AUTOMATIC CODE GENERATOR (ACG) FOR CONSTRUCTING USER-DEFINED BIOGEOCHEMICAL REACTION NETWORKS

version 1.2

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INPUT TYPES

000 : Sections that should be modified by the user
000 : Sections that should NOT be modified by the user

000 : comments
000 : Maple input
000 : Maple output (appears only after you have executed the spreadsheet)
000 : Maple input entries that have to be specified by the user

www : Hyperlink to the Knowledge Book

Maple specific info

```
> restart ;
  #with(Spread) :
>  precision := double :
```

Summary and governing equations

Governing equation

The governing equation solved is of the form :

theta(x)*dC/dt = -d(Fdiff+Fadv)/dx + R,
where
- dX/dp is the partial derivative of X with respect to p [M/L^3/[p]]
- theta(x) = A(x)*por(x) for dissolved, and A(x)*(1-por(x)) for solid species [L^2]
- Fdiff = -(D(x)*theta(x)*dC/dx) [M/L^2/T]
- Fadv = (v*theta(x)*C)[M/L^2/T]
- A is the cross section area [L^2], por is porosity [-]
- v is the advection velocity [L/T], the sum of
the water flow velocity (vwat = water flow q in [L^3/T]/theta(x), solutes only) and
an advective velocity w acting upon both solids and solutes (e.g. movement due to fixed reference frame)
- D is the effective diffusion coefficient [L^2/T], the sum of
the molecular diffusion coefficient (Dmol, solutes only),
the bioturbation coefficient (Db) and
the dispersion coefficient (Disp = aL*|vwat|, solutes only, aL in [L]).
- R is the sum of the reaction terms [M/L^3/T] as specified in the reaction network established below

Caveats

- for real numbers you should add a point after the number.
- make sure all units match.
e.g. rates and dXdt, or flux boundary conditions and concentrations
for the conversion of solid to solute units,
one may define temporary variables that can be used in the rate laws below:
s_dens := 2.5; # solid density in [g/cm_solid^3]
sd := 1000. * s_dens * (1. - por(j)) / por(j);
the factor 1.d03 converts cm^3 to liter, e.g. [g/cm^3] to [g/l].
note that you need to refer to porosity exactly as por(j).

Physics - Parameters

The list of length **nparphys & nparphys2** *is given by* **phys_name & phys_name2***; the values collected in* **phys_val & phys_val2.**

Spatial and temporal domain size

tot_time: total length of simulation (T, e.g. years)
depth_max: spatial extent, e.g. total depth of simulation (L, e.g. cm)

```
>

  ### Start conditions for GSA ###

  TOC_wt := 1.0 ;
```

```
SedRate:= 0.5;
SWI_pH := 8.1;
Log_a  := 1.0;

DTime:= 0.005;

SWI_a  := 10**Log_a ;
SWI_TOC:= TOC_wt*2.5/12/100 ;



depth_max := 100.4 ;
tot_time := 2*depth_max/SedRate ;

##################################
```

```
                        TOC_wt := 1.0
                        SedRate := 0.5
                        SWI_pH := 8.1
                        Log_a := 1.0
                        DTime := 0.005
                        SWI_a := 10.
                 SWI_TOC := 0.002083333333
                     depth_max := 100.4
                  tot_time := 401.6000000                    (3.1.1)
```

Temperature and salinity

T_C: temperature (Celsius)

S : salinity (PSU)

T and S are used to calculate the molecular diffusion coefficients

T: absolute temperature (Kelvin)

```
> T_C := 10.3 ;
  T := T_C + 273.15 ;
  S := 35.0 ;
  Depth:= 100.0;
  P := Depth*9.81*1027./100000.;
  R := 83.145;
```

```
                        T_C := 10.3
                        T := 283.45
                         S := 35.0
                      Depth := 100.0
                    P := 10.07487000
                        R := 83.145                          (3.1.1.1)
```

Transport coefficients

vaL: longitudinal dispersivity (L). The dispersion coefficient is calculated as Disp = aL*|vwat|
viq: depth dependency of flow. 0: constant, else changing with depth (i.e. distance)
vq0: water flow (either constant or else at x=0, L^3/T)
viw: depth dependency of w. 0: constant, else changing with depth (i.e. distance)
vw0: advection velocity working on solids and solutes (either constant or else at x=0, L/T)
viDb: depth dependency of Db. 0: constant, else changing with depth (i.e. distance)
vDb0: bioturbation coefficient working on solids and solutes (either constant or else at x=0, L^2/T)

- user specified profiles of q(x), w(x) or Db(x) must be defined in the fortran subroutines advcoeff.f and diffcoeff.f, respectively.
- the molecular diffusion coefficients for the species used are specified further below

```
> val  := 0.0 ;
  viq  := 0 ;
  vq0  := 0. ;
  viw  := 0 ;
  vw0  := SedRate; #3.3*10.0^(-0.87478367-0.00043512*
  Depth);
  viDb  := 1 ;
  vDb0  := 5.2*(10.0^(0.7624-0.0003972*Depth));
  #Middelburg (water depth)
  #vDb0  := 15.7*(vw0^0.69) ; #Boudreau (sedimentation
  rate)
```

$$\begin{gathered} val := 0. \\ viq := 0 \\ vq0 := 0. \\ viw := 0 \\ vw0 := 0.5 \\ viDb := 1 \\ vDb0 := 27.45891316 \end{gathered} \tag{3.2.1}$$

Porosity profile and cross section area

vipor: depth dependency of porosity. 0: constant, else changing with depth (i.e. distance)
vpor0: porosity value (either constant or else at x=0)
viarea: depth dependency of cross section area. 0: constant, else changing with depth (i.e. distance)
varea0: cross section area (either constant or else at x=0, L^2)
- user specified profiles of por(x) or area(x) must be defined in

the fortran subroutine porarea.f.

```
> vipor := 1 ;
  vpor0 := 0.85 ;
  viarea := 0 ;
  varea0 := 1.0 ;
```

```
                    vipor := 1
                   vpor0 := 0.85
                    viarea := 0
                   varea0 := 1.0                          (3.3.1)
```

Grid and discretization

Dt: time step of numerical integration (T).
note that there are options defined in drivervalues.f that allow automatical selection of timestep
nnodes: number of nodes in the spatial domain.
for a regular grid, the grid spacing of the concentration profile is then depth_max/(nnodes-1)
vigridv: type of grid.
0 is for regular, evenly spaced grid,
else the user needs to specify the grid in the fortran subroutine gridsetup.f

```
> Dt := DTime;
  nnodes := 121;
  vigrid := 1;
```

```
                    Dt := 0.005
                   nnodes := 121
                    vigrid := 1                           (3.5.1)
```

Reaction Network - Size and Variables

Size of reaction network

nsolids : number of solid species
ndissolved : number of dissolved species
ncompo : total number of species
nreactions : total number of reactions (including equilibrium rxns)
neqrxns : number of equilibrium reaction

```
> nsolids := 26;
  ndissolved := 29;
  ncompo := nsolids + ndissolved;
  nreactions := 60;
  neqrxns := 13 ;
```

```
                   nsolids := 26
```

```
ndissolved := 29
ncompo := 55
nreactions := 60
neqrxns := 13                                        (4.1.1)
```

List of variables

variables: list of variables to model. example:
listsolids: species number which is a SOLID species.
note: all other variables are temporary and are NOT parsed to the ACG

Example:
variables:=[O2, so4, MnOx, FeOx, hco3, co3, hplus, hs];
listsolids: = [3,4];

```
> variables := [ch2o, o2, no3, mno2, feoh3, so4, ch4,
  nh4, po4, mn, fe, h2s, hs, ch4g, h2co3, hco3, co3,
  boh4, boh3, hplus, caco3, ca, snh4, spo4, fes, feco3,
  s0, fes2, sfe, sfp, mnco3, age, mno2pr, feoh3mr,
  feoh3pr, arago, mgcal, mg, BSi, DSi, sfSi, al, aloh,
  aloh2, aloh3, aloh4, glass, plagio, na, kplus, olive,
  pyrox, illite, smect, kaoli] ;

  listsolids := [1, 4, 5, 21, 23, 24, 25, 26, 28, 29,
  30, 31, 32, 33, 34, 35, 36, 37, 39, 41, 47, 48, 51,
  52, 53, 54, 55] ;
```

```
variables := [ch2o, o2, no3, mno2, feoh3, so4, ch4, nh4, po4, mn, fe, h2s, hs, ch4g,
    h2co3, hco3, co3, boh4, boh3, hplus, caco3, ca, snh4, spo4, fes, feco3, s0, fes2, sfe,
    sfp, mnco3, age, mno2pr, feoh3mr, feoh3pr, arago, mgcal, mg, BSi, DSi, sfSi, al,
    aloh, aloh2, aloh3, aloh4, glass, plagio, na, kplus, olive, pyrox, illite, smect, kaoli]
listsolids := [1, 4, 5, 21, 23, 24, 25, 26, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 39, 41, 47,   (4.2.1)
    48, 51, 52, 53, 54, 55]
```

Biogeochemistry - Rate laws

Definition of **kinetic rate laws**
rate.i : array of rates.
- For equilibrium rate expression, a kinetic rate MUST be specified as well. It will be overwritten in the equilibrium section below, but you need it as space holder and stoichiometry. Furthermore, the steadystate module uses detailed balancing method with fast kinetics. Therefore, in the example below, kf will have to be defined as a rather large number and kb = kf*Keq
note: all other variables are temporary and are NOT parsed to the ACG
- ***conditional statements***: if a rate law depends on a conditional statement you need to make use of the subroutine switches.f. Example: dissolution (Rd) is only to take place at undersaturation, thus Rd=

f(saturation). If saturation > 1, Rd>0, else Rd=0. This canbe implemented as Rd:=k*H1*saturation, where H1 is toggled between 0 and 1. Rather than giving the condition here in maple, for now you need to do this in "switches.f", where you program the conditions for H1, e.g. *H1=0, If (A*B/K>1) then H1 = 1.*

example:
*rate1 := 1000.*O2*hs; # rate law for 2O2 + HS -> SO4 + Hplus*
*rate2 := kf*hplus*co3 - kb*hco3; # kinetic rate law for HCO3 = CO3 + Hplus (equilibrium)*

Primary redox reactions www

```
> #primary redox
  #attpor:=5.0e-1;
  #porX:=0.70;

  #age   :=sw01*1e-10 + (1.0-sw01)*(((1-porX)*(x_pos-
  xbiot)+1.0/attpor*(vpor0-porX)*(exp(-attpor*(x_pos-
  xbiot))-1.0))/(vw0*(1-vpor0)));
  fo2   :=(sw02+(1.0-sw02)*o2/kmo2);
  fno3  :=sw03*(1.0-fo2)*(sw04+(1.0-sw04)*no3/kmno3);
  fmno2 :=sw05*(1.0-fo2-fno3)*(sw06+(1.0-sw06)*
  mno2/kmmno2);
  ffeoh3:=sw07*(1.0-fo2-fno3-fmno2)*(sw08+(1.0-sw08)*
  feoh3/kmfeoh3);
  fso4  :=sw09*(1.0-fo2-fno3-fmno2-ffeoh3)*(sw10+(1.0-
  sw10)*so4/kmso4);
  fch4  :=sw11*(1.0-fo2-fno3-fmno2-ffeoh3-fso4);

  rate1 := 0.0; # nu/(inita+age)*ch2o;
  rate2 := nu/(inita+age)*ch2o*fo2;
  rate3 := nu/(inita+age)*ch2o*fno3;
  rate4 := nu/(inita+age)*ch2o*fmno2;
  rate5 := nu/(inita+age)*ch2o*ffeoh3;
  rate6 := nu/(inita+age)*ch2o*fso4;
  rate7 := nu/(inita+age)*ch2o*fch4;


  #secondary redox
  rate8 := knit*nh4*o2;
  rate9 := kmnox*mn*o2;
  rate10:= kfemno2*fe*mno2;
```

```
rate37:= kfemno2pr*fe*mno2pr; # FSF PR MnO2
rate11:= kfeo2*fe*o2;
rate12:= kh2so2*(h2s+hs)*o2;
rate13:= kh2smno2*mno2*(hs+h2s);
rate38:= kh2smno2pr*mno2pr*(hs+h2s); # FSF PR MnO2
rate14:= kh2sfeoh3*feoh3*(hs+h2s);
rate40:= kh2sfeoh3mr*feoh3mr*(hs+h2s); # FSF MR FeOH3
rate41:= kh2sfeoh3pr*feoh3pr*(hs+h2s); # FSF PR FeOH3
rate15:= kaom*ch4*so4;
rate16:= kaomo2*ch4*o2;
rate17:= kfeso2*fes*o2;

#mineral
rate18:= kmnco3precip*sw12*((mn*co3/KsMnCO3)-1.0);
rate19:= kfesprecip*sw13*(((fe*hs)/(hplus*KsFeS))-1.0)
;
rate20:= kfesdiss*(1.0-sw13)*fes*(1.0-((fe*hs)/(hplus*
KsFeS)));
rate21:= kfeco3precip*sw14*((fe*co3/KsFeCO3)-1.0);
rate22:= kpyr*fes*(h2s+hs);
rate23:= kfess0*fes*s0;
rate24:= sw15*kcaldiss *caco3* ((1.0 - (ca*(co3)
/kspcal)));
rate25:= sw16*kapa*(po4-po4_eq);
rate43:= sw20*kcalppt*((ca*co3/kspcal)-5.0); #FSF
CaCO3 (calcite) precipitation
rate44:= sw21*karadis *arago* ((1.0 - (ca*co3/kspara))
);
rate45:= sw22*karappt*((ca*co3/kspara)-5.0);
rate46:= sw23*kmgcdis *mgcal* ((1.0 - (ca*co3/kspmgc))
); #Ikaite
rate47:= sw24*kmgcppt*((ca*co3/kspmgc)-1.0); #Ikaite

#misc
rate26:= (1.0-sw17)*kdis*sw18*(ch4g)*(ch4eq-(ch4));
rate27:= sw17*kgas*(ch4-ch4eq);
rate28:= kdi*sw19*s0;
rate39:= kmnage*mno2; #FSF HR MnO2 ageing into unreac
MnO2
rate42:= kfeage*feoh3; #FSF HR FeOH3 ageing into MR
FeOH3
```

```
#Silicon

#Biogenic Silica dissolution
kBSidis_z := (kBSidis*bd) + ((kBSidis - kBSidis*bd)*
exp(-ad*x_pos));
rate48 := sw25*kBSidis_z*BSi*(1.0-DSi/BSisat) ;

#eq
rate29:= kf1*hplus*hco3-kb1*h2co3;
rate30:= kf2*hplus*co3-kb2*hco3;
rate31:= kf3*hplus*hs-kb3*h2s ;
rate32:= kf4*hplus*boh4-kb4*boh3;
rate33:= kf5*po4*por(j) - kb5*spo4*(1. - por(j));
rate34:= kf6*nh4*por(j) - kb6*snh4*(1. - por(j));
rate35:= kf7*(feoh3+feoh3mr+feoh3pr)*po4- kb7*sfp;
#FSF Iron fractions;
rate36:= kf8*fe*por(j)  - kb8*sfe*(1. - por(j));

#eq Silicon
rate49:= kf9*(feoh3+feoh3mr+feoh3pr)*(DSi) - kb9*
(sfSi);

#eq aluminium
rate50:= kf10*aloh*hplus - kb10*al;
rate51:= kf11*aloh2*hplus**2 - kb11*al;
rate52:= kf12*aloh3*hplus**3 - kb12*al;
rate53:= kf13*aloh4*hplus**4 - kb13*al;

#Silicate weathering
rate54:= sw26*kglass*glass*(hplus**3/al)**(1/3) * (1.0
- DSi*al**0.36/hplus**1.08/kspglass);
rate55:= sw27*kplagio*plagio*(hplus**3/al)**0.35 *
(1.0 - DSi**2.3*aloh4**1.7*na**0.3*ca**0.7/kspplagio);
rate56:= sw28*kolive*olive * (1.0 - DSi*mg**1.6*fe**
0.4/hplus**4/kspolive);
rate57:= sw29*kpyrox*pyrox * (1.0 - DSi**2 * fe**0.46
* mg**0.84 * ca**0.7 / hplus**4 / ksppyrox);

#Silicate reverse weathering
rate58:= sw30*killite * (DSi**3.5 * al**2.3 * kplus**
0.6 * mg**0.25 / hplus**8 / kspillite - 1.0);
rate59:= sw31*ksmect * (ca**0.165 * mg**0.33 * al**1.7
* DSi**4 /hplus**6 / kspsmect - 1.0);
rate60:= sw32*kkaoli * (al**2 * DSi**2 / hplus**6/
kspkaoli - 1.0);
```

$$fo2 := sw02 + \frac{(1.0 - sw02)\, o2}{kmo2}$$

$$fno3 := sw03 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2}\right) \left(sw04 + \frac{(1.0 - sw04)\, no3}{kmno3}\right)$$

$$fmno2 := sw05 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2} - sw03 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2}\right) \left(sw04 + \frac{(1.0 - sw04)\, no3}{kmno3}\right)\right) \left(sw06 + \frac{(1.0 - sw06)\, mno2}{kmmno2}\right)$$

$$ffeoh3 := sw07 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2} - sw03 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2}\right) \left(sw04 + \frac{(1.0 - sw04)\, no3}{kmno3}\right) - sw05 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2} - sw03 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2}\right) \left(sw04 + \frac{(1.0 - sw04)\, no3}{kmno3}\right)\right) \left(sw06 + \frac{(1.0 - sw06)\, mno2}{kmmno2}\right)\right) \left(sw08 + \frac{(1.0 - sw08)\, feoh3}{kmfeoh3}\right)$$

$$fso4 := sw09 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2} - sw03 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2}\right) \left(sw04 + \frac{(1.0 - sw04)\, no3}{kmno3}\right) - sw05 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2} - sw03 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2}\right) \left(sw04 + \frac{(1.0 - sw04)\, no3}{kmno3}\right)\right) \left(sw06 + \frac{(1.0 - sw06)\, mno2}{kmmno2}\right) - sw07 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2} - sw03 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2}\right) \left(sw04 + \frac{(1.0 - sw04)\, no3}{kmno3}\right) - sw05 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2} - sw03 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2}\right) \left(sw04 + \frac{(1.0 - sw04)\, no3}{kmno3}\right)\right) \left(sw06 + \frac{(1.0 - sw06)\, mno2}{kmmno2}\right)\right) \left(sw08 + \frac{(1.0 - sw08)\, feoh3}{kmfeoh3}\right)\right) \left(sw10 + \frac{(1.0 - sw10)\, so4}{kmso4}\right)$$

$$fch4 := sw11 \left(1.0 - sw02 - \frac{(1.0 - sw02)\, o2}{kmo2} - sw03 \left(1.0 - sw02 \right.\right.$$

$$-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)-\mathit{sw05}\,\bigg(1.0-\mathit{sw02}$$

$$-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}-\mathit{sw03}\,\bigg(1.0-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}$$

$$+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)\bigg)\bigg(\mathit{sw06}+\frac{(1.0-\mathit{sw06})\,\mathit{mno2}}{\mathit{kmmno2}}\bigg)-\mathit{sw07}\,\bigg(1.0-\mathit{sw02}$$

$$-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}-\mathit{sw03}\,\bigg(1.0-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}$$

$$+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)-\mathit{sw05}\,\bigg(1.0-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}-\mathit{sw03}\,\bigg(1.0$$

$$-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)\bigg)\bigg(\mathit{sw06}$$

$$+\frac{(1.0-\mathit{sw06})\,\mathit{mno2}}{\mathit{kmmno2}}\bigg)\bigg)\bigg(\mathit{sw08}+\frac{(1.0-\mathit{sw08})\,\mathit{feoh3}}{\mathit{kmfeoh3}}\bigg)-\mathit{sw09}\,\bigg(1.0-\mathit{sw02}$$

$$-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}-\mathit{sw03}\,\bigg(1.0-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}$$

$$+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)-\mathit{sw05}\,\bigg(1.0-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}-\mathit{sw03}\,\bigg(1.0$$

$$-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)\bigg)\bigg(\mathit{sw06}$$

$$+\frac{(1.0-\mathit{sw06})\,\mathit{mno2}}{\mathit{kmmno2}}\bigg)-\mathit{sw07}\,\bigg(1.0-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}-\mathit{sw03}\,\bigg(1.0$$

$$-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)-\mathit{sw05}\,\bigg(1.0$$

$$-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}-\mathit{sw03}\,\bigg(1.0-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}$$

$$+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)\bigg)\bigg(\mathit{sw06}+\frac{(1.0-\mathit{sw06})\,\mathit{mno2}}{\mathit{kmmno2}}\bigg)\bigg)\bigg(\mathit{sw08}$$

$$+\frac{(1.0-\mathit{sw08})\,\mathit{feoh3}}{\mathit{kmfeoh3}}\bigg)\bigg)\bigg(\mathit{sw10}+\frac{(1.0-\mathit{sw10})\,\mathit{so4}}{\mathit{kmso4}}\bigg)\bigg)$$

$$\mathit{rate1} := 0.$$

$$\mathit{rate2} := \frac{\nu\,\mathit{ch2o}\,\bigg(\mathit{sw02}+\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)}{\mathit{inita}+\mathit{age}}$$

$$\mathit{rate3} := \frac{1}{\mathit{inita}+\mathit{age}}\bigg(\nu\,\mathit{ch2o}\,\mathit{sw03}\,\bigg(1.0-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}$$

$$+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)\bigg)$$

$$\mathit{rate4} := \frac{1}{\mathit{inita}+\mathit{age}}\bigg(\nu\,\mathit{ch2o}\,\mathit{sw05}\,\bigg(1.0-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}-\mathit{sw03}\,\bigg(1.0$$

$$-\mathit{sw02}-\frac{(1.0-\mathit{sw02})\,\mathit{o2}}{\mathit{kmo2}}\bigg)\bigg(\mathit{sw04}+\frac{(1.0-\mathit{sw04})\,\mathit{no3}}{\mathit{kmno3}}\bigg)\bigg)\bigg(\mathit{sw06}$$

$$+\frac{(1.0-\mathit{sw06})\,\mathit{mno2}}{\mathit{kmmno2}}\bigg)\bigg)$$

$$\begin{aligned}
\mathit{rate5} := {} & \frac{1}{\mathit{inita} + \mathit{age}} \left(\nu\, \mathit{ch2o}\, \mathit{sw07} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 \right.\right.\right. \\
& \left. - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) - \mathit{sw05} \left(1.0 \right. \\
& - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} \right. \\
& \left.\left.\left. + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) \right) \left(\mathit{sw06} + \frac{(1.0 - \mathit{sw06})\, \mathit{mno2}}{\mathit{kmmno2}} \right) \right) \left(\mathit{sw08} \right. \\
& \left.\left. + \frac{(1.0 - \mathit{sw08})\, \mathit{feoh3}}{\mathit{kmfeoh3}} \right) \right)
\end{aligned}$$

$$\begin{aligned}
\mathit{rate6} := {} & \frac{1}{\mathit{inita} + \mathit{age}} \left(\nu\, \mathit{ch2o}\, \mathit{sw09} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 \right.\right.\right. \\
& \left. - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) - \mathit{sw05} \left(1.0 \right. \\
& - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} \right. \\
& \left.\left. + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) \right) \left(\mathit{sw06} + \frac{(1.0 - \mathit{sw06})\, \mathit{mno2}}{\mathit{kmmno2}} \right) - \mathit{sw07} \left(1.0 - \mathit{sw02} \right. \\
& - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} \right. \\
& \left. + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) - \mathit{sw05} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 \right.\right. \\
& \left.\left. - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) \right) \left(\mathit{sw06} \right. \\
& \left.\left. + \frac{(1.0 - \mathit{sw06})\, \mathit{mno2}}{\mathit{kmmno2}} \right) \right) \left(\mathit{sw08} + \frac{(1.0 - \mathit{sw08})\, \mathit{feoh3}}{\mathit{kmfeoh3}} \right) \right) \left(\mathit{sw10} \right. \\
& \left.\left. + \frac{(1.0 - \mathit{sw10})\, \mathit{so4}}{\mathit{kmso4}} \right) \right)
\end{aligned}$$

$$\begin{aligned}
\mathit{rate7} := {} & \frac{1}{\mathit{inita} + \mathit{age}} \left(\nu\, \mathit{ch2o}\, \mathit{sw11} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 \right.\right.\right. \\
& \left. - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) - \mathit{sw05} \left(1.0 \right. \\
& - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} \right. \\
& \left.\left. + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) \right) \left(\mathit{sw06} + \frac{(1.0 - \mathit{sw06})\, \mathit{mno2}}{\mathit{kmmno2}} \right) - \mathit{sw07} \left(1.0 - \mathit{sw02} \right. \\
& - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} \right. \\
& \left. + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) - \mathit{sw05} \left(1.0 - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} - \mathit{sw03} \left(1.0 \right.\right. \\
& \left.\left. - \mathit{sw02} - \frac{(1.0 - \mathit{sw02})\, \mathit{o2}}{\mathit{kmo2}} \right) \left(\mathit{sw04} + \frac{(1.0 - \mathit{sw04})\, \mathit{no3}}{\mathit{kmno3}} \right) \right) \left(\mathit{sw06} \right. \\
& \left.\left. + \frac{(1.0 - \mathit{sw06})\, \mathit{mno2}}{\mathit{kmmno2}} \right) \right) \left(\mathit{sw08} + \frac{(1.0 - \mathit{sw08})\, \mathit{feoh3}}{\mathit{kmfeoh3}} \right) - \mathit{sw09} \left(1.0 - \mathit{sw02} \right.
\end{aligned}$$

$$- \frac{(1.0 - sw02)\ o2}{kmo2} - sw03 \bigg(1.0 - sw02 - \frac{(1.0 - sw02)\ o2}{kmo2}\bigg) \bigg(sw04$$

$$+ \frac{(1.0 - sw04)\ no3}{kmno3}\bigg) - sw05 \bigg(1.0 - sw02 - \frac{(1.0 - sw02)\ o2}{kmo2} - sw03 \bigg(1.0$$

$$- sw02 - \frac{(1.0 - sw02)\ o2}{kmo2}\bigg) \bigg(sw04 + \frac{(1.0 - sw04)\ no3}{kmno3}\bigg)\bigg) \bigg(sw06$$

$$+ \frac{(1.0 - sw06)\ mno2}{kmmno2}\bigg) - sw07 \bigg(1.0 - sw02 - \frac{(1.0 - sw02)\ o2}{kmo2} - sw03 \bigg(1.0$$

$$- sw02 - \frac{(1.0 - sw02)\ o2}{kmo2}\bigg) \bigg(sw04 + \frac{(1.0 - sw04)\ no3}{kmno3}\bigg) - sw05 \bigg(1.0$$

$$- sw02 - \frac{(1.0 - sw02)\ o2}{kmo2} - sw03 \bigg(1.0 - sw02 - \frac{(1.0 - sw02)\ o2}{kmo2}\bigg) \bigg(sw04$$

$$+ \frac{(1.0 - sw04)\ no3}{kmno3}\bigg)\bigg) \bigg(sw06 + \frac{(1.0 - sw06)\ mno2}{kmmno2}\bigg)\bigg) \bigg(sw08$$

$$+ \frac{(1.0 - sw08)\ feoh3}{kmfeoh3}\bigg)\bigg) \bigg(sw10 + \frac{(1.0 - sw10)\ so4}{kmso4}\bigg)\bigg)\bigg)$$

$$rate8 := knit\ nh4\ o2$$

$$rate9 := kmnox\ mn\ o2$$

$$rate10 := kfemno2\ fe\ mno2$$

$$rate37 := kfemno2pr\ fe\ mno2pr$$

$$rate11 := kfeo2\ fe\ o2$$

$$rate12 := kh2so2\ (h2s + hs)\ o2$$

$$rate13 := kh2smno2\ mno2\ (h2s + hs)$$

$$rate38 := kh2smno2pr\ mno2pr\ (h2s + hs)$$

$$rate14 := kh2sfeoh3\ feoh3\ (h2s + hs)$$

$$rate40 := kh2sfeoh3mr\ feoh3mr\ (h2s + hs)$$

$$rate41 := kh2sfeoh3pr\ feoh3pr\ (h2s + hs)$$

$$rate15 := kaom\ ch4\ so4$$

$$rate16 := kaomo2\ ch4\ o2$$

$$rate17 := kfeso2\ fes\ o2$$

$$rate18 := kmnco3precip\ sw12 \left(\frac{mn\ co3}{KsMnCO3} - 1.0\right)$$

$$rate19 := kfesprecip\ sw13 \left(\frac{fe\ hs}{hplus\ KsFeS} - 1.0\right)$$

$$rate20 := kfesdiss\ (1.0 - sw13)\ fes \left(1.0 - \frac{fe\ hs}{hplus\ KsFeS}\right)$$

$$rate21 := kfeco3precip\ sw14 \left(\frac{fe\ co3}{KsFeCO3} - 1.0\right)$$

$$rate22 := kpyr\ fes\ (h2s + hs)$$

$$rate23 := kfess0\ fes\ s0$$

$$rate24 := sw15\ kcaldiss\ caco3 \left(1.0 - \frac{ca\ co3}{kspcal}\right)$$

$$rate25 := sw16\ kapa\ (po4 - po4\_eq)$$

$$rate43 := sw20\ kcalppt \left(\frac{ca\ co3}{kspcal} - 5.0\right)$$

$$rate44 := sw21\, karadis\, arago \left(1.0 - \frac{ca\, co3}{kspara}\right)$$

$$rate45 := sw22\, karappt \left(\frac{ca\, co3}{kspara} - 5.0\right)$$

$$rate46 := sw23\, kmgcdis\, mgcal \left(1.0 - \frac{ca\, co3}{kspmgc}\right)$$

$$rate47 := sw24\, kmgcppt \left(\frac{ca\, co3}{kspmgc} - 1.0\right)$$

$$rate26 := (1.0 - sw17)\, kdis\, sw18\, ch4g\, (ch4eq - ch4)$$

$$rate27 := sw17\, kgas\, (ch4 - ch4eq)$$

$$rate28 := kdi\, sw19\, s0$$

$$rate39 := kmnage\, mno2$$

$$rate42 := kfeage\, feoh3$$

$$kBSidis\_z := kBSidis\, bd + (-bd\, kBSidis + kBSidis)\, \mathrm{e}^{-ad\, x\_pos}$$

$$rate48 := sw25\, \left(kBSidis\, bd + (-bd\, kBSidis + kBSidis)\, \mathrm{e}^{-ad\, x\_pos}\right) BSi \left(1.0 - \frac{DSi}{BSisat}\right)$$

$$rate29 := hco3\, hplus\, kf1 - h2co3\, kb1$$

$$rate30 := co3\, hplus\, kf2 - hco3\, kb2$$

$$rate31 := hplus\, hs\, kf3 - h2s\, kb3$$

$$rate32 := boh4\, hplus\, kf4 - boh3\, kb4$$

$$rate33 := kf5\, po4\, por(j) - kb5\, spo4\, (1. - por(j))$$

$$rate34 := kf6\, nh4\, por(j) - kb6\, snh4\, (1. - por(j))$$

$$rate35 := kf7\, (feoh3 + feoh3mr + feoh3pr)\, po4 - kb7\, sfp$$

$$rate36 := kf8\, fe\, por(j) - kb8\, sfe\, (1. - por(j))$$

$$rate49 := kf9\, (feoh3 + feoh3mr + feoh3pr)\, DSi - kb9\, sfSi$$

$$rate50 := aloh\, hplus\, kf10 - al\, kb10$$

$$rate51 := aloh2\, hplus^{2}\, kf11 - al\, kb11$$

$$rate52 := aloh3\, hplus^{3}\, kf12 - al\, kb12$$

$$rate53 := aloh4\, hplus^{4}\, kf13 - al\, kb13$$

$$rate54 := sw26\, kglass\, glass \left(\frac{hplus^{3}}{al}\right)^{1/3} \left(1.0 - \frac{DSi\, al^{0.36}}{hplus^{1.08}\, kspglass}\right)$$

$$rate55 := sw27\, kplagio\, plagio \left(\frac{hplus^{3}}{al}\right)^{0.35} \left(1.0 - \frac{DSi^{2.3}\, aloh4^{1.7}\, na^{0.3}\, ca^{0.7}}{kspplagio}\right)$$

$$rate56 := sw28\, kolive\, olive \left(1.0 - \frac{DSi\, mg^{1.6}\, fe^{0.4}}{hplus^{4}\, kspolive}\right)$$

$$rate57 := sw29\, kpyrox\, pyrox \left(1.0 - \frac{DSi^{2}\, fe^{0.46}\, mg^{0.84}\, ca^{0.7}}{hplus^{4}\, ksppyrox}\right)$$

$$rate58 := sw30\, killite \left(\frac{DSi^{3.5}\, al^{2.3}\, kplus^{0.6}\, mg^{0.25}}{hplus^{8}\, kspillite} - 1.0\right)$$

$$rate59 := sw31\, ksmect \left(\frac{ca^{0.165}\, mg^{0.33}\, al^{1.7}\, DSi^{4}}{hplus^{6}\, kspsmect} - 1.0\right)$$

(5.1.1)

$$rate60 := sw32\ kkaoli\left(\frac{al^{2}\ DSi^{2}}{hplus^{6}\ kspkaoli} - 1.0\right) \tag{5.1.1}$$

Biogeochemistry - Stoichiometry

Stoichiometry of the biogeochemical reactions
d.sp.dt : rates of change of sp due to the sum of biogeochemical reactions
note that rateX must be referred to as rX

example:
*dO2dt := -2*r1;*
dhco3dt = -r2;

```
> SD := (1.0 - por(j)) / por(j);
  SD1:= 1/por(j);
  x  := 106;
  y  :=  12;
  z  :=   1;
```

$$SD := \frac{1.0 - por(j)}{por(j)}$$

$$SD1 := \frac{1}{por(j)}$$

$$x := 106$$

$$y := 12$$

$$z := 1 \tag{6.1}$$

```
> dch2odt := 0.0; # PP
  dagedt  := 0.0; # PP
  do2dt   := -(x+2*y)/x*SD*r2-2.0*r8-2.0*r16-2.0*r12-0.25*
  r11-2.0*SD*r17-0.5*r9;
  dno3dt  := -(4.0*x+3.0*y)/(5.0*x)*SD*r3+r8;
  dmno2dt := -2.0*r4+r9/SD-r10-r13-r39; # FSF (r39 =
  ageing);
  dmno2prdt := -r37-r38+r39; # FSF PR MnO2 rate
  dfeoh3dt:= -4*r5-2.0*r14+1.0*r11/SD+2.0*r10+2.0*r37-r42;
  #FSF (r42 = ageing);
  dfeoh3mrdt:= -2.0*r40+r42; #FSF MR FeOH3 rate;
  dfeoh3prdt:= -2.0*r41; #FSF PR FeOH3 rate;
  dso4dt  := -0.5*SD*r6-r15+0.5*r12+SD*r17;#+r28;
  dch4dt  :=  0.5*SD*r7-r15-r16+r26-r27;
  dch4gdt := -r26+r27;
```

```
dnh4dt  := y/x*SD*( (r2+r3+r4+r5+r6+r7) -r3)-r8-r34*SD1;
# PP
dpo4dt  := z/x*SD*( r2+r3+r4+r5+r6+r7 )-r25-r33*SD1-r35*
SD1; # PP

#dnh4dt  := y/x*SD*(r1-r3)-r8-r34*SD1;
#dpo4dt  := z/x*SD*(r1)-r25-r33*SD1-r35*SD1;


dmndt   := 2.0*SD*r4-r9+(r10+r37)*SD+(r13+r38)*SD-1.0*
r18*SD; #FSF
dfedt   := 4.0*SD*r5+2.0*SD*(r14+r40+r41)-1.0*r11+SD*r17
-1.0*r19-1.0*SD*r21+SD*r20-r36*SD1-2.0*(r10+r37)*
SD+0.46*SD*r67 +0.4*SD*r66; #FSF

dh2sdt  := 0.5*SD*r6+r15-r12+r31-1.0*SD*(r14+r40+r41)
-1.0*r19-1.0*SD*r22+3.0*r28+SD*r20-(r13+r38)*SD; #FSF
dhsdt   := -r31;

dh2co3dt:=((x+y+2.0*z)/x)*SD*r2   +((x-3.0*y+10.0*z)/
(5.0*x))*SD*r3   -(3.0*x+y-2.0*z)*SD*r4/x   -((y-2.0*z)
/x)*SD*r6   +((x-2.0*y+4.0*z)/(2.0*x))*SD*r7   -(7.0*x+
y-2.0*z)/x*SD*r5   +2.0*r8   -r15   +r16   +2.0*r12
-4.0*SD*(r14+r40+r41)   +r29   +2.0*r11   +2.0*r19
+2.0*r28   -2.0*SD*r20   +2.0*r9   +2.0*(r10+r37)*SD
-2.0*(r13+r38)*SD   ; #FSF +r18+1.0*r21

dhco3dt:=-((y+2.0*z)/x)*SD*r2   +((4.0*x+3.0*y-10.0*z)/
(5.0*x))*SD*r3   +(4.0*x+y-2.0*z)*SD*r4/x   +((x+y-2.0*
z)/x)*SD*r6   +((y-2.0*z)/x)*SD*r7   +(8.0*x+y-2.0*z)/x*
SD*r5   -2.0*r8   +2.0*r15   -2.0*r12   +4.0*SD*(r14+
r40+r41)   -r29   +r30   -2.0*r11   -2.0*r19   -2.0*r28
 +2.0*SD*r20   -2.0*r9   -2.0*(r10+r37)*SD   +2.0*(r13+
r38)*SD  ; #-2.0*r18*SD-2.0*SD*r21

dco3dt:=-r30+SD*r24-r43+SD*r44-r45+SD*r46-r47-r18-r21;
#FSF r43: CaCO3 prec

dboh4dt:=-r32;
dboh3dt:=r32;

dhplusdt:=-r29-r30-r31-r32-r50-2.0*r51-3.0*r52-4.0*r53
```

```
-1.08*SD*r54+8.0*r58-4.0*SD*r57-4.0*SD*r56+6.0*r59+6.0*
r60;

dcaco3dt:=-r24+1.0*r43/SD; #FSF r43: CaCO3 prec
dcadt:=SD*r24-r43+SD*r44-r45+SD*r46-r47+0.7*SD*r57+0.7*
SD*r55-0.165*r59; #FSF r43: CaCO3 prec ##
dsnh4dt:=r34/(1.0-por(j));
dspo4dt:=r33/(1.0-por(j));
dfesdt:=(1.0*r19/SD-1.0*r17-1.0*r22-1.0*r23-r20);
dfeco3dt:=(1.0*r21/SD);
dmnco3dt:=(1.0*r18/SD);
dfes2dt:=1.0*r22+1.0*r23;
ds0dt:=1.0*SD*(r14+r40+r41)-4.0*r28-1.0*SD*r23+1.0*SD*
(r13+r38); #FSF
dsfedt:=r36/(1.0-por(j));
dsfpdt:=r35/(1.0-por(j));

daragodt:=-r44+r45/SD;
dmgcaldt:=-r46+r47/SD ;  ## Ikaite
dmgdt:=0.84*SD*r57 +1.6*SD*r56-0.25*r58-0.33*r59;



dBSidt := -r48;

dDSidt := r48*SD-r49*SD1+SD*r56+r54*SD+2.3*SD*r55-3.5*
r58+2.0*SD*r57-4.0*r59-2.0*r60;

dsfSidt:= r49/(1.0 - por(j));


daldt   := r50+r51+r52+r53+0.36*SD*r54-2.3*r58+0.0025*
SD*r48-1.7*r59-2.0*r60;
dalohdt := -r50;
daloh2dt:= -r51;
daloh3dt:= -r52;
daloh4dt:= -r53+1.7*SD*r55;

dglassdt:= -r54;
dplagiodt:= -r55;
dolivedt:= -r56;
dpyroxdt:= -r57;
```

```
dillitedt:= r58/SD;
dsmectdt:= r59/SD;
dkaolidt:= r60/SD;

dnadt := 0.3*SD*r55;
dkplusdt := -0.6*r58;
```

$$\mathit{dch2odt} := 0.$$

$$\mathit{dagedt} := 0.$$

$$\mathit{do2dt} := -\frac{65}{53}\,\frac{(1.0-\mathit{por}(j))\,\mathit{r2}}{\mathit{por}(j)} - 2.0\,\mathit{r8} - 2.0\,\mathit{r16} - 2.0\,\mathit{r12} - 0.25\,\mathit{r11} - \frac{2.0\,(1.0-\mathit{por}(j))\,\mathit{r17}}{\mathit{por}(j)} - 0.5\,\mathit{r9}$$

$$\mathit{dno3dt} := -\frac{0.8679245284\,(1.0-\mathit{por}(j))\,\mathit{r3}}{\mathit{por}(j)} + \mathit{r8}$$

$$\mathit{dmno2dt} := -2.0\,\mathit{r4} + \frac{\mathit{r9}\,\mathit{por}(j)}{1.0-\mathit{por}(j)} - \mathit{r10} - \mathit{r13} - \mathit{r39}$$

$$\mathit{dmno2prdt} := -\mathit{r37} - \mathit{r38} + \mathit{r39}$$

$$\mathit{dfeoh3dt} := -4\,\mathit{r5} - 2.0\,\mathit{r14} + \frac{1.0\,\mathit{r11}\,\mathit{por}(j)}{1.0-\mathit{por}(j)} + 2.0\,\mathit{r10} + 2.0\,\mathit{r37} - \mathit{r42}$$

$$\mathit{dfeoh3mrdt} := -2.0\,\mathit{r40} + \mathit{r42}$$

$$\mathit{dfeoh3prdt} := -2.0\,\mathit{r41}$$

$$\mathit{dso4dt} := -\frac{0.5\,(1.0-\mathit{por}(j))\,\mathit{r6}}{\mathit{por}(j)} - \mathit{r15} + 0.5\,\mathit{r12} + \frac{(1.0-\mathit{por}(j))\,\mathit{r17}}{\mathit{por}(j)}$$

$$\mathit{dch4dt} := \frac{0.5\,(1.0-\mathit{por}(j))\,\mathit{r7}}{\mathit{por}(j)} - \mathit{r15} - \mathit{r16} + \mathit{r26} - \mathit{r27}$$

$$\mathit{dch4gdt} := -\mathit{r26} + \mathit{r27}$$

$$\mathit{dnh4dt} := \frac{6}{53}\,\frac{(1.0-\mathit{por}(j))\,(\mathit{r2}+\mathit{r4}+\mathit{r5}+\mathit{r6}+\mathit{r7})}{\mathit{por}(j)} - \mathit{r8} - \frac{\mathit{r34}}{\mathit{por}(j)}$$

$$\mathit{dpo4dt} := \frac{1}{106}\,\frac{(1.0-\mathit{por}(j))\,(\mathit{r2}+\mathit{r3}+\mathit{r4}+\mathit{r5}+\mathit{r6}+\mathit{r7})}{\mathit{por}(j)} - \mathit{r25} - \frac{\mathit{r33}}{\mathit{por}(j)} - \frac{\mathit{r35}}{\mathit{por}(j)}$$

$$\mathit{dmndt} := \frac{2.0\,(1.0-\mathit{por}(j))\,\mathit{r4}}{\mathit{por}(j)} - \mathit{r9} + \frac{(\mathit{r10}+\mathit{r37})\,(1.0-\mathit{por}(j))}{\mathit{por}(j)} + \frac{(\mathit{r13}+\mathit{r38})\,(1.0-\mathit{por}(j))}{\mathit{por}(j)} - \frac{1.0\,\mathit{r18}\,(1.0-\mathit{por}(j))}{\mathit{por}(j)}$$

$$\mathit{dfedt} := \frac{4.0\,(1.0-\mathit{por}(j))\,\mathit{r5}}{\mathit{por}(j)} + \frac{2.0\,(1.0-\mathit{por}(j))\,(\mathit{r14}+\mathit{r40}+\mathit{r41})}{\mathit{por}(j)} - 1.0\,\mathit{r11} + \frac{(1.0-\mathit{por}(j))\,\mathit{r17}}{\mathit{por}(j)} - 1.0\,\mathit{r19} - \frac{1.0\,(1.0-\mathit{por}(j))\,\mathit{r21}}{\mathit{por}(j)} + \frac{(1.0-\mathit{por}(j))\,\mathit{r20}}{\mathit{por}(j)}$$

$$-\frac{r36}{por(j)}-\frac{2.0\,(r10+r37)\,(1.0-por(j))}{por(j)}+\frac{0.46\,(1.0-por(j))\,r67}{por(j)}$$
$$+\frac{0.4\,(1.0-por(j))\,r66}{por(j)}$$

$$\mathit{dh2sdt}:=\frac{0.5\,(1.0-por(j))\,r6}{por(j)}+r15-r12+r31$$
$$-\frac{1.0\,(1.0-por(j))\,(r14+r40+r41)}{por(j)}-1.0\,r19-\frac{1.0\,(1.0-por(j))\,r22}{por(j)}$$
$$+3.0\,r28+\frac{(1.0-por(j))\,r20}{por(j)}-\frac{(r13+r38)\,(1.0-por(j))}{por(j)}$$

$$\mathit{dhsdt}:=-r31$$

$$\mathit{dh2co3dt}:=\frac{1.132075472\,(1.0-por(j))\,r2}{por(j)}+\frac{0.1509433962\,(1.0-por(j))\,r3}{por(j)}$$
$$-\frac{3.094339623\,(1.0-por(j))\,r4}{por(j)}-\frac{0.09433962264\,(1.0-por(j))\,r6}{por(j)}$$
$$+\frac{0.4056603774\,(1.0-por(j))\,r7}{por(j)}-\frac{7.094339623\,(1.0-por(j))\,r5}{por(j)}+2.0\,r8$$
$$-r15+r16+2.0\,r12-\frac{4.0\,(1.0-por(j))\,(r14+r40+r41)}{por(j)}+r29+2.0\,r11$$
$$+2.0\,r19+2.0\,r28-\frac{2.0\,(1.0-por(j))\,r20}{por(j)}+2.0\,r9$$
$$+\frac{2.0\,(r10+r37)\,(1.0-por(j))}{por(j)}-\frac{2.0\,(r13+r38)\,(1.0-por(j))}{por(j)}$$

$$\mathit{dhco3dt}:=-\frac{0.1320754717\,(1.0-por(j))\,r2}{por(j)}+\frac{0.8490566038\,(1.0-por(j))\,r3}{por(j)}$$
$$+\frac{4.094339623\,(1.0-por(j))\,r4}{por(j)}+\frac{1.094339623\,(1.0-por(j))\,r6}{por(j)}$$
$$+\frac{0.09433962264\,(1.0-por(j))\,r7}{por(j)}+\frac{8.094339623\,(1.0-por(j))\,r5}{por(j)}-2.0\,r8$$
$$+2.0\,r15-2.0\,r12+\frac{4.0\,(1.0-por(j))\,(r14+r40+r41)}{por(j)}-r29+r30-2.0\,r11$$
$$-2.0\,r19-2.0\,r28+\frac{2.0\,(1.0-por(j))\,r20}{por(j)}-2.0\,r9$$
$$-\frac{2.0\,(r10+r37)\,(1.0-por(j))}{por(j)}+\frac{2.0\,(r13+r38)\,(1.0-por(j))}{por(j)}$$

$$\mathit{dco3dt}:=\frac{(1.0-por(j))\,r24}{por(j)}+\frac{(1.0-por(j))\,r44}{por(j)}+\frac{(1.0-por(j))\,r46}{por(j)}-r18$$
$$-r21-r30-r43-r45-r47$$

$$\mathit{dboh4dt}:=-r32$$

$$\mathit{dboh3dt}:=r32$$

$$\mathit{dhplusdt}:=-r29-r30-r31-r32-r50-2.0\,r51-3.0\,r52-4.0\,r53$$
$$-\frac{1.08\,(1.0-por(j))\,r54}{por(j)}+8.0\,r58-\frac{4.0\,(1.0-por(j))\,r57}{por(j)}$$
$$-\frac{4.0\,(1.0-por(j))\,r56}{por(j)}+6.0\,r59+6.0\,r60$$

$$\mathit{dcaco3dt} := -\mathit{r24} + \frac{1.0\ \mathit{r43}\ \mathit{por}(j)}{1.0 - \mathit{por}(j)}$$

$$\begin{aligned}\mathit{dcadt} := {} & \frac{(1.0 - \mathit{por}(j))\ \mathit{r24}}{\mathit{por}(j)} - \mathit{r43} + \frac{(1.0 - \mathit{por}(j))\ \mathit{r44}}{\mathit{por}(j)} - \mathit{r45} \\ & + \frac{(1.0 - \mathit{por}(j))\ \mathit{r46}}{\mathit{por}(j)} - \mathit{r47} + \frac{0.7\ (1.0 - \mathit{por}(j))\ \mathit{r57}}{\mathit{por}(j)} + \frac{0.7\ (1.0 - \mathit{por}(j))\ \mathit{r55}}{\mathit{por}(j)} \\ & - 0.165\ \mathit{r59}\end{aligned}$$

$$\mathit{dsnh4dt} := \frac{\mathit{r34}}{1.0 - \mathit{por}(j)}$$

$$\mathit{dspo4dt} := \frac{\mathit{r33}}{1.0 - \mathit{por}(j)}$$

$$\mathit{dfesdt} := \frac{1.0\ \mathit{r19}\ \mathit{por}(j)}{1.0 - \mathit{por}(j)} - 1.0\ \mathit{r17} - 1.0\ \mathit{r22} - 1.0\ \mathit{r23} - \mathit{r20}$$

$$\mathit{dfeco3dt} := \frac{1.0\ \mathit{r21}\ \mathit{por}(j)}{1.0 - \mathit{por}(j)}$$

$$\mathit{dmnco3dt} := \frac{1.0\ \mathit{r18}\ \mathit{por}(j)}{1.0 - \mathit{por}(j)}$$

$$\mathit{dfes2dt} := 1.0\ \mathit{r22} + 1.0\ \mathit{r23}$$

$$\begin{aligned}\mathit{ds0dt} := {} & \frac{1.0\ (1.0 - \mathit{por}(j))\ (\mathit{r14} + \mathit{r40} + \mathit{r41})}{\mathit{por}(j)} - 4.0\ \mathit{r28} - \frac{1.0\ (1.0 - \mathit{por}(j))\ \mathit{r23}}{\mathit{por}(j)} \\ & + \frac{1.0\ (\mathit{r13} + \mathit{r38})\ (1.0 - \mathit{por}(j))}{\mathit{por}(j)}\end{aligned}$$

$$\mathit{dsfedt} := \frac{\mathit{r36}}{1.0 - \mathit{por}(j)}$$

$$\mathit{dsfpdt} := \frac{\mathit{r35}}{1.0 - \mathit{por}(j)}$$

$$\mathit{daragodt} := -\mathit{r44} + \frac{\mathit{r45}\ \mathit{por}(j)}{1.0 - \mathit{por}(j)}$$

$$\mathit{dmgcaldt} := -\mathit{r46} + \frac{\mathit{r47}\ \mathit{por}(j)}{1.0 - \mathit{por}(j)}$$

$$\mathit{dmgdt} := \frac{0.84\ (1.0 - \mathit{por}(j))\ \mathit{r57}}{\mathit{por}(j)} + \frac{1.6\ (1.0 - \mathit{por}(j))\ \mathit{r56}}{\mathit{por}(j)} - 0.25\ \mathit{r58} - 0.33\ \mathit{r59}$$

$$\mathit{dBSidt} := -\mathit{r48}$$

$$\begin{aligned}\mathit{dDSidt} := {} & \frac{\mathit{r48}\ (1.0 - \mathit{por}(j))}{\mathit{por}(j)} - \frac{\mathit{r49}}{\mathit{por}(j)} + \frac{(1.0 - \mathit{por}(j))\ \mathit{r56}}{\mathit{por}(j)} \\ & + \frac{(1.0 - \mathit{por}(j))\ \mathit{r54}}{\mathit{por}(j)} + \frac{2.3\ (1.0 - \mathit{por}(j))\ \mathit{r55}}{\mathit{por}(j)} - 3.5\ \mathit{r58} \\ & + \frac{2.0\ (1.0 - \mathit{por}(j))\ \mathit{r57}}{\mathit{por}(j)} - 4.0\ \mathit{r59} - 2.0\ \mathit{r60}\end{aligned}$$

$$\mathit{dsfSidt} := \frac{\mathit{r49}}{1.0 - \mathit{por}(j)}$$

$$\begin{aligned}\mathit{daldt} := {} & \mathit{r50} + \mathit{r51} + \mathit{r52} + \mathit{r53} + \frac{0.36\ (1.0 - \mathit{por}(j))\ \mathit{r54}}{\mathit{por}(j)} - 2.3\ \mathit{r58} \\ & + \frac{0.0025\ \mathit{r48}\ (1.0 - \mathit{por}(j))}{\mathit{por}(j)} - 1.7\ \mathit{r59} - 2.0\ \mathit{r60}\end{aligned}$$

$$dalohdt := -r50$$
$$daloh2dt := -r51$$
$$daloh3dt := -r52$$
$$daloh4dt := -r53 + \frac{1.7\ (1.0 - por(j))\ r55}{por(j)}$$
$$dglassdt := -r54$$
$$dplagiodt := -r55$$
$$dolivedt := -r56$$
$$dpyroxdt := -r57$$
$$dillitedt := \frac{r58\ por(j)}{1.0 - por(j)}$$
$$dsmectdt := \frac{r59\ por(j)}{1.0 - por(j)}$$
$$dkaolidt := \frac{r60\ por(j)}{1.0 - por(j)}$$
$$dnadt := \frac{0.3\ (1.0 - por(j))\ r55}{por(j)}$$
$$dkplusdt := -0.6\ r58 \tag{6.2}$$

Biogeochemistry - Equilibria

Specification of equilibrium constraints
eqrxnsId : set of kinetic reactions which are overuled by a thermodynamic constraint
equilibriumseqns[i] : Equilibrium constraint for reaction i

example:
eqrxnID := [r2,rX];
*equilibriumeqns[1] := hplus*co3 - Keq*hco3;*
equilibriumeqns[2] := ...;

```
> eqrxnId := [r29, r30, r31, r32, r33, r34, r35, r36, r49,
  r50, r51, r52, r53] ;
> equilibriumeqns[1] := hplus*hco3-keq1*h2co3 ;
  equilibriumeqns[2] := hplus*co3-keq2*hco3  ;
  equilibriumeqns[3] := hplus*hs-keq3*h2s ;
  equilibriumeqns[4] := hplus*boh4-keq4*boh3;
  equilibriumeqns[5] := kspo4*po4*por(j) - spo4*(1. - por
  (j)) ;
  equilibriumeqns[6] := ksnh4*nh4*por(j) - snh4*(1. - por
  (j)) ;
  equilibriumeqns[7] := ksfp*(feoh3+feoh3mr+feoh3pr)*po4 -
  sfp ; #(assume forward reaction is dictated by solid
  phase)#FSF Iron fractions;
  equilibriumeqns[8] := ksfe*fe*por(j) - sfe*(1. - por(j))
  ;
```

```
equilibriumeqns[9] := ksfsi*(feoh3+feoh3mr+feoh3pr)*
(DSi) - (sfSi) ; #(assume forward reaction is dictated
by solid phase);
equilibriumeqns[10]:= aloh*hplus - eq1_al*al;
equilibriumeqns[11]:= aloh2*hplus**2 - eq2_al*al;
equilibriumeqns[12]:= aloh3*hplus**3 - eq3_al*al;
equilibriumeqns[13]:= aloh4*hplus**4 - eq4_al*al;
```

$$eqrxnId := [r29, r30, r31, r32, r33, r34, r35, r36, r49, r50, r51, r52, r53]$$

$$equilibriumeqns_1 := -h2co3\ keq1 + hco3\ hplus$$

$$equilibriumeqns_2 := co3\ hplus - hco3\ keq2$$

$$equilibriumeqns_3 := -h2s\ keq3 + hplus\ hs$$

$$equilibriumeqns_4 := -boh3\ keq4 + boh4\ hplus$$

$$equilibriumeqns_5 := kspo4\ po4\ por(j) - spo4\ (1. - por(j))$$

$$equilibriumeqns_6 := ksnh4\ nh4\ por(j) - snh4\ (1. - por(j))$$

$$equilibriumeqns_7 := ksfp\ (feoh3 + feoh3mr + feoh3pr)\ po4 - sfp$$

$$equilibriumeqns_8 := ksfe\ fe\ por(j) - sfe\ (1. - por(j))$$

$$equilibriumeqns_9 := ksfsi\ (feoh3 + feoh3mr + feoh3pr)\ DSi - sfSi$$

$$equilibriumeqns_{10} := -al\ eq1\_al + aloh\ hplus$$

$$equilibriumeqns_{11} := aloh2\ hplus^2 - al\ eq2\_al$$

$$equilibriumeqns_{12} := aloh3\ hplus^3 - al\ eq3\_al$$

$$equilibriumeqns_{13} := aloh4\ hplus^4 - al\ eq4\_al \qquad \textbf{(7.1)}$$

Biogeochemistry - Parameters

Values of rates constants and parameters

In this section, all parameters defined in section 'Rate laws' should be defined.

nparam: number of parameters to define

The list is given by **bio_name**; the values collected in **bio_val.**

note that for double precision, 10 should be written as 10.

```
example:
nparam:=4;
bio_name:=[kmo2hs,kf,kb,Keq];
vkf :=1.0*10^(5);
vKeq:=1.0*10^(-10.4);
vkb :=vkf*vKeq;
bio_val:=[1000.,vkf,vkb,vKeq];
```

```
> nparam := 139;
```

$$nparam := 139 \qquad \textbf{(8.1)}$$

```
> # calculate the dissociation constants, etc, based on
  temp and salinity (baseline P = 0) from Millero (1995)
  lnKC1_0 := 2.83655 - 2307.1266/ T - 1.5529413* ln(T) +
  (- (0.20760841 + 4.0484/ T)* sqrt(S)) + (0.08468345* S -
  0.00654208* S* sqrt(S)) + (ln(1 - 0.001005* S));
  lnKC2_0 :=-9.226508 - 3351.6106/ T - 0.2005743* ln(T)+
  (-0.106901773 - 23.9722/ T)* sqrt(S)+(0.1130822* S -
  0.00846934* S^1.5 + ln(1 - 0.001005 * S));
  lnKS_0 := 225.838 - 13275.3/T - 34.6435*ln(T) + 0.3449*
  S^0.5 - 0.0274*S ;
  lnKB_0:=(-8966.90-2890.53*sqrt(S)-77.942*S+1.728*S^
  (3.0/2.0)-0.0996*S*S)/T+(148.0248+137.1942*sqrt(S)
  +1.62142*S)+((-24.4344-25.085*sqrt(S)-0.2474*S)*ln(T))+
  (0.053105*sqrt(S)*T);

  # Now apply conversion for P (Millero 1995).
  # units are M

  deltav:=  -25.5 + 0.1271*T_C + 0.0*T_C*T_C;
  deltak:= (-3.08e-3 + 0.0877e-3*T_C + 0.0*T_C*T_C);
  lnkpok0:= -(deltav/(R*T))*P + (0.5*deltak/(R*T))*P*P;
  val_kkeq1 := exp(lnKC1_0)*exp(lnkpok0);


  deltav:=  -15.82  -0.0219*T_C;
  deltak:=  (1.13e-3 -0.1475e-3*T_C);
  lnkpok0:= -(deltav/(R*T))*P + (0.5*deltak/(R*T))*P*P;
  val_kkeq2:= exp(lnKC2_0)*exp(lnkpok0);

  val_kkeq3 := exp(lnKS_0 + ((14.8  - 0.002*T_C + 0.0004
  *T_C^2)*P + 0.5* (2.89 + 0.054*T_C) *P^2/1.01345)/R/T);

  deltav:=  -29.48 + 0.1622*T_C -2.608e-3*T_C*T_C;
  deltak:= (-2.84e-3+ 0.0794e-3*T_C);
  lnkpok0:= -(deltav/(R*T))*P + (0.5*deltak/(R*T))*P*P;
  val_kkeq4:= exp(lnKB_0)*exp(lnkpok0);

  lnKC3_0:= -13847.26/T + 148.96502 - 23.6521* log(T)+
  (118.67/T - 5.977 + 1.0495*log(T))*sqrt(S) - 0.01615*S;
> deltav:=  -25.6 +0.2324*T_C-3.6246e-3*T_C**2;
> deltak:=  (5.13e-3 +0.07945e-3*T_C);
> lnkpok0:= -(deltav/(R*T))*P + (0.5*deltak/(R*T))*P*P;
> val_kkeq5:= exp(lnKC3_0)*exp(lnkpok0);
> 
  # calculate the solubility product for caco3
  readlib(log10) :
  tmp1 := -171.9065-0.077993*T+2839.319/T+71.595*log10(T);
  tmp2 := +(-0.77712+0.0028426*T+178.34/T)*sqrt(S);
  tmp3 := -0.07711*S+0.0041249*S^1.5;
  log10Kspc := tmp1 + tmp2 + tmp3;
  ksca := 10.0^(log10Kspc);

  deltav:=   -48.7600 + 0.5304*T_C;
  deltak:= (-0.0118 +  3.6920e-4*T_C);
  lnkpok0:= -(deltav/(R*T))*P + (0.5*deltak/(R*T))*P*P;
  val_kksca:= ksca * exp(lnkpok0);

  # calculate the solubility product for aragonite
  readlib(log10) :
  tmp4 := -171.945-0.077993*T+2903.293/T+71.595*log10(T);
  tmp5 := +(-0.068393+0.0017276*T+88.135/T)*sqrt(S);
  tmp6 := -0.10018*S+0.0059415*S^1.5;
  log10Kspa := tmp4 + tmp5 + tmp6;
  ksar := 10.0^(log10Kspa);

  deltav:=   -35.0 + 0.5304*T_C;
  deltak:= (-0.0118 +  3.6920e-4*T_C);
  lnkpok0:= -(deltav/(R*T))*P + (0.5*deltak/(R*T))*P*P;
  val_kksar:= ksar * exp(lnkpok0);


  # calculate the solubility product for ikaite
  readlib(log10) :
  LogKspi := 0.15981 - 2011.1/T ; #Bischoff et al., 1993
  ksik := 10**LogKspi ;
  gammaCO3:= 0.0508; #CO3 activity coefficient (T/S) from
  Pierot & Millero,  2017
  gammaCa2:= 0.2053; #Ca2+ activity coefficient (T/S) from
  Pierot & Millero,  2017
  val_kksik:= ksik/(gammaCO3*gammaCa2);


  # aluminium equilibrium constants (logK)
  # LogK @ 5oC SUPERCRIPT database
  # LogK' corrected to 10 oC / sal 35 (Pierrot and
  Millero, 2017)
  # unit correction: (mol/L) to (mol/cm3) applied
  accordingly
  LogK1_al := -5.297;
  LogK2_al := -12.438;
  LogK3_al := -19.012;
  LogK4_al := -24.584;

  kk1_al := (10**LogK1_al)*1.0e-3; # **mol/cm-3
  conversion**
  kk2_al := (10**LogK2_al)*1.0e-6; # **mol/cm-3
  conversion**
  kk3_al := (10**LogK3_al)*1.0e-9; # **mol/cm-3
  conversion**
  kk4_al := (10**LogK4_al)*1.0e-12; # **mol/cm-3
  conversion**

  # silicate minerals solubility constants
  # Ksp values multiplied by a factor to convert to ***mol
  cm-3***

  ## Basaltic glass: (0.36*Al + H4SiO4) ### from Gislason
  and Oelkers, 2003 (SiO2 + 0.36Gibbsite = SiAl(0.36)O2(OH
  (1.08))
  ## Ksp @ 10 oC SUPERCRPT
  ## corrected to 10 oC / sal 35 (Pierrot and Millero,
  2017)
  LogKspglass:= 0.756 ;
  Kspglass:= (10**LogKspglass)*0.144544; # ** conversion
  (mol/L)^n to (mol/cm3)^n **

  ## Plagioclase - An70Ab30: (0.7*Ca + 0.3*Na + 1.7*AlOH4
  + 2.3*H4SiO4)
  ## Ksp @ 5oC after Stefansson 2001
  ## corrected to K'sp @ 5 oC / sal 35 (Pierrot and
  Millero, 2017)
  LogKspplagio := -18.248;
  Kspplagio := (10**LogKspplagio)*1.0e-15 ; # **
  conversion (mol/L)^n to (mol/cm3)^n **

  ## Olivine - Fo80Fa20 (1.6*Mg + 0.4*Fe + H4SiO4)
```

```
  ## Ksp @ 10oC after Stefansson 2001
  ## corrected to K'sp @ 10 oC / sal 35 (Pierrot and
  Millero, 2017)
  Log_Ksolive := 29.317 ;
  Kspolive := (10**Log_Ksolive)*1.0e3 ; # ** conversion
  (mol/L)^n to (mol/cm3)^n **

  ## Clinopyroxene - Di45Hed25En19Fs11:
  ## Ksp @ 5oC after Stefansson 2001
  ## corrected K'sp to 5 oC / sal 35 (Pierrot and Millero,
  2017)
  LogKspyrox := 24.916 ;
  Ksppyrox := (10**LogKspyrox)*1.0; # ** conversion
  (mol/L)^n to (mol/cm3)^n **

  ##Illite ... ### 0.6K+ + 0.25Mg2+ + 2.3Al3+ +3.5H4SiO4!!
  !
  ## Ksp @ 10 oC from SUPERCRIPT database
  ## corrected K'sp to 10 oC / sal 35 (Pierrot and
  Millero, 2017)
  LogKsillite:= 13.044 ;
  Kspillite:= (10**LogKsillite)*1.122*1.0e4; # **
  conversion (mol/L)^n to (mol/cm3)^n **

  ##Smectite # Ca-Montmorillonite
  ##Ksp @ 5oC from SUPERCRIPT database
  ##corrected K'sp to 5oC / sal 35 (Pierrot and Millero,
  2017)
  LogKssmect:= 6.244 ;
  Kspsmect:= (10**LogKssmect)*2.6002e-1; #** conversion
  (mol/L) to (mol/cm3) **

  ##Kaolinite #Al2Si2O5(OH)4
  ##Ksp @ 5oC from SUPERCRIPT database
  ##Corrected K'sp to 5oC / sal 35 (Pierrot and Millero,
  2017)
  LogKskaoli:= 8.176 ;
  Kspkaoli:= (10**LogKskaoli)* 1.0e6; #**conversion
  (mol/L) to (mol/cm3)**

>
  #______________________________________________________
```

$$lnKC1\_0 := -13.81164725$$
$$lnKC2\_0 := -21.14789969$$
$$lnKS\_0 := -15.54834188$$
$$lnKB\_0 := -20.20576891$$
$$deltav := -24.19087$$
$$deltak := -0.00217669$$
$$lnkpok0 := 0.01033668884$$
$$val\_kkeq1 := 0.000001014301296$$
$$deltav := -16.04557$$
$$deltak := -0.00038925$$
$$lnkpok0 := 0.006858496573$$
$$val\_kkeq2 := 6.585101419\ 10^{-10}$$
$$val\_kkeq3 := 1.792144094\ 10^{-7}$$
$$deltav := -28.08602272$$
$$deltak := -0.00202218$$
$$lnkpok0 := 0.01200216383$$
$$val\_kkeq4 := 1.698081511\ 10^{-9}$$
$$lnKC3\_0 := -31.83859080$$
$$deltav := -23.59081381$$
$$deltak := 0.005948335$$
$$lnkpok0 := 0.01009766720$$
$$val\_kkeq5 := 1.503353334\ 10^{-14}$$
$$tmp1 := -8.4115624$$
$$tmp2 := 3.891545170$$
$$tmp3 := -1.844736688$$
$$log10Kspc := -6.364753918$$
$$ksca := 4.317636555\ 10^{-7}$$
$$deltav := -43.29688$$
$$deltak := -0.007997240$$
$$lnkpok0 := 0.01849179953$$
$$val\_kksca := 4.398220198\ 10^{-7}$$
$$tmp4 := -8.2243647$$
$$tmp5 := 4.331942300$$
$$tmp6 := -2.276036419$$
$$log10Kspa := -6.168458819$$
$$ksar := 6.784864534\ 10^{-7}$$
$$deltav := -29.53688$$
$$deltak := -0.007997240$$
$$lnkpok0 := 0.01260952505$$
$$val\_kksar := 6.870960123\ 10^{-7}$$
$$LogKspi := -6.935268498$$
$$ksik := 1.160730782\ 10^{-7}$$
$$gammaCO3 := 0.0508$$
$$gammaCa2 := 0.2053$$

$$val\_kksik := 0.00001112958166$$
$$LogK1\_al := -5.297$$
$$LogK2\_al := -12.438$$
$$LogK3\_al := -19.012$$
$$LogK4\_al := -24.584$$
$$kk1\_al := 5.046612976\ 10^{-9}$$
$$kk2\_al := 3.647539469\ 10^{-19}$$
$$kk3\_al := 9.727472238\ 10^{-29}$$
$$kk4\_al := 2.606153550\ 10^{-37}$$
$$LogKspglass := 0.756$$
$$Kspglass := 0.8241382458$$
$$LogKspplagio := -18.248$$
$$Kspplagio := 5.649369748\ 10^{-34}$$
$$Log\_Ksolive := 29.317$$
$$Kspolive := 2.074913517\ 10^{32}$$
$$LogKspyrox := 24.916$$
$$Ksppyrox := 8.241381150\ 10^{24}$$
$$LogKsillite := 13.044$$
$$Kspillite := 1.241631886\ 10^{17}$$
$$LogKssmect := 6.244$$
$$Kspsmect := 4.560440081\ 10^{5}$$
$$LogKskaoli := 8.176$$
$$Kspkaoli := 1.499684836\ 10^{14} \qquad \textbf{(8.2)}$$

```
> #units mol, l, yr
```

```
> val_xbiot        :=10.0;
  val_inita        :=SWI_a;
  val_nu           :=0.1;
  val_kmo2         :=8.0e-9;
  val_kmno3        :=5.0e-9;
  val_kmmno2       :=5.0e-6;
  val_kmfeoh3      :=1.25e-5;
  val_kmso4        :=100.0e-9;
  val_knit         :=1.0e7;
  val_kmnox        :=5.0e7;
  val_kfemno2      :=3.0e6;
  val_kfemno2pr    :=3.0e2; #FSF
  val_kfeo2        :=5.0e9;
  val_kh2so2       :=1.0e7;
  val_kh2smno2     :=1.0e2;
  val_kh2smno2pr   :=1.0e-1; #FSF
  val_kh2sfeoh3    :=1.0e2;
  val_kh2sfeoh3mr  :=1.0e-2; #FSF
  val_kh2sfeoh3pr  :=1.0e-4; #FSF
  val_kaom         :=5.0e6;
```

```
val_kaomo2      :=1.0e13;
val_kfeso2      :=1.0e9;
val_kmnco3precip:=0.1e-7;
val_KsMnCO3     :=3.2e-15;
val_kfesprecip  :=5.0e-9;
val_kfesdiss    :=1.0e-3;
val_KsFeS       :=6.3e-6/0.77;
val_kfeco3precip:=1.0e-9;
val_KsFeCO3     :=4.0e-15;
val_kcaldiss    :=0.1e0;
val_kcalppt     :=0.1e-1; #FSF
val_karadis     :=0.1e0;
val_karappt     :=0.1e-1;
val_kmgcdis     :=0.1e0; ## Ikaite
val_kmgcppt     :=0.1e-1; ## Ikaite
val_kpyr        :=60.0e6;
val_kfess0      :=2.5e4;
val_kapa        :=1.0e0;
val_po4_eq      :=10.0e-9;
val_kdis        :=0.0e0;
val_ch4eq       :=0.1e5;
val_kgas        :=0.0e0;
val_kdi         :=0.1e-2;
val_h2sstar     :=0.1e-4;
val_ksnh4       :=0.16e1;
val_kspo4       :=0.18e1;
val_ksfp        :=100.0;
val_ksfe        :=400.0;
val_kmnage      :=0.6; #FSF
val_kfeage      :=0.6; #FSF

val_keq1 := val_kkeq1*1e-3;
val_keq2 := val_kkeq2*1e-3;
val_keq3 := val_kkeq3*1e-3;
val_keq4 := val_kkeq4*1e-3;
val_keq5 := val_kkeq5*1e-6; #cst ionisation water Kw=10
-14mol/l; 10-20mol/cm3


val_kf1 := 1.0;
val_kb1 := val_keq1;
val_kf2 := 1.0 ;
```

```
val_kb2 := val_keq2;
val_kf3 := 1.0;
val_kb3 := val_keq3;
val_kf4 := 1.0;
val_kb4 := val_keq4;
val_kf5 := val_kspo4;
val_kb5 := 1.0;
val_kf6 := val_ksnh4;
val_kb6 := 1.0;
val_kf7 := val_ksfp;
val_kb7 := 1.0;
val_kf8 := val_ksfe;
val_kb8 := 1.0;
val_kspcal := val_kksca*1e-6;
val_kspara := val_kksar*1e-6;
val_kspmgc := val_kksik*1e-6; #Ikaite ##for MgCal,
val_kspmgc := val_kspara*1.21;

val_kBSidis := 0.1e-2;
val_ad := 0.2;
val_bd := 0.05;
val_BSisat := 8.0e-7;

val_ksfsi:= 0.0 ; #0.5e7;
val_kf9 := val_ksfsi;
val_kb9 := 1.0;

val_eq1_al:= kk1_al;
val_eq2_al:= kk2_al;
val_eq3_al:= kk3_al;
val_eq4_al:= kk4_al;
val_kf10  := 1.0;
val_kb10  := val_eq1_al;
val_kf11  := 1.0;
val_kb11  := val_eq2_al;
val_kf12  := 1.0;
val_kb12  := val_eq3_al;
val_kf13  := 1.0;
val_kb13  := val_eq4_al;

val_kspglass := Kspglass;
val_kglass:= 0.0; #0.2e1;
```

```
val_kspplagio:= Kspplagio;
val_kplagio := 0.0 ; #0.1e0;

val_kspolive:= Kspolive;
val_kolive := 0.0; #0.15e-3;

val_ksppyrox:= Ksppyrox;
val_kpyrox := 0.0 ; #0.1e-6;

val_kspillite:= Kspillite;
val_killite := 0.0; #0.2e-9;

val_kspsmect:= Kspsmect;
val_ksmect:= 0.0 ; #0.1e-15;

val_kspkaoli:= Kspkaoli;
val_kkaoli:= 0.0 ; #0.1e-15;
```

$$\mathit{val\_xbiot} := 10.0$$
$$\mathit{val\_inita} := 10.$$
$$\mathit{val\_nu} := 0.1$$
$$\mathit{val\_kmo2} := 8.0\ 10^{-9}$$
$$\mathit{val\_kmno3} := 5.0\ 10^{-9}$$
$$\mathit{val\_kmmno2} := 0.0000050$$
$$\mathit{val\_kmfeoh3} := 0.0000125$$
$$\mathit{val\_kmso4} := 1.000\ 10^{-7}$$
$$\mathit{val\_knit} := 1.0\ 10^{7}$$
$$\mathit{val\_kmnox} := 5.0\ 10^{7}$$
$$\mathit{val\_kfemno2} := 3.0\ 10^{6}$$
$$\mathit{val\_kfemno2pr} := 300.$$
$$\mathit{val\_kfeo2} := 5.0\ 10^{9}$$
$$\mathit{val\_kh2so2} := 1.0\ 10^{7}$$
$$\mathit{val\_kh2smno2} := 100.$$
$$\mathit{val\_kh2smno2pr} := 0.10$$
$$\mathit{val\_kh2sfeoh3} := 100.$$
$$\mathit{val\_kh2sfeoh3mr} := 0.010$$
$$\mathit{val\_kh2sfeoh3pr} := 0.00010$$
$$\mathit{val\_kaom} := 5.0\ 10^{6}$$
$$\mathit{val\_kaomo2} := 1.0\ 10^{13}$$
$$\mathit{val\_kfeso2} := 1.0\ 10^{9}$$
$$\mathit{val\_kmnco3precip} := 1.\ 10^{-8}$$
$$\mathit{val\_KsMnCO3} := 3.2\ 10^{-15}$$
$$\mathit{val\_kfesprecip} := 5.0\ 10^{-9}$$
$$\mathit{val\_kfesdiss} := 0.0010$$
$$\mathit{val\_KsFeS} := 0.000008181818182$$

$$\mathit{val\_kfeco3precip} := 1.0\ 10^{-9}$$
$$\mathit{val\_KsFeCO3} := 4.0\ 10^{-15}$$
$$\mathit{val\_kcaldiss} := 0.1$$
$$\mathit{val\_kcalppt} := 0.01$$
$$\mathit{val\_karadis} := 0.1$$
$$\mathit{val\_karappt} := 0.01$$
$$\mathit{val\_kmgcdis} := 0.1$$
$$\mathit{val\_kmgcppt} := 0.01$$
$$\mathit{val\_kpyr} := 6.00\ 10^{7}$$
$$\mathit{val\_kfess0} := 25000.$$
$$\mathit{val\_kapa} := 1.0$$
$$\mathit{val\_po4\_eq} := 1.00\ 10^{-8}$$
$$\mathit{val\_kdis} := 0.$$
$$\mathit{val\_ch4eq} := 10000.$$
$$\mathit{val\_kgas} := 0.$$
$$\mathit{val\_kdi} := 0.001$$
$$\mathit{val\_h2sstar} := 0.00001$$
$$\mathit{val\_ksnh4} := 1.6$$
$$\mathit{val\_kspo4} := 1.8$$
$$\mathit{val\_ksfp} := 100.0$$
$$\mathit{val\_ksfe} := 400.0$$
$$\mathit{val\_kmnage} := 0.6$$
$$\mathit{val\_kfeage} := 0.6$$
$$\mathit{val\_keq1} := 1.014301296\ 10^{-9}$$
$$\mathit{val\_keq2} := 6.585101419\ 10^{-13}$$
$$\mathit{val\_keq3} := 1.792144094\ 10^{-10}$$
$$\mathit{val\_keq4} := 1.698081511\ 10^{-12}$$
$$\mathit{val\_keq5} := 1.503353334\ 10^{-20}$$
$$\mathit{val\_kf1} := 1.0$$
$$\mathit{val\_kb1} := 1.014301296\ 10^{-9}$$
$$\mathit{val\_kf2} := 1.0$$
$$\mathit{val\_kb2} := 6.585101419\ 10^{-13}$$
$$\mathit{val\_kf3} := 1.0$$
$$\mathit{val\_kb3} := 1.792144094\ 10^{-10}$$
$$\mathit{val\_kf4} := 1.0$$
$$\mathit{val\_kb4} := 1.698081511\ 10^{-12}$$
$$\mathit{val\_kf5} := 1.8$$
$$\mathit{val\_kb5} := 1.0$$
$$\mathit{val\_kf6} := 1.6$$
$$\mathit{val\_kb6} := 1.0$$
$$\mathit{val\_kf7} := 100.0$$
$$\mathit{val\_kb7} := 1.0$$
$$\mathit{val\_kf8} := 400.0$$
$$\mathit{val\_kb8} := 1.0$$
$$\mathit{val\_kspcal} := 4.398220198\ 10^{-13}$$
$$\mathit{val\_kspara} := 6.870960123\ 10^{-13}$$

$val\_kspmgc := 1.112958166\ 10^{-11}$

$val\_kBSidis := 0.001$

$val\_ad := 0.2$

$val\_bd := 0.05$

$val\_BSisat := 8.0\ 10^{-7}$

$val\_ksfsi := 0.$

$val\_kf9 := 0.$

$val\_kb9 := 1.0$

$val\_eq1\_al := 5.046612976\ 10^{-9}$

$val\_eq2\_al := 3.647539469\ 10^{-19}$

$val\_eq3\_al := 9.727472238\ 10^{-29}$

$val\_eq4\_al := 2.606153550\ 10^{-37}$

$val\_kf10 := 1.0$

$val\_kb10 := 5.046612976\ 10^{-9}$

$val\_kf11 := 1.0$

$val\_kb11 := 3.647539469\ 10^{-19}$

$val\_kf12 := 1.0$

$val\_kb12 := 9.727472238\ 10^{-29}$

$val\_kf13 := 1.0$

$val\_kb13 := 2.606153550\ 10^{-37}$

$val\_kspglass := 0.8241382458$

$val\_kglass := 2.$

$val\_kspplagio := 5.649369748\ 10^{-34}$

$val\_kplagio := 0.$

$val\_kspolive := 2.074913517\ 10^{32}$

$val\_kolive := 0.00015$

$val\_ksppyrox := 8.241381150\ 10^{24}$

$val\_kpyrox := 0.$

$val\_kspillite := 1.241631886\ 10^{17}$

$val\_killite := 2.\ 10^{-10}$

$val\_kspsmect := 4.560440081\ 10^{5}$

$val\_ksmect := 0.$

$val\_kspkaoli := 1.499684836\ 10^{14}$

$val\_kkaoli := 0.$ **(8.3)**

```
> bio_name := [sw01, sw02, sw03, sw04, sw05, sw06, sw07,
  sw08, sw09, sw10, sw11, sw12, sw13, sw14, sw15, sw16,
  sw17, sw18, sw19, sw20, sw21, sw22, sw23, sw24, sw25,
  sw26, sw27, sw28, sw29, sw30, sw31, sw32, xbiot, inita,
  nu, kmo2, kmno3, kmmno2, kmfeoh3, kmso4, knit, kmnox,
  kfemno2, kfeo2, kh2so2, kh2smno2, kh2sfeoh3, kaom,
  kaomo2, kfeso2, kmnco3precip, KsMnCO3, kfesprecip,
  kfesdiss, KsFeS, kfeco3precip, KsFeCO3, kcaldiss,
  kcalppt, karadis, karappt, kmgcdis, kmgcppt, kpyr,
  kfess0, kapa, po4_eq, kdis, h2sstar, ch4eq, kgas, kdi,
  ksnh4, kspo4, ksfp, ksfe, kf1, kb1, kf2, kb2, kf3, kb3,
  kf4, kb4, kf5, kb5, kf6, kb6, kf7, kb7, kf8, kb8,
  kspcal, kspara, kspmgc, keq1, keq2, keq3, keq4,
  kfemno2pr, kh2smno2pr, kmnage, kh2sfeoh3mr, kh2sfeoh3pr,
  kfeage, keq5, kBSidis, ad, bd, BSisat, ksfsi, kf9, kb9,
  eq1_al, eq2_al, eq3_al, eq4_al, kf10, kb10, kf11, kb11,
  kf12, kb12, kf13, kb13, kspglass, kglass, kspplagio,
  kplagio, kspolive, kolive, ksppyrox, kpyrox, kspillite,
  killite, kspsmect, ksmect, kspkaoli, kkaoli];
```

```
bio_name := [sw01, sw02, sw03, sw04, sw05, sw06, sw07, sw08, sw09, sw10, sw11, sw12,      (8.4)
    sw13, sw14, sw15, sw16, sw17, sw18, sw19, sw20, sw21, sw22, sw23, sw24, sw25, sw26,
    sw27, sw28, sw29, sw30, sw31, sw32, xbiot, inita, ν, kmo2, kmno3, kmmno2, kmfeoh3,
    kmso4, knit, kmnox, kfemno2, kfeo2, kh2so2, kh2smno2, kh2sfeoh3, kaom, kaomo2, kfeso2,
    kmnco3precip, KsMnCO3, kfesprecip, kfesdiss, KsFeS, kfeco3precip, KsFeCO3, kcaldiss,
    kcalppt, karadis, karappt, kmgcdis, kmgcppt, kpyr, kfess0, kapa, po4_eq, kdis, h2sstar,
    ch4eq, kgas, kdi, ksnh4, kspo4, ksfp, ksfe, kf1, kb1, kf2, kb2, kf3, kb3, kf4, kb4, kf5, kb5, kf6,
    kb6, kf7, kb7, kf8, kb8, kspcal, kspara, kspmgc, keq1, keq2, keq3, keq4, kfemno2pr,
    kh2smno2pr, kmnage, kh2sfeoh3mr, kh2sfeoh3pr, kfeage, keq5, kBSidis, ad, bd, BSisat,
    ksfsi, kf9, kb9, eq1_al, eq2_al, eq3_al, eq4_al, kf10, kb10, kf11, kb11, kf12, kb12, kf13,
    kb13, kspglass, kglass, kspplagio, kplagio, kspolive, kolive, ksppyrox, kpyrox, kspillite,
    killite, kspsmect, ksmect, kspkaoli, kkaoli]
```

```
> bio_val :=[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, val_xbiot, val_inita, val_nu, val_kmo2, val_kmno3,
  val_kmmno2, val_kmfeoh3, val_kmso4, val_knit, val_kmnox,
  val_kfemno2, val_kfeo2, val_kh2so2, val_kh2smno2,
  val_kh2sfeoh3, val_kaom, val_kaomo2, val_kfeso2,
  val_kmnco3precip, val_KsMnCO3, val_kfesprecip,
  val_kfesdiss, val_KsFeS, val_kfeco3precip, val_KsFeCO3,
  val_kcaldiss, val_kcalppt, val_karadis, val_karappt,
  val_kmgcdis, val_kmgcppt, val_kpyr, val_kfess0,
  val_kapa, val_po4_eq, val_kdis, val_h2sstar, val_ch4eq,
  val_kgas, val_kdi, val_ksnh4, val_kspo4, val_ksfp,
  val_ksfe, val_kf1, val_kb1, val_kf2, val_kb2, val_kf3,
  val_kb3, val_kf4, val_kb4, val_kf5, val_kb5, val_kf6,
  val_kb6, val_kf7, val_kb7, val_kf8, val_kb8, val_kspcal,
  val_kspara, val_kspmgc, val_keq1, val_keq2, val_keq3,
  val_keq4, val_kfemno2pr, val_kh2smno2pr, val_kmnage,
  val_kh2sfeoh3mr, val_kh2sfeoh3pr, val_kfeage, val_keq5,
  val_kBSidis, val_ad, val_bd, val_BSisat, val_ksfsi,
  val_kf9, val_kb9, val_eq1_al, val_eq2_al, val_eq3_al,
val_eq4_al, val_kf10, val_kb10, val_kf11, val_kb11,
val_kf12, val_kb12, val_kf13, val_kb13, val_kspglass,
val_kglass, val_kspplagio, val_kplagio, val_kspolive,
val_kolive, val_ksppyrox, val_kpyrox, val_kspillite,
val_killite, val_kspsmect, val_ksmect, val_kspkaoli,
val_kkaoli];
```

$$\begin{aligned}
&\mathit{bio\_val} := [0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., \qquad \textbf{(8.5)}\\
&\quad 0., 0., 0., 0., 0., 0., 10.0, 10., 0.1, 8.0\ 10^{-9}, 5.0\ 10^{-9}, 0.0000050, 0.0000125, 1.000\ 10^{-7},\\
&\quad 1.0\ 10^{7}, 5.0\ 10^{7}, 3.0\ 10^{6}, 5.0\ 10^{9}, 1.0\ 10^{7}, 100., 100., 5.0\ 10^{6}, 1.0\ 10^{13}, 1.0\ 10^{9}, 1.\ 10^{-8},\\
&\quad 3.2\ 10^{-15}, 5.0\ 10^{-9}, 0.0010, 0.000008181818182, 1.0\ 10^{-9}, 4.0\ 10^{-15}, 0.1, 0.01, 0.1, 0.01,\\
&\quad 0.1, 0.01, 6.00\ 10^{7}, 25000., 1.0, 1.00\ 10^{-8}, 0., 0.00001, 10000., 0., 0.001, 1.6, 1.8, 100.0,\\
&\quad 400.0, 1.0, 1.014301296\ 10^{-9}, 1.0, 6.585101419\ 10^{-13}, 1.0, 1.792144094\ 10^{-10}, 1.0,\\
&\quad 1.698081511\ 10^{-12}, 1.8, 1.0, 1.6, 1.0, 100.0, 1.0, 400.0, 1.0, 4.398220198\ 10^{-13},\\
&\quad 6.870960123\ 10^{-13}, 1.112958166\ 10^{-11}, 1.014301296\ 10^{-9}, 6.585101419\ 10^{-13},\\
&\quad 1.792144094\ 10^{-10}, 1.698081511\ 10^{-12}, 300., 0.10, 0.6, 0.010, 0.00010, 0.6,\\
&\quad 1.503353334\ 10^{-20}, 0.001, 0.2, 0.05, 8.0\ 10^{-7}, 0., 0., 1.0, 5.046612976\ 10^{-9},\\
&\quad 3.647539469\ 10^{-19}, 9.727472238\ 10^{-29}, 2.606153550\ 10^{-37}, 1.0, 5.046612976\ 10^{-9}, 1.0,\\
&\quad 3.647539469\ 10^{-19}, 1.0, 9.727472238\ 10^{-29}, 1.0, 2.606153550\ 10^{-37}, 0.8241382458, 2.,\\
&\quad 5.649369748\ 10^{-34}, 0., 2.074913517\ 10^{32}, 0.00015, 8.241381150\ 10^{24}, 0.,\\
&\quad 1.241631886\ 10^{17}, 2.\ 10^{-10}, 4.560440081\ 10^{5}, 0., 1.499684836\ 10^{14}, 0.]
\end{aligned}$$

Switches

Switches can be used in the rate equations. Specify in **nswitches**, how many switches are in use, name them and define the switch expressions. The switch names must also appear in **bio_name** and must be assigned a dummy value there. The switch equals 1 if the switch expression is >0, 0 otherwise. To reference the coordinates in the domain, use x_pos, y_pos and z_pos.

```
> nswitches := 32;
```

$$\mathit{nswitches} := 32 \qquad \textbf{(8.1.1)}$$

```
> switchlist := [sw01, sw02, sw03, sw04, sw05, sw06,
  sw07, sw08, sw09, sw10, sw11, sw12, sw13, sw14, sw15,
  sw16, sw17, sw18, sw19, sw20, sw21, sw22, sw23, sw24,
  sw25, sw26, sw27, sw28, sw29, sw30, sw31, sw32] ;
```

$$\begin{aligned}
&\mathit{switchlist} := [\mathit{sw01}, \mathit{sw02}, \mathit{sw03}, \mathit{sw04}, \mathit{sw05}, \mathit{sw06}, \mathit{sw07}, \mathit{sw08}, \mathit{sw09}, \mathit{sw10}, \mathit{sw11}, \qquad \textbf{(8.1.2)}\\
&\quad \mathit{sw12}, \mathit{sw13}, \mathit{sw14}, \mathit{sw15}, \mathit{sw16}, \mathit{sw17}, \mathit{sw18}, \mathit{sw19}, \mathit{sw20}, \mathit{sw21}, \mathit{sw22}, \mathit{sw23}, \mathit{sw24},\\
&\quad \mathit{sw25}, \mathit{sw26}, \mathit{sw27}, \mathit{sw28}, \mathit{sw29}, \mathit{sw30}, \mathit{sw31}, \mathit{sw32}]
\end{aligned}$$

```
> switchcrit := [(xbiot-x_pos), (o2-kmo2), -(sw02-1.0),
  sw03*(no3-kmno3), -sw03*(sw04-1.0), sw05*(mno2-
kmmno2),-sw05*(sw06-1.0), sw07*(feoh3-kmfeoh3), -sw07*
(sw08-1.0), sw09*(so4-kmso4), -sw09*(sw10-1.0), ((mn*
co3/KsMnCO3)-1.0), ((fe*hs)/(KsFeS*hplus)-1.0), ((fe*
co3/KsFeCO3)-1.0), (1.0-(ca*co3/kspcal)), (po4-
po4_eq), (ch4-ch4eq), (ch4-0.0), (h2sstar-(h2s+hs)), (
(ca*co3/kspcal)-5.0), (1.0-(ca*co3/kspara)), ((ca*
co3/kspara)-5.0), (1.0-(ca*co3/kspmgc)), ((ca*
co3/kspmgc)-1.0), -(DSi-BSisat), (1.0 - DSi*al**
0.36/hplus**1.08/kspglass), (1.0 - DSi**2.3*aloh4**
1.7*na**0.3*ca**0.7/kspplagio), (1.0 - DSi*mg**1.6*fe*
*0.4/hplus**4/kspolive), (1.0 - DSi**2 * fe**0.46 *
mg**0.84 * ca**0.7 / hplus**4 / ksppyrox), (DSi**3.5 *
al**2.3 * kplus**0.6 * mg**0.25 / hplus**8 / kspillite
- 1.0), (ca**0.165 * mg**0.33 * al**1.7 * DSi**4 /
hplus**6 / kspsmect - 1.0), (al**2 * DSi**2 / hplus**6
/ kspkaoli - 1.0)];
```

$$\begin{aligned}
switchcrit := \Big[& xbiot - x\_pos,\ o2 - kmo2,\ 1.0 - sw02,\ sw03\ (no3 - kmno3), \\
& -sw03\ (sw04 - 1.0),\ sw05\ (mno2 - kmmno2),\ -sw05\ (sw06 - 1.0), \\
& sw07\ (feoh3 - kmfeoh3),\ -sw07\ (sw08 - 1.0),\ sw09\ (so4 - kmso4), \\
& -sw09\ (sw10 - 1.0),\ \frac{mn\ co3}{KsMnCO3} - 1.0,\ \frac{fe\ hs}{hplus\ KsFeS} - 1.0,\ \frac{fe\ co3}{KsFeCO3} - 1.0, \\
& 1.0 - \frac{ca\ co3}{kspcal},\ po4 - po4\_eq,\ ch4 - ch4eq,\ ch4,\ h2sstar - h2s - hs,\ \frac{ca\ co3}{kspcal} \\
& - 5.0,\ 1.0 - \frac{ca\ co3}{kspara},\ \frac{ca\ co3}{kspara} - 5.0,\ 1.0 - \frac{ca\ co3}{kspmgc},\ \frac{ca\ co3}{kspmgc} - 1.0,\ -DSi \\
& + BSisat,\ 1.0 - \frac{DSi\ al^{0.36}}{hplus^{1.08}\ kspglass},\ 1.0 - \frac{DSi^{2.3}\ aloh4^{1.7}\ na^{0.3}\ ca^{0.7}}{kspplagio},\ 1.0 \\
& - \frac{DSi\ mg^{1.6}\ fe^{0.4}}{hplus^{4}\ kspolive},\ 1.0 - \frac{DSi^{2}\ fe^{0.46}\ mg^{0.84}\ ca^{0.7}}{hplus^{4}\ ksppyrox},\ \frac{DSi^{3.5}\ al^{2.3}\ kplus^{0.6}\ mg^{0.25}}{hplus^{8}\ kspillite} \\
& - 1.0,\ \frac{ca^{0.165}\ mg^{0.33}\ al^{1.7}\ DSi^{4}}{hplus^{6}\ kspsmect} - 1.0,\ \frac{al^{2}\ DSi^{2}}{hplus^{6}\ kspkaoli} - 1.0\Big]
\end{aligned} \tag{8.1.3}$$

Transport - Molecular Diffusion

Spec ification of the molecular diffusion coefficients
diffdata: molecular diffusion coefficient at 0 degree celsius (cm^2/yr)

alphadata: temperature dependence of the diffusion coefficient (1/K)

the in situ molecular diffusion coefficient, corrected for tortuosity is calculated as:
D(T,sal) = [(0.95-0.001*sal)* D(T=0,sal=0)*(1 + muc*T[C])]/(1-ln (por^2))
example:
diffdata := [100., 304.,0.,0.,100.];
alphadata:= [0.006, 0.04,0.,0.,.0.05];
[ch2o, o2, no3, mno2, feoh3, so4, ch4, nh4, po4, mn, fe, h2s, hs, ch4g, h2co3, hco3, co3, boh4, boh3, hplus, caco3, ca, snh4, spo4, fes, feco3, s0, fes2, sfe, sfp, mnco3]

```
> diffdata := [0.0, 380.449545, 394.5878727, 0.0, 0.0,
  173.9205889, 263.9351889, 395.8731752, 112.35777,
  123.3890416, 136.2420668, 331.6080494, 392.0172677,
  5000.0, 320.0403267, 217.2161254, 176.0864448,
  96.29573485, 110.0522684, 600.0, 0.0, 150.3803945, 0.0,
  0.0, 0.0, 0.0, 173.9205889, 0.0, 0.0, 0.0, 0.0 , 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 112.26816, 0.0, 125.0, 0.0,
  87.9966, 87.9966, 140.6684, 140.6684, 140.6684, 0.0,
  0.0, 197.73072, 310.94496, 0.0, 0.0, 0.0, 0.0, 0.0];

  alphadata := [0.0, 0.06, 0.038, 0.0, 0.0, 0.045, 0.0520,
  0.041, 0.054, 0.05, 0.044, 0.06, 0.031, 0.0, 0.06,
  0.048, 0.047, 0.048, 0.048, 0.06, 0.0, 0.045, 0.0, 0.0,
  0.0, 0.0, 0.045, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0] ;
```

```
diffdata := [0., 380.449545, 394.5878727, 0., 0., 173.9205889, 263.9351889, 395.8731752,
    112.35777, 123.3890416, 136.2420668, 331.6080494, 392.0172677, 5000.0,
    320.0403267, 217.2161254, 176.0864448, 96.29573485, 110.0522684, 600.0, 0.,
    150.3803945, 0., 0., 0., 0., 173.9205889, 0., 0., 0., 0., 0., 0., 0., 0., 0., 112.26816, 0.,
    125.0, 0., 87.9966, 87.9966, 140.6684, 140.6684, 140.6684, 0., 0., 197.73072, 310.94496,
    0., 0., 0., 0., 0.]
alphadata := [0., 0.06, 0.038, 0., 0., 0.045, 0.0520, 0.041, 0.054, 0.05, 0.044, 0.06, 0.031, 0.,   (9.1)
    0.06, 0.048, 0.047, 0.048, 0.048, 0.06, 0., 0.045, 0., 0., 0., 0., 0.045, 0., 0., 0., 0., 0., 0., 0.,
    0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.]
```

Transport - Boundary Conditions

Specification of upper and lower boundary conditions for each species.
There are 3 options
0. kmnown concentration (Dirichlet, M/L^3)
1. kmnown concentration gradient (Neumann, M/L^3*L)

2. kmnown total (diffusive and advective) flux (Robin, M/L^2/T)
technical note: option 1 and 2 involve ghost points outside the domain. If the mixing parameters vary with depth, one needs to assign a mixing intensities at the ghost points. By default this is done by linear extrapolation. To ovrwrite this, the user has to edit gridsetup.f and advdiffcoeff.f (both at the bottom; explanations are given there)

type_up: array defining the type of condition for each species at the upper boundary (0, 1 or 2)

bnddata_up: array containing the values specified at the upper boundary.

type_down: array defining the type of condition for each species at the lower boundary

bnddata_down: array containing the values specified at the upper boundary.

example:
type_up := [0,0,2];
bnddata_up := [1.4,0.001,0.001];
type_down := [1,1,1];
bnddata_down := [0.,0.,0.];
[ch2o, o2, no3, mno2, feoh3, so4, ch4, nh4, po4, mn, fe, h2s, hs, ch4g, h2co3, hco3, co3, boh4, boh3, hplus, caco3, ca, snh4, spo4, fes, feco3, s0, fes2, sfe, sfp, mnco3] ;

```
> #set upper boundary cond TCup from given TAup and
  hplusup
  #by def: keq4=(hplus*BOH4)/BOH3; keq3=(hplus*HS)/H2S ;
  and keq5=hplus*OHminus
  #TAup and hplusup to be set by the user:
  TAup :=2.306e-6;  #mol/cm3
  TBup := 0.416e-6;
  TSup := 0.0;
  hplusup := 10**(-SWI_pH)*1e-3; ## value in brackets is
  'the actual pH-value #FSF

  term1 := -(val_keq4*TBup)/(hplusup+val_keq4)-(val_keq3*
  TSup)/(hplusup+val_keq3)-val_keq5/hplusup+hplusup;
  term2 := 1+val_keq1/hplusup+(val_keq1*val_keq2)/
  (hplusup*hplusup);
  term3 := val_keq1/hplusup+(2*val_keq1*val_keq2)/
  (hplusup*hplusup);
  TCup := (TAup+term1)*term2/term3;


  co3up := TCup*val_keq1*val_keq2/(val_keq1*val_keq2+
  val_keq1*hplusup+hplusup*hplusup);
  hco3up := TCup*val_keq1*hplusup/(val_keq1*val_keq2+
  val_keq1*hplusup+hplusup*hplusup);
  h2co3up := TCup - co3up - hco3up;

  boh4up := TBup*hplusup/(val_keq4+hplusup);
  boh3up := TBup-boh4up;

  ohup := val_keq5/hplusup;
  caup := 10.0e-6;        #report manually the value from
  bnddata_up
  Omegaup := (co3up*caup)/val_kspcal;


  ## Set upper boundary conditions for Aluminium species
  based on T_Al and pH ##
  ## Al eq constants LogK_Al defined in parameters above

  T_Al_up:= 200.0e-12; ## Total dissolved aluminium
  concentration at the SWI

  ## Al_DNT = common denominator for Al speciation
  Al_DNT := hplusup**4 + kk1_al*hplusup**3 + kk2_al*
  hplusup**2 + kk3_al*hplusup + kk4_al ;

  AlOH_up:= (T_Al_up*kk1_al*hplusup**3)/Al_DNT;

  AlOH2_up:= (T_Al_up*kk2_al*hplusup**2)/Al_DNT;

  AlOH3_up:= (T_Al_up*kk3_al*hplusup)/Al_DNT;

  AlOH4_up:= (T_Al_up*kk4_al)/Al_DNT;

  Al_up   := (T_Al_up*hplusup**4)/Al_DNT;

  type_up := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0] ;

  bnddata_up := [SWI_TOC, 195.0e-9, 17.3e-9, 1.36e-4,
  2.21e-4, 28.0e-6, 0.0, 0.0, 1.0e-9, 0.0, 0.0, 0.0, 0.0,
  0.0, h2co3up, hco3up, co3up, boh3up, boh4up, hplusup,
  1.78e-3, caup, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 1.36e-4, 2.21e-4, 2.21e-4, 9.53e-4, 0.0,
  0.523e-4, 1.5e-03, 17.3e-9, 0.0, Al_up, AlOH_up,
  AlOH2_up, AlOH3_up, AlOH4_up, 2.4e-3, 0.0, 469.1e-6,
  10.2e-6, 0.85e-3, 0.0, 0.0, 0.0, 0.0] ;

  type_down := [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
  1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
  1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
  1, 1, 1] ;

  bnddata_down := [0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0] ;
```

$$TAup := 0.000002306$$

$$TBup := 4.16\ 10^{-7}$$

$$TSup := 0.$$

$$hplusup := 7.943282347\ 10^{-12}$$

$$term1 := -7.515250686\ 10^{-8}$$

$$term2 := 139.2789082$$

$$term3 := 148.8648487$$

$$TCup := 0.000002087195237$$

$$co3up := 1.586379795\ 10^{-7}$$

$$hco3up := 0.000001913571534$$

$$h2co3up := 1.4985724\ 10^{-8}$$

$$boh4up := 3.427321595\ 10^{-7}$$

$$boh3up := 7.32678405\ 10^{-8}$$

$$ohup := 1.892609715\ 10^{-9}$$

$$caup := 0.0000100$$

$$Omegaup := 3.606867605$$

$$T\_Al\_up := 2.000\ 10^{-10}$$

$$Al\_DNT := 2.614135833\ 10^{-37}$$

$$AlOH\_up := 1.935093015\ 10^{-15}$$

$$AlOH2\_up := 1.760766819\ 10^{-14}$$

$$AlOH3\_up := 5.911556509\ 10^{-13}$$

$$AlOH4\_up := 1.993892985\ 10^{-10}$$

$$Al\_up := 3.045803248\ 10^{-18}$$

$$type\_up := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$$

bnddata_up := [0.002083333333, 1.950 10^{-7}, 1.73 10^{-8}, 0.000136, 0.000221, 0.0000280, 0., 0., 1.0 10^{-9}, 0., 0., 0., 0., 0., 1.4985724 10^{-8}, 0.000001913571534, 1.586379795 10^{-7}, 7.32678405 10^{-8}, 3.427321595 10^{-7}, 7.943282347 10^{-12}, 0.00178, 0.0000100, 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.000136, 0.000221, 0.000221, 0.000953, 0., 0.0000523, 0.0015, 1.73 10^{-8}, 0., 3.045803248 10^{-18}, 1.935093015 10^{-15}, 1.760766819 10^{-14}, 5.911556509 10^{-13}, 1.993892985 10^{-10}, 0.0024, 0., 0.0004691, 0.0000102, 0.00085, 0., 0., 0., 0.]

type_down := [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]

bnddata_down := [0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.] **(10.1)**

Transport - Identify species that are not transported

nrnotransp: number of species that are not getting transported at all
notransp: list of species that are not getting transported at all (i.e. for which the above defined dispersion and advection velocities are not used!)

example:
nrnotransp:=3;
notransp := [1,3,4];

```
> nrnotransp := 1;
  listnotransp := [20] ;
```

nrnotransp := 1
listnotransp := [20] **(11.1)**

Initial conditions

vic: options to select initial guesses
- 1: read from a file "initialconc.txt", which contains the columns z, conc(species1), conc(species2)....
- 2: fixed concentration, defined in the array **iniconc**
- 3: individual files for each species. listinput contains the species number (lenght: number of species), filenames are given in "file_in_names".inp, containing in column 1 the conc, in column 2 depth.

example (only relevant input data is given for each option, assuming 17 species):
NOTE that you have to provide something for all ncomp species in the arrays iniconc, listinput and file_in_names, EVEN IF YOU DON'T USE IT WITH THE OPTION YOU SELECTED
vic:=1;

vic:=2;iniconc:=[0.,2.,...];
vic:=3;listinput:=[1,2,...,17];file_in_names:=[o2,no3,...,sp17];

```
> vic := 2 ;
  iniconc := [SWI_TOC, 195.0e-9, 17.3e-9, 0.0, 0.0,
  28.0e-6, 0.0, 0.0, 1.0e-9, 0.0, 0.0, 0.0, 0.0, 0.0,
  h2co3up, hco3up, co3up, boh3up, boh4up, hplusup,
  1.78e-3, caup, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
  0.0, 0.0, 0.0, 0.0, 0.0, 9.53e-4, 0.0, 0.523e-4,
  1.5e-03, 17.3e-9, 0.0, Al_up, AlOH_up, AlOH2_up,
  AlOH3_up, AlOH4_up, 0.72e-3, 0.0, 469.1e-6, 10.2e-6,
  0.17e-3, 0.0, 0.0, 0.0, 0.0] ;

  listinput := [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13,
  14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27,
  28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41,
  42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55]
  ;

  file_in_names := [dummy_1, dummy_2, dummy_3, dummy_4,
  dummy_5, dummy_6, dummy_7, dummy_8, dummy_9, dummy_10,
  dummy_11, dummy_12, dummy_13, dummy_14, dummy_15,
  dummy_16, dummy_17, dummy_18, dummy_19, dummy_20,
  dummy_21, dummy_22, dummy_23, dummy_24, dummy_25,
  dummy_26, dummy_27, dummy_28, dummy_29, dummy_30,
  dummy_31, dummy_32, dummy_33, dummy_34, dummy_35,
  dummy_36, dummy_37, dummy_38, dummy_39, dummy_40,
  dummy_41, dummy_42, dummy_43, dummy_44, dummy_45,
  dummy_46, dummy_47, dummy_48, dummy_49,  dummy_50,
  dummy_51, dummy_52, dummy_53, dummy_54, dummy_55];
```

vic := 2

iniconc := [0.002083333333, 1.950 10^{-7}, 1.73 10^{-8}, 0., 0., 0.0000280, 0., 0., 1.0 10^{-9}, 0., 0.,
0., 0., 0., 1.4985724 10^{-8}, 0.000001913571534, 1.586379795 10^{-7}, 7.32678405 10^{-8},
3.427321595 10^{-7}, 7.943282347 10^{-12}, 0.00178, 0.0000100, 0., 0., 0., 0., 0., 0., 0., 0., 0.,
0., 0., 0., 0., 0.000953, 0., 0.0000523, 0.0015, 1.73 10^{-8}, 0., 3.045803248 10^{-18},
1.935093015 10^{-15}, 1.760766819 10^{-14}, 5.911556509 10^{-13}, 1.993892985 10^{-10}, 0.00072,
0., 0.0004691, 0.0000102, 0.00017, 0., 0., 0., 0.]

listinput := [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24,
25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47,
48, 49, 50, 51, 52, 53, 54, 55]

file_in_names := [*dummy_1*, *dummy_2*, *dummy_3*, *dummy_4*, *dummy_5*, *dummy_6*, **(12.1)**
dummy_7, *dummy_8*, *dummy_9*, *dummy_10*, *dummy_11*, *dummy_12*, *dummy_13*,
dummy_14, *dummy_15*, *dummy_16*, *dummy_17*, *dummy_18*, *dummy_19*, *dummy_20*,
dummy_21, *dummy_22*, *dummy_23*, *dummy_24*, *dummy_25*, *dummy_26*, *dummy_27*,
dummy_28, *dummy_29*, *dummy_30*, *dummy_31*, *dummy_32*, *dummy_33*, *dummy_34*,

dummy_35, dummy_36, dummy_37, dummy_38, dummy_39, dummy_40, dummy_41,
dummy_42, dummy_43, dummy_44, dummy_45, dummy_46, dummy_47, dummy_48,
dummy_49, dummy_50, dummy_51, dummy_52, dummy_53, dummy_54, dummy_55]

Output

noutput: number of species to be printed
nroutput: number of rates to be printed
listoutput: species number to print
listroutput: rate number to print
file_names: Respective file name for each of the species to print
file_rnames: Respective file name for each of the rates to print
time_iniout: First time (in years) for which a printout is requested
time_intvout: time interval (in years) at which the printing is performed, starting from time_iniout

example:
noutput:=4;
listoutput:=[1,2,3,5];
file_names:=[o2, so4, MnOx, hco3];
time_iniout:=10.;
time_intvout:= 100.;

```
> noutput := 55;
  nroutput := 60;
  listoutput := [1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,
  17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,
  35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,
  53,54,55] ;

  listroutput := [1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,
  17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,
  35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,
  53,54,55,56,57,58,59,60] ;

  file_names := [ch2o, zzo2, zno3, mno2, feoh3, zso4,
  zch4, znh4, zpo4, zzmn, zzfe, zh2s, zzhs, ch4g, h2co,
  hco3, zco3, boh4, boh3, zzph, caco, zzca, snh4, spo4,
  zfes, feco, zzs0, fes2, zsfe, zfp, mnco, age, mno2pr,
  feoh3mr, feoh3pr, arago, mgcal, mg, BSi, DSi, sfSi, al,
  aloh, aloh2, aloh3, aloh4, glass, plagio, na, kplus,
  olive, pyrox, illite, smect, kaoli] ;

  file_rnames := [xrate1, xrate2, xrate3, xrate4, xrate5,
  xrate6, xrate7, xrate8, xrate9, xrate10, xrate11,
  xrate12, xrate13, xrate14, xrate15, xrate16, xrate17,
  xrate18, xrate19, xrate20, xrate21, xrate22, xrate23,
  xrate24, xrate25, xrate26, xrate27, xrate28, xrate29,
  xrate30, xrate31, xrate32, xrate33, xrate34, xrate35,
  xrate36, xrate37, xrate38,xrate39, xrate40, xrate41,
  xrate42,xrate43,xrate44,xrate45,xrate46,xrate47,xrate48,
  xrate49,xrate50,xrate51,xrate52,xrate53,xrate54,xrate55,
  xrate56,xrate57,xrate58,xrate59,xrate60] ;

  time_iniout := 0.9*tot_time ;
  time_intvout := tot_time/10.0 ;
```

```
                          noutput := 55
                          nroutput := 60
listoutput := [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24,
    25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47,
    48, 49, 50, 51, 52, 53, 54, 55]
listroutput := [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23,
    24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46,
    47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]
file_names := [ch2o, zzo2, zno3, mno2, feoh3, zso4, zch4, znh4, zpo4, zzmn, zzfe, zh2s,
    zzhs, ch4g, h2co, hco3, zco3, boh4, boh3, zzph, caco, zzca, snh4, spo4, zfes, feco, zzs0,
    fes2, zsfe, zfp, mnco, age, mno2pr, feoh3mr, feoh3pr, arago, mgcal, mg, BSi, DSi, sfSi,
    al, aloh, aloh2, aloh3, aloh4, glass, plagio, na, kplus, olive, pyrox, illite, smect, kaoli]
file_rnames := [xrate1, xrate2, xrate3, xrate4, xrate5, xrate6, xrate7, xrate8, xrate9,
    xrate10, xrate11, xrate12, xrate13, xrate14, xrate15, xrate16, xrate17, xrate18, xrate19,
    xrate20, xrate21, xrate22, xrate23, xrate24, xrate25, xrate26, xrate27, xrate28, xrate29,
    xrate30, xrate31, xrate32, xrate33, xrate34, xrate35, xrate36, xrate37, xrate38, xrate39,
    xrate40, xrate41, xrate42, xrate43, xrate44, xrate45, xrate46, xrate47, xrate48, xrate49,
    xrate50, xrate51, xrate52, xrate53, xrate54, xrate55, xrate56, xrate57, xrate58, xrate59,
    xrate60]
                    time_iniout := 361.4400000
                    time_intvout := 40.16000000                          (13.1)
```

Optimization

there are several optimization options available. here you can specify what needs to be optimized and where the data is stored. to identify what kind of algorithm you want to use please select the appropriate options in drivervalues.f

nopt_v: number of parameters to be optimized

ntopt_v: number of time points where measurements are available

nparam_opt: total number of parameters. can include the nparam but also the physical parameters.

maxxmeas_v: maximum number of depth points at any given time measured (used to make array sizes)

```
maxspmeas_v: maximum number of species measured at any given time
(used to make array sizes)
opt_name: names of the parameters. they have to match the names
given above, so best you make a copy paste!
idpar_v: identify the parameters to be optimized from the parameter
list opt_name
filemeas_name: name of the files containing the measured data
if nopt_v is set to 0 then the rest of the input doesn't matter
```

example:
nopt_v := 2; # number of parameters to be optimized
ntopt_v := 3; # number of timepoints with measurements
nparam_opt := nparam; # total number of parameters, set equal to all parameters except physcial ones
maxxmeas_v:=20; # maximum 20 points in a profile at any given time
maxspmeas_v :=2; # maximum 2 species measured at one timepoint
opt_name := bioname; # (note that this does not include the physical parameters! if you want them to be adapted you need to specify them explicitly)
idpar_v:= [1,3]; # optimize parameters 1 and 3 in the above list
filemeas_name:= [meas1.dat, meas2.dat, meas3.dat]; # filenames with measurements at timepoints

```
> nopt_v := 0 ;
  ntopt_v := 0 ;
  nparam_opt := 0 ;
  maxxmeas_v := 0;
  maxspmeas_v := 0;
  opt_name := [];
  idpar_v := [];
  filemeas_name := [];
```

$$\begin{gathered} nopt\_v := 0 \\ ntopt\_v := 0 \\ nparam\_opt := 0 \\ maxxmeas\_v := 0 \\ maxspmeas\_v := 0 \\ opt\_name := [\ ] \\ idpar\_v := [\ ] \\ filemeas\_name := [\ ] \end{gathered} \tag{14.1}$$

Maple specific info

```
dir_f: directory where the FORTRAN routines and Maple spread.m files
are parsed
format Mac: "Macinthosh HD:UU:...:code"
format PC: "C:\\maple\\...\\code"
```

WAS: dir_f := "C:\\Dokumente und Einstellungen\\centler\\Desktop\\Labor\\Simulations":
currentdir(dir_f):
save "spread.m" ;

```
> dir_f := "C:/BRNS/BRNS_source_Sep2018" :
  currentdir(dir_f) :
  parse(sprintf("save %q,\"spread.m\";",anames()),
  statement) ;
> "now execute processor - make sure the directories are
  set correctly";
```

```
           "now execute processor - make sure the directories are set correctly"                (15.1)
```