg    total mass of the oceans
2      Vol   1.34e+18     m^3    total volume of the oceans
3  VolSurf  1.81e+16     m^3    volume of the surface ocean (0-50m)
4  VolDeep  9.44e+17     m^3    volume of the deep ocean (>1200m)
5      Area  3.58e+14     m^2    total area of the oceans
6  AreaIF  3.32e+14     m^2    annual mean ice-free area of the oceans
7  AreaAtl  7.5e+13     m^2    area of the Atlantic ocean, >45dgS
8  AreaPac  1.51e+14     m^2    area of the Pacific ocean, >45dgS
9  AreaInd  5.7e+13     m^2    area of the Indian ocean, >45dgS
10  AreaArct  9.6e+12     m^2    area of the Arctic ocean
11  AreaEncl  4.5e+12     m^2    area of enclosed seas (e.g. Mediterranean)
12      Depth     3690      m    mean depth of the oceans
13 RiverFlow  3.7e+13 m^3/yr          Total river flow
```

2.3. World bathymetric data

data set `Bathymetry` from the **marelac** package can be used to generate the bathymetry (and hypsometry) of the world oceans (and land):

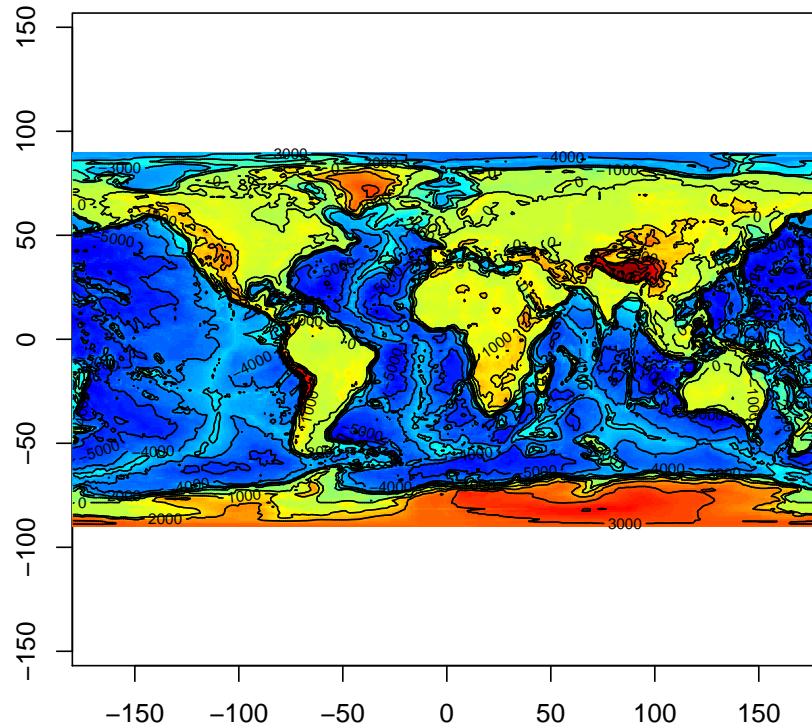


Figure 1: Image plot of ocean bathymetry - see text for R-code

```
> require(marelac)
> image(Bathymetry$x,Bathymetry$y,Bathymetry$z,col=femmecol(100),
+       asp=TRUE,xlab="",ylab="")
> contour(Bathymetry$x,Bathymetry$y,Bathymetry$z,add=TRUE)
```

2.4. AtomicWeight

Dataset `AtomicWeight` holds the atomic weight of various chemical elements, as in (Wieser 2006); The data set contains NA for elements which have no stable isotopes (except U, Th, Pa). The data set can be called in two versions. `AtomicWeight` shows the full table and `atomicweight` can be used for symbolic computations with the elements.

```
> AtomicWeight
```

Number		Name	Symbol	Weight	Footnotes
1	1	hydrogen	H	1.00794(7)	gmr

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2	2	helium	He	4.002602(2)	gr
3	3	lithium	Li	6.941(2)	+gmr
4	4	beryllium	Be	9.012182(3)	
5	5	boron	B	10.811(7)	gmr
6	6	carbon	C	12.0107(8)	gr
7	7	nitrogen	N	14.0067(2)	gr
8	8	oxygen	O	15.9994(3)	gr
9	9	fluorine	F	18.9984032(5)	
10	10	neon	Ne	20.1797(6)	gm
11	11	sodium	Na	22.98976928(2)	
12	12	magnesium	Mg	24.3050(6)	
13	13	aluminium	Al	26.9815386(8)	
14	14	silicon	Si	28.0855(3)	r
15	15	phosphorus	P	30.973762(2)	
16	16	sulfur	S	32.065(5)	gr
17	17	chlorine	Cl	35.453(2)	+gmr
18	18	argon	Ar	39.948(1)	gr
19	19	potassium	K	39.0983(1)	
20	20	calcium	Ca	40.078(4)	g
21	21	scandium	Sc	44.955912(6)	
22	22	titanium	Ti	47.867(1)	
23	23	vanadium	V	50.9415(1)	
24	24	chromium	Cr	51.9961(6)	
25	25	manganese	Mn	54.938045(5)	
26	26	iron	Fe	55.845(2)	
27	27	cobalt	Co	58.933195(5)	
28	28	nickel	Ni	58.6934(2)	
29	29	copper	Cu	63.546(3)	r
30	30	zinc	Zn	65.409(4)	
31	31	gallium	Ga	69.723(1)	
32	32	germanium	Ge	72.64(1)	
33	33	arsenic	As	74.92160(2)	
34	34	selenium	Se	78.96(3)	r
35	35	bromine	Br	79.904(1)	
36	36	krypton	Kr	83.798(2)	gm
37	37	rubidium	Rb	85.4678(3)	g
38	38	strontium	Sr	87.62(1)	gr
39	39	yttrium	Y	88.90585(2)	
40	40	zirconium	Zr	91.224(2)	g
41	41	niobium	Nb	92.90638(2)	
42	42	molybdenum	Mo	95.94(2)	g
43	43	technetium	Tc		*
44	44	ruthenium	Ru	101.07(2)	g
45	45	rhodium	Rh	102.90550(2)	
46	46	palladium	Pd	106.42(1)	g
47	47	silver	Ag	107.8682(2)	g
48	48	cadmium	Cd	112.411(8)	g

49	49	indium	In	114.818(3)	
50	50	tin	Sn	118.710(7)	g
51	51	antimony	Sb	121.760(1)	g
52	52	tellurium	Te	127.60(3)	g
53	53	iodine	I	126.90447(3)	
54	54	xenon	Xe	131.293(6)	gm
55	55	caesium	Cs	132.9054519(2)	
56	56	barium	Ba	137.327(7)	
57	57	lanthanum	La	138.90547(7)	g
58	58	cerium	Ce	140.116(1)	g
59	59	praseodymium	Pr	140.90765(2)	
60	60	neodymium	Nd	144.242(3)	g
61	61	promethium	Pm		*
62	62	samarium	Sm	150.36(2)	g
63	63	euroopium	Eu	151.964(1)	g
64	64	gadolinium	Gd	157.25(3)	g
65	65	terbium	Tb	158.92535(2)	
66	66	dysprosium	Dy	162.500(1)	g
67	67	holmium	Ho	164.93032(2)	
68	68	erbium	Er	167.259(3)	g
69	69	thulium	Tm	168.93421(2)	
70	70	ytterbium	Yb	173.04(3)	g
71	71	lutetium	Lu	174.967(1)	g
72	72	hafnium	Hf	178.49(2)	
73	73	tantalum	Ta	180.94788(2)	
74	74	tungsten	W	183.84(1)	
75	75	rhenium	Re	186.207(1)	
76	76	osmium	Os	190.23(3)	g
77	77	iridium	Ir	192.217(3)	
78	78	platinum	Pt	195.084(9)	
79	79	gold	Au	196.966569(4)	
80	80	mercury	Hg	200.59(2)	
81	81	thallium	Tl	204.3833(2)	
82	82	lead	Pb	207.2(1)	gr
83	83	bismuth	Bi	208.98040(1)	
84	84	polonium	Po		*
85	85	astatine	At		*
86	86	radon	Rn		*
87	87	francium	Fr		*
88	88	radium	Ra		*
89	89	actinium	Ac		*
90	90	thorium	Th	232.03806(2)	*g
91	91	protactinium	Pa	231.03588(2)	*
92	92	uranium	U	238.02891(3)	*gm
93	93	neptunium	Np		*
94	94	plutonium	Pu		*
95	95	americium	Am		*

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```
96      96      curium      Cm          *
97      97      berkelium    Bk          *
98      98      californium  Cf          *
99      99      einsteinium  Es          *
100     100     fermium      Fm          *
101     101     mendelevium  Md          *
102     102     nobelium     No          *
103     103     lawrencium   Lr          *
104     104     rutherfordium Rf          *
105     105     dubnium     Db          *
106     106     seaborgium   Sg          *
107     107     bohrium      Bh          *
108     108     hassium      Hs          *
109     109     meitnerium   Mt          *
110     110     darmstadtium Ds          *
111     111     roentgenium Rg          *
```

```
> AtomicWeight[8,]
```

Number	Name	Symbol	Weight	Footnotes
8	oxygen	O	15.9994(3)	gr

```
> (W_H2O<- with (atomicweight, 2 * H + O))
```

```
[1] 18.01528
```

2.5. atmospheric composition

The atmospheric composition, given in units of the moles of each gas to the total of moles of gas in dry air is in function `atmComp`:

```
> atmComp("O2")
```

```
O2
0.20946
```

```
> atmComp()
```

He	Ne	N2	O2	Ar	Kr
5.2400e-06	1.8180e-05	7.8084e-01	2.0946e-01	9.3400e-03	1.1400e-06
CH4	C02	N20	H2	Xe	C0
1.7450e-06	3.6500e-04	3.1400e-07	5.5000e-07	8.7000e-08	5.0000e-08
O3					
1.0000e-08					

```
> sum(atmComp())      #!
```

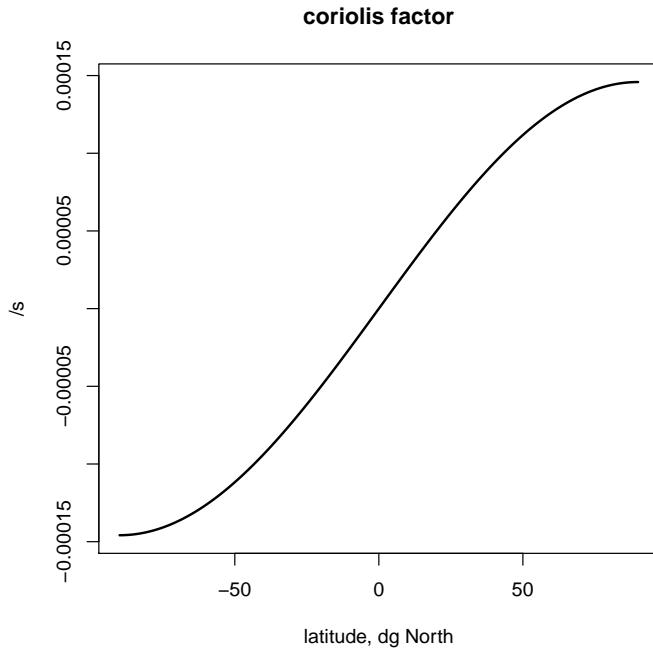


Figure 2: The coriolis function

```
[1] 1.000032
```

3. physical functions

3.1. coriolis

Function `coriolis` estimates the coriolis factor, f , units sec^{-1} according to the formula:
 $f = 2 * \omega * \sin(lat)$, where $\omega = 7.292e^{-5}\text{radianssec}^{-1}$

```
> plot(-90:90,coriolis(-90:90),xlab="latitude, dg North",
+       ylab= "/s" , main = "coriolis factor",type="l",lwd=2)
```

3.2. molecular diffusion coefficients

In function `diffcoeff` the molecular and ionic diffusion coefficients (m^2s^{-1}), for several species at given salinity (S) temperature (t) and pressure (P) is estimated. The implementation is based on the code "CANDI" by Bernie Boudreau (Boudreau 1996).

```
> diffcoeff(S=15,t=15)*24*3600*1e4 # cm2/day
```

	O2	CO2	NH3	H2S	CH4	HC03	CO3
1	1.429209	1.205459	1.422551	1.229482	1.133013	0.7693278	0.6126982

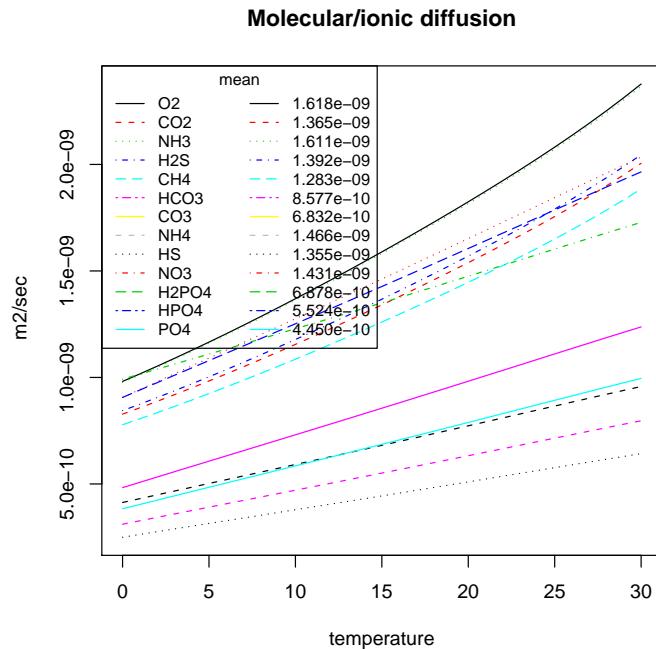


Figure 3: molecular diffusion coefficients as a function of temperature

```

NH4      HS      NO3      H2PO4      HPO4      PO4      H
1 1.314600 1.214089 1.283190 0.6168861 0.4954354 0.3991123 6.51018
      OH      Ca      Mg      Fe      Mn      SO4      H3PO4
1 3.543850 0.5264263 0.4682136 0.4657009 0.4610941 0.7002265 0.555835
      BOH3     BOH4     H4SiO4
1 0.7602404 0.6652104 0.6882134

> diffcoeff(t=10)$O2
[1] 1.369619e-09

> difftemp <- diffcoeff(t=0:30)[,1:13]
> diffsal <- diffcoeff(S=0:35)[,1:13]

> matplot(0:30,difftemp,xlab="temperature",ylab=" m2/sec",
+           main="Molecular/ionic diffusion",type="l")
> legend("topleft",ncol=2,cex=0.8,title="mean",col=1:13,lty=1:13,
+           legend=cbind(names(difftemp),format(colMeans(difftemp),digits=4)))

```

3.3. shear viscosity of water

viscosity calculates the shear viscosity of water, in centipoise ($gm^{-1}sec^{-1}$). Valid for $0 < t < 30$ and $0 < S < 36$.

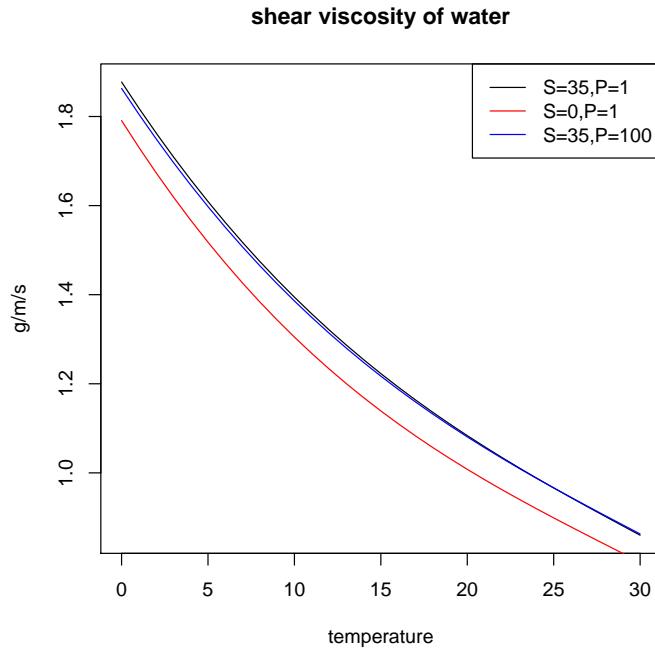


Figure 4: shear viscosity of water as a function of temperature

```
> plot(0:30,viscosity(S=35,t=0:30,P=1),xlab="temperature",ylab="g/m/s",
+       main="shear viscosity of water",type="l")
> lines(0:30,viscosity(S=0,t=0:30,P=1),col="red")
> lines(0:30,viscosity(S=35,t=0:30,P=100),col="blue")
> legend("topright",col=c("black","red","blue"),lty=1,
+        legend=c("S=35,P=1","S=0,P=1","S=35,P=100"))
```

4. dissolved gasses

4.1. saturated oxygen concentrations

gas_O2sat estimates the saturated concentration of oxygen:

```
> gas_O2sat(t = 20)

[1] 7.374404

> t <- seq(0, 30, 0.1)

> plot(t, gas_O2sat(t = t), type = "l", ylim = c(0, 15), lwd=2,
+       main="Oxygen saturation", ylab = "mg/l", xlab="temperature")
> lines(t, gas_O2sat(S = 0, t = t, method = "Weiss"), col = "green",
```

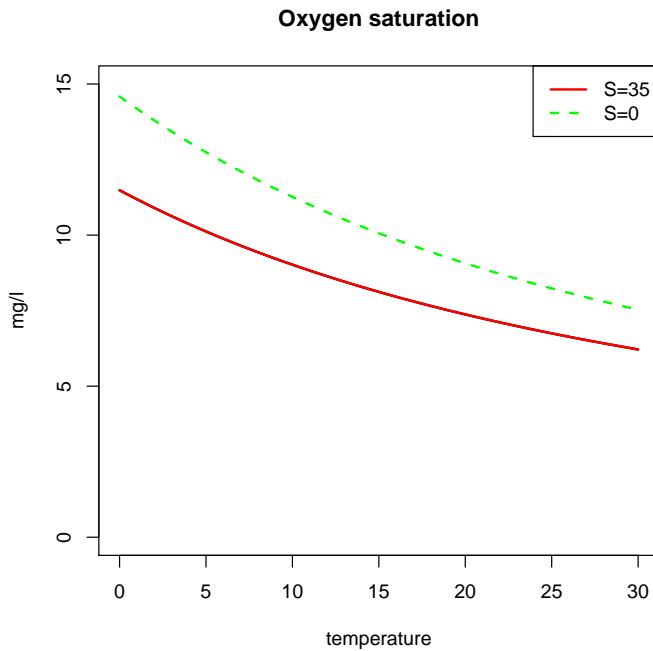


Figure 5: Oxygen saturated concentration as a function of temperature, and for different salinities

```
+      lwd = 2, lty = "dashed")
> lines(t, gas_O2sat(S = 35, t = t, method = "Weiss"), col = "red", lwd = 2)
> legend("topright", c("S=35", "S=0"), col=c("red", "green"), lty=c(1,2), lwd=2)
```

4.2. solubilities and saturated concentrations

More solubilities and saturated concentrations are in functions `gas_solubility` and `gas_satconc`.

```
> gas_satconc(species="O2")
          O2
[1,] 210.9798

> Temp<-seq(from=0,to=30,by=0.1)
> Sal <- seq(from=0,to=35,by=0.1)

> #
> mf  <-par(mfrow=c(2,2))
> #
> gs  <-gas_solubility(t=Temp)
> species <- c("CC14", "CO2", "N2O", "Rn", "CCl2F2")
> matplot(Temp,gs[,species],type="l",lty=1,lwd=2,xlab="temperature",
```

```

+      ylab="mmol/m3",main="solubility (S=35)")
> legend("topright",col=1:5,lwd=2,legend=species)
> #
> species2 <- c("Kr","CH4","Ar","O2","N2","Ne")
> matplot(Temp,gs[,species2],type="l",lty=1,lwd=2,xlab="temperature",
+      ylab="mmol/m3",main="solubility (S=35)")
> legend("topright",col=1:6,lwd=2,legend=species2)
> #
>
> species <- c("N2","CO2","O2","CH4","N2O")
> gsat <-gas_satconc(t=Temp,species=species)
> matplot(Temp,gsat,type="l",xlab="temperature",log="y", lty=1,
+      ylab="mmol/m3",main="Saturated conc (S=35)",lwd=2)
> legend("right",col=1:5,lwd=2,legend=species)
> #
> gsat <-gas_satconc(S=Sal,species=species)
> matplot(Sal,gsat,type="l",xlab="salinity",log="y", lty=1,
+      ylab="mmol/m3",main="Saturated conc (T=20)",lwd=2)
> legend("right",col=1:5,lwd=2,legend=species)
> #
> par("mfrow"=mf)

```

4.3. partial pressure of water vapor

`vapor` estimates the partial pressure of water vapor, divided by the atmospheric pressure.

```

> plot(0:30, vapor(t = 0:30), xlab = "Temperature, dgC", ylab = "pH2O/P",
+      type ="l")

```

4.4. Schmidt number and gas transfer velocity

The Schmidt number of a gas (`gas_schmidt`) is an essential quantity in the gas transfer velocity calculation (`gas_transfer`). The latter also depends on wind velocity (as measured 10 metres above sealevel).

```

> gas_schmidt(species="CO2",t=20)
[1] 665.988

> useq <- 0:15

> plot(useq,gas_transfer(u10=useq,species="O2"),type="l",lwd=2,xlab="u10,m/s",
+      ylab="m/s", main="O2 gas transfer velocity",ylim=c(0,3e-4))
> lines(useq,gas_transfer(u10=useq,species="O2",method="Nightingale"),lwd=2,lty=2)
> lines(useq,gas_transfer(u10=useq,species="O2",method="Wanninkhof1"),lwd=2,lty=3)
> lines(useq,gas_transfer(u10=useq,species="O2",method="Wanninkhof2"),lwd=2,lty=4)
> legend("topleft",lty=1:4,lwd=2,legend=c("Liss and Merlivat 1986",
+ "Nightingale et al. 2000","Wanninkhof 1992","Wanninkhof and McGillis 1999"))

```

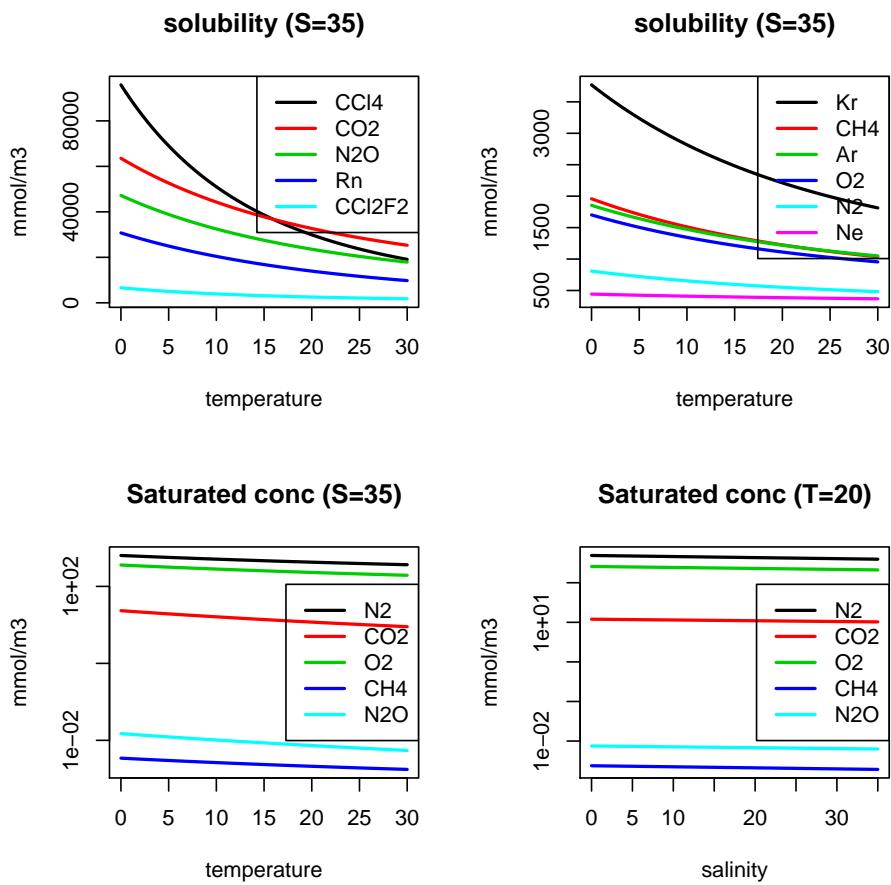


Figure 6: Saturated concentrations and solubility as a function of temperature and salinity, and for different species

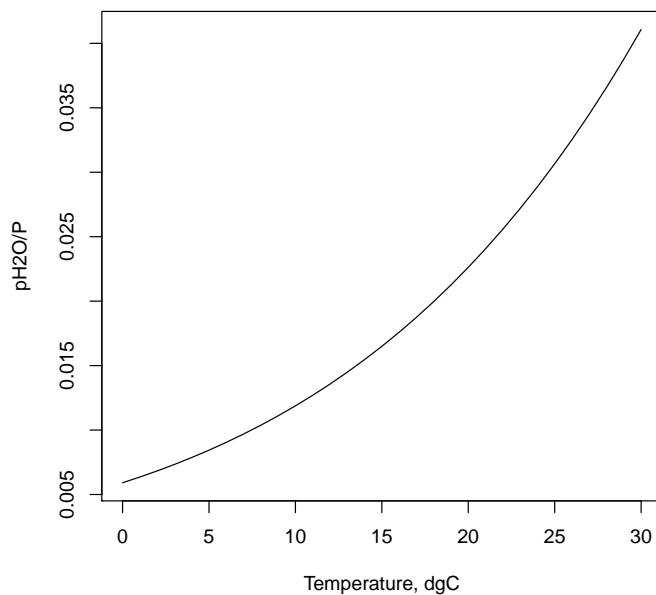


Figure 7: partial pressure of water in saturated air as a function of temperature

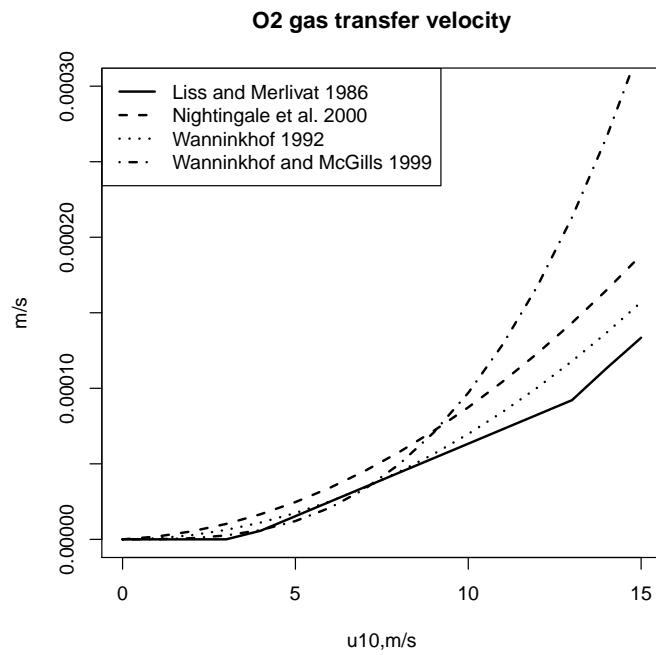


Figure 8: gas transfer velocity for seawater

5. seawater properties

5.1. Concentration of conservative species in seawater

Borate, calcite, sulphate and fluoride concentrations can be estimated as a function of the seawater salinity:

```
> sw_conserv(S=seq(0,35,by=5))
```

	Borate	Calcite	Sulphate	Fluoride
1	0.00000	0.000	0.000	0.000000
2	59.42857	1468.571	4033.633	9.760629
3	118.85714	2937.143	8067.267	19.521257
4	178.28571	4405.714	12100.900	29.281886
5	237.71429	5874.286	16134.534	39.042515
6	297.14286	7342.857	20168.167	48.803144
7	356.57143	8811.429	24201.801	58.563772
8	416.00000	10280.000	28235.434	68.324401

5.2. Thermophysical seawater properties

marelac also implements several thermodynamic properties of seawater. Either one can choose the formulation based on the UNESCO polynomial ([Fofonoff and Millard 1983](#)), which has served the oceanographic community for decades, or the more recent derivation as in ([Feistel 2008](#)). In the latter case the estimates are based on three individual thermodynamic potentials for fluid water, for ice and for the saline contribution of seawater (the Helmholtz function for pure water, an equation of state for salt-free ice, in the form of a Gibbs potential function, and the saline part of the Gibbs potential).

Note that the formulations use a new salinity scale, termed "Reference composition salinity" ([Millero, Feistel, Wright, and McDougall 2008](#)).

```
> sw_cp(S=40,t=1:20)
```

```
[1] 3958.545 3959.028 3959.576 3960.180 3960.831 3961.523 3962.247
[8] 3962.997 3963.768 3964.553 3965.348 3966.148 3966.949 3967.747
[15] 3968.540 3969.324 3970.098 3970.859 3971.605 3972.336
```

```
> sw_cp(S=40,t=1:20,UNESCO=TRUE)
```

```
[1] 3956.080 3955.898 3955.883 3956.021 3956.296 3956.697 3957.209
[8] 3957.819 3958.516 3959.288 3960.124 3961.013 3961.945 3962.911
[15] 3963.900 3964.906 3965.918 3966.931 3967.936 3968.927
```

Below we plot all implemented thermophysical properties as a function of salinity and temperature. We first define a function that does that

```

> plotST <- function(fun,title)
+ {
+   Sal <- seq(0,40,by=0.5)
+   Temp<- seq(-5,40,by=0.5)
+
+   Val <- outer(X=Sal,Y=Temp,FUN=function(X,Y) fun(S=X, t=Y))
+   contour(Sal,Temp,Val,xlab="Salinity",ylab="temperature",
+           main=title,nlevel=20)
+ }
> par (mfrow=c(3,2))
> par(mar=c(4,4,3,2))
> plotST(sw_gibbs,"Gibbs function")
> plotST(sw_cp,"Heat capacity")
> plotST(sw_entropy,"Entropy")
> plotST(sw_enthalpy,"Enthalpy")
> plotST(sw_dens,"Density")
> plotST(sw_svel,"Sound velocity")

> par (mfrow=c(3,2))
> par(mar=c(4,4,3,2))
> plotST(sw_kappa,"Isentropic compressibility")
> plotST(sw_kappa_t,"Isothermal compressibility")
> plotST(sw_alpha,"Thermal expansion coefficient")
> plotST(sw_beta,"Haline contraction coefficient")
> plotST(sw_adtgrad,"Adiabatic temperature gradient")
> par (mfrow=c(1,1))

```

6. conversions

Finally, several functions are included to convert between units of certain properties.

6.1. gram, mol, liter conversions

marelac function `molweight` converts from gram to moles and vice versa

```
> 1/molweight("CO3")
```

```
CO3
0.01666419
```

```
> 1/molweight("HC03")
```

```
HC03
0.01638892
```

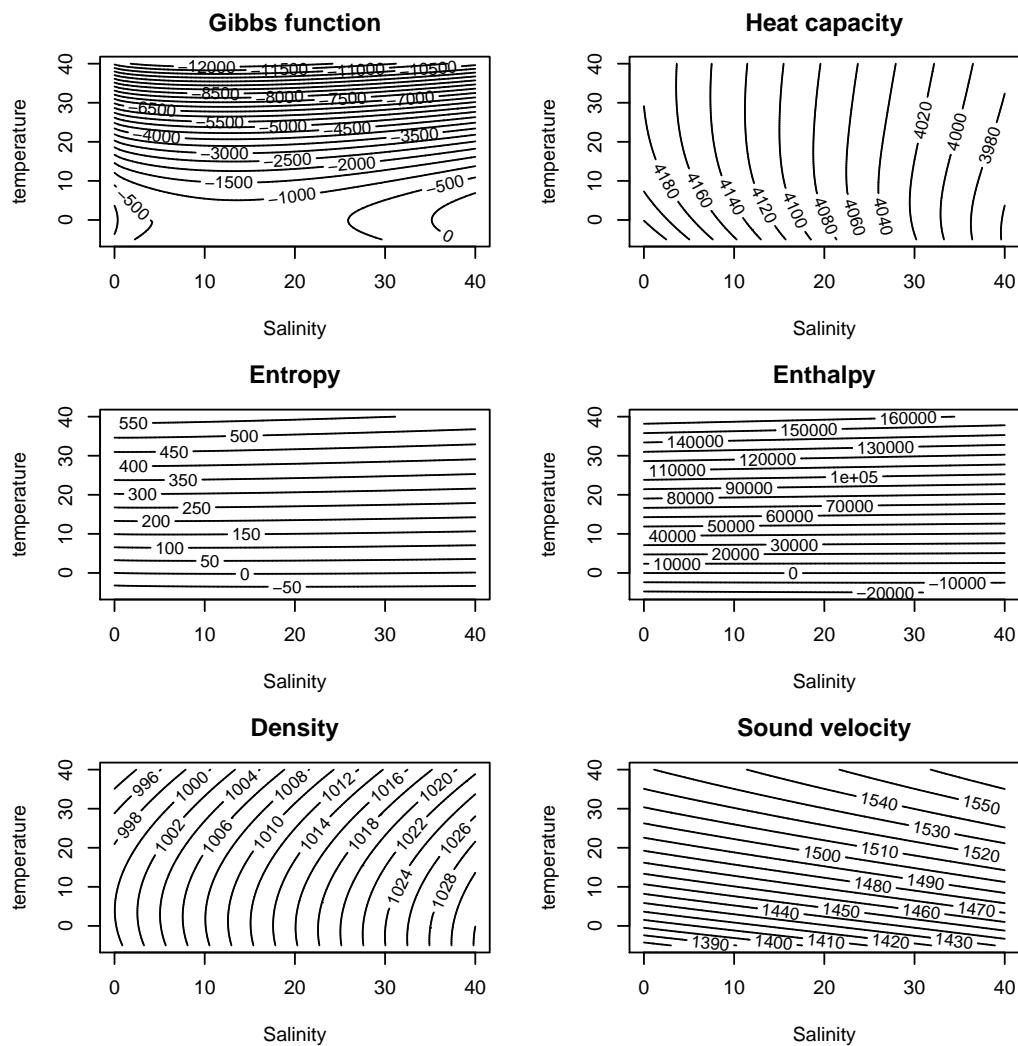


Figure 9: seawater properties as a function of salinity and temperature - see text for R-code

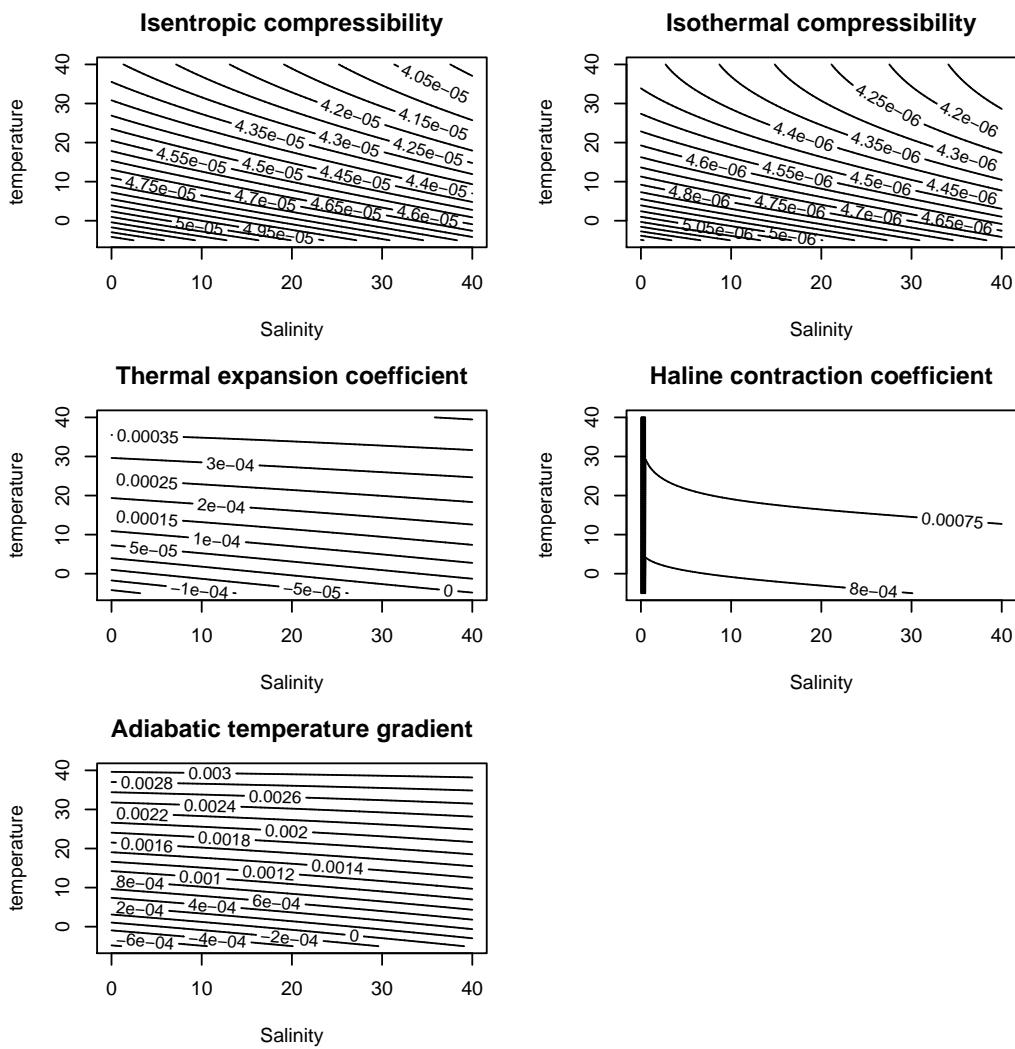


Figure 10: seawater properties as a function of salinity and temperature - continued - see text for R-code

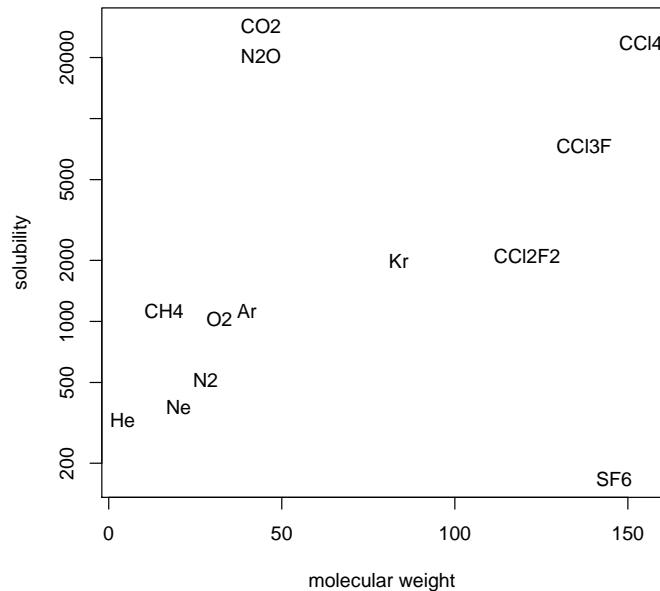


Figure 11: Gas solubility as a function of molecular weight see text for R-code

```
> 1/molweight(c("C2H5OH", "CO2", "H2O"))
C2H5OH          CO2          H2O
0.02170683  0.02272237  0.05550844

> molweight(c("SiOH4", "NaHC03", "C6H12O6", "Ca(HC03)2", "Pb(N03)2", "(NH4)2S04"))
SiOH4      NaHC03      C6H12O6 Ca(HC03)2 Pb(N03)2 (NH4)2S04
48.11666   84.00661  180.15588 162.11168 331.20980 132.13952
```

We can use that to estimate the importance of molecular weight on certain physical properties:

```
> gs <- gas_solubility()
> species <- colnames(gs)
> mw <- molweight(species)

> plot(mw,gs,type="n",xlab="molecular weight", ylab="solubility", log="y")
> text(mw,gs,species)
```

molvol estimates the volume of one liter of a gas. molar volume of an ideal gas

```
> molvol(species="ideal")
```

```
ideal
24.46536
```

```
> molvol(species="ideal", t=1:10)

    ideal
[1,] 22.49599
[2,] 22.57804
[3,] 22.66010
[4,] 22.74216
[5,] 22.82421
[6,] 22.90627
[7,] 22.98833
[8,] 23.07039
[9,] 23.15244
[10,] 23.23450

> 1/molvol(species="O2", t=0)*1000

    O2
44.67259

> 1/molvol(species="O2", q=1:6, t=0)

    O2
[1,] 0.044672589
[2,] 0.022336294
[3,] 0.014890860
[4,] 0.011168149
[5,] 0.008934518
[6,] 0.007445432

> 1/molvol(t=1:5, species=c("CO2", "O2", "N2O"))

      CO2        O2        N2O
[1,] 0.04468587 0.04450899 0.04469987
[2,] 0.04452145 0.04434659 0.04453529
[3,] 0.04435824 0.04418537 0.04437192
[4,] 0.04419623 0.04402533 0.04420975
[5,] 0.04403541 0.04386644 0.04404877
```

6.2. pressure conversions

`convert_p` converts between the different barometric scales:

```
> convert_p(1, "atm")

      Pa      bar      at atm      torr
1 101325.3 1.013253 1.033214   1 760.0008
```

6.3. temperature conversions

while `convert_T` converts between the different temperature scales (Kelvin, Celsius, Fahrenheit):

```
> convert_T(1, "C")
```

	K	C	F
1	274.15	1	33.8

6.4. salinity and chlorinity

The relationship between Salinity, chlorinity and conductivity is in various functions:

```
> convert_StoCl(S=35)
```

```
[1] 19.37394
```

```
> convert_RtoS(R=1)
```

```
[1] 27.59808
```

```
> convert_StoR(S=35)
```

```
[1] 1.236537
```

7. finally

This vignette was made with Sweave ([Leisch 2002](#)).

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Affiliation:

Karline Soetaert
 Centre for Estuarine and Marine Ecology (CEME)
 Netherlands Institute of Ecology (NIOO)
 4401 NT Yerseke, Netherlands
 E-mail: k.soetaert@nioo.knaw.nl
 URL: <http://www.nioo.knaw.nl/ppages/ksoetaert>

Thomas Petzoldt

Institut für Hydrobiologie
Technische Universität Dresden
01062 Dresden, Germany
E-mail: thomas.petzoldt@tu-dresden.de
URL: <http://tu-dresden.de/Members/thomas.petzoldt/>

Filip Meysman
Centre for Estuarine and Marine Ecology (CEME)
Netherlands Institute of Ecology (NIOO)
4401 NT Yerseke, Netherlands
E-mail: f.meysman@nioo.knaw.nl