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 2009a).

2. Constants and datasets

2.1. Physical constants

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

```
> 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/s2        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    m3                  total volume of the oceans
3    VolSurf 1.81e+16    m3         volume of the surface ocean (0-50m)
4    VolDeep 9.44e+17    m3           volume of the deep ocean (>1200m)
5       Area 3.58e+14    m2                    total area of the oceans
6     AreaIF 3.32e+14    m2    annual mean ice-free area of the oceans
7    AreaAtl  7.5e+13    m2         area of the Atlantic ocean, >45dgS
8    AreaPac 1.51e+14    m2          area of the Pacific ocean, >45dgS
9    AreaInd  5.7e+13    m2           area of the Indian ocean, >45dgS
10  AreaArct  9.6e+12    m2                    area of the Arctic ocean
11  AreaEncl  4.5e+12    m2 area of enclosed seas (e.g. Mediterranean)
12     Depth     3690     m                    mean depth of the oceans
13 RiverFlow  3.7e+13 m3/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):

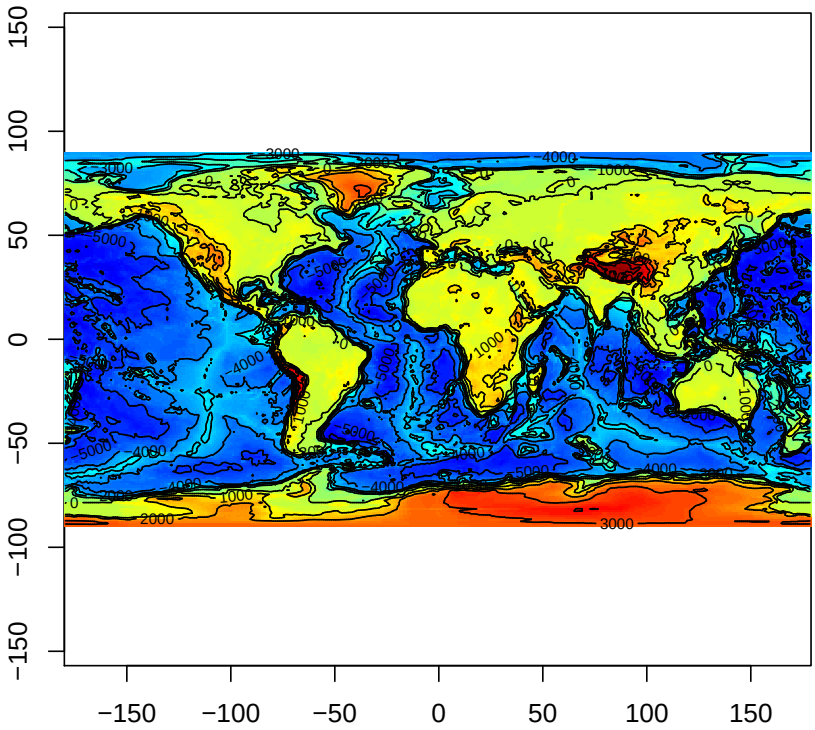

Figure 1: Image plot of ocean bathymetry - see text for R-code

```
> 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. Surface of 1 dg by 1 dg grid cells of the earth

Function `earth_surf` estimates the surface (m^2) of the bathymetric grid cells of 1dg by 1dg, based on their latitude.

We use it to estimate the surface of the earth; the true surface is 510072000 km^2:

```
> SURF <- outer(X=Bathymetry$x,
+                Y=Bathymetry$y,
+                FUN <- function(X,Y) earth_surf(Y,X))
> sum(SURF)
```

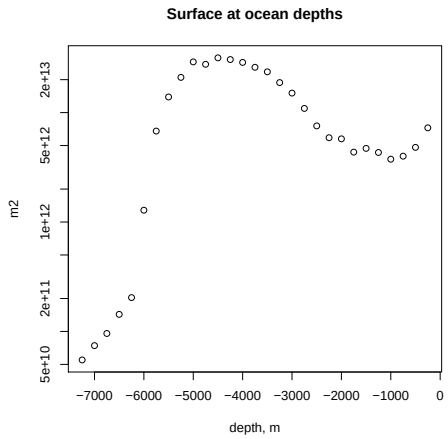

Figure 2: Earth surface at certain ocean depths - see text for R-code

```
[1] 5.100718e+14
```

Similarly, we can estimate the surface and volume of the oceans; it should be $3.58e^{14}$ and $1.34e^{+18}$ respectively.

```
>  sum(SURF*(Bathymetry$z<0))

[1] 3.618831e+14

> - sum(SURF*Bathymetry$z*(Bathymetry$z<0))

[1] 1.336255e+18
```

Combined with the dataset `Bathymetry`, function `earth_surf` allows to estimate the total earth surface at certain water depths:

```
> SurfDepth <- vector()
> dseq <- seq(-7500,-250,by=250)
> for (i in 2:length(dseq)) {
+   ii <- which (Bathymetry$z>dseq[i-1]&Bathymetry$z<=dseq[i])
+   SurfDepth[i-1]<-sum(SURF[ii])
+ }

> plot(dseq[-1],SurfDepth, xlab="depth, m", log="y",
+      ylab = "m2", main = "Surface at ocean depths")
```

2.5. AtomicWeight

Dataset `AtomicWeight` holds the atomic weight of most chemical elements according to the IUPAC table (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 (see also `molweight`).

```
> AtomicWeight
```

	Number	Name	Symbol	Weight	Footnotes
1	1	hydrogen	H	1.00794(7)	gmr
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	europium	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                      *
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      8 oxygen      O 15.9994(3)        gr
```

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

```
[1] 18.01528
```

2.6. 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()
```

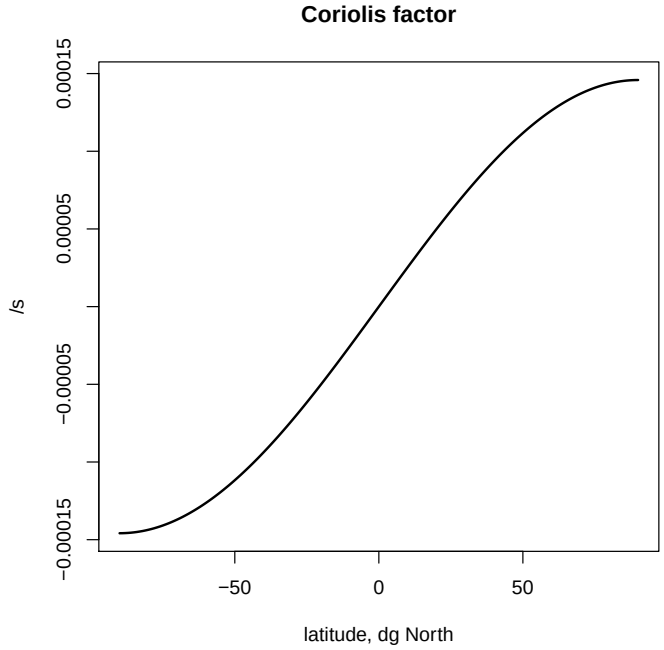

Figure 3: The Coriolis function

```
        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         CO2         N2O          H2          Xe          CO
1.7450e-06 3.6500e-04 3.1400e-07 5.5000e-07 8.7000e-08 5.0000e-08
        O3
1.0000e-08
```

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

```
[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 $\omega = 7.292e^{-5}$radians $\sec^{-1}$

```
> 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

       H2O       O2      CO2       H2      CH4       DMS       He       Ne
1 1.478897 1.570625 1.241991 3.429952 1.198804 0.8770747 5.186823 2.749411
        Ar       Kr        Xe        Rn       N2      H2S      NH3
1 1.554712 1.166917 0.9126865 0.8079991 1.190863 1.180685 1.467438
        NO      N2O       CO      SO2       OH         F       Cl       Br
1 1.500764 1.164872 1.195000 1.035560 3.543847 0.9577852 1.354384 1.391657
         I      HCO3       CO3     H2PO4     HPO4       PO4       HS
1 1.364436 0.7693272 0.6126977 0.6168857 0.495435 0.3991121 1.214088
       HSO3       SO3      HSO4      SO4       IO3      NO2      NO3
1 0.8836584 0.7379176 0.8874275 0.700226 0.7069267 1.278582 1.283189
         H        Li        Na         K       Cs       Ag      NH4
1 6.510175 0.6738419 0.8807268 0.8807268 1.385375 1.106039 1.314599
         Ca        Mg        Fe        Mn        Ba        Be        Cd
1 0.5264259 0.4682133 0.4657005 0.4610938 0.5611859 0.3911549 0.4682133
         Co        Cu        Hg        Ni        Sr      Pb        Ra
1 0.4682133 0.4824524 0.5653738 0.4447608 0.5214003 0.62233 0.5775189
         Zn        Al        Ce        La        Pu    H3PO4      BOH3
1 0.4669569 0.4497863 0.4116759 0.4037188 0.3777535 0.555835 0.7602404
       BOH4    H4SiO4
1 0.6652104 0.6882134

> diffcoeff(t=10)$O2

[1] 1.539783e-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 ($gm^{-1}sec^{-1}$). The formula is valid for $0 < t < 30$ and $0 < S < 36$.

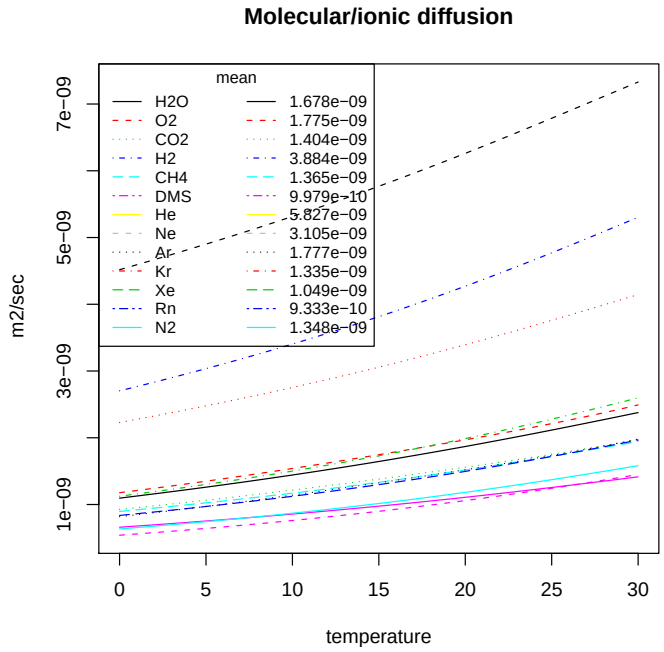

Figure 4: Molecular diffusion coefficients as a function of temperature

```
> 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 in mgL^{-1}. Method APHA (American Public Health Association 1992) is the standard formula in Limnology, the method after Weiss (1970) the traditional formula used in marine sciences.

```
> gas_O2sat(t = 20)

[1] 7.374404

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

Conversion to $mmolm^{-3}$ can be done via:

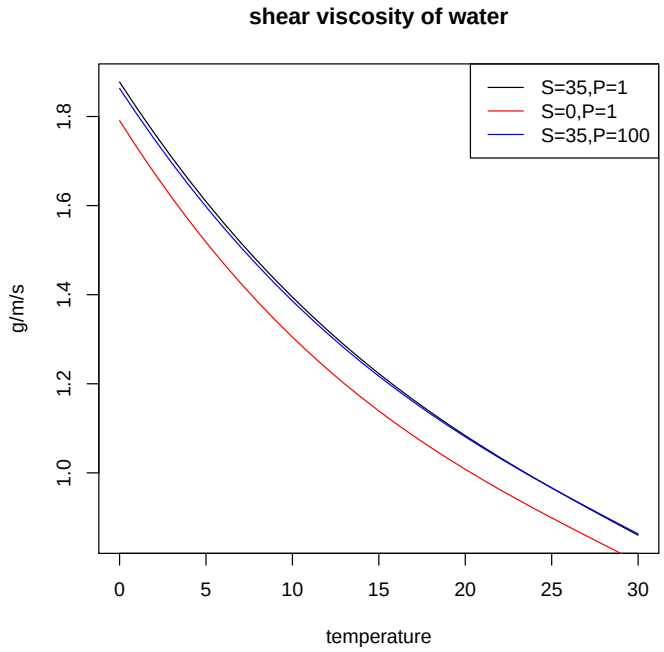

Figure 5: Shear viscosity of water as a function of temperature

```
> gas_O2sat(S=35, t=20)*1000/molweight("O2")

      O2
230.4588

>   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",
+         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 (in mmolm^{-3}) 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)
```

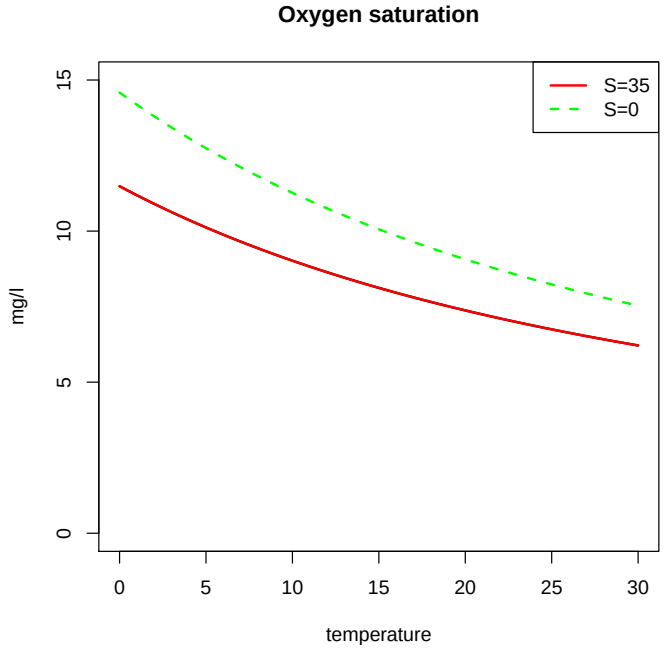

Figure 6: Oxygen saturated concentration as a function of temperature, and for different salinities

```
> #
> mf  <-par(mfrow=c(2,2))
> #
> gs  <-gas_solubility(t=Temp)
> species   <- c("CCl4","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,
```

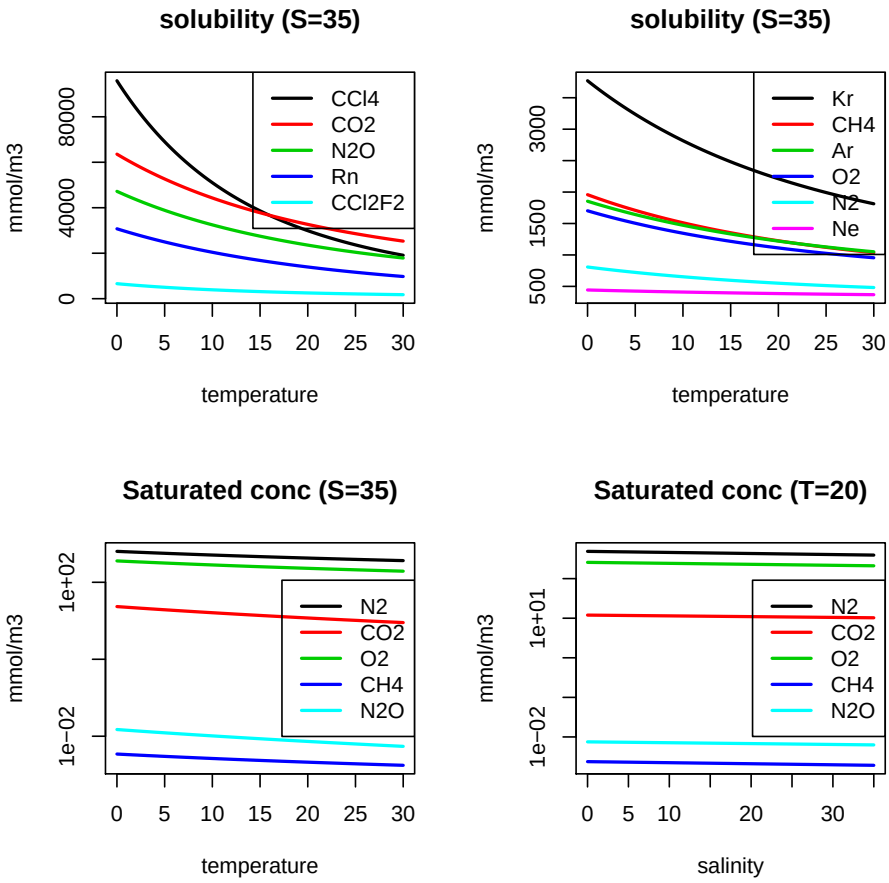

Figure 7: Saturated concentrations and solubility as a function of temperature and salinity, and for different species

```
+      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 pessure 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

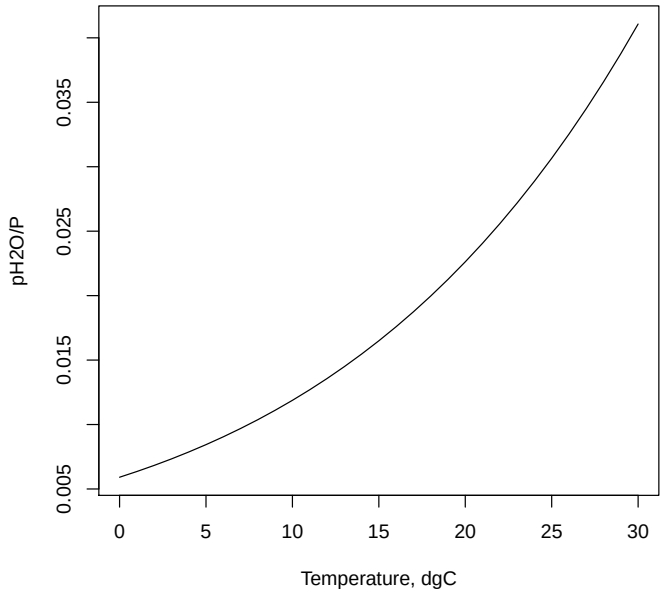

Figure 8: Partial pressure of water in saturated air as a function of temperature

velocity calculation (`gas_transfer`). The latter also depends on wind velocity (as measured 10 metres above sea level).

```
> 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 McGills 1999"))
```

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:

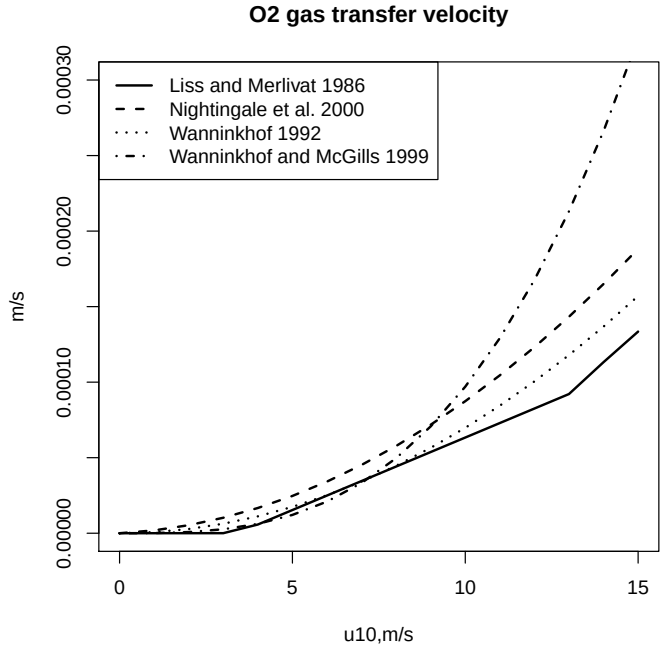

Figure 9: Gas transfer velocity for seawater

```
> 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. Two salinity scales

Millero, Feistel, Wright, and McDougall (2008) and McDougall, Jackett, and Millero (2009b) provide a function to derive absolute salinity (expressed in g kg^{-1}) from measures of practical salinity. Absolute salinity is to be used as the concentration variable entering the thermodynamic functions of seawater (see next section).

The conversion between salinity scales is done with functions:

- `convert_AStoPS` from absolute to practical salinity and
- `convert_PStoAS` from practical to absolute salinity

For example:

```
> convert_AStoPS(S=35)

[1] 34.83573

> convert_PStoAS(S=35)

[1] 35.16504
```

These functions have as extra arguments the gauge pressure (`p`), latitude (`lat`) and longitude (`lon`), and -optional- the dissolved Si concentration (`DSi`) and the ocean (`Ocean`).

When one of these arguments are provided, they also correct for inconsistencies due to local composition anomalies.

When `DSi` is not given, the correction makes use of a conversion table that estimates the salinity variations as a function of present-day local seawater composition. The conversion in Ruses the FORTRAN code developed by D. Jackett (http://www.marine.csiro.au/~jackett/TEOS-10/).

The correction factors are in a data set called `sw_sfac`, a list with the properties used in the conversion functions.

Below we first convert from practical to absolute salinity, for different longitudes, and then plot the correction factors as a function of latitude and longitude and at the seawater surface (i.e. for `p=0`)[1].

```
> convert_PStoAS(S=35,lat=-10,lon=0)

[1] 35.16525

> convert_PStoAS(S=35,lat=0,lon=0)

[1] 35.16558

> convert_PStoAS(S=35,lat=10,lon=0)

[1] 35.16504

> convert_PStoAS(S=35,lat=-10,lon=0)

[1] 35.16525

> convert_PStoAS(S=35,lat=-10, DSi=1:10, Ocean="Pacific")
```

[1] Before plotting, the negative numbers in the salinity anomaly table `sw_sfac` are converted to `NA` (not available). In the data set, numbers not available are denoted with `-99`.

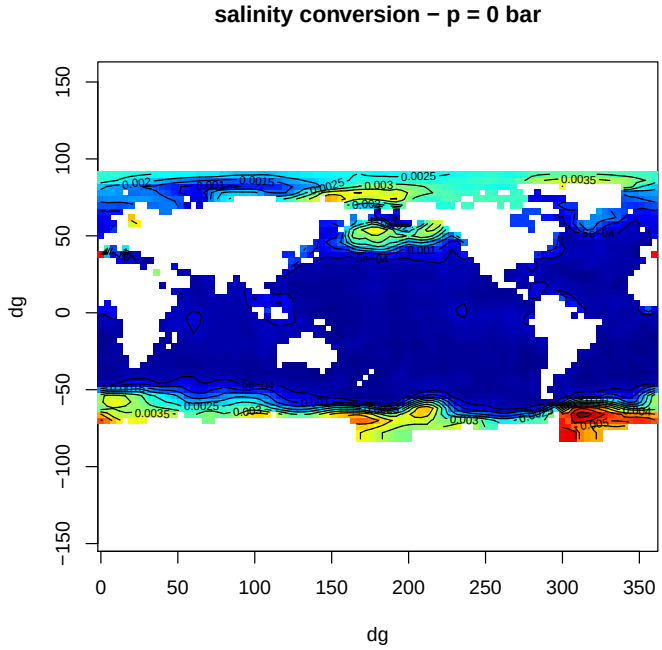

Figure 10: Salinity anomaly to convert from practical to absolute salinity and vice versa

```
 [1] 35.16513 35.16523 35.16532 35.16541 35.16550 35.16560 35.16569
 [8] 35.16578 35.16588 35.16597
```

```
> dsal <- t(sw_sfac$del_sa[1,,])
> dsal [dsal < -90]<-NA

> image(sw_sfac$longs, sw_sfac$lats, dsal, col=femmecol(100),
+       asp=TRUE, xlab="dg", ylab="dg",
+       main="salinity conversion - p = 0 bar")
> contour(sw_sfac$longs, sw_sfac$lats, dsal, asp=TRUE, add=TRUE)
```

5.3. 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 from Feistel (2008) use the absolute salinity scale (Millero *et al.* 2008), while the UNESCO polynomial uses practical salinity.

```
> 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,method="UNESCO")

 [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
```

The precision of the calculations can be assessed by comparing them to some test values:

```
> t  <-  25.5
> p  <- 1023/10  # pressure in bar
> S  <- 35.7
> sw_alpha(S,t,p)               -0.0003098378393192645

[1] 1.167598e-13

> sw_beta(S,t,p)                -0.0007257297978386655

[1] 2.555374e-12

> sw_cp(S,t,p)                  -3974.42541259729

[1] -5.945121e-07

> sw_tpot(S,t,p)                -25.2720983155409

[1] 5.203708e-05

> sw_dens(S,t,p)                -1027.95249315662

[1] 9.467044e-08

> sw_enthalpy(S,t,p)            -110776.712408975

[1] -2.050104e-05

> sw_entropy(S,t,p)             -352.81879771528

[1] -9.916204e-08

> sw_kappa(S,t,p)               -4.033862685464779e-6

[1] -1.068645e-15
```

```
> sw_kappa_t(S,t,p)              -4.104037946151349e-6

[1] -1.011721e-15

> sw_svel(S,t,p)                 -1552.93372863425

[1] 1.341919e-07
```

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))
```

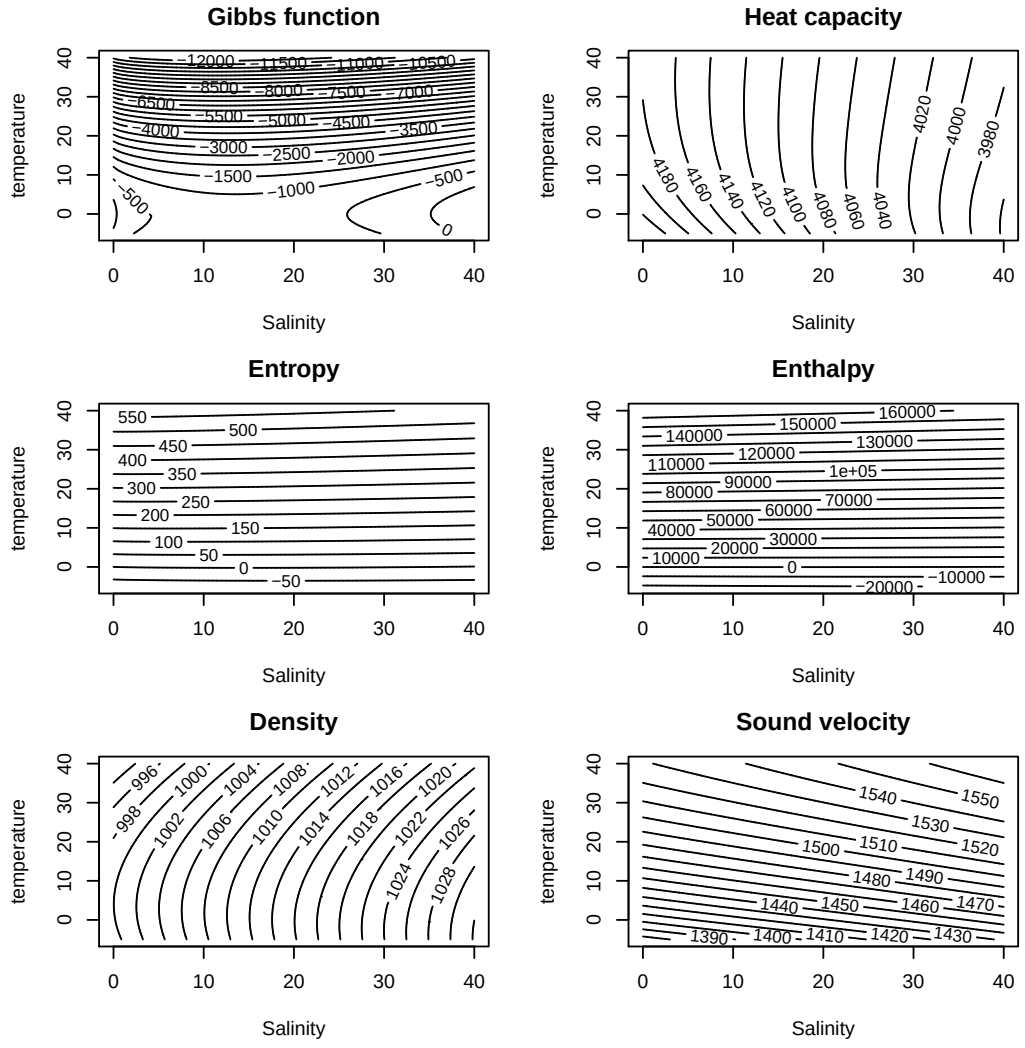

Figure 11: Seawater properties as a function of salinity and temperature - see text for R-code

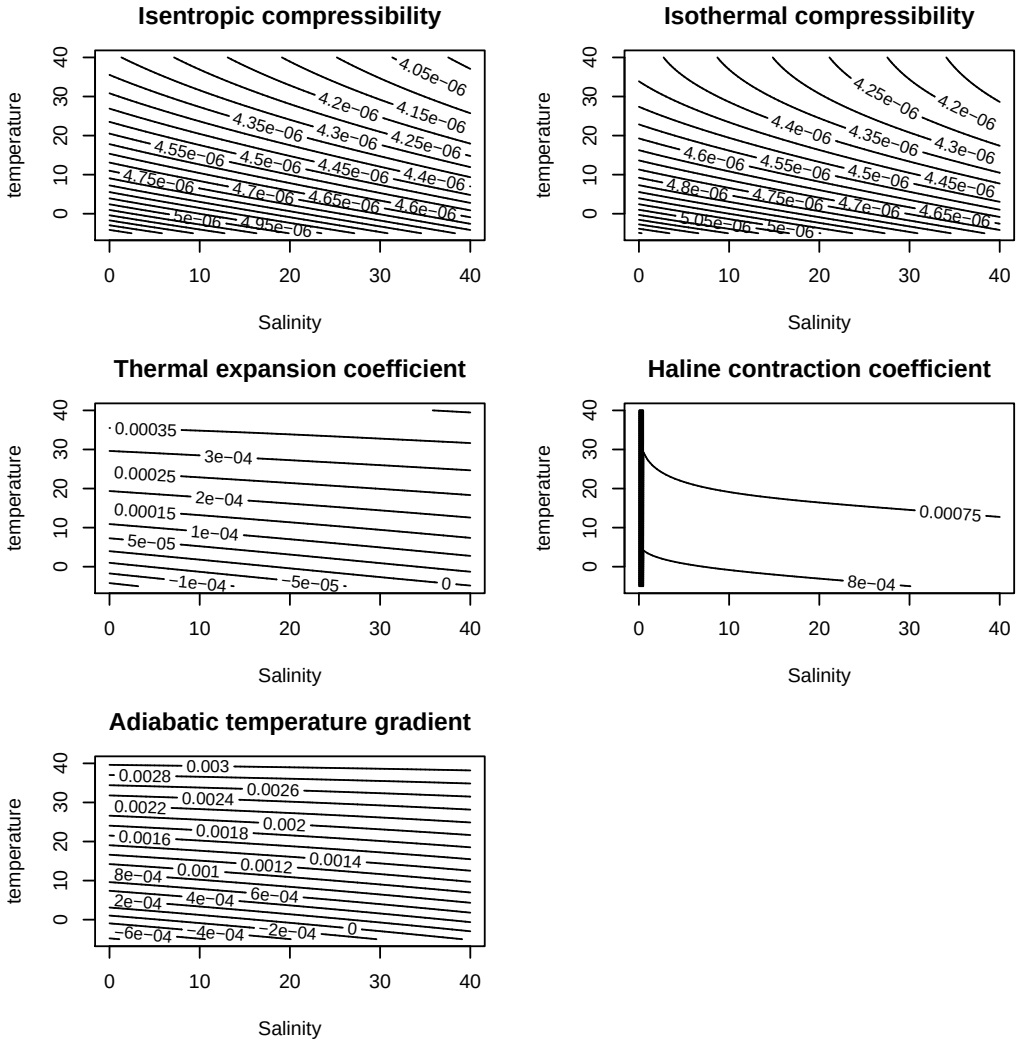

Figure 12: Seawater properties as a function of salinity and temperature - continued - see text for R-code

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. The function is based ona lexical parser and the IUPAC table of atomic weights, so it should be applicable to arbitrary chemical formulae:

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

       CO3
0.01666419

> 1/molweight("HCO3")

      HCO3
0.01638892

> 1/molweight(c("C2H5OH", "CO2", "H2O"))

    C2H5OH        CO2        H2O
0.02170683 0.02272237 0.05550844

> molweight(c("SiOH4", "NaHCO3", "C6H12O6", "Ca(HCO3)2", "Pb(NO3)2", "(NH4)2SO4"))

    SiOH4    NaHCO3   C6H12O6 Ca(HCO3)2  Pb(NO3)2 (NH4)2SO4
 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 or the molar volume of an ideal gas.

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

   ideal
24.46536
```

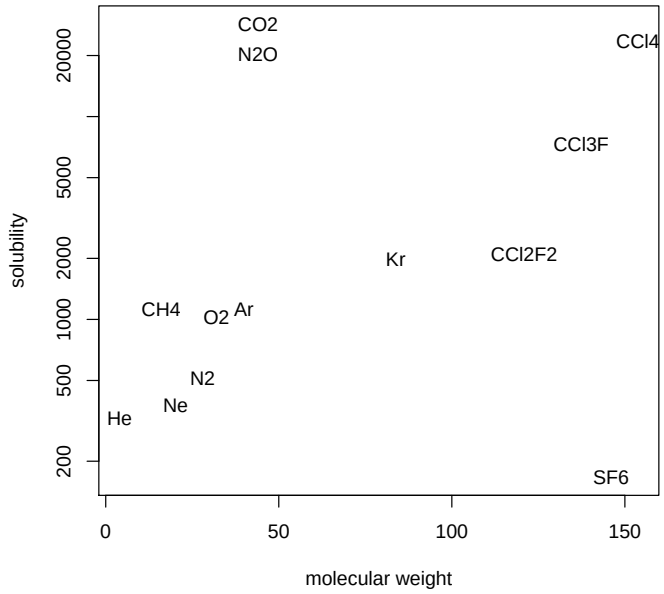

Figure 13: Gas solubility as a function of molecular weight see text for R-code

```
> 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

Function `convert_T` converts between 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/users/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