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 Ris 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"))
> ll <- lm(log(SCOC[,2])~ log(SCOC[,1]))
> rr <- summary(ll)$r.squared
> A  <- exp(coef(ll)[1])
> B  <- (coef(ll)[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

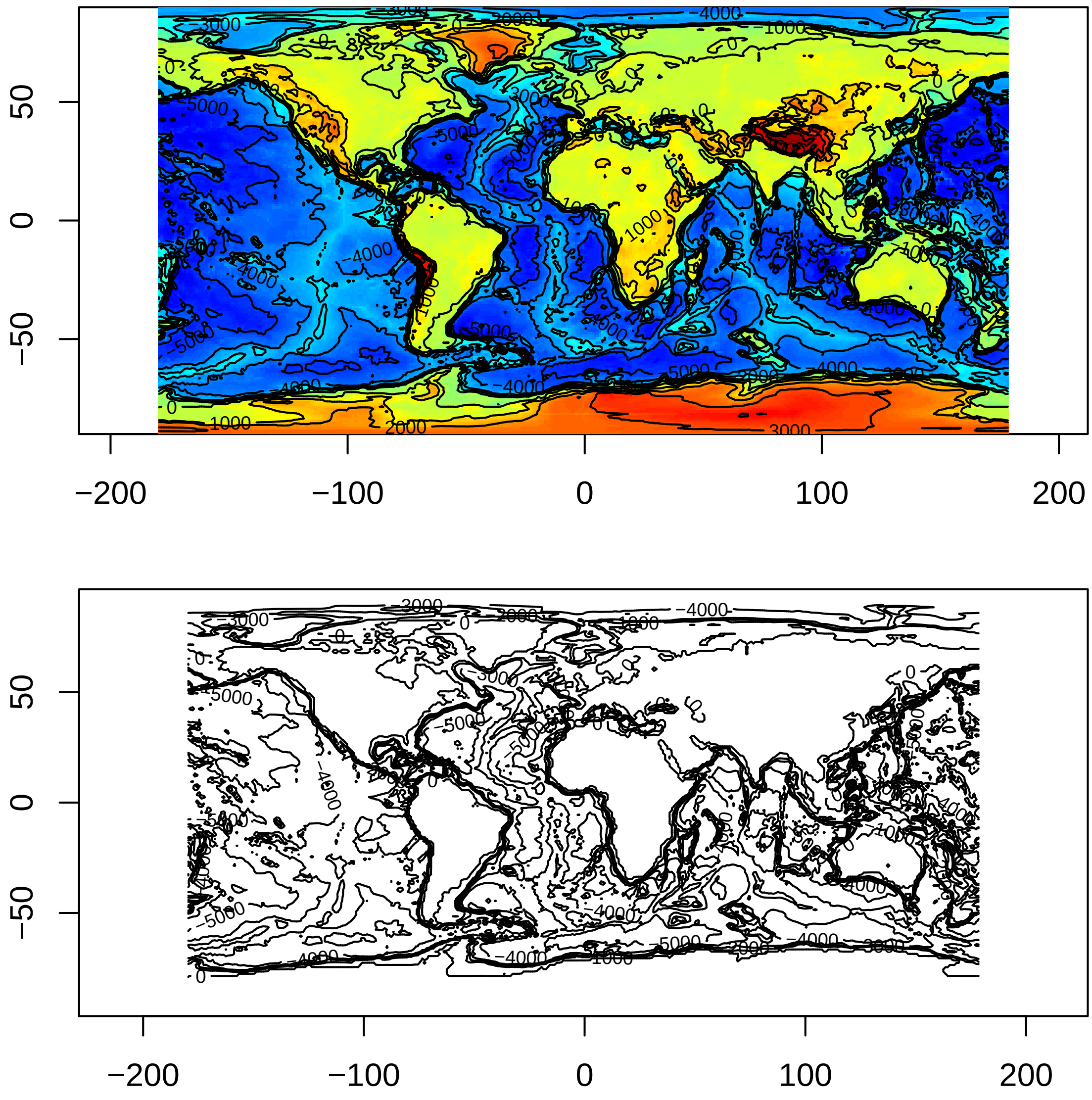

Figure 1: Bathymetry and hypsometry of the world's ocean.

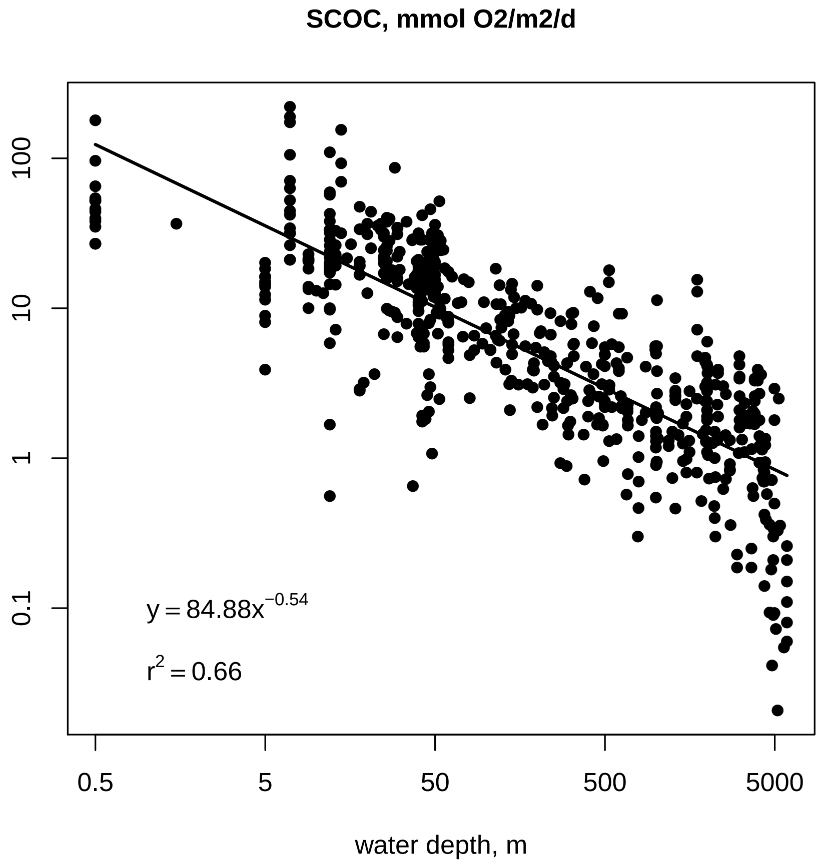

Figure 2: Sediment community oxygen consumption rate as a function of water depth

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$Group),col=1:6,pch=15:20)
> ll <- lm(log(Zoogrowth[,2])~ log(Zoogrowth[,1]))
> rr <- summary(ll)$r.squared
> A  <- exp(coef(ll)[1])
> B  <- (coef(ll)[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
```

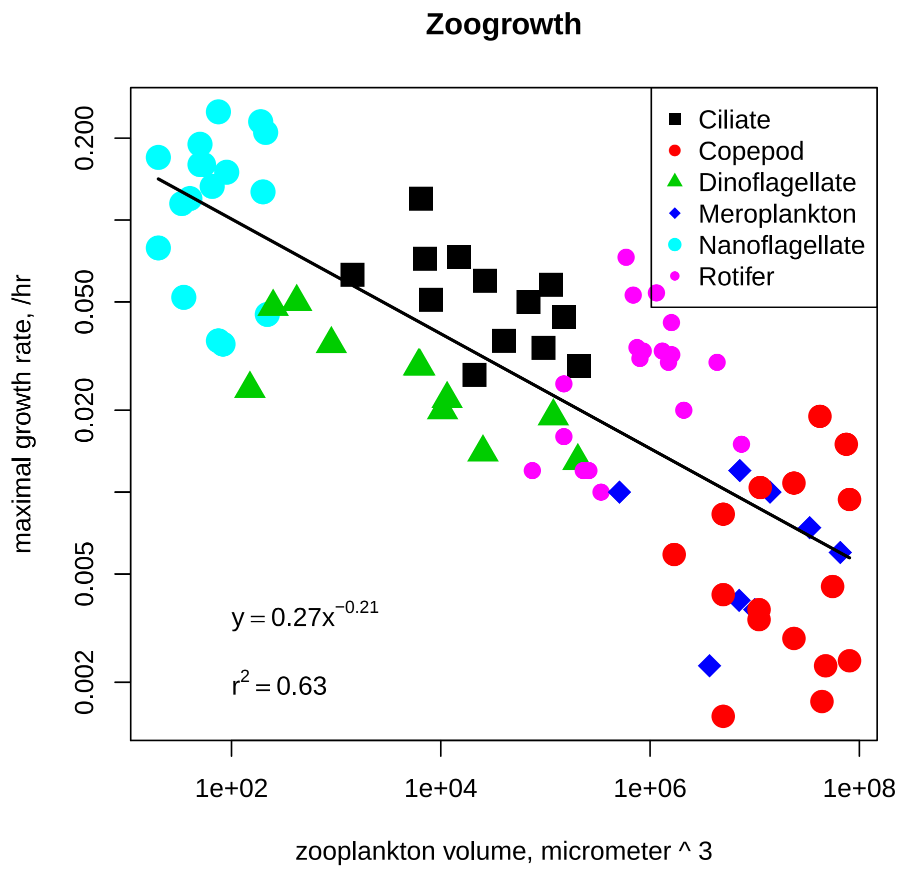

Figure 3: maximal growth rates of zooplankton as a function of body volume

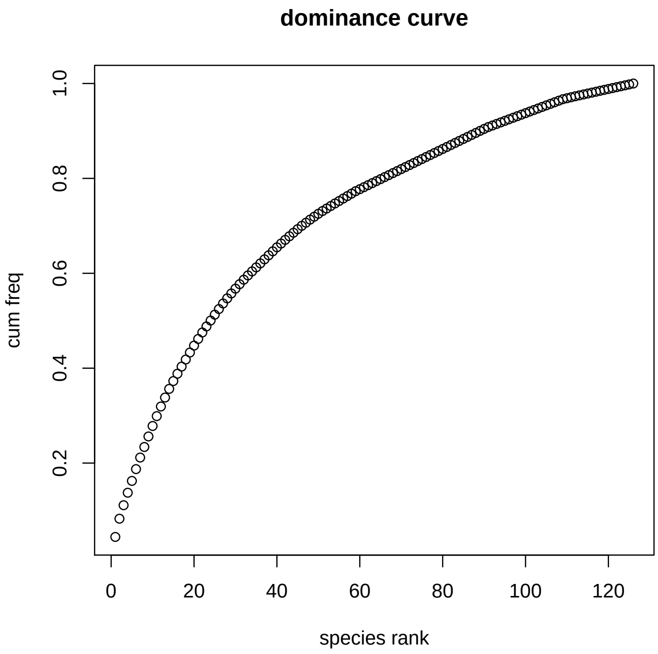

Figure 4: Species dominance curves for a sediment at 160 m depth in the Mediterranean Sea

```
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 + O))

[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(lat), where omega=7.292e-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
```

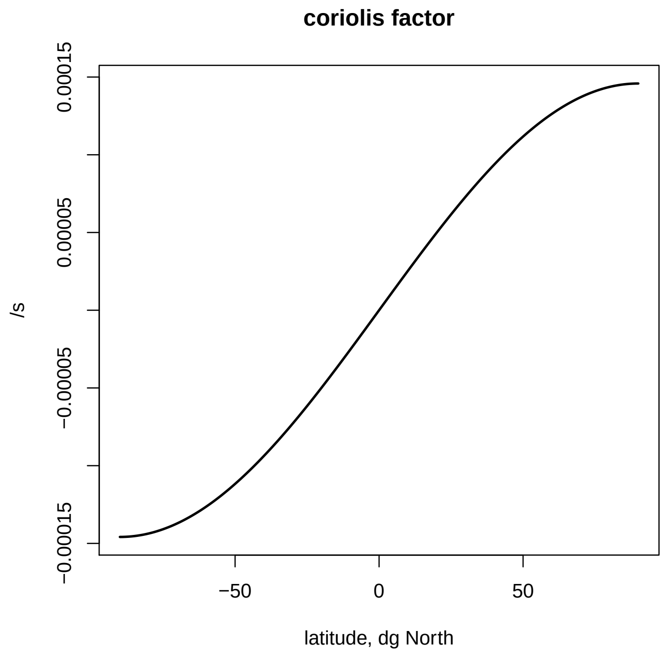

Figure 5: The coriolis function

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      HCO3       CO3
1 1.429208 1.205458 1.422550 1.229481 1.133012 0.7693272 0.6126977
       NH4        HS       NO3     H2PO4      HPO4       PO4         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]
```

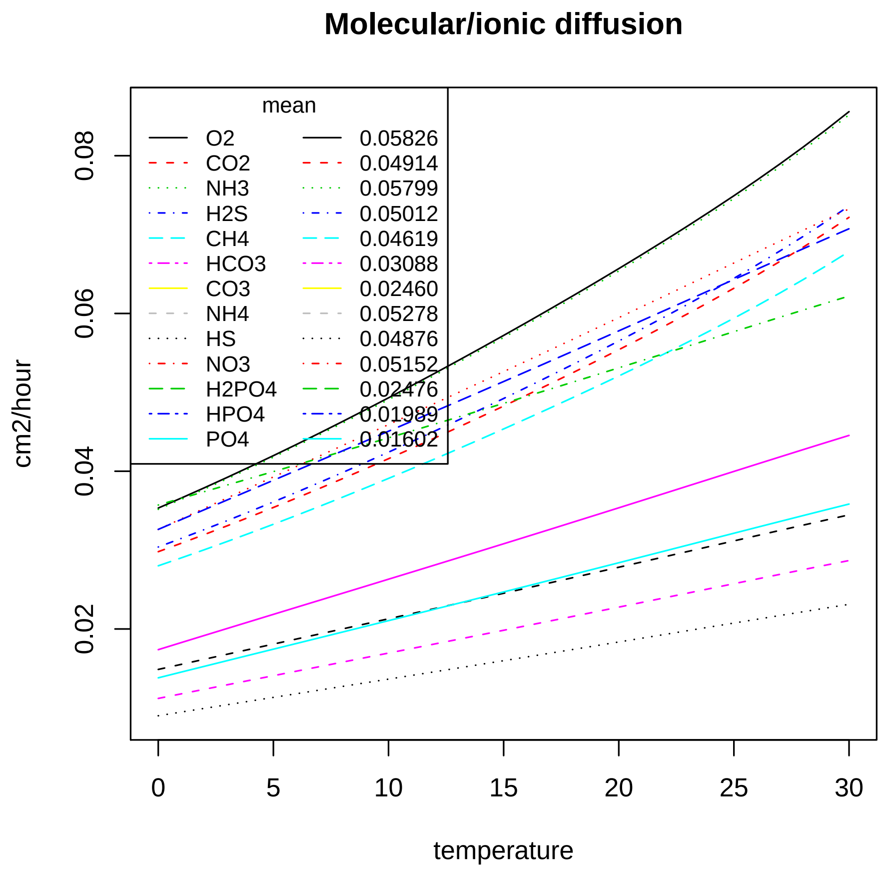

Figure 6: molecular diffusion coefficients as a function of temperature

```
> 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"))
```

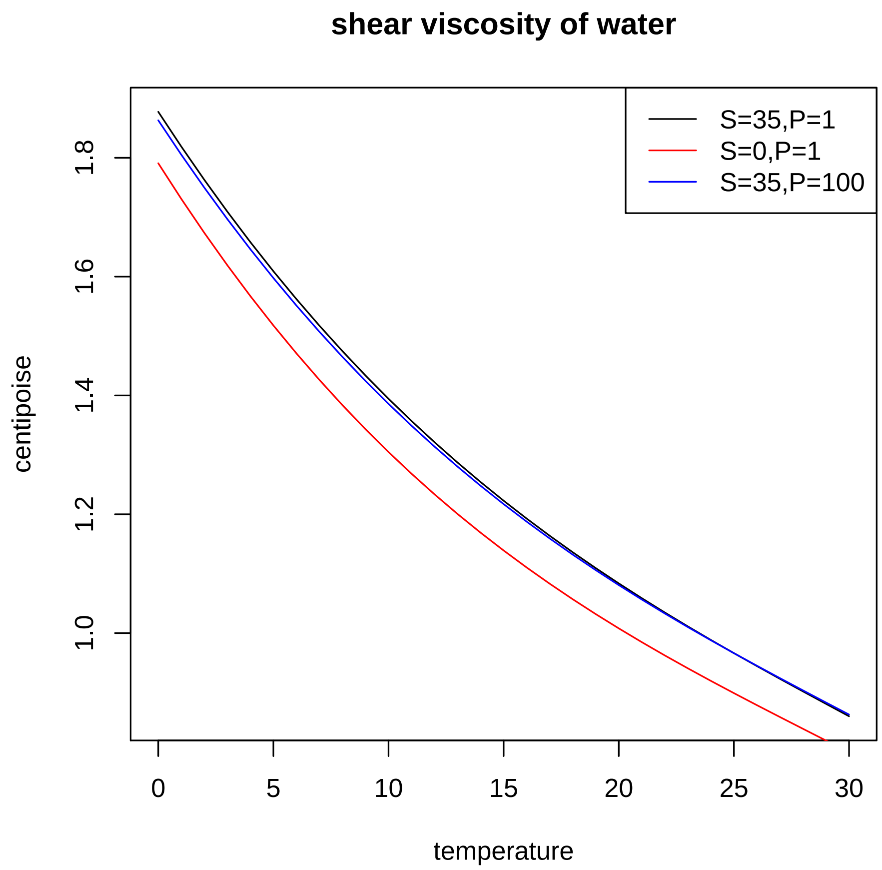

Figure 7: shear viscosity of water as a function of temperature

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

```
> l2mol(x=8,a=1.382,b=0.03186,T=0)*1000
```

```
[1] 357.3925
```

```
> l2mol(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

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