

R-package **marelac** : utilities for the marine and lacustrine sciences

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Abstract

Rpackage **marelac** ([Soetaert and Meysman 2008](#)) contains datasets, chemical and physical constants and functions, routines for unit conversion, and other utilities useful for marine (oceans, seas) and lacustrine (lakes) sciences.

The package also contains lecture notes for novice R-users.

Keywords: marine, lacustrine, science, datasets, constants, conversion, R.

1. Introduction

Whereas R is predominantly used as a statistical package, it is also very well suited for scientific computing, e.g. ([Soetaert and Herman 2009](#)).

R-package **marelac** has been designed as a tool for use by scientists working in the marine and lacustrine sciences.

It contains:

- data sets. These are mainly used in the lecture notes "Using R for scientific computing" ([Soetaert 2008](#)), written as an introductory course for students that follow our course in ecological modelling, taught at the universities of Ghent and Brussels (by Filip Meysman and myself).
- chemical and physical constants, e.g. atomic weights, gas constants.
- conversion factors, e.g. gram to mol to liter conversions.
- functions, e.g. to estimate concentrations of conservative substances as a function of salinity, ...

2. data sets

To date, there are 3 datasets

2.1. Bathymetry

This dataset, as used by ([Andersson, Wijsman, Herman, Middelburg, Soetaert, and Heip](#)

2004) contains elevations, in metres of the world at 1 dg intervals. Positive values are altitudes, negative values are ocean depths.

Used to demonstrate R's image and contouring capabilities:

```
> par(mfrow=c(2,1))
> par(mar=c(2,2,2,2))
> image(Bathymetry$x,Bathymetry$y,Bathymetry$z,col=femmecol(100),
+       asp=TRUE,xlab="dg",ylab="dg")
> contour(Bathymetry$x,Bathymetry$y,Bathymetry$z,asp=TRUE,add=TRUE)
> # remove land and only contours.
> zz      <- Bathymetry$z
> zz[zz>0]<-0
> contour(Bathymetry$x,Bathymetry$y,zz,asp=TRUE)
> par(mfrow=c(1,1))
> par(mar=c(5.1,4.1,4.1,2.1))
```

2.2. SCOC

This literature dataset, as compiled by (Andersson *et al.* 2004) contains 584 measurements of sediment community oxygen consumption rates, as a function of water depth, and performed in deep-water sediments, either by in situ incubations or via modelling of oxygen microprofiles.

These SCOC values are good estimates of organic matter deposition to the ocean floor. It is used to demonstrate the order-of-magnitude of deposition flux with water depth.

A log-log regression with water depth explains the data quite well.

```
> plot(SCOC[,1],SCOC[,2],log="xy",xlab="water depth, m",ylab="",
+       main="SCOC, mmol O2/m2/d",pch=16,xaxt="n",yaxt="n",cex.main=1)
> axis(1,at=c(0.5,5,50,500,5000),labels=c("0.5","5","50","500","5000"))
> axis(2,at=c(0.1,1,10,100),labels=c("0.1","1","10","100"))
> l1 <- lm(log(SCOC[,2]) ~ log(SCOC[,1]))
> rr <- summary(l1)$r.squared
> A <- exp(coef(l1)[1])
> B <- (coef(l1)[2])
> curve(A*x^B,add=TRUE,lwd=2)
> AA <- round(A*100)/100
> BB <- round(B*100)/100
> expr <- substitute(y==A*x^B,list(A=AA,B=BB))
> text(1,.1,expr,adj=0)
> expr2 <- substitute(r^2==rr,list(rr=round(rr*100)/100))
> text(1,0.04,expr2, adj=0)
```

2.3. Zoogrowth

This literature dataset, as compiled by (Hansen, Bjornsen, and Hansen 1997) contains 84 measurements of maximal growth rates as a function of organism volume and temperature

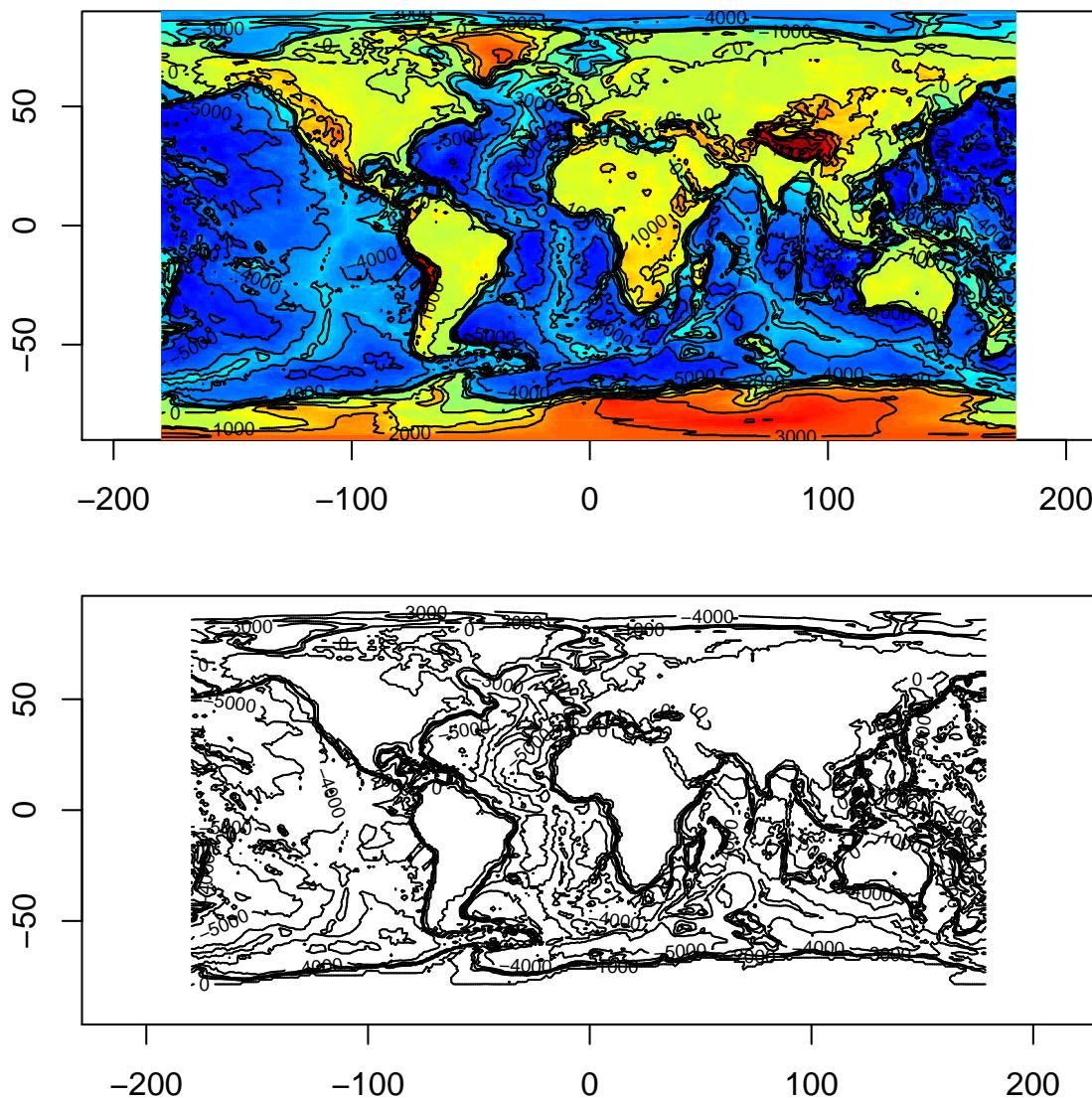


Figure 1: Bathymetry and hypsometry of the world's ocean.

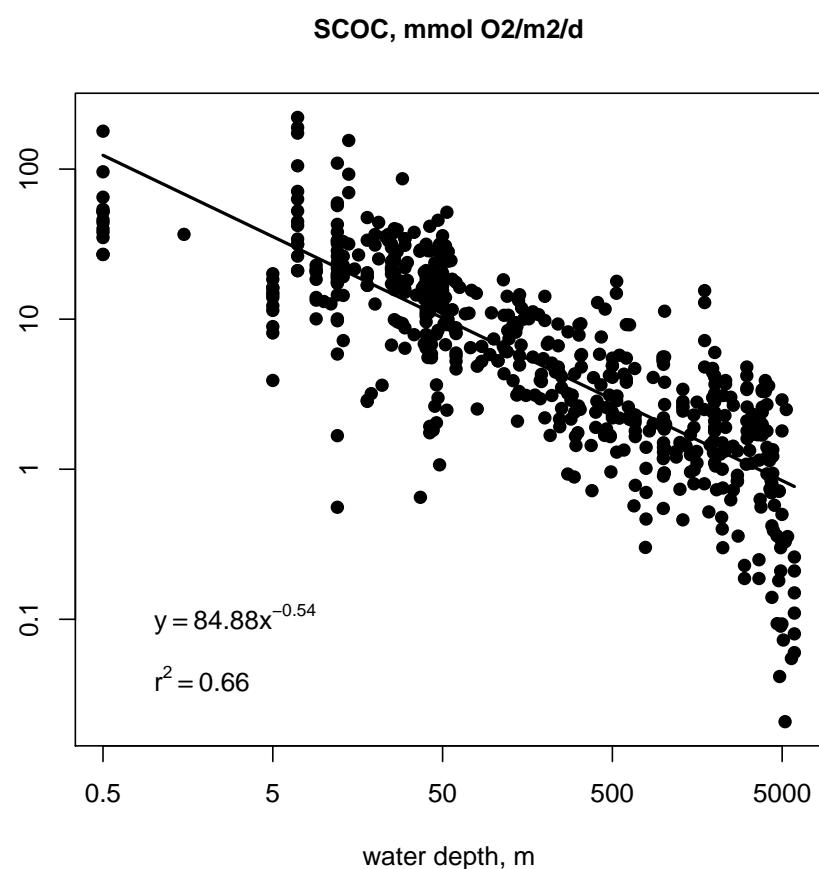


Figure 2: Sediment community oxygen consumption rate as a function of water depth

for various species of zooplankton. The maximal growth rates were obtained from laboratory experiments.

It is used to demonstrate R's graphical capabilities.

```
> plot(Zoogrowth$Volume,Zoogrowth$Mumax,log="xy",
+       xlab="zooplankton volume, micrometer ^ 3",
+       ylab="maximal growth rate, /hr",main="Zoogrowth",cex=2,
+       pch=(15:20)[Zoogrowth$Group],col=(1:6)[Zoogrowth$Group])
> legend("topright",legend=levels(Zoogrowth$Group),col=1:6,pch=15:20)
> l1 <- lm(log(Zoogrowth[,2]) ~ log(Zoogrowth[,1]))
> rr <- summary(l1)$r.squared
> A <- exp(coef(l1)[1])
> B <- (coef(l1)[2])
> curve(A*x^B,add=TRUE,lwd=2)
> AA <- round(A*100)/100
> BB <- round(B*100)/100
> expr <- substitute(y==A*x^B,list(A=AA,B=BB))
> text(100,.0035,expr,adj=0)
> expr2 <- substitute(r^2==rr,list(rr=round(rr*100)/100))
> text(100,0.002,expr2, adj=0)
```

2.4. Nemaspec

Dataset of (Soetaert, Heip, and Vincx 1991) with nematode species densities in Mediterranean deep-sea sediments, at depths ranging from 160 m to 1220 m.

The densities are expressed in individuals per 10 cm².

Nematodes are small free-living worms (<1mm long), generally very abundant in all aquatic sediments.

This data set is used in the lecture notes, to estimate diversity indices.

As an example here, we use it to draw species-dominance curves.

```
> head(Nemaspec)
```

	SPECIES	M160a	M160b	M280a	M280b	M530a	
1	Acantholaimus	0	6.580261	0.000000	1.120782	1.315487	
2	Acantholaimus elegans	0	0.000000	1.439706	0.000000	3.956836	
3	Acantholaimus iubilus	0	0.000000	0.000000	0.000000	0.000000	
4	Acantholaimus M1	0	5.919719	0.000000	3.628518	0.000000	
5	Acantholaimus M10	0	0.000000	0.000000	1.120782	0.000000	
6	Acantholaimus M11	0	0.000000	0.000000	0.000000	0.000000	
	M530b	M820a	M820b	M990a	M990b	M1220a	M1220b
1	1.727387	3.417313	3.748096	2.447545	3.728838	4.369345	4.787512
2	0.000000	0.000000	2.198407	5.080900	5.330997	3.644567	3.494481
3	1.193131	0.000000	0.000000	1.270450	1.372789	0.000000	0.000000
4	1.193131	1.155307	0.000000	5.052036	6.225598	0.000000	1.166825

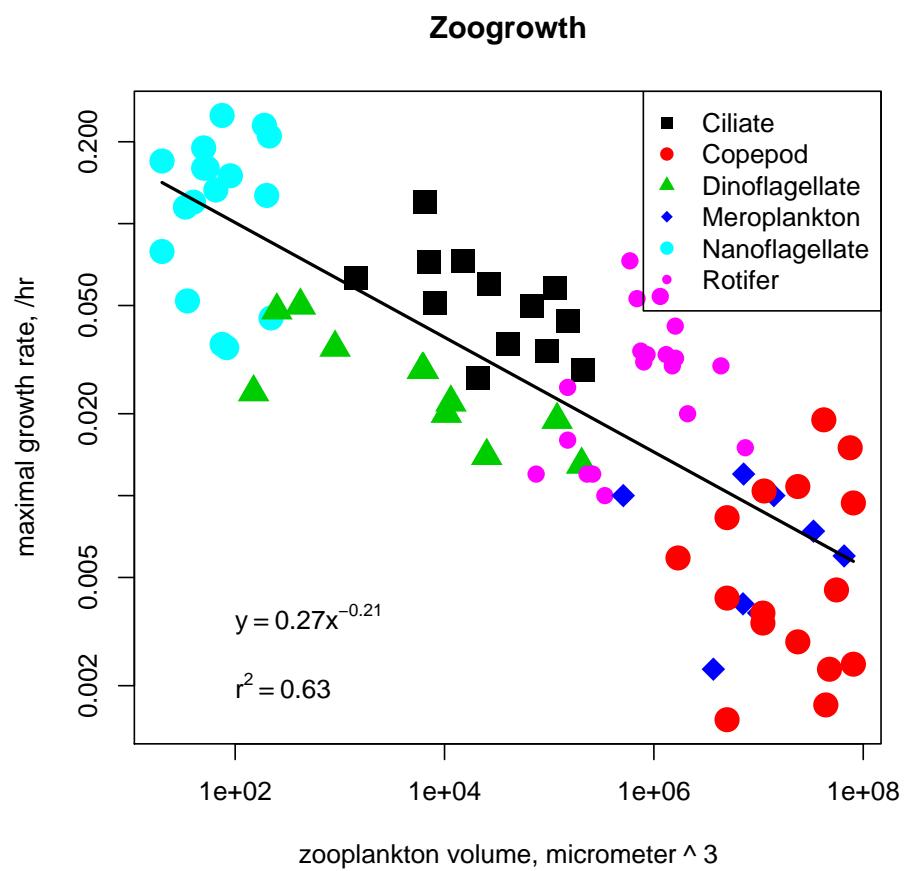


Figure 3: maximal growth rates of zooplankton as a function of body volume

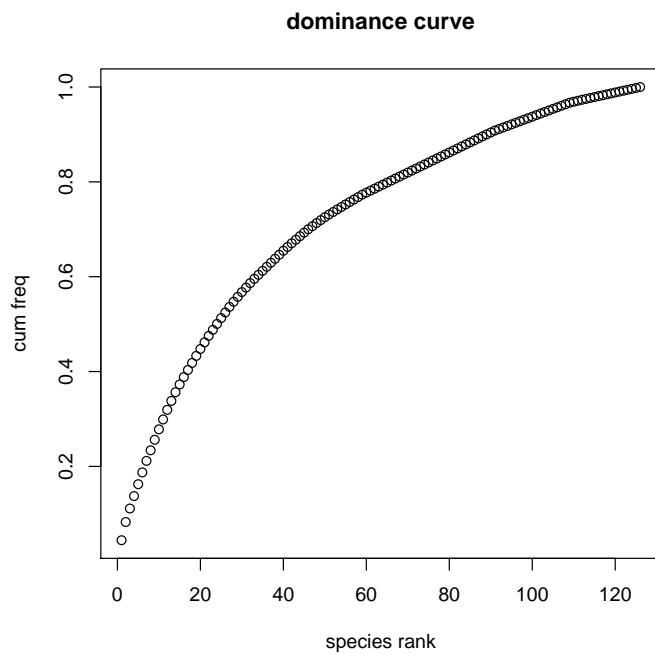


Figure 4: Species dominance curves for a sediment at 160 m depth in the Mediterranean Sea

```

5 0.000000 0.000000 0.000000 0.000000 0.000000 1.115981 0.000000
6 0.000000 0.000000 0.000000 0.000000 2.285694 0.000000 0.000000

> # select densities of species present in M160b
> st160b<-data.frame(Nemaspec$SPECIES,dens=Nemaspec$M160b)
> st160b<-st160b[st160b$dens!=0,]

> plot(cumsum(rev(sort(st160b$dens)/sum(st160b$dens))),main="dominance curve",
+       xlab="species rank",ylab="cum freq")

```

3. constants

3.1. AtomicWeight

```

> AtomicWeight

      H     Li      B      C      N      O      F      Na      Mg
1 1.00794 6.941 10.811 12.011 14.0067 15.9994 18.9984 22.98977 24.305
      Si      P      S     Cl      K      Ca      Mn      Fe      Cu
1 28.0855 30.9737 32.066 35.4527 39.0983 40.078 54.938 55.847 63.546
      Zn      Br      Sr      Ag      I      Ba      La
1 65.392 79.905 87.52 107.868 126.9 137.33 138.9055

```

```
> AtomicWeight$H
[1] 1.00794
> (W_H2O<- with (AtomicWeight, 2*H + 0))
[1] 18.01528
```

3.2. Constants

```
> 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    atm     101325       Pa    pressure conversion
6    bar      1e+05       Pa    pressure conversion
7     B1  1.3806504e-23       J/K    Boltzmann constant
8     B2  8.617343e-05       eV/K    Boltzmann constant
```

4. functions

4.1. coriolis

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

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

4.2. heat capacity

Estimates the heat capacity of seawater, using the UNESCO 1983 polynomial ([Fofonoff and Millard 1983](#))

```
> cp(S=40,T=1:20)
[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
```

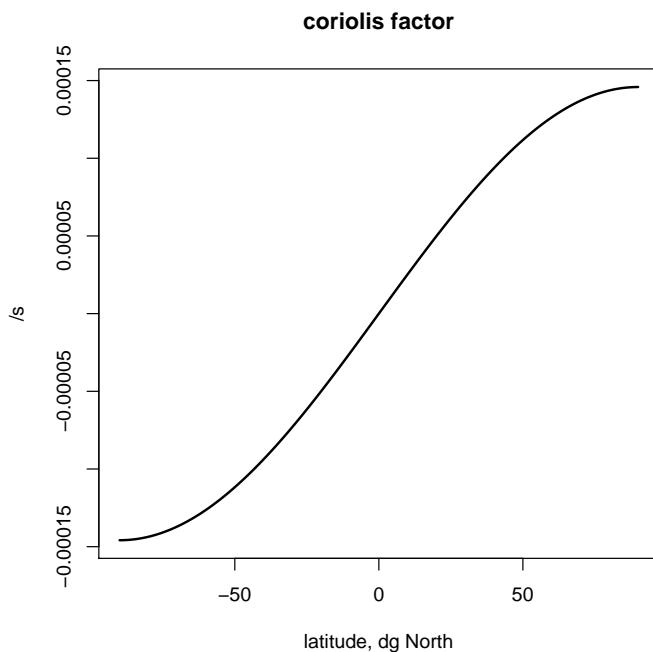


Figure 5: The coriolis function

4.3. molecular diffusion coefficients

Calculates molecular and ionic diffusion coefficients (cm²/hour), for several species at given salinity (S) temperature (T) and pressure (P).

Based on the code "CANDI" by Bernie Boudreau ([Boudreau 1996](#)).

```
> diffcoeff(S=15,T=15)*24 # cm2/day

      O2      CO2      NH3      H2S      CH4      HC03      C03
1 1.429208 1.205458 1.422550 1.229481 1.133012 0.7693272 0.6126977
      NH4      HS      NO3      H2PO4     HP04      P04       H
1 1.314599 1.214088 1.283189 0.6168857 0.495435 0.3991121 6.510175
      OH      Ca      Mg      Fe      Mn      SO4      H3PO4
1 3.543847 0.5264259 0.4682133 0.4657005 0.4610938 0.700226 0.5558346
      BOH3     BOH4     H4SiO4
1 0.7602399 0.6652099 0.6882129

> diffcoeff(T=10)$O2
[1] 0.04930624

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

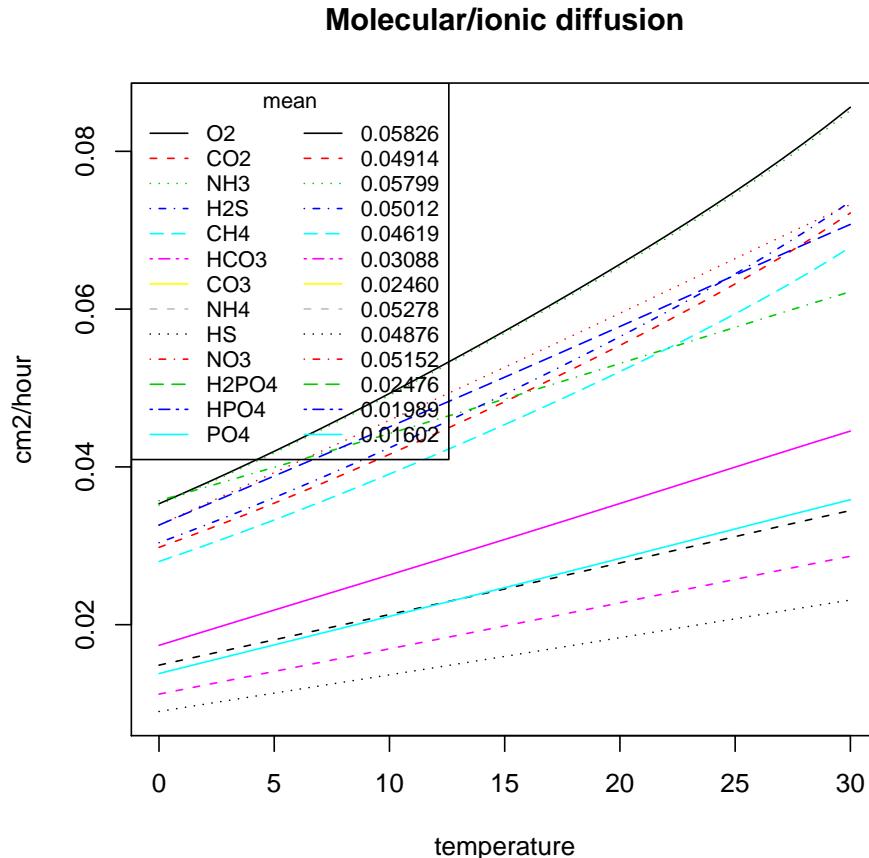


Figure 6: molecular diffusion coefficients as a function of temperature

```
> matplot(0:30,difftemp,xlab="temperature",ylab="cm2/hour",
+           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)))
```

4.4. molecular diffusion coefficients

Calculates the shear viscosity of water, in centipoise. Valid for 0 < T < 30 and 0 < S < 36.

Based on the code "CANDI" by Bernie Boudreau ([Boudreau 1996](#)).

```
> plot(0:30,viscosity(S=35,T=0:30,P=1),xlab="temperature",ylab="centipoise",
+       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"))
```

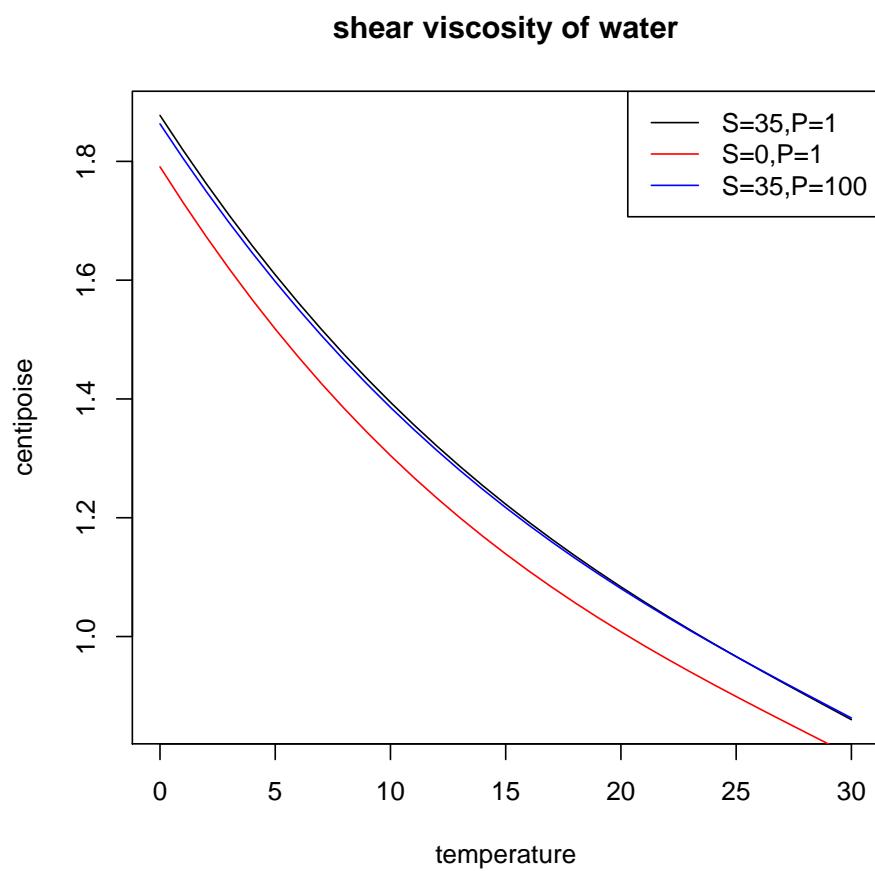


Figure 7: shear viscosity of water as a function of temperature

4.5. Concentration of conservative species in seawater

```
> salconc(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

4.6. Saturated concentration of O₂, N₂ and Ar

```
> satconc(S=35,T=seq(0,20,by=5))
```

	O2	N2	Ar
1	358.9267	633.2110	17.44495
2	310.5971	554.2451	15.13654
3	271.9429	490.5970	13.28185
4	240.5663	438.5412	11.76977
5	214.7383	395.3705	10.51985

5. conversions

5.1. gram, mol, liter conversions

gram to moles

```
> g2mol("CO3")
```

```
[1] 0.01666411
```

```
> g2mol("hCO3")
```

```
[1] 0.01638884
```

```
> g2mol("H")
```

```
[1] 0.9921225
```

liter to moles

```
> 12mol(x=8,a=1.382,b=0.03186,T=0)*1000  
[1] 357.3925  
  
> 12mol(x=1:6)  
[1] 0.04087373 0.08174746 0.12262119 0.16349492 0.20436864 0.24524237
```

molar volume of an ideal gas

```
> mol.vol()  
[1] 24.46559  
  
> mol.vol(T=1:10)  
[1] 22.49620 22.57826 22.66032 22.74237 22.82443 22.90649 22.98855  
[8] 23.07061 23.15266 23.23472
```

molecular weight of a chemical species

```
> mol.weight("CO3")
```

```
[1] 60.0092
```

```
> mol.weight("HCO3")
```

```
[1] 61.01714
```

```
> mol.weight("H")
```

```
[1] 1.00794
```

5.2. salinity and chlorinity

```
> sal2cl(S=35)
```

```
[1] 19.37394
```

6. finally

This vignette is mainly a Sweave ([Leisch 2002](#)) translation of part of the **marelac** help files.

References

- Andersson H, Wijsman J, Herman P, Middelburg J, Soetaert K, Heip C (2004). “Respiration patterns in the deep ocean.” *Geophysical Research Letters*, **31**, LO3304.
- Boudreau B (1996). “A method-of-lines code for carbon and nutrient diagenesis in aquatic sediments.” *Computers and Geosciences*, **22** (5), 479–496.
- Fofonoff P, Millard RJ (1983). *Algorithms for computation of fundamental properties of seawater.*, volume 44. Unesco. 53 pp.
- Hansen P, Bjornsen P, Hansen B (1997). “Zooplankton grazing and growth: Scaling within the 2-2,000-mu m body size range.” *Limnology and Oceanography*, **42**, 687–704.
- Leisch F (2002). “Sweave: Dynamic Generation of Statistical Reports Using Literate Data Analysis.” In W Härdle, B Rönz (eds.), “Compstat 2002 - Proceedings in Computational Statistics,” pp. 575–580. Physica Verlag, Heidelberg. ISBN 3-7908-1517-9, URL <http://www.stat.uni-muenchen.de/~leisch/Sweave>.
- Soetaert K (2008). *using R for scientific computing*. NIOO-CEME, Yerseke.
- Soetaert K, Heip C, Vincx M (1991). “Diversity of nematode assemblages along a mediterranean deep-sea transect.” *Marine Ecology Progress Series*, **75**, 275–282.
- Soetaert K, Herman PMJ (2009). *A Practical Guide to Ecological Modelling. Using Ras a Simulation Platform*. Springer. ISBN 978-1-4020-8623-6.
- Soetaert K, Meysman F (2008). *marelac: Datasets, constants, conversion factors, utilities for the marine and lacustrine sciences*. R package version 1.1.

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