

ERGOM (SED 1.0) Documentation

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1 Introduction

This is an automatically generated description of the ecosystem model ERGOM version SED 1.0 . Model formulation is provided by text files in compliance with the rules of the Code Generation Tool (CGT) by Hagen Radtke (see www.ergom.net).

The model consists of a set of state variables, the so called tracers. They are defined and described in Chapter 2.

The following Chapter 3 is the main part of this model description document, since it describes the processes which change the tracer concentrations over time. They are defined analog to chemical processes, two components describe their action:

- A process equation which describes the transformation from precursors (on the left-hand side) to products (on the right-hand side), and
- a turnover rate, describing how fast the process runs.

The rate at which a process changes a tracer can then easily be determined by multiplying the process turnover rate with the stoichiometric ratio in which it consumes or produces the tracer according to the reaction equation.

We structured the documentation into different process types to keep the documentation readable. So all processes belonging to one type (e.g. phytoplankton assimilation) are listed together with their constants and auxiliary variables they depend on. This means that some constants, such as stoichiometric ratios, will occur several times in this documentation, making it longer. We take this compromise for the sake of readability, keeping all information required to understand a specific process in its own section.

The classical way of describing an ecosystem model is by giving the tracer equations. We still do this in the last chapter for the sake of completeness, but rather suggest to stick to Chapter 3 to understand the model, and see Chapter 4 as a supplement only.

2 Description of model state variables (tracers)

Tracers in the water column only	
t_don	autochthonous dissolved organic nitrogen (mol/kg)
t_spp	small-cell phytoplankton (mol/kg)
opacity =	30.0 m ² /mol
t_zoo	zooplankton (mol/kg)
t_ipw	suspended iron phosphate (mol/kg)
vertical speed =	-1.0 m/day
t_lpp	large-cell phytoplankton (mol/kg)
vertical speed =	-0.5 m/day
opacity =	30.0 m ² /mol
t_cya	diazotroph cyanobacteria (mol/kg)
vertical speed =	0.1 m/day
opacity =	30.0 m ² /mol
t_det_1	detritus fractions_1 (mol/kg)
vertical speed =	-4.5 m/day
opacity =	45.0 m ² /mol
t_det_2	detritus fractions_2 (mol/kg)
vertical speed =	-4.5 m/day
opacity =	45.0 m ² /mol
t_det_3	detritus fractions_3 (mol/kg)
vertical speed =	-4.5 m/day
opacity =	45.0 m ² /mol
t_det_4	detritus fractions_4 (mol/kg)
vertical speed =	-4.5 m/day
opacity =	45.0 m ² /mol
t_det_5	detritus fractions_5 (mol/kg)
vertical speed =	-4.5 m/day
opacity =	45.0 m ² /mol
continued on next page...	

Tracers in the water column only, continued from previous page	
t_det_6	detritus fractions__6 (mol/kg)
vertical speed =	-4.5 m/day
opacity =	45.0 m ² /mol
t_ihw	suspended iron hydroxide (mol/kg)
vertical speed =	-1.0 m/day
t_mow	suspended manganese oxide (mol/kg)
vertical speed =	-1.0 m/day
t_detp_1	phosphate in detritus fractions__1 (mol/kg)
vertical speed =	-4.5 m/day
t_detp_2	phosphate in detritus fractions__2 (mol/kg)
vertical speed =	-4.5 m/day
t_detp_3	phosphate in detritus fractions__3 (mol/kg)
vertical speed =	-4.5 m/day
t_detp_4	phosphate in detritus fractions__4 (mol/kg)
vertical speed =	-4.5 m/day
t_detp_5	phosphate in detritus fractions__5 (mol/kg)
vertical speed =	-4.5 m/day
t_detp_6	phosphate in detritus fractions__6 (mol/kg)
vertical speed =	-4.5 m/day
t_poc	particulate organic carbon (mol/kg)
vertical speed =	-0.5 m/day
Tracers in water and pore water	
t_n2	dissolved molecular nitrogen (mol/kg)
t_o2	dissolved molecular oxygen (mol/kg)
t_dic	dissolved inorganic carbon (mol/kg)
t_nh4	ammonium (mol/kg)
t_no3	nitrate (mol/kg)
t_po4	phosphate (mol/kg)
t_h2s	hydrogen sulfide (mol/kg)
continued on next page...	

Tracers in water and pore water, continued from previous page	
t_sul	sulfur (mol/kg)
t_alk	total alkalinity (mol/kg)
t_so4	sulfate (mol/kg)
t_fe2	ferrous iron (mol/kg)
t_ca2	dissolved calcium (mol/kg)
t_mn2	dissolved manganese-II (mol/kg)
t_ohm_quickdiff	OH- ions with realistically quick diffusion (mol/kg)
t_ohm_slowdiff	OH- ions which move unrealistically slow with alkalinity (mol/kg)
t_sil	silicate (mol/kg)
Tracers in fluff and sediment	
t_ips	iron-bound phosphate in the sediment (mol/m ²)
t_sed_1	sedimentary detritus fractions_1 (mol/m ²)
t_sed_2	sedimentary detritus fractions_2 (mol/m ²)
t_sed_3	sedimentary detritus fractions_3 (mol/m ²)
t_sed_4	sedimentary detritus fractions_4 (mol/m ²)
t_sed_5	sedimentary detritus fractions_5 (mol/m ²)
t_sed_6	sedimentary detritus fractions_6 (mol/m ²)
t_ihs	iron hydroxide in the sediment (mol/m ²)
t_pyr	pyrite (mol/m ²)
t_ims	iron monosulphide (mol/m ²)
t_mos	manganese oxide in the sediments (mol/m ²)
t_rho	rhodochrosite (mol/m ²)
continued on next page...	

Tracers in fluff and sediment, continued from previous page	
t_iim	iron-II adsorbed to illite-montmorillonite mixed layer minerals (mol/m ²)
t_i3i	potentially reducible iron-III in illite-montmorillonite mixed layer minerals (mol/m ²)
t_ihc	iron hydroxide in the sediment - crystalline phase (mol/m ²)
t_pim	phosphate adsorbed to illite-montmorillonite (mol/m ²)
t_aim	ammonium adsorbed to illite-montmorillonite (mol/m ²)
t_sedp_1	phosphate in sedimentary detritus fractions_1 (mol/m ²)
t_sedp_2	phosphate in sedimentary detritus fractions_2 (mol/m ²)
t_sedp_3	phosphate in sedimentary detritus fractions_3 (mol/m ²)
t_sedp_4	phosphate in sedimentary detritus fractions_4 (mol/m ²)
t_sedp_5	phosphate in sedimentary detritus fractions_5 (mol/m ²)
t_sedp_6	phosphate in sedimentary detritus fractions_6 (mol/m ²)

3 Description of model processes, ordered by process type

3.1 Process type BGC/benthic/bioresuspension

Processes
bio resuspension of sedimentary detritus (index 1 to 6) (sediment only) [mol/m ² /day] t_sed_1 -> t_det_1 p_sed_1_biores_det = (r_biores*t_sed_1*(1.0-cgt_in_sediment))*lim_t_o2_7* = lim_t_sed_1_22
bio resuspension of sedimentary detritus (index 1 to 6) (sediment only) [mol/m ² /day] t_sedp_1 -> t_detp_1 (r_biores*t_sedp_1*(1.0-cgt_in_sediment))*lim_t_o2_7* p_sedp_1_biores_detplim_t_sedp_1_46 =
bio resuspension of iron PO4 (sediment only) [mol/m ² /day] t_ips -> t_ipw p_ips_biores_ipw = (r_biores*t_ips*(1.0-cgt_in_sediment))*lim_t_o2_7* lim_t_ips_52
bio resuspension of iron hydroxyde (sediment only) [mol/m ² /day] t_ihs -> t_ihw p_ihs_biores_ihw = (r_biores*t_ihs*(1.0-cgt_in_sediment))*lim_t_o2_7* lim_t_ihs_53
bio resuspension of iron hydroxyde (sediment only) [mol/m ² /day] t_ihc -> t_ihw p_ihc_biores_ihw = (r_biores*t_ihc*(1.0-cgt_in_sediment))*lim_t_o2_7* lim_t_ihc_54
bio resuspension of iron monosulfide (sediment only) [mol/m ² /day] 0.125*t_so4 + 0.25*h3oplu + 2.25*h2o + t_ims -> t_ihw + 1.125*t_h2s p_ims_biores_ihw = (r_biores*t_ims*(1.0-cgt_in_sediment))*lim_t_o2_7* lim_t_so4_28*lim_t_ims_57
bio resuspension of pyrite (sediment only) [mol/m ² /day]
continued on next page...

Processes, continued from previous page	
$t_{\text{pyr}} + 3.75 \cdot h_{2o} \rightarrow 0.25 \cdot h_{3oplus} + 1.875 \cdot t_{h2s} + 0.125 \cdot t_{so4} + t_{ihw}$	
$p_{\text{pyr_biores_ihw}} = (r_{\text{biores}} \cdot t_{\text{pyr}} \cdot (1.0 - \text{cgt_in_sediment})) \cdot \text{lim_t_o2_7} \cdot \text{lim_t_pyr_58}$	
bio resuspension of manganese oxide (sediment only) [mol/m²/day]	
$t_{\text{mos}} \rightarrow t_{\text{mow}}$	
$p_{\text{mos_biores_mow}} = (r_{\text{biores}} \cdot t_{\text{mos}} \cdot (1.0 - \text{cgt_in_sediment})) \cdot \text{lim_t_o2_7} \cdot \text{lim_t_mos_59}$	
bio resuspension of rhodochrosite (sediment only) [mol/m²/day]	
$0.25 \cdot t_{so4} + 1.7 \cdot h_{3oplus} + t_{rho} \rightarrow t_{mow} + 0.25 \cdot t_{h2s} + 2.3 \cdot h_{2o} + 0.6 \cdot t_{ca2} + 1.6 \cdot t_{dic}$	
$p_{\text{rho_biores_mow}} = (r_{\text{biores}} \cdot t_{rho} \cdot (1.0 - \text{cgt_in_sediment})) \cdot \text{lim_t_o2_7} \cdot \text{lim_t_so4_28} \cdot \text{lim_t_rho_60}$	
bio resuspension of iron in clay minerals (sediment only) [mol/m²/day]	
$0.125 \cdot t_{so4} + 0.25 \cdot h_{2o} + 0.25 \cdot h_{3oplus} + t_{iim} \rightarrow t_{ihw} + 0.125 \cdot t_{h2s}$	
$p_{\text{iim_biores_ihw}} = (r_{\text{biores}} \cdot t_{iim} \cdot (1.0 - \text{cgt_in_sediment})) \cdot \text{lim_t_o2_7} \cdot \text{lim_t_so4_28} \cdot \text{lim_t_iim_61}$	
Auxiliary variables	
Constants	
oxygen half-saturation constant for recycling of sediment detritus using oxygen [mol/kg]	
$o2_{\text{min_sed_resp}} = 2.0E-5$	
bio-resuspension rate [1/day]	
$r_{\text{biores}} = 0.03$	
Process limitation factors	
$\text{lim_t_o2_7} = t_{o2} \cdot t_{o2} / (t_{o2} \cdot t_{o2} + o2_{\text{min_sed_resp}} \cdot o2_{\text{min_sed_resp}})$	
$\text{lim_t_ips_52} = \text{theta}(t_{\text{ips}} - 0.0)$	
$\text{lim_t_so4_28} = \text{theta}(t_{so4} - 0.0)$	
$\text{lim_t_sed_1_22} = \text{theta}(t_{\text{sed_1}} - 0.0)$	
$\text{lim_t_sed_2_23} = \text{theta}(t_{\text{sed_2}} - 0.0)$	
$\text{lim_t_sed_3_24} = \text{theta}(t_{\text{sed_3}} - 0.0)$	
$\text{lim_t_sed_4_25} = \text{theta}(t_{\text{sed_4}} - 0.0)$	
$\text{lim_t_sed_5_26} = \text{theta}(t_{\text{sed_5}} - 0.0)$	
continued on next page...	

Process limitation factors, continued from previous page

```
lim_t_sed_6_27 = theta(t_sed_6-0.0)
```

```
lim_t_ihs_53 = theta(t_ihs-0.0)
```

```
lim_t_pyr_58 = theta(t_pyr-0.0)
```

```
lim_t_ims_57 = theta(t_ims-0.0)
```

```
lim_t_mos_59 = theta(t_mos-0.0)
```

```
lim_t_rho_60 = theta(t_rho-0.0)
```

```
lim_t_iim_61 = theta(t_iim-0.0)
```

```
lim_t_ihc_54 = theta(t_ihc-0.0)
```

```
lim_t_sedp_1_46 = theta(t_sedp_1-0.0)
```

```
lim_t_sedp_2_47 = theta(t_sedp_2-0.0)
```

```
lim_t_sedp_3_48 = theta(t_sedp_3-0.0)
```

```
lim_t_sedp_4_49 = theta(t_sedp_4-0.0)
```

```
lim_t_sedp_5_50 = theta(t_sedp_5-0.0)
```

```
lim_t_sedp_6_51 = theta(t_sedp_6-0.0)
```

3.2 Process type BGC/benthic/mineralization

Processes
<p>recycling of sedimentary detritus to ammonium using oxygen (respiration) (index 1 to 6) (sediment only) [mol/m²/day]</p> $\text{h3oplus} + \text{rfr_pc_enrichment_det} * 6.625 * \text{t_o2} + \text{t_sed_1} \rightarrow \text{rfr_si} * \text{t_sil} + (1.0 + 6.625 * \text{rfr_pc_enrichment_det}) * \text{h2o} + \text{rfr_pc_enrichment_det} * \text{rfr_c} * \text{t_dic} + \text{t_nh4}$ $\text{p_sed_1_resp_nh4} = (\text{t_sed_1} * \text{r_det_1_rec} * \exp(\text{q10_det_rec} * \text{cgt_temp})) * \text{lim_t_o2_12} * \text{lim_t_sed_1_22}$
<p>recycling of sedimentary detritus to ammonium using nitrate (denitrification) (index 1 to 6) (sediment only) [mol/m²/day]</p> $\text{t_sed_1} + (1.0 + 5.3 * \text{rfr_pc_enrichment_det}) * \text{h3oplus} + \text{rfr_pc_enrichment_det} * 5.3 * \text{t_no3} \rightarrow \text{rfr_pc_enrichment_det} * \text{rfr_c} * \text{t_dic} + \text{t_nh4} + \text{rfr_pc_enrichment_det} * 2.65 * \text{t_n2} + (1.0 + 14.575 * \text{rfr_pc_enrichment_det}) * \text{h2o} + \text{rfr_si} * \text{t_sil}$ $\text{p_sed_1_denit_nh4} = (\text{t_sed_1} * \text{r_det_1_rec} * \exp(\text{q10_det_rec} * \text{cgt_temp})) * \text{pH_inhibition_ironred} * (1.0 - \text{lim_t_o2_2}) * \text{lim_t_no3_3} * \text{lim_t_sed_1_22}$
<p>recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (index 1 to 6) (sediment only) [mol/m²/day]</p> $(1.0 + \text{rfr_pc_enrichment_det} * 6.625) * \text{h3oplus} + \text{rfr_pc_enrichment_det} * 3.3125 * \text{t_so4} + \text{t_sed_1} \rightarrow (1.0 + \text{rfr_pc_enrichment_det} * 13.25) * \text{h2o} + \text{rfr_pc_enrichment_det} * 3.3125 * \text{t_h2s} + \text{rfr_pc_enrichment_det} * \text{rfr_c} * \text{t_dic} + \text{t_nh4} + \text{rfr_si} * \text{t_sil}$ $\text{p_sed_1_sulf_nh4} = (\text{t_sed_1} * \text{r_det_1_rec} * \exp(\text{q10_det_rec} * \text{cgt_temp})) * \max(\text{t_so4}, 0.0) / (\max(\text{t_so4}, 0.0) + \text{so4_min_det_sulf}) * \text{pH_inhibition_ironred} * (1.0 - \text{lim_t_o2_2}) * (1.0 - \text{lim_t_no3_3}) * (1.0 - \text{lim_t_ihs_4}) * (1.0 - \text{lim_t_mos_5}) * (1.0 - \text{lim_t_i3i_6}) * \text{lim_t_so4_28} * \text{lim_t_sed_1_22}$
<p>recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction) (index 1 to 6) (sediment only) [mol/m²/day]</p> $\text{t_sed_1} + (1.0 + 26.5 * \text{rfr_pc_enrichment_det}) * \text{h3oplus} + 13.25 * \text{rfr_pc_enrichment_det} * \text{t_mos} \rightarrow \text{rfr_si} * \text{t_sil} + (1.0 + 46.375 * \text{rfr_pc_enrichment_det}) * \text{h2o} + 13.25 * \text{rfr_pc_enrichment_det} * \text{t_mn2} + \text{t_nh4} + \text{rfr_pc_enrichment_det} * \text{rfr_c} * \text{t_dic}$ $\text{p_sed_1_mnred_mn2} = (\text{t_sed_1} * \text{r_det_1_rec} * \exp(\text{q10_det_rec} * \text{cgt_temp})) * \text{pH_inhibition_ironred} * (1.0 - \text{lim_t_o2_2}) * (1.0 - \text{lim_t_no3_3}) * \text{lim_t_mos_5} * \text{lim_t_sed_1_22}$
<p>recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (index 1 to 6) (sediment only) [mol/m²/day]</p> $26.5 * \text{rfr_pc_enrichment_det} * \text{t_h2s} + 26.5 * \text{rfr_pc_enrichment_det} * \text{t_ihs} + \text{h3oplus} + \text{t_sed_1} \rightarrow \text{rfr_pc_enrichment_det} * \text{rfr_c} * \text{t_dic} + \text{t_nh4} + 26.5 * \text{rfr_pc_enrichment_det} * \text{t_ims} + (1.0 + 72.875 * \text{rfr_pc_enrichment_det}) * \text{h2o} + \text{rfr_si} * \text{t_sil}$
continued on next page...

Processes, continued from previous page

```
p_sed_1_irred_ims = (t_sed_1*r_det_1_rec*exp(q10_det_rec*cgt_temp)*
    t_ihs/max(fe3_sed,epsilon)*fe2_ims_is_smallest*
    pH_inhibition_ironred)*(1.0-lim_t_o2_2)*(1.0-lim_t_no3_3)*
    (1.0-lim_t_mos_5)*lim_t_ihs_4*lim_t_h2s_29*lim_t_sed_1_22
```

recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction) (index 1 to 6) (sediment only) [mol/m²/day]

```
26.5*rfr_pc_enrichment_det*t_ips + (1.0+159.1875*rfr_pc_enrichment_det)*h3oplus
+ 86.125*rfr_pc_enrichment_det*h2o + t_sed_1 + 26.5*rfr_pc_enrichment_det*t_h2s
-> rfr_si*t_sil + rfr_pc_enrichment_det*rfr_c*t_dic + t_nh4 + 26.5*
rfr_pc_enrichment_det*t_ims + h2o + 26.5*rfr_pc_enrichment_det*t_po4 +
238.6875*rfr_pc_enrichment_det*h3oplus
    (t_sed_1*r_det_1_rec*exp(q10_det_rec*cgt_temp)*
p_sed_1_irredips_imst_ips/max(fe3_sed,epsilon)*fe2_ims_is_smallest*
=
    pH_inhibition_ironred)*(1.0-lim_t_o2_2)*(1.0-lim_t_no3_3)*
    (1.0-lim_t_mos_5)*lim_t_ihs_4*lim_t_ips_52*lim_t_sed_1_22*
    lim_t_h2s_29
```

recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (index 1 to 6) (sediment only) [mol/m²/day]

```
53.0*rfr_pc_enrichment_det*h3oplus + t_sed_1 + h3oplus + 26.5*
rfr_pc_enrichment_det*t_ihs + 53*rfr_pc_enrichment_det*ohminus -> rfr_si*t_sil
+ 125.875*rfr_pc_enrichment_det*h2o + h2o + 26.5*rfr_pc_enrichment_det*t_iim +
t_nh4 + rfr_pc_enrichment_det*rfr_c*t_dic
p_sed_1_irred_iim = (t_sed_1*r_det_1_rec*exp(q10_det_rec*cgt_temp)*
    t_ihs/max(fe3_sed,epsilon)*fe2_iim_is_smallest*
    pH_inhibition_ironred)*(1.0-lim_t_o2_2)*(1.0-lim_t_no3_3)*
    (1.0-lim_t_mos_5)*lim_t_ihs_4*lim_t_sed_1_22
```

recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (index 1 to 6) (sediment only) [mol/m²/day]

```
26.5*rfr_pc_enrichment_det*t_ips + t_sed_1 + (1+53.0*rfr_pc_enrichment_det)*
h3oplus + 33.125*rfr_pc_enrichment_det*h2o + 53*rfr_pc_enrichment_det*ohminus -
> rfr_si*t_sil + rfr_pc_enrichment_det*rfr_c*t_dic + rfr_pc_enrichment_det*
26.5*t_po4 + t_nh4 + 26.5*rfr_pc_enrichment_det*t_iim + h2o + 79.5*
rfr_pc_enrichment_det*h3oplus
    (t_sed_1*r_det_1_rec*exp(q10_det_rec*cgt_temp)*
p_sed_1_irredips_iimt_ips/max(fe3_sed,epsilon)*fe2_iim_is_smallest*
=
    pH_inhibition_ironred)*(1.0-lim_t_o2_2)*(1.0-lim_t_no3_3)*
    (1.0-lim_t_mos_5)*lim_t_ihs_4*lim_t_ips_52*lim_t_sed_1_22
```

recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction) (index 1 to 6) (sediment only) [mol/m²/day]

continued on next page...

Processes, continued from previous page

```

t_sed_1 + h3oplus + 26.5*rfr_pc_enrichment_det*t_i3i -> rfr_si*t_sil + (1.0+
19.875*rfr_pc_enrichment_det)*h2o + 26.5*rfr_pc_enrichment_det*i2i + t_nh4 +
rfr_pc_enrichment_det*rfr_c*t_dic
p_i3i_1_irred_i2i = (t_sed_1*r_det_1_rec*exp(q10_det_rec*cgt_temp)*
pH_inhibition_ironred)*(1.0-lim_t_o2_2)*(1.0-lim_t_no3_3)*
(1.0-lim_t_mos_5)*(1.0-lim_t_ihs_4)*lim_t_i3i_6*
lim_t_sed_1_22

```

recycling of sediment detrital phosphate (index 1 to 6) (sediment only)

[mol/m²/day]

```

t_sedp_1 + 3*rfr_pc_enrichment_det*rfr_p*h2o -> 3*rfr_pc_enrichment_det*rfr_p*
h3oplus + rfr_pc_enrichment_det*rfr_p*t_po4
p_sedp_1_remin_po4 (t_sedp_1*r_det_1_rec*exp(q10_det_rec*cgt_temp)*(1.0+
= (factor_pref_remin_p-1.0)*o2_min_sed_resp/(t_o2 +
o2_min_sed_resp)))*lim_t_sedp_1_46

```

Auxiliary variables

absolute temperature [K]

```
temp_k = cgt_temp + 273.15
```

temporary value assumed for pH [1]

```
ph_temp = 0.0-log(min(max(h3o,1.0e-12),1.0e-2))/log(10.0)
```

calculated iteratively, 10 iterations, initial value = 0.0

self-ionization constant of Water [mol²/kg²]

```

k_water = exp( -13847.26 / temp_k + 148.96502 - 23.6521 * log(temp_k)
+ (118.67/temp_k - 5.977 + 1.0495 * log(temp_k)) *
sqrt(cgt_sali) - 0.01615 * cgt_sali)

```

Acid dissociation constant CO₂ + 2 H₂O <-> HCO₃⁻ + H₃O⁺ [mol/kg]

```

k1_co2 = power(10.0,( -3633.86 / temp_k + 61.2172 - 9.6777 *
log(temp_k) + 0.011555 * cgt_sali - 0.0001152 * cgt_sali *
cgt_sali))

```

Acid dissociation constant HCO₃⁻ + H₂O <-> [CO₃ 2⁻] + H₃O⁺ [mol/kg]

```

k2_co2 = power(10.0,( -471.78 / temp_k - 25.929 + 3.16967 *
log(temp_k)+ 0.01781 * cgt_sali - 0.0001122 * cgt_sali *
cgt_sali))

```

Acid dissociation constant of boric acid [mol/kg]

```

k_boron = exp(( -8966.9 - 2890.53*sqrt(cgt_sali) - 77.942*cgt_sali +
1.728*cgt_sali*sqrt(cgt_sali) - 0.0996*cgt_sali*cgt_sali) /
temp_k + 148.0248 + 137.1942*sqrt(cgt_sali) + 1.62142*
cgt_sali + (-24.4344 - 25.085*sqrt(cgt_sali) - 0.2474*
cgt_sali)*log(temp_k) + 0.053105*sqrt(cgt_sali)*temp_k )

```

continued on next page...

Auxiliary variables, continued from previous page

Acid dissociation constant $\text{H}_3\text{PO}_4 + \text{H}_2\text{O} \rightleftharpoons [\text{H}_2\text{PO}_4^-] + \text{H}_3\text{O}^+$ [mol/kg]

$$k1_po4 = \exp(-4576.752/\text{temp_k} + 115.525 - 18.453 \cdot \log(\text{temp_k}) + (0.69171 - 106.736/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.01844 + 0.65643/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $[\text{H}_2\text{PO}_4^-] + \text{H}_2\text{O} \rightleftharpoons [\text{HPO}_4^{2-}] + \text{H}_3\text{O}^+$ [mol/kg]

$$k2_po4 = \exp(-8814.715/\text{temp_k} + 172.0883 - 27.927 \cdot \log(\text{temp_k}) + (1.35660 - 160.340/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.05778 - 0.37335/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $[\text{HPO}_4^{2-}] + \text{H}_2\text{O} \rightleftharpoons [\text{PO}_4^{3-}] + \text{H}_3\text{O}^+$ [mol/kg]

$$k3_po4 = \exp(-3070.75/\text{temp_k} - 18.141 + (2.81197 + 17.27039/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.09984 + 44.99486/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $\text{H}_2\text{S} + \text{H}_2\text{O} \rightleftharpoons \text{HS}^- + \text{H}_3\text{O}^+$ [mol/kg]

$$k1_h2s = \exp(-3131.42/\text{temp_k} - 5.818 + 0.368 \cdot (\text{power}(\max(0.0, \text{cgt_sali}), (1.0/3.0))))$$

total concentration of boron [mol/kg]

$$\text{boron_total} = 0.000416 \cdot \text{cgt_sali}/35.0$$

boron alkalinity [mol/kg]

$$\text{alk_boron} = \text{boron_total} \cdot k_boron / (k_boron + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

hydrogen sulfide alkalinity [mol/kg]

$$\text{alk_h2s} = t_h2s \cdot k1_h2s / (k1_h2s + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

water alkalinity [mol/kg]

$$\text{alk_water} = k_water / h3o - h3o$$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in phosphate alkalinity formula [mol³/kg³]

$$\text{alk_po4_denominator} = (h3o \cdot h3o \cdot h3o + k1_po4 \cdot h3o \cdot h3o + k1_po4 \cdot k2_po4 \cdot h3o + k1_po4 \cdot k2_po4 \cdot k3_po4)$$

calculated iteratively, 10 iterations, initial value = 0.0

phosphate alkalinity [mol/kg]

$$\text{alk_po4} = (t_po4 \cdot (k1_po4 \cdot k2_po4 \cdot h3o + 2.0 \cdot k1_po4 \cdot k2_po4 \cdot k3_po4 - h3o \cdot h3o \cdot h3o)) / \text{alk_po4_denominator}$$

calculated iteratively, 10 iterations, initial value = 0.0

continued on next page...

Auxiliary variables, continued from previous page

denominator in carbonate alkalinity formula [mol²/kg²]

```
alk_co2_denominator (h3o*h3o + k1_co2*h3o + k1_co2*k2_co2)
=
calculated iteratively, 10 iterations, initial value = 0.0
```

carbonate alkalinity [mol/kg]

```
alk_co2 = t_dic*k1_co2*(h3o+2*k2_co2)/alk_co2_denominator
calculated iteratively, 10 iterations, initial value = 0.0
```

error in total alkalinity calculation at the assumed pH [mol/kg]

```
alk_residual = t_alk - alk_co2 - alk_po4 - alk_boron - alk_h2s - alk_water
calculated iteratively, 10 iterations, initial value = 0.0
```

derivative of phosphate alkalinity with respect to h3o [1]

```
dalkp_dh3o = t_po4*(0.0-k1_po4*h3o*h3o*h3o-h3o-4*k1_po4*k2_po4*h3o*h3o*
h3o-(k1_po4*k1_po4*k2_po4+9*k1_po4*k2_po4*k3_po4)*h3o*h3o-
4*k1_po4*k1_po4*k2_po4*k3_po4*h3o-k1_po4*k1_po4*k2_po4*
k2_po4*k3_po4)/(alk_po4_denominator*alk_po4_denominator)
calculated iteratively, 10 iterations, initial value = 0.0
```

derivative of carbonate alkalinity with respect to h3o [1]

```
dalkc_dh3o = t_dic*(0.0-k1_co2*h3o*h3o-k1_co2*k1_co2*k2_co2-4*k1_co2*
k2_co2*h3o)/(alk_co2_denominator*alk_co2_denominator)
calculated iteratively, 10 iterations, initial value = 0.0
```

derivative of residual_alk with respect to pH [mol/kg]

```
dalkresidual_dpH = 0.0-log(10.0)*h3o*(alk_boron/(k_boron+h3o)+alk_h2s/(k1_h2s+
h3o)+k_water/(h3o*h3o)+1-dalkp_dh3o-dalkc_dh3o)
calculated iteratively, 10 iterations, initial value = 0.0
```

newly determined pH value [1]

```
temp1 = alk_residual/dalkresidual_dpH
ph = ph_temp - temp1 + theta(abs(temp1) - 1)*0.5*temp1
calculated iteratively, 10 iterations, initial value = 0.0
```

h3o ion concentration [mol/kg]

```
h3o = power(10.0,0.0-max(1.0,min(13.0,ph)))
calculated iteratively, 10 iterations, initial value = 1.0e-8
```

Acid dissociation constant H2S + H2O <-> HS- + H3O+ [mol/kg]

```
k1_h2s_sed = exp( -3131.42/temp_k - 5.818 + 0.368*
(power(max(0.0,cgt_sali),(1.0/3.0))))
```

iron hydroxide half-saturation constant converted to [mol/m²]

continued on next page...

Auxiliary variables, continued from previous page	
ih _s _min_sed_irred_2d	ih _s _min_sed_irred*cgt_cellheight*cgt_density
=	
manganese oxide half-saturation constant converted to [mol/m ²]	
mos_min_sed_irred_2d	mos_min_sed_irred*cgt_cellheight*cgt_density
=	
sum of Fe-III in the sediment [mol/m ²]	
fe3_sed =	t_ips+t_ihs
ionic strength of the solution [mol/kg]	
ionic_strength =	0.02*cgt_sali
dielectric constant of seawater [F/m]	
temp1 =	cgt_sali*(1.707e-2+1.205e-5*cgt_sali+4.058e-9*
	power(cgt_sali,2.0))
temp2 =	1.0-0.2551*temp1+5.151e-2*temp1*temp1-6.889e-3*temp1*temp1*
	temp1
temp3 =	87.74-0.40008*temp_k+9.398e-4*temp_k*temp_k+1.401e-6*
	temp_k*temp_k*temp_k
dielectric_constant	temp2*temp3
=	
concentration of HS ⁻ ions [mol/kg]	
hsminus =	t_h2s * k1_h2s_sed / (k1_h2s_sed + h3o)
parameter A for the Davies formula [mol ^{0.5} l ^{-0.5}]	
davies_parameter_a	1.82e6*power(dielectric_constant*temp_k,-1.5)
=	
activity to concentration ratio of ions with a charge of +1/-1 [1]	
activity_coefficient/(1+sqrt(ionic_strength))-0.3*ionic_strength)	power(10.0,0.0-davies_parameter_a*1*(sqrt(ionic_strength)
=	
activity to concentration ratio of ions with a charge of +2/-2 [1]	
activity_coefficient/(1+sqrt(ionic_strength))-0.3*ionic_strength)	power(10.0,0.0-davies_parameter_a*2*(sqrt(ionic_strength)
=	
activity of H ₃ O ⁺ ions (concentration corrected by ionic strength) [mol/kg]	
activity_h3oplus =	h3o*activity_coefficient_1
Fe-II concentration in equilibrium with iron monosulfide precipitation [mol/kg]	
fe2_eq_ims =	power(10.0,-2.95)*activity_h3oplus/max(hsminus*
	activity_coefficient_1,1.0e-3*epsilon)
	/activity_coefficient_2
continued on next page...	

Auxiliary variables, continued from previous page

Fe-II concentration in equilibrium with iron adsorbed to illite-montmorillonite mixed layer minerals [mol/kg]

```
temp1 = 2.7 * max(vol_fraction_im*(1.0-POR),epsilon)
fe2_eq_iim = (max(t_iim,epsilon)/cgt_cellheight/cgt_density)/(100*temp1)
+1000*(1.0-cgt_in_sediment)
```

siderite is the favoured species for precipitation (0 or 1) [1]

```
fe2_ims_is_smallest theta(fe2_eq_iim-fe2_eq_ims)
=
```

minnesotaite is the favoured species for precipitation (0 or 1) [1]

```
fe2_iim_is_smallest theta(fe2_eq_ims-fe2_eq_iim)
=
```

factor for inhibition of iron / sulfate reduction at large pH [1]

```
1.0+0.0*(theta(pH_opt_ironred-pH)+theta(pH-pH_opt_ironred)*
ph_inhibition_ironredmax((pH_max_ironred-pH)/(pH_max_ironred-pH_opt_ironred)
= ,0.0))
```

Constants

no division by 0

```
epsilon = 4.5E-17
```

iron hydroxide half-saturation concentration for detritus remineralization by iron reduction [mol/kg]

```
ihs_min_sed_irred = 0.0065
```

iron hydroxide half-saturation concentration for detritus remineralization by iron reduction [mol/kg]

```
mos_min_sed_irred = 0.0004
```

nitrate half-saturation concentration for denitrification in the water column [mol/kg]

```
no3_min_sed_denit = 4.0E-6
```

oxygen half-saturation constant for recycling of sediment detritus using oxygen [mol/kg]

```
o2_min_sed_resp = 2.0E-5
```

q10 rule factor for recycling [1/K]

```
q10_det_rec = 0.15
```

redfield ratio C/N

```
rfr_c = 6.625
```

continued on next page...

 Constants, continued from previous page

redfield ratio P/N

rfr_p = 0.0625

enrichment factor for P and C in detritus [1]
 1.5
 rfr_pc_enrichment_de
 =
minimum sulfate concentration for sulfate reduction [mol/kg]

so4_min_det_sulf = 1.0E-6

detritus recycling rates [1/d]

r_det_1_rec = 0.0647

detritus recycling rates [1/d]

r_det_2_rec = 0.00924

detritus recycling rates [1/d]

r_det_3_rec = 0.00136

detritus recycling rates [1/d]

r_det_4_rec = 0.000108

detritus recycling rates [1/d]

r_det_5_rec = 1.62E-5

detritus recycling rates [1/d]

r_det_6_rec = 0.0

porosity

por = 0.77

optimal pH for iron reduction [1]

pH_opt_ironred = 7.2

maximum pH for iron reduction [1]

pH_max_ironred = 20.0

average ratio Si/N [1]

rfr_si = 0.9375

fraction of illite-montmorillonite mixed layer minerals on volume of all minerals [1]

vol_fraction_im = 0.5

 continued on next page...

Constants, continued from previous page	
acceleration factor for preferential mineralization of P compared to N under hypoxic conditions [1]	
factor_pref_remin_p	10.0
=	
Process limitation factors	
lim_t_o2_2 =	$1.0 - \exp(-t_{o2}/o2_{min_sed_resp})$
lim_t_o2_12 =	$\theta(t_{o2} - 0.0)$
lim_t_no3_3 =	$1.0 - \exp(-t_{no3}/no3_{min_sed_denit})$
lim_t_h2s_29 =	$\theta(t_{h2s} - 0.0)$
lim_t_ips_52 =	$\theta(t_{ips} - 0.0)$
lim_t_so4_28 =	$\theta(t_{so4} - 0.0)$
lim_t_sed_1_22 =	$\theta(t_{sed_1} - 0.0)$
lim_t_sed_2_23 =	$\theta(t_{sed_2} - 0.0)$
lim_t_sed_3_24 =	$\theta(t_{sed_3} - 0.0)$
lim_t_sed_4_25 =	$\theta(t_{sed_4} - 0.0)$
lim_t_sed_5_26 =	$\theta(t_{sed_5} - 0.0)$
lim_t_sed_6_27 =	$\theta(t_{sed_6} - 0.0)$
lim_t_ihs_4 =	$1.0 - \exp(-t_{ihs}/ihs_{min_sed_irred_2d})$
lim_t_mos_5 =	$1.0 - \exp(-t_{mos}/mos_{min_sed_irred_2d})$
lim_t_i3i_6 =	$1.0 - \exp(-t_{i3i}/ihs_{min_sed_irred_2d})$
lim_t_sedp_1_46 =	$\theta(t_{sedp_1} - 0.0)$
lim_t_sedp_2_47 =	$\theta(t_{sedp_2} - 0.0)$
lim_t_sedp_3_48 =	$\theta(t_{sedp_3} - 0.0)$
lim_t_sedp_4_49 =	$\theta(t_{sedp_4} - 0.0)$
continued on next page...	

Process limitation factors, continued from previous page

```
lim_t_sedp_5_50 = theta(t_sedp_5-0.0)
```

```
lim_t_sedp_6_51 = theta(t_sedp_6-0.0)
```

3.3 Process type BGC/benthic/precipitation

Processes	
transformation of amorphous iron oxyhydroxides to crystalline phase (sediment only) [mol/m²/day]	
t_ihs -> t_ihc	
p_ihs_trans_ihc =	(r_ihs_trans_ihc*t_ihs)*lim_t_ihs_53
manganese-II precipitation to rhodochrosite (sediment only) [mol/m²/day]	
4.8*h2o + 0.6*t_ca2 + t_mn2 + 1.6*t_dic -> t_rho + 3.2*h3oplus	
p_mn2_prec_rho =	(0.1*t_mn2*theta(saturation_rhodochrosite-1.0)* cgt_in_sediment*cgt_cellheight*cgt_density)*lim_t_ca2_56* lim_t_mn2_62*lim_t_dic_13
Auxiliary variables	
absolute temperature [K]	
temp_k =	cgt_temp + 273.15
temporary value assumed for pH [1]	
ph_temp =	0.0-log(min(max(h3o,1.0e-12),1.0e-2))/log(10.0)
calculated iteratively, 10 iterations, initial value = 0.0	
self-ionization constant of Water [mol²/kg²]	
k_water =	exp(-13847.26 / temp_k + 148.96502 - 23.6521 * log(temp_k) + (118.67/temp_k - 5.977 + 1.0495 * log(temp_k)) * sqrt(cgt_sali) - 0.01615 * cgt_sali)
Solubility of CO2 [mol/kg/Pa]	
k0_co2 =	exp(9345.17 / temp_k - 60.2409 + 23.3585 * (log(temp_k) - 4.605170186) + cgt_sali*(0.023517 - 0.00023656 * temp_k + 0.00000047036 *temp_k*temp_k))/101325.0
Acid dissociation constant CO2 + 2 H2O <-> HCO3- + H3O+ [mol/kg]	
k1_co2 =	power(10.0,(-3633.86 / temp_k + 61.2172 - 9.6777 * log(temp_k) + 0.011555 * cgt_sali - 0.0001152 * cgt_sali * cgt_sali))
Acid dissociation constant HCO3- + H2O <-> [CO3 2-] + H3O+ [mol/kg]	
k2_co2 =	power(10.0,(-471.78 / temp_k - 25.929 + 3.16967 * log(temp_k) + 0.01781 * cgt_sali - 0.0001122 * cgt_sali * cgt_sali))
Acid dissociation constant of boric acid [mol/kg]	
k_boron =	exp((-8966.9 - 2890.53*sqrt(cgt_sali) - 77.942*cgt_sali + 1.728*cgt_sali*sqrt(cgt_sali) - 0.0996*cgt_sali*cgt_sali) / temp_k + 148.0248 + 137.1942*sqrt(cgt_sali) + 1.62142* cgt_sali + (-24.4344 - 25.085*sqrt(cgt_sali) - 0.2474* cgt_sali)*log(temp_k) + 0.053105*sqrt(cgt_sali)*temp_k)
continued on next page...	

Auxiliary variables, continued from previous page

Acid dissociation constant $\text{H}_3\text{PO}_4 + \text{H}_2\text{O} \rightleftharpoons [\text{H}_2\text{PO}_4^-] + \text{H}_3\text{O}^+$ [mol/kg]

$$k1_po4 = \exp(-4576.752/\text{temp_k} + 115.525 - 18.453 \cdot \log(\text{temp_k}) + (0.69171 - 106.736/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.01844 + 0.65643/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $[\text{H}_2\text{PO}_4^-] + \text{H}_2\text{O} \rightleftharpoons [\text{HPO}_4^{2-}] + \text{H}_3\text{O}^+$ [mol/kg]

$$k2_po4 = \exp(-8814.715/\text{temp_k} + 172.0883 - 27.927 \cdot \log(\text{temp_k}) + (1.35660 - 160.340/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.05778 - 0.37335/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $[\text{HPO}_4^{2-}] + \text{H}_2\text{O} \rightleftharpoons [\text{PO}_4^{3-}] + \text{H}_3\text{O}^+$ [mol/kg]

$$k3_po4 = \exp(-3070.75/\text{temp_k} - 18.141 + (2.81197 + 17.27039/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.09984 + 44.99486/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $\text{H}_2\text{S} + \text{H}_2\text{O} \rightleftharpoons \text{HS}^- + \text{H}_3\text{O}^+$ [mol/kg]

$$k1_h2s = \exp(-3131.42/\text{temp_k} - 5.818 + 0.368 \cdot (\text{power}(\max(0.0, \text{cgt_sali}), (1.0/3.0))))$$

total concentration of boron [mol/kg]

$$\text{boron_total} = 0.000416 \cdot \text{cgt_sali}/35.0$$

boron alkalinity [mol/kg]

$$\text{alk_boron} = \text{boron_total} \cdot k_boron / (k_boron + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

hydrogen sulfide alkalinity [mol/kg]

$$\text{alk_h2s} = t_h2s \cdot k1_h2s / (k1_h2s + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

water alkalinity [mol/kg]

$$\text{alk_water} = k_water / h3o - h3o$$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in phosphate alkalinity formula [mol³/kg³]

$$\text{alk_po4_denominator} = (h3o \cdot h3o \cdot h3o + k1_po4 \cdot h3o \cdot h3o + k1_po4 \cdot k2_po4 \cdot h3o + k1_po4 \cdot k2_po4 \cdot k3_po4)$$

calculated iteratively, 10 iterations, initial value = 0.0

phosphate alkalinity [mol/kg]

$$\text{alk_po4} = (t_po4 \cdot (k1_po4 \cdot k2_po4 \cdot h3o + 2.0 \cdot k1_po4 \cdot k2_po4 \cdot k3_po4 - h3o \cdot h3o \cdot h3o)) / \text{alk_po4_denominator}$$

calculated iteratively, 10 iterations, initial value = 0.0

continued on next page...

Auxiliary variables, continued from previous page

denominator in carbonate alkalinity formula [mol²/kg²]

alk_co2_denominator (h3o*h3o + k1_co2*h3o + k1_co2*k2_co2)
=
calculated iteratively, 10 iterations, initial value = 0.0

carbonate alkalinity [mol/kg]

alk_co2 = t_dic*k1_co2*(h3o+2*k2_co2)/alk_co2_denominator
calculated iteratively, 10 iterations, initial value = 0.0

error in total alkalinity calculation at the assumed pH [mol/kg]

alk_residual = t_alk - alk_co2 - alk_po4 - alk_boron - alk_h2s - alk_water
calculated iteratively, 10 iterations, initial value = 0.0

derivative of phosphate alkalinity with respect to h3o [1]

dalkp_dh3o = t_po4*(0.0-k1_po4*h3o*h3o*h3o-h3o-4*k1_po4*k2_po4*h3o*h3o*
h3o-(k1_po4*k1_po4*k2_po4+9*k1_po4*k2_po4*k3_po4)*h3o*h3o-
4*k1_po4*k1_po4*k2_po4*k3_po4*h3o-k1_po4*k1_po4*k2_po4*
k2_po4*k3_po4)/(alk_po4_denominator*alk_po4_denominator)
calculated iteratively, 10 iterations, initial value = 0.0

derivative of carbonate alkalinity with respect to h3o [1]

dalkc_dh3o = t_dic*(0.0-k1_co2*h3o*h3o-k1_co2*k1_co2*k2_co2-4*k1_co2*
k2_co2*h3o)/(alk_co2_denominator*alk_co2_denominator)
calculated iteratively, 10 iterations, initial value = 0.0

derivative of residual_alk with respect to pH [mol/kg]

dalkresidual_dpH = 0.0-log(10.0)*h3o*(alk_boron/(k_boron+h3o)+alk_h2s/(k1_h2s+
h3o)+k_water/(h3o*h3o)+1-dalkp_dh3o-dalkc_dh3o)
calculated iteratively, 10 iterations, initial value = 0.0

newly determined pH value [1]

temp1 = alk_residual/dalkresidual_dpH
ph = ph_temp - temp1 + theta(abs(temp1) - 1)*0.5*temp1
calculated iteratively, 10 iterations, initial value = 0.0

h3o ion concentration [mol/kg]

h3o = power(10.0,0.0-max(1.0,min(13.0,ph)))
calculated iteratively, 10 iterations, initial value = 1.0e-8

co2 partial pressure [Pa]

pco2 = t_dic / k0_co2 / (1 + k1_co2/h3o + k1_co2*k2_co2/h3o/h3o)

ionic strength of the solution [mol/kg]

ionic_strength = 0.02*cgt_sali

continued on next page...

Auxiliary variables, continued from previous page

dielectric constant of seawater [F/m]

```
temp1 = cgt_sali*(1.707e-2+1.205e-5*cgt_sali+4.058e-9*
          power(cgt_sali,2.0))
temp2 = 1.0-0.2551*temp1+5.151e-2*temp1*temp1-6.889e-3*temp1*temp1*
          temp1
temp3 = 87.74-0.40008*temp_k+9.398e-4*temp_k*temp_k+1.401e-6*
          temp_k*temp_k*temp_k
dielectric_constant temp2*temp3
=
```

CO2 concentration in the surface layer [mol/kg]

```
co2 = pco2*k0_co2
```

parameter A for the Davies formula [mol^{0.5} l^{-0.5}]

```
davies_parameter_a 1.82e6*power(dielectric_constant*temp_k,-1.5)
=
```

concentration of HCO₃⁻ ions

```
hco3minus = co2*k1_co2/h3o
```

activity to concentration ratio of ions with a charge of +2/-2 [1]

```
power(10.0,0.0-davies_parameter_a*2*(sqrt(ionic_strength)
activity_coefficient/(1+sqrt(ionic_strength))-0.3*ionic_strength))
=
```

concentration of CO₃⁻⁻ ions

```
co32minus = hco3minus*k2_co2/h3o
```

activity of CO₃⁻⁻ ions (concentration corrected by ionic strength) [mol/kg]

```
activity_co32minus co32minus*activity_coefficient_2
=
```

relative saturation of rhodochrosite [1]

```
t_mn2*activity_coefficient_2*
saturation_rhodochroactivity_co32minus/power(10.0,-9.5)
=
```

Constants

transformation rate from amorphous to crystalline iron hydroxide [1/d]

```
r_ihs_trans_ihc = 0.00164
```

Process limitation factors

```
lim_t_dic_13 = theta(t_dic-0.0)
```

```
lim_t_ihs_53 = theta(t_ihs-0.0)
```

continued on next page...

Process limitation factors, continued from previous page

```
lim_t_ca2_56 =      theta(t_ca2-0.0)
```

```
lim_t_mn2_62 =      theta(t_mn2-0.0)
```

3.4 Process type BGC/benthic/reoxidation

Processes
nitrification in the sediment [mol/kg/day] $t_{nh4} + 2*t_{o2} + h2o \rightarrow t_{no3} + 2*h3oplus$ $p_{nh4_nit_no3_sed} = (t_{nh4}*t_{o2}*k_{nh4_o2}*exp(q10_nit*cgt_temp))*cgt_in_sediment*lim_t_o2_1*lim_t_nh4_16$
oxidation of hydrogen sulfide with oxygen [mol/kg/day] $t_{h2s} + 0.5*t_{o2} \rightarrow t_{sul} + h2o$ $p_{h2s_oxo2_sul} = (t_{h2s}*t_{o2}*k_{h2s_o2}*exp(q10_h2s*cgt_temp))*lim_t_h2s_29*lim_t_o2_12$
oxidation of hydrogen sulfide with nitrate [mol/kg/day] $0.4*h3oplus + 0.4*t_{no3} + t_{h2s} \rightarrow 0.2*t_{n2} + 1.6*h2o + t_{sul}$ $p_{h2s_oxno3_sul} = (t_{h2s}*t_{no3}*k_{h2s_no3}*exp(q10_h2s*cgt_temp))*lim_t_no3_14*lim_t_h2s_29$
oxidation of elemental sulfur with oxygen [mol/kg/day] $3*h2o + 1.5*t_{o2} + t_{sul} \rightarrow 2*h3oplus + t_{so4}$ $p_{sul_oxo2_so4} = (t_{sul}*t_{o2}*k_{sul_o2}*exp(q10_h2s*cgt_temp))*lim_t_o2_12*lim_t_sul_30$
oxidation of elemental sulfur with nitrate [mol/kg/day] $1.2*h2o + 1.2*t_{no3} + t_{sul} \rightarrow 0.6*t_{n2} + 0.8*h3oplus + t_{so4}$ $p_{sul_oxno3_so4} = (t_{sul}*t_{no3}*k_{sul_no3}*exp(q10_h2s*cgt_temp))*lim_t_no3_14*lim_t_sul_30$
oxidation of Fe²⁺ to iron hydroxide in the sediment (sediment only) [mol/m²/day] $t_{fe2} + 4.5*h2o + 0.25*t_{o2} \rightarrow 2*h3oplus + t_{ihs}$ $p_{fe2_ox_ihs} = (k_{feo2}*t_{fe2}*t_{o2}*oh*oh*cgt_in_sediment*cgt_cellheight*cgt_density)*lim_t_fe2_55*lim_t_o2_12$
reduction of sedimentary iron hydroxide to iron-II (sediment only) [mol/m²/day] $t_{h2s} + 8.0*t_{ihs} \rightarrow 8.0*t_{iim} + 2*h2o + t_{so4} + 2.0*h3oplus$ $p_{ihs_red_iim} = (k_{h2s_ihs}*t_{h2s}*ihs_conc_pw*fe2_iim_is_smallest)*lim_t_ihs_4*lim_t_h2s_29$
reduction of sedimentary iron hydroxide to iron-II (sediment only) [mol/m²/day] $9.0*t_{h2s} + 8.0*t_{ihs} \rightarrow 8.0*t_{ims} + 18*h2o + t_{so4} + 2.0*h3oplus$ $p_{ihs_red_ims} = (k_{h2s_ihs}*t_{h2s}*ihs_conc_pw*fe2_ims_is_smallest)*lim_t_ihs_4*lim_t_h2s_29$
oxidation of Mn²⁺ to manganese oxide in the sediment (sediment only) [mol/m²/day]
continued on next page...

Processes, continued from previous page

$$t_{mn2} + 0.5*t_{o2} + 3*h2o \rightarrow 2*h3oplus + t_{mos}$$

$$p_{mn2_ox_mos} = (k_{mno2}*t_{mn2}*t_{o2}*cgt_in_sediment*cgt_cellheight*cgt_density)*lim_t_{mn2_62}*lim_t_{o2_12}$$

oxidation of pyrite by manganese oxide to iron oxyhydroxide (sediment only)
[mol/m²/day]

$$t_{mos} + t_{pyr} + 1.25*h3oplus + 1.25*h2o \rightarrow 0.375*t_{so4} + 1.625*t_{h2s} + t_{ihs} + t_{mn2}$$

$$p_{pyr_oxmos_ihs} = (cgt_in_sediment*max(r_{max_lib_mn2_pyrox}/cgt_cellheight/cgt_density, r_{max_ox_pyr}*t_{pyr}))*lim_t_{mos_59}*lim_t_{pyr_58}$$

oxidation of pyrite by manganese oxide to iron oxyhydroxide (sediment only)
[mol/m²/day]

$$0.25*t_{o2} + t_{pyr} + 4*h2o \rightarrow 1.75*t_{h2s} + 0.25*t_{so4} + 0.5*h3oplus + t_{ihs}$$

$$p_{pyr_oxo2_ihs} = (cgt_in_sediment*t_{o2}*pyr_conc_pw*k_{o2_pyr}*cgt_cellheight*cgt_density)*lim_t_{o2_12}*lim_t_{pyr_58}$$

oxidation of minnesotaite by oxygen to iron oxyhydroxide (sediment only)
[mol/m²/day]

$$0.25*t_{o2} + t_{iim} + 0.5*h2o \rightarrow t_{ihs}$$

$$p_{imm_oxo2_ihs} = (cgt_in_sediment*t_{o2}*iim_conc_pw*k_{o2_pyr}*cgt_cellheight*cgt_density)*lim_t_{o2_12}*lim_t_{iim_61}$$

oxidation of iron-II in illite-montmorillonite mixed layer minerals to iron-III (sediment only) [mol/m²/day]

$$0.5*h2o + 0.25*t_{o2} + i2i \rightarrow t_{i3i}$$

$$p_{i2i_oxo2_i3i} = (cgt_in_sediment*max(i3i_max-t_{i3i}, 0.0)*r_{i2i_ox})*lim_t_{o2_2}$$

reduction of iron-III in clay minerals to iron-II consuming h2s (sediment only)
[mol/m²/day]

$$8*t_{i3i} + t_{h2s} \rightarrow t_{so4} + 2*h3oplus + 2*h2o + 8*i2i$$

$$p_{i3i_redh2s_i2i} = (r_{h2s_ox_i3i}*t_{h2s})*lim_t_{i3i_6}*lim_t_{h2s_29}$$

reduction of sedimentary iron hydroxide to iron-II (sediment only) [mol/m²/day]

$$t_{h2s} + 8.0*t_{ihc} \rightarrow 8.0*t_{iim} + 2*h2o + t_{so4} + 2.0*h3oplus$$

$$p_{ihc_red_iim} = (k_{h2s_ihs}*t_{h2s}*ihc_conc_pw*fe2_iim_is_smallest)*lim_t_{ihc_10}*lim_t_{h2s_29}$$

reduction of sedimentary iron hydroxide to iron-II (sediment only) [mol/m²/day]

$$9.0*t_{h2s} + 8.0*t_{ihc} \rightarrow 8.0*t_{ims} + 18*h2o + t_{so4} + 2.0*h3oplus$$

$$p_{ihc_red_ims} = (k_{h2s_ihs}*t_{h2s}*ihc_conc_pw*fe2_ims_is_smallest)*lim_t_{ihc_10}*lim_t_{h2s_29}$$

continued on next page...

Processes, continued from previous page

oxidation of Fe²⁺ by reduction of MnO₂ (sediment only) [mol/m²/day]

```
t_mos + 2.0*t_fe2 + 6.0*h2o -> 2.0*h3oplus + t_mn2 + 2.0*t_ihs
p_fe2_mnox_ihs = (t_fe2*mos_conc_pw*k_mno2_fe2*cgt_cellheight*cgt_density)*
lim_t_mos_59*lim_t_fe2_55
```

oxidation of h₂s by reduction of MnO₂ (sediment only) [mol/m²/day]

```
0.25*t_h2s + 1.5*h3oplus + t_mos -> t_mn2 + 2.5*h2o + 0.25*t_so4
p_h2s_mnox_so4 = (t_h2s*mos_conc_pw*k_mno2_h2s*cgt_cellheight*cgt_density)*
lim_t_h2s_29*lim_t_mos_59
```

iron monosulfide oxidation to iron oxihydroxides (sediment only) [mol/m²/day]

```
t_ims + 2.25*t_o2 + 4.5*h2o -> t_so4 + t_ihs + 2*h3oplus
p_ims_oxo2_ihs = (k_ims_o2*ims_conc_pw*t_o2*cgt_cellheight*cgt_density)*
lim_t_ims_57*lim_t_o2_12
```

Auxiliary variables**absolute temperature [K]**

```
temp_k = cgt_temp + 273.15
```

temporary value assumed for pH [1]

```
ph_temp = 0.0-log(min(max(h3o,1.0e-12),1.0e-2))/log(10.0)
calculated iteratively, 10 iterations, initial value = 0.0
```

self-ionization constant of Water [mol²/kg²]

```
k_water = exp( -13847.26 / temp_k + 148.96502 - 23.6521 * log(temp_k)
+ (118.67/temp_k - 5.977 + 1.0495 * log(temp_k)) *
sqrt(cgt_sali) - 0.01615 * cgt_sali)
```

Acid dissociation constant CO₂ + 2 H₂O <-> HCO₃⁻ + H₃O⁺ [mol/kg]

```
k1_co2 = power(10.0,( -3633.86 / temp_k + 61.2172 - 9.6777 *
log(temp_k) + 0.011555 * cgt_sali - 0.0001152 * cgt_sali *
cgt_sali))
```

Acid dissociation constant HCO₃⁻ + H₂O <-> [CO₃²⁻] + H₃O⁺ [mol/kg]

```
k2_co2 = power(10.0,( -471.78 / temp_k - 25.929 + 3.16967 *
log(temp_k)+ 0.01781 * cgt_sali - 0.0001122 * cgt_sali *
cgt_sali))
```

Acid dissociation constant of boric acid [mol/kg]

```
k_boron = exp(( -8966.9 - 2890.53*sqrt(cgt_sali) - 77.942*cgt_sali +
1.728*cgt_sali*sqrt(cgt_sali) - 0.0996*cgt_sali*cgt_sali) /
temp_k + 148.0248 + 137.1942*sqrt(cgt_sali) + 1.62142*
cgt_sali + (-24.4344 - 25.085*sqrt(cgt_sali) - 0.2474*
cgt_sali)*log(temp_k) + 0.053105*sqrt(cgt_sali)*temp_k )
```

continued on next page...

Auxiliary variables, continued from previous page

Acid dissociation constant $\text{H}_3\text{PO}_4 + \text{H}_2\text{O} \rightleftharpoons [\text{H}_2\text{PO}_4^-] + \text{H}_3\text{O}^+$ [mol/kg]

$$k1_po4 = \exp(-4576.752/\text{temp_k} + 115.525 - 18.453 \cdot \log(\text{temp_k}) + (0.69171 - 106.736/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.01844 + 0.65643/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $[\text{H}_2\text{PO}_4^-] + \text{H}_2\text{O} \rightleftharpoons [\text{HPO}_4^{2-}] + \text{H}_3\text{O}^+$ [mol/kg]

$$k2_po4 = \exp(-8814.715/\text{temp_k} + 172.0883 - 27.927 \cdot \log(\text{temp_k}) + (1.35660 - 160.340/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.05778 - 0.37335/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $[\text{HPO}_4^{2-}] + \text{H}_2\text{O} \rightleftharpoons [\text{PO}_4^{3-}] + \text{H}_3\text{O}^+$ [mol/kg]

$$k3_po4 = \exp(-3070.75/\text{temp_k} - 18.141 + (2.81197 + 17.27039/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.09984 + 44.99486/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $\text{H}_2\text{S} + \text{H}_2\text{O} \rightleftharpoons \text{HS}^- + \text{H}_3\text{O}^+$ [mol/kg]

$$k1_h2s = \exp(-3131.42/\text{temp_k} - 5.818 + 0.368 \cdot (\text{power}(\max(0.0, \text{cgt_sali}), (1.0/3.0))))$$

total concentration of boron [mol/kg]

$$\text{boron_total} = 0.000416 \cdot \text{cgt_sali}/35.0$$

boron alkalinity [mol/kg]

$$\text{alk_boron} = \text{boron_total} \cdot k_boron / (k_boron + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

hydrogen sulfide alkalinity [mol/kg]

$$\text{alk_h2s} = t_h2s \cdot k1_h2s / (k1_h2s + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

water alkalinity [mol/kg]

$$\text{alk_water} = k_water / h3o - h3o$$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in phosphate alkalinity formula [mol³/kg³]

$$\text{alk_po4_denominator} = (h3o \cdot h3o \cdot h3o + k1_po4 \cdot h3o \cdot h3o + k1_po4 \cdot k2_po4 \cdot h3o + k1_po4 \cdot k2_po4 \cdot k3_po4)$$

calculated iteratively, 10 iterations, initial value = 0.0

phosphate alkalinity [mol/kg]

$$\text{alk_po4} = (t_po4 \cdot (k1_po4 \cdot k2_po4 \cdot h3o + 2.0 \cdot k1_po4 \cdot k2_po4 \cdot k3_po4 - h3o \cdot h3o \cdot h3o)) / \text{alk_po4_denominator}$$

calculated iteratively, 10 iterations, initial value = 0.0

continued on next page...

Auxiliary variables, continued from previous page

denominator in carbonate alkalinity formula [mol²/kg²]

```
alk_co2_denominator (h3o*h3o + k1_co2*h3o + k1_co2*k2_co2)
=
calculated iteratively, 10 iterations, initial value = 0.0
```

carbonate alkalinity [mol/kg]

```
alk_co2 = t_dic*k1_co2*(h3o+2*k2_co2)/alk_co2_denominator
calculated iteratively, 10 iterations, initial value = 0.0
```

error in total alkalinity calculation at the assumed pH [mol/kg]

```
alk_residual = t_alk - alk_co2 - alk_po4 - alk_boron - alk_h2s - alk_water
calculated iteratively, 10 iterations, initial value = 0.0
```

derivative of phosphate alkalinity with respect to h3o [1]

```
dalkp_dh3o = t_po4*(0.0-k1_po4*h3o*h3o*h3o-h3o-4*k1_po4*k2_po4*h3o*h3o*
h3o-(k1_po4*k1_po4*k2_po4+9*k1_po4*k2_po4*k3_po4)*h3o*h3o-
4*k1_po4*k1_po4*k2_po4*k3_po4*h3o-k1_po4*k1_po4*k2_po4*
k2_po4*k3_po4)/(alk_po4_denominator*alk_po4_denominator)
calculated iteratively, 10 iterations, initial value = 0.0
```

derivative of carbonate alkalinity with respect to h3o [1]

```
dalkc_dh3o = t_dic*(0.0-k1_co2*h3o*h3o-k1_co2*k1_co2*k2_co2-4*k1_co2*
k2_co2*h3o)/(alk_co2_denominator*alk_co2_denominator)
calculated iteratively, 10 iterations, initial value = 0.0
```

derivative of residual_alk with respect to pH [mol/kg]

```
dalkresidual_dpH = 0.0-log(10.0)*h3o*(alk_boron/(k_boron+h3o)+alk_h2s/(k1_h2s+
h3o)+k_water/(h3o*h3o)+1-dalkp_dh3o-dalkc_dh3o)
calculated iteratively, 10 iterations, initial value = 0.0
```

newly determined pH value [1]

```
temp1 = alk_residual/dalkresidual_dpH
ph = ph_temp - temp1 + theta(abs(temp1) - 1)*0.5*temp1
calculated iteratively, 10 iterations, initial value = 0.0
```

h3o ion concentration [mol/kg]

```
h3o = power(10.0,0.0-max(1.0,min(13.0,ph)))
calculated iteratively, 10 iterations, initial value = 1.0e-8
```

h3o ion concentration [mol/kg]

```
oh = power(10.0,log(k_water)/log(10.0)+max(1.0,min(13.0,ph)))
```

Acid dissociation constant H₂S + H₂O <-> HS⁻ + H₃O⁺ [mol/kg]

```
k1_h2s_sed = exp( -3131.42/temp_k - 5.818 + 0.368*
(power(max(0.0,cgt_sali),(1.0/3.0))))
```

continued on next page...

Auxiliary variables, continued from previous page

iron hydroxide half-saturation constant converted to [mol/m²]

```

            ihs_min_sed_irred*cgt_cellheight*cgt_density
ihs_min_sed_irred_2d
=

```

ionic strength of the solution [mol/kg]

```

ionic_strength = 0.02*cgt_sali

```

dielectric constant of seawater [F/m]

```

temp1 = cgt_sali*(1.707e-2+1.205e-5*cgt_sali+4.058e-9*
            power(cgt_sali,2.0))
temp2 = 1.0-0.2551*temp1+5.151e-2*temp1*temp1-6.889e-3*temp1*temp1*
            temp1
temp3 = 87.74-0.40008*temp_k+9.398e-4*temp_k*temp_k+1.401e-6*
            temp_k*temp_k*temp_k
dielectric_constant temp2*temp3
=

```

concentration of HS- ions [mol/kg]

```

hsminus = t_h2s * k1_h2s_sed / (k1_h2s_sed + h3o)

```

rate constant iron-II oxidation by o₂ [kg³/mol³/d]

```

k_feo2 = power(10.0,21.56-1545.0/temp_k-3.29*
            power(ionic_strength,0.5)+1.52*ionic_strength)

```

parameter A for the Davies formula [mol^{0.5} l^{-0.5}]

```

davies_parameter_a 1.82e6*power(dielectric_constant*temp_k,-1.5)
=

```

activity to concentration ratio of ions with a charge of +1/-1 [1]

```

            power(10.0,0.0-davies_parameter_a*1*(sqrt(ionic_strength)
activity_coefficient/(1+sqrt(ionic_strength))-0.3*ionic_strength))
=

```

activity to concentration ratio of ions with a charge of +2/-2 [1]

```

            power(10.0,0.0-davies_parameter_a*2*(sqrt(ionic_strength)
activity_coefficient/(1+sqrt(ionic_strength))-0.3*ionic_strength))
=

```

activity of H₃O⁺ ions (concentration corrected by ionic strength) [mol/kg]

```

activity_h3oplus = h3o*activity_coefficient_1

```

amount of structural iron in illite-montmorillonite mixed-layer minerals that can be oxidized or reduced [mol/m²]

```

temp1 = 2.7 * max(vol_fraction_im*(1.0-POR),epsilon)

```

continued on next page...

Auxiliary variables, continued from previous page	
temp2 =	temp1*fe_content_im
temp3 =	temp2/55.0
i3i_max =	temp3 * 1000 * cgt_cellheight*cgt_density
Fe-II concentration in equilibrium with iron monosulfide precipitation [mol/kg]	
fe2_eq_ims =	power(10.0,-2.95)*activity_h3oplus/max(hsminus* activity_coefficient_1,1.0e-3*epsilon) /activity_coefficient_2
Fe-II concentration in equilibrium with iron adsorbed to illite-montmorillonite mixed layer minerals [mol/kg]	
temp1 =	2.7 * max(vol_fraction_im*(1.0-POR),epsilon)
fe2_eq_iim =	(max(t_iim,epsilon)/cgt_cellheight/cgt_density)/(100*temp1) +1000*(1.0-cgt_in_sediment)
siderite is the favoured species for precipitation (0 or 1) [1]	
fe2_ims_is_smallest	theta(fe2_eq_iim-fe2_eq_ims)
=	
minnesotaite is the favoured species for precipitation (0 or 1) [1]	
fe2_iim_is_smallest	theta(fe2_eq_ims-fe2_eq_iim)
=	
pyrite concentration if all was dissolved in the pore water [mol/kg]	
pyr_conc_pw =	t_pyr/cgt_cellheight/cgt_density/max(POR,epsilon)
potential iron-II adsorbed to illite-montmorillonite mixed-layer minerals concentration if all was dissolved in the pore water [mol/kg]	
iim_conc_pw =	t_iim/cgt_cellheight/cgt_density/max(POR,epsilon)
potential amorphous iron hydroxide concentration if all was dissolved in the pore water [mol/kg]	
ihs_conc_pw =	t_ihs/cgt_cellheight/cgt_density/max(POR,epsilon)
potential crystalline iron hydroxide concentration if all was dissolved in the pore water [mol/kg]	
ihc_conc_pw =	t_ihc/cgt_cellheight/cgt_density/max(POR,epsilon)
potential manganese oxide concentration if all was dissolved in the pore water [mol/kg]	
mos_conc_pw =	t_mos/cgt_cellheight/cgt_density/max(POR,epsilon)
potential iron monosulfide concentration if all was dissolved in the pore water [mol/kg]	
continued on next page...	

Auxiliary variables, continued from previous page	
ims_conc_pw =	t_ims/cgt_cellheight/cgt_density/max(POR,epsilon)
Constants	
no division by 0	
epsilon =	4.5E-17
iron hydroxide half-saturation concentration for detritus remineralization by iron reduction [mol/kg]	
ihs_min_sed_irred =	0.0065
reaction constant h2s oxidation with no3 [kg/mol/day]	
k_h2s_no3 =	438.0
reaction constant h2s oxidation with o2 [kg/mol/day]	
k_h2s_o2 =	438.0
reaction constant sul oxidation with no3 [kg/mol/day]	
k_sul_no3 =	20000.0
reaction constant sul oxidation with o2 [kg/mol/day]	
k_sul_o2 =	20000.0
oxygen half-saturation constant for nitrification [mol/kg]	
o2_min_nit =	1.0E-6
oxygen half-saturation constant for recycling of sediment detritus using oxygen [mol/kg]	
o2_min_sed_resp =	2.0E-5
q10 rule factor for oxidation of h2s and sul [1/K]	
q10_h2s =	0.0693
q10 rule factor for nitrification [1/K]	
q10_nit =	0.11
nitrification rate for ammonium in the sediment at 0°C [1/d]	
k_nh4_o2 =	274000.0
porosity	
por =	0.77
rate constant for hydrogen sulfide oxidation in presence of iron-III minerals [1/d]	
k_h2s_ihs =	21.9
continued on next page...	

Constants, continued from previous page	
oxidation constant for manganese-II [kg³/mol³/d]	
k_mno2 =	548000.0
fraction of illite-montmorillonite mixed layer minerals on volume of all minerals [1]	
vol_fraction_im =	0.5
potentially reducible iron content of illite-montmorillonite mixed layer minerals [g/g]	
fe_content_im =	0.001
maximum rate of mn2 liberation due to pyrite reduction [mol/kg/d]	
r_max_lib_mn2_pyrox	1.0E-5
maximum oxidation rate of pyrite [1/d]	
r_max_ox_pyr =	0.1
rate coefficient for oxygen consumption by pyrite oxidation [kg/mol/d]	
k_o2_pyr =	2.73
rate of oxidation of iron-II in illite-montmorillonite mixed-layer minerals [1/d]	
r_i2i_ox =	0.1
rate of h2s reduction by i3i oxidation [1/d]	
r_h2s_ox_i3i =	0.1
rate constant for MnO2 reduction by Fe2+ [kg/mol/d]	
k_mno2_fe2 =	5.48
rate constant for ims oxidation by O2 [kg/mol/d]	
k_ims_o2 =	822.0
rate constant for manganese oxide reduction by h2s [kg/mol/d]	
k_mno2_h2s =	58.4
Process limitation factors	
lim_t_o2_1 =	t_o2/(t_o2+o2_min_nit)
lim_t_o2_2 =	1.0-exp(-t_o2/o2_min_sed_resp)
lim_t_o2_12 =	theta(t_o2-0.0)
lim_t_nh4_16 =	theta(t_nh4-0.0)
lim_t_no3_14 =	theta(t_no3-0.0)
continued on next page...	

Process limitation factors, continued from previous page	
lim_t_h2s_29 =	theta(t_h2s-0.0)
lim_t_sul_30 =	theta(t_sul-0.0)
lim_t_ihs_4 =	1.0-exp(-t_ihs/ihs_min_sed_irred_2d)
lim_t_fe2_55 =	theta(t_fe2-0.0)
lim_t_pyr_58 =	theta(t_pyr-0.0)
lim_t_ims_57 =	theta(t_ims-0.0)
lim_t_mos_59 =	theta(t_mos-0.0)
lim_t_mn2_62 =	theta(t_mn2-0.0)
lim_t_iim_61 =	theta(t_iim-0.0)
lim_t_i3i_6 =	1.0-exp(-t_i3i/ihs_min_sed_irred_2d)
lim_t_ihc_10 =	1.0-exp(-t_ihc/ihs_min_sed_irred_2d)

3.5 Process type BGC/pelagic/mineralization

Processes
mineralization of DON [mol/kg/day] $t_{don} \rightarrow t_{nh4}$ $p_{don_rec_nh4} = (t_{don} * r_{don_rec}) * lim_t_{don_21}$
recycling of detritus to ammonium using oxygen (respiration) (index 1 to 6) [mol/kg/day] $h3oplus + rfr_pc_enrichment_det * 6.625 * t_{o2} + t_{det_1} \rightarrow (1.0 + 6.625 * rfr_pc_enrichment_det) * h2o + rfr_pc_enrichment_det * rfr_c * t_{dic} + t_{nh4} + 0 * h3oplus + 0 * h2o$ $p_{det_1_resp_nh4} = (t_{det_1} * r_{det_1_rec} * exp(q10_det_rec * cgt_temp) * (1.0 - cgt_in_sediment)) * lim_t_{o2_8} * lim_t_{det_1_31}$
recycling of detritus to ammonium using nitrate (denitrification) (index 1 to 6) [mol/kg/day] $rfr_pc_enrichment_det * 5.3 * t_{no3} + (1.0 + 5.3 * rfr_pc_enrichment_det) * h3oplus + t_{det_1} \rightarrow (1.0 + 14.575 * rfr_pc_enrichment_det) * h2o + rfr_pc_enrichment_det * 2.65 * t_{n2} + t_{nh4} + rfr_pc_enrichment_det * rfr_c * t_{dic}$ $p_{det_1_denit_nh4} = (t_{det_1} * r_{det_1_rec} * exp(q10_det_rec * cgt_temp) * (1.0 - cgt_in_sediment)) * (1.0 - lim_t_{o2_8}) * lim_t_{no3_9} * lim_t_{det_1_31}$
recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (index 1 to 6) [mol/kg/day] $(1.0 + rfr_pc_enrichment_det * 6.625) * h3oplus + rfr_pc_enrichment_det * 3.3125 * t_{so4} + t_{det_1} \rightarrow (1.0 + rfr_pc_enrichment_det * 13.25) * h2o + rfr_pc_enrichment_det * 3.3125 * t_{h2s} + rfr_pc_enrichment_det * rfr_c * t_{dic} + t_{nh4}$ $p_{det_1_sulf_nh4} = (t_{det_1} * r_{det_1_rec} * exp(q10_det_rec * cgt_temp) * max(t_{so4}, 0.0) / (max(t_{so4}, 0.0) + so4_min_det_sulf) * (1.0 - cgt_in_sediment)) * (1.0 - lim_t_{o2_8}) * (1.0 - lim_t_{no3_9}) * lim_t_{so4_28} * lim_t_{det_1_31}$
recycling of detritus to ammonium using oxygen (respiration) (index 1 to 6) [mol/kg/day] $t_{detp_1} + 3 * rfr_pc_enrichment_det * rfr_p * h2o \rightarrow 3 * rfr_pc_enrichment_det * rfr_p * h3oplus + rfr_pc_enrichment_det * rfr_p * t_{po4}$ $p_{detp_1_remin_po4} = (t_{detp_1} * r_{det_1_rec} * exp(q10_det_rec * cgt_temp) * (1.0 - cgt_in_sediment) * (1.0 + (factor_pref_remin_p - 1.0) * o2_min_sed_resp / (t_{o2} + o2_min_sed_resp))) * lim_t_{detp_1_37}$
respiration of POC [mol/kg/day] $t_{o2} + t_{poc} \rightarrow h2o + t_{dic}$ $p_{poc_resp} = (t_{poc} * r_{poc_rec} * exp(q10_det_rec * cgt_temp)) * lim_t_{o2_8} * lim_t_{poc_68}$
continued on next page...

Processes, continued from previous page

recycling of POC using nitrate (denitrification) [mol/kg/day]

$$0.8 \cdot h3oplus + 0.8 \cdot t_{no3} + t_{poc} \rightarrow 0.4 \cdot t_{n2} + 2.2 \cdot h2o + t_{dic}$$

$$p_{poc_denit} = (t_{poc} \cdot r_{poc_rec} \cdot \exp(q10_det_rec \cdot cgt_temp)) \cdot (1.0 - \lim_{t_o2_8}) \cdot \lim_{t_no3_9} \cdot \lim_{t_poc_68}$$
Mineralization of POC, e-acceptor sulfate (sulfate reduction) [mol/kg/day]

$$h3oplus + 0.5 \cdot t_{so4} + t_{poc} \rightarrow 2 \cdot h2o + 0.5 \cdot t_{h2s} + t_{dic}$$

$$p_{poc_sulf} = (t_{poc} \cdot r_{poc_rec} \cdot \exp(q10_det_rec \cdot cgt_temp)) \cdot (1.0 - \lim_{t_o2_8}) \cdot (1.0 - \lim_{t_no3_9}) \cdot \lim_{t_so4_28} \cdot \lim_{t_poc_68}$$
Auxiliary variables**Constants****minimum no3 concentration for recycling of detritus using nitrate (denitrification)**

$$no3_min_det_denit = 1.0E-9$$
oxygen half-saturation constant for detritus recycling [mol/kg]

$$o2_min_det_resp = 1.0E-5$$
oxygen half-saturation constant for recycling of sediment detritus using oxygen [mol/kg]

$$o2_min_sed_resp = 2.0E-5$$
q10 rule factor for recycling [1/K]

$$q10_det_rec = 0.15$$
redfield ratio C/N

$$rfr_c = 6.625$$
redfield ratio P/N

$$rfr_p = 0.0625$$
enrichment factor for P and C in detritus [1]

$$rfr_pc_enrichment_de = 1.5$$
rate constant mineralizing DON into NH4 [1/d]

$$r_don_rec = 0.01$$
minimum sulfate concentration for sulfate reduction [mol/kg]

$$so4_min_det_sulf = 1.0E-6$$
detritus recycling rates [1/d]

continued on next page...

Constants, continued from previous page	
r_det_1_rec =	0.0647
detritus recycling rates [1/d]	
r_det_2_rec =	0.00924
detritus recycling rates [1/d]	
r_det_3_rec =	0.00136
detritus recycling rates [1/d]	
r_det_4_rec =	0.000108
detritus recycling rates [1/d]	
r_det_5_rec =	1.62E-5
detritus recycling rates [1/d]	
r_det_6_rec =	0.0
acceleration factor for preferential mineralization of P compared to N under hypoxic conditions [1]	
factor_pref_remin_p	10.0
=	
recycling rate of particulate organic carbon (TEP) at 0 degC [1/day]	
r_poc_rec =	0.003
Process limitation factors	
lim_t_don_21 =	theta(t_don-0.0)
lim_t_o2_8 =	1.0-exp(-t_o2/o2_min_det_resp)
lim_t_no3_9 =	1.0-exp(-t_no3/no3_min_det_denit)
lim_t_so4_28 =	theta(t_so4-0.0)
lim_t_det_1_31 =	theta(t_det_1-0.0)
lim_t_det_2_32 =	theta(t_det_2-0.0)
lim_t_det_3_33 =	theta(t_det_3-0.0)
lim_t_det_4_34 =	theta(t_det_4-0.0)
lim_t_det_5_35 =	theta(t_det_5-0.0)
lim_t_det_6_36 =	theta(t_det_6-0.0)
continued on next page...	

Process limitation factors, continued from previous page

```
lim_t_detp_1_37 = theta(t_detp_1-0.0)
```

```
lim_t_detp_2_38 = theta(t_detp_2-0.0)
```

```
lim_t_detp_3_39 = theta(t_detp_3-0.0)
```

```
lim_t_detp_4_40 = theta(t_detp_4-0.0)
```

```
lim_t_detp_5_41 = theta(t_detp_5-0.0)
```

```
lim_t_detp_6_42 = theta(t_detp_6-0.0)
```

```
lim_t_poc_68 = theta(t_poc-0.0)
```

3.6 Process type BGC/pelagic/phytoplankton

Processes
assimilation of nitrate by large-cell phytoplankton [mol/kg/day] $t_{no3} + rfr_p*t_{po4} + rfr_c*t_{dic} + 6.4375*h2o + 1.1875*h3oplus \rightarrow t_{lpp} + 8.625*t_{o2}$ $p_{no3_assim_lpp} = (lpp_plus_lpp0*lr_assim_lpp*t_{no3}/(din+epsilon))*lim_t_{no3_14}*lim_t_{po4_15}*lim_t_{dic_13}$
assimilation of ammonium by large-cell phytoplankton [mol/kg/day] $7.4375*h2o + rfr_c*t_{dic} + rfr_p*t_{po4} + t_{nh4} \rightarrow 0.8125*h3oplus + 6.625*t_{o2} + t_{lpp}$ $p_{nh4_assim_lpp} = (lpp_plus_lpp0*lr_assim_lpp*t_{nh4}/(din+epsilon))*lim_t_{dic_13}*lim_t_{po4_15}*lim_t_{nh4_16}$
assimilation of nitrate by small-cell phytoplankton [mol/kg/day] $t_{no3} + rfr_p*t_{po4} + rfr_c*t_{dic} + 6.4375*h2o + 1.1875*h3oplus \rightarrow t_{spp} + 8.625*t_{o2}$ $p_{no3_assim_spp} = (spp_plus_spp0*lr_assim_spp*t_{no3}/(din+epsilon))*lim_t_{no3_14}*lim_t_{po4_15}*lim_t_{dic_13}$
assimilation of ammonium by small-cell phytoplankton [mol/kg/day] $t_{nh4} + rfr_p*t_{po4} + rfr_c*t_{dic} + 0*h2o + 7.4375*h2o \rightarrow t_{spp} + 6.625*t_{o2} + 0.8125*h3oplus$ $p_{nh4_assim_spp} = (spp_plus_spp0*lr_assim_spp*t_{nh4}/(din+epsilon))*lim_t_{nh4_16}*lim_t_{po4_15}*lim_t_{dic_13}$
fixation of dinitrogen by diazotroph cyanobacteria [mol/kg/day] $0.1875*h3oplus + 0.5*t_{n2} + rfr_p*t_{po4} + rfr_c*t_{dic} + 7.9375*h2o \rightarrow t_{cya} + 7.375*t_{o2}$ $p_{n2_assim_cya} = (cya_plus_cya0*lr_assim_cya)*lim_t_{n2_11}*lim_t_{po4_15}*lim_t_{dic_13}$
respiration of large-cell phytoplankton [mol/kg/day] $t_{lpp} + 6.625*t_{o2} + 0.8125*h3oplus \rightarrow don_fraction*t_{don} + (1-don_fraction)*t_{nh4} + rfr_p*t_{po4} + rfr_c*t_{dic} + 7.4375*h2o$ $p_{lpp_resp_nh4} = (t_{lpp}*r_{lpp_resp}*(1.0-cgt_in_sediment))*lim_t_{lpp_17}*lim_t_{o2_12}$
respiration of small-cell phytoplankton [mol/kg/day] $0.8125*h3oplus + 6.625*t_{o2} + t_{spp} \rightarrow 7.4375*h2o + rfr_c*t_{dic} + rfr_p*t_{po4} + (1-don_fraction)*t_{nh4} + don_fraction*t_{don}$ $p_{spp_resp_nh4} = (t_{spp}*r_{spp_resp}*(1.0-cgt_in_sediment))*lim_t_{o2_12}*lim_t_{spp_18}$
continued on next page...

Processes, continued from previous page

respiration of diazotroph cyanobacteria [mol/kg/day]

```
0.8125*h3oplus + 6.625*t_o2 + t_cya -> 7.4375*h2o + rfr_c*t_dic + rfr_p*t_po4 +
don_fraction*t_don + (1-don_fraction)*t_nh4
p_cya_resp_nh4 = (t_cya*r_cya_resp*(1.0-cgt_in_sediment))*lim_t_o2_12*
lim_t_cya_19
```

mortality of large-cell phytoplankton (index 1 to 6) [mol/kg/day]

```
(1.0-(1.0/rfr_pc_enrichment_det))*h3oplus + t_lpp -> (1.0-
(1.0/rfr_pc_enrichment_det))*h2o + (1.0-(1.0/rfr_pc_enrichment_det))*t_nh4 +
(1.0/rfr_pc_enrichment_det)*t_det_1 + (1.0/rfr_pc_enrichment_det)*t_detp_1
p_lpp_mort_det_1 = (frac_det_1*t_lpp*r_pp_mort*(1+9*theta(5.0e-6-t_o2)))*
lim_t_lpp_17
```

mortality of small-scale phytoplankton (index 1 to 6) [mol/kg/day]

```
(1.0-(1.0/rfr_pc_enrichment_det))*h3oplus + t_spp -> (1.0-
(1.0/rfr_pc_enrichment_det))*h2o + (1.0-(1.0/rfr_pc_enrichment_det))*t_nh4 +
(1.0/rfr_pc_enrichment_det)*t_det_1 + (1.0/rfr_pc_enrichment_det)*t_detp_1
p_spp_mort_det_1 = (frac_det_1*t_spp*r_pp_mort*(1+9*theta(5.0e-6-t_o2)))*
lim_t_spp_18
```

mortality of diazotroph cyanobacteria (index 1 to 6) [mol/kg/day]

```
t_cya + (1.0-(1.0/rfr_pc_enrichment_det))*h3oplus ->
(1.0/rfr_pc_enrichment_det)*t_detp_1 + (1.0/rfr_pc_enrichment_det)*t_det_1 +
(1.0-(1.0/rfr_pc_enrichment_det))*t_nh4 + (1.0-(1.0/rfr_pc_enrichment_det))*h2o
p_cya_mort_det_1 = (frac_det_1*t_cya*r_pp_mort*(1+9*theta(5.0e-6-t_o2)))*
lim_t_cya_19
```

Production of POC by LPP [mol/kg/day]

```
h2o + t_dic -> t_o2 + t_poc
p_assim_lpp_poc = (rfr_c * lpp_plus_lpp0 * lr_assim_lpp_poc)*lim_t_dic_13
```

Production of POC by SPP [mol/kg/day]

```
h2o + t_dic -> t_o2 + t_poc
p_assim_spp_poc = (rfr_c * spp_plus_spp0 * lr_assim_spp_poc)*lim_t_dic_13
```

Production of POC by CYA [mol/kg/day]

```
t_dic + h2o -> t_poc + t_o2
p_assim_cya_poc = (rfr_c * cya_plus_cya0 * lr_assim_cya_poc)*lim_t_dic_13
```

Auxiliary variables**square of positive temperature [°C * °C]**

```
temp_sq = max(0.0,cgt_temp)*max(0.0,cgt_temp)
```

dissolved inorganic nitrogen [mol/kg]

```
din = t_no3+t_nh4
```

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Auxiliary variables, continued from previous page	
squared phosphate [mol**2/kg**2]	
po4_sq =	t_po4*t_po4
large-cell phytoplankton plus seed concentration [mol/kg]	
lpp_plus_lpp0 =	t_lpp+lpp0
small-cell phytoplankton plus seed concentration [mol/kg]	
spp_plus_spp0 =	t_spp+spp0
diazotroph cyanobacteria plus seed concentration [mol/kg]	
cya_plus_cya0 =	t_cya+cya0
light limitation factor for large-cell phytoplankton growth [1]	
lim_light_lpp =	cgt_light/max(cgt_light/2.0,light_opt_lpp)*exp(1- cgt_light/max(cgt_light/2.0,light_opt_lpp))
light limitation factor for small-cell phytoplankton growth [1]	
temp1 =	max(cgt_light/2.0,light_opt_spp)
lim_light_spp =	cgt_light/temp1*exp(1-cgt_light/temp1)
squared DIN [mol2/kg2]	
din_sq =	din*din
growth rate of diazotroph cyanobacteria, limited by DIP, light, oxygen, temperature and salinity [1/day]	
lr_assim_cya =	r_cya_assim*theta(t_o2-2*t_h2s)*min(po4_sq/(po4_sq+ dip_min_cya*dip_min_cya),lim_light_spp)*(1/(1+ exp(temp_min_cya-cgt_temp)))*(1/(1+exp(cgt_sali- sali_max_cya)))*(1/(1+exp(sali_min_cya-cgt_sali)))
growth rate of large-cell phytoplankton, limited by DIN, DIP, light and oxygen [1/day]	
lr_assim_lpp =	r_lpp_assim*theta(t_o2-2*t_h2s)*min(din_sq/(din_sq+ din_min_lpp*din_min_lpp),min(po4_sq/(po4_sq+din_min_lpp* din_min_lpp*rfr_p*rfr_p),lim_light_lpp))
growth rate of small-cell phytoplankton, limited by DIN, DIP, light, oxygen and temperature [1/day]	
lr_assim_spp =	r_spp_assim*theta(t_o2-2*t_h2s)*min(din_sq/(din_sq+ din_min_spp*din_min_spp),min(po4_sq/(po4_sq+din_min_spp* din_min_spp*rfr_p*rfr_p),lim_light_spp))*(1+ temp_sq/(temp_sq+temp_min_spp*temp_min_spp))
continued on next page...	

Auxiliary variables, continued from previous page

production rate of POC by LPP

```
lr_assim_lpp_poc = fac_poc_assim * r_lpp_assim * theta(t_o2-2*t_h2s) *
min(max(1 - din_sq/(din_sq+din_min_lpp*din_min_lpp), 1 -
po4_sq/(din_min_lpp*din_min_lpp*rfr_p*rfr_p + po4_sq)),
lim_light_lpp)
```

production rate of POC by LPP

```
lr_assim_spp_poc = fac_poc_assim * r_lpp_assim * theta(t_o2-2*t_h2s) *
min(max(1 - din_sq/(din_sq+din_min_lpp*din_min_lpp), 1 -
po4_sq/(din_min_lpp*din_min_lpp*rfr_p*rfr_p + po4_sq)),
lim_light_lpp)
```

production rate of POC by CYA

```
lr_assim_cya_poc = fac_poc_assim * r_cya_assim*theta(t_o2-2*t_h2s)*min(1 -
po4_sq/(po4_sq+dip_min_cya*dip_min_cya),lim_light_spp)*
(1/(1+exp(temp_min_cya-cgt_temp)))*(1/(1+exp(cgt_sali-
sali_max_cya)))*(1/(1+exp(sali_min_cya-cgt_sali)))
```

Constants

seed concentration for diazotroph cyanobacteria [mol/kg]

cya0 = 4.5E-9

DIN half saturation constant for large-cell phytoplankton growth [mol/kg]

din_min_lpp = 1.125E-6

DIN half saturation constant for small-cell phytoplankton growth [mol/kg]

din_min_spp = 4.5E-7

DIP half saturation constant for diazotroph cyanobacteria growth [mol/kg]

dip_min_cya = 1.125E-7

no division by 0

epsilon = 4.5E-17

optimal light for large-cell phytoplankton growth [W/m**2]

light_opt_lpp = 35.0

optimal light for small-cell phytoplankton growth [W/m**2]

light_opt_spp = 50.0

seed concentration for large-cell phytoplankton [mol/kg]

lpp0 = 4.5E-9

maximum rate for nutrient uptake of diazotroph cyanobacteria [1/day]

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Constants, continued from previous page	
r_cya_assim =	0.75
respiration rate of cyanobacteria to ammonium [1/day]	
r_cya_resp =	0.01
maximum rate for nutrient uptake of large-cell phytoplankton [1/day]	
r_lpp_assim =	1.4
respiration rate of large phytoplankton to ammonium [1/day]	
r_lpp_resp =	0.06
mortality rate of phytoplankton [1/day]	
r_pp_mort =	0.02
maximum rate for nutrient uptake of small-cell phytoplankton [1/day]	
r_spp_assim =	0.46
respiration rate of small phytoplankton to ammonium [1/day]	
r_spp_resp =	0.015
redfield ratio C/N	
rfr_c =	6.625
redfield ratio P/N	
rfr_p =	0.0625
enrichment factor for P and C in detritus [1]	
rfr_pc_enrichment_de =	1.5
upper salinity limit - diazotroph cyanobacteria [psu]	
sali_max_cya =	10.0
lower salinity limit - diazotroph cyanobacteria [psu]	
sali_min_cya =	1.0
seed concentration for small-cell phytoplankton [mol/kg]	
spp0 =	4.5E-9
lower temperature limit - diazotroph cyanobacteria [°C]	
temp_min_cya =	13.5
lower temperature limit - small-cell phytoplankton [°C]	
temp_min_spp =	10.0
continued on next page...	

Constants, continued from previous page

fraction of DON in respiration products
--

don_fraction = 0.1

fraction of this detritus class in total detritus production [1]

frac_det_1 = 0.26

fraction of this detritus class in total detritus production [1]

frac_det_2 = 0.16

fraction of this detritus class in total detritus production [1]

frac_det_3 = 0.16

fraction of this detritus class in total detritus production [1]

frac_det_4 = 0.16

fraction of this detritus class in total detritus production [1]

frac_det_5 = 0.08

fraction of this detritus class in total detritus production [1]

frac_det_6 = 0.18

which fraction of DIC assimilation continues and causes POC production if nutrients are depleted [1]

fac_poc_assim = 1.0

Process limitation factors

lim_t_n2_11 = theta(t_n2-0.0)

lim_t_o2_12 = theta(t_o2-0.0)

lim_t_dic_13 = theta(t_dic-0.0)

lim_t_nh4_16 = theta(t_nh4-0.0)

lim_t_no3_14 = theta(t_no3-0.0)

lim_t_po4_15 = theta(t_po4-0.0)

lim_t_spp_18 = theta(t_spp-0.0)

lim_t_lpp_17 = theta(t_lpp-0.0)

lim_t_cya_19 = theta(t_cya-0.0)

continued on next page...

Process limitation factors, continued from previous page

3.7 Process type BGC/pelagic/reoxidation

Processes	
nitrification [mol/kg/day]	
$\text{h2o} + 2*\text{t_o2} + \text{t_nh4} \rightarrow 2*\text{h3oplus} + \text{t_no3}$	
$\text{p_nh4_nit_no3} =$	$(\text{t_nh4}*\text{r_nh4_nitrif}*\exp(\text{q10_nit}*\text{cgt_temp})*(1.0-\text{cgt_in_sediment}))*\text{lim_t_o2_0}*\text{lim_t_nh4_16}$
oxidation of Fe2+ to iron hydroxide in the sediment [mol/kg/day]	
$0.25*\text{t_o2} + 4.5*\text{h2o} + \text{t_fe2} \rightarrow \text{t_ihw} + 2*\text{h3oplus}$	
$\text{p_fe2_ox_ihw} =$	$(\text{k_feo2}*\text{t_fe2}*\text{t_o2}*\text{oh}*\text{oh}*(1.0-\text{cgt_in_sediment}))*\text{lim_t_o2_12}*\text{lim_t_fe2_55}$
nitrification in the sediment (sediment only) [mol/m²/day]	
$2*\text{t_o2} + \text{t_aim} \rightarrow \text{h3oplus} + \text{t_no3}$	
$\text{p_aim_nit_no3_sed} =$	$(\text{t_aim}*\text{t_o2}*\text{k_nh4_o2}*\exp(\text{q10_nit}*\text{cgt_temp})*\text{cgt_in_sediment})*\text{lim_t_o2_1}*\text{lim_t_aim_67}$
Auxiliary variables	
absolute temperature [K]	
$\text{temp_k} =$	$\text{cgt_temp} + 273.15$
temporary value assumed for pH [1]	
$\text{ph_temp} =$	$0.0-\log(\min(\max(\text{h3o}, 1.0\text{e-}12), 1.0\text{e-}2))/\log(10.0)$
calculated iteratively, 10 iterations, initial value = 0.0	
self-ionization constant of Water [mol²/kg²]	
$\text{k_water} =$	$\exp(-13847.26 / \text{temp_k} + 148.96502 - 23.6521 * \log(\text{temp_k}) + (118.67/\text{temp_k} - 5.977 + 1.0495 * \log(\text{temp_k})) * \sqrt{\text{cgt_sali}} - 0.01615 * \text{cgt_sali})$
Acid dissociation constant CO₂ + 2 H₂O <-> HCO₃⁻ + H₃O⁺ [mol/kg]	
$\text{k1_co2} =$	$\text{power}(10.0, (-3633.86 / \text{temp_k} + 61.2172 - 9.6777 * \log(\text{temp_k}) + 0.011555 * \text{cgt_sali} - 0.0001152 * \text{cgt_sali} * \text{cgt_sali}))$
Acid dissociation constant HCO₃⁻ + H₂O <-> [CO₃²⁻] + H₃O⁺ [mol/kg]	
$\text{k2_co2} =$	$\text{power}(10.0, (-471.78 / \text{temp_k} - 25.929 + 3.16967 * \log(\text{temp_k}) + 0.01781 * \text{cgt_sali} - 0.0001122 * \text{cgt_sali} * \text{cgt_sali}))$
Acid dissociation constant of boric acid [mol/kg]	
$\text{k_boron} =$	$\exp((-8966.9 - 2890.53*\sqrt{\text{cgt_sali}} - 77.942*\text{cgt_sali} + 1.728*\text{cgt_sali}*\sqrt{\text{cgt_sali}} - 0.0996*\text{cgt_sali}*\text{cgt_sali}) / \text{temp_k} + 148.0248 + 137.1942*\sqrt{\text{cgt_sali}} + 1.62142*\text{cgt_sali} + (-24.4344 - 25.085*\sqrt{\text{cgt_sali}} - 0.2474*\text{cgt_sali})*\log(\text{temp_k}) + 0.053105*\sqrt{\text{cgt_sali}}*\text{temp_k})$
continued on next page...	

Auxiliary variables, continued from previous page

Acid dissociation constant $\text{H}_3\text{PO}_4 + \text{H}_2\text{O} \rightleftharpoons [\text{H}_2\text{PO}_4^-] + \text{H}_3\text{O}^+$ [mol/kg]

$$k1_po4 = \exp(-4576.752/\text{temp_k} + 115.525 - 18.453 \cdot \log(\text{temp_k}) + (0.69171 - 106.736/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.01844 + 0.65643/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $[\text{H}_2\text{PO}_4^-] + \text{H}_2\text{O} \rightleftharpoons [\text{HPO}_4^{2-}] + \text{H}_3\text{O}^+$ [mol/kg]

$$k2_po4 = \exp(-8814.715/\text{temp_k} + 172.0883 - 27.927 \cdot \log(\text{temp_k}) + (1.35660 - 160.340/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.05778 - 0.37335/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $[\text{HPO}_4^{2-}] + \text{H}_2\text{O} \rightleftharpoons [\text{PO}_4^{3-}] + \text{H}_3\text{O}^+$ [mol/kg]

$$k3_po4 = \exp(-3070.75/\text{temp_k} - 18.141 + (2.81197 + 17.27039/\text{temp_k}) \cdot \sqrt{\text{cgt_sali}} - (0.09984 + 44.99486/\text{temp_k}) \cdot \text{cgt_sali})$$

Acid dissociation constant $\text{H}_2\text{S} + \text{H}_2\text{O} \rightleftharpoons \text{HS}^- + \text{H}_3\text{O}^+$ [mol/kg]

$$k1_h2s = \exp(-3131.42/\text{temp_k} - 5.818 + 0.368 \cdot (\text{power}(\max(0.0, \text{cgt_sali}), (1.0/3.0))))$$

total concentration of boron [mol/kg]

$$\text{boron_total} = 0.000416 \cdot \text{cgt_sali}/35.0$$

boron alkalinity [mol/kg]

$$\text{alk_boron} = \text{boron_total} \cdot k_boron / (k_boron + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

hydrogen sulfide alkalinity [mol/kg]

$$\text{alk_h2s} = t_h2s \cdot k1_h2s / (k1_h2s + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

water alkalinity [mol/kg]

$$\text{alk_water} = k_water / h3o - h3o$$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in phosphate alkalinity formula [mol³/kg³]

$$\text{alk_po4_denominator} = (h3o \cdot h3o \cdot h3o + k1_po4 \cdot h3o \cdot h3o + k1_po4 \cdot k2_po4 \cdot h3o + k1_po4 \cdot k2_po4 \cdot k3_po4)$$

calculated iteratively, 10 iterations, initial value = 0.0

phosphate alkalinity [mol/kg]

$$\text{alk_po4} = (t_po4 \cdot (k1_po4 \cdot k2_po4 \cdot h3o + 2.0 \cdot k1_po4 \cdot k2_po4 \cdot k3_po4 - h3o \cdot h3o \cdot h3o)) / \text{alk_po4_denominator}$$

calculated iteratively, 10 iterations, initial value = 0.0

continued on next page...

Auxiliary variables, continued from previous page

denominator in carbonate alkalinity formula [mol²/kg²]

alk_co2_denominator (h3o*h3o + k1_co2*h3o + k1_co2*k2_co2)
=

calculated iteratively, 10 iterations, initial value = 0.0

carbonate alkalinity [mol/kg]

alk_co2 = t_dic*k1_co2*(h3o+2*k2_co2)/alk_co2_denominator

calculated iteratively, 10 iterations, initial value = 0.0

error in total alkalinity calculation at the assumed pH [mol/kg]

alk_residual = t_alk - alk_co2 - alk_po4 - alk_boron - alk_h2s - alk_water

calculated iteratively, 10 iterations, initial value = 0.0

derivative of phosphate alkalinity with respect to h3o [1]

dalkp_dh3o = t_po4*(0.0-k1_po4*h3o*h3o*h3o-h3o-4*k1_po4*k2_po4*h3o*h3o*
h3o-(k1_po4*k1_po4*k2_po4+9*k1_po4*k2_po4*k3_po4)*h3o*h3o-
4*k1_po4*k1_po4*k2_po4*k3_po4*h3o-k1_po4*k1_po4*k2_po4*
k2_po4*k3_po4)/(alk_po4_denominator*alk_po4_denominator)

calculated iteratively, 10 iterations, initial value = 0.0

derivative of carbonate alkalinity with respect to h3o [1]

dalkc_dh3o = t_dic*(0.0-k1_co2*h3o*h3o-k1_co2*k1_co2*k2_co2-4*k1_co2*
k2_co2*h3o)/(alk_co2_denominator*alk_co2_denominator)

calculated iteratively, 10 iterations, initial value = 0.0

derivative of residual_alk with respect to pH [mol/kg]

dalkresidual_dpH = 0.0-log(10.0)*h3o*(alk_boron/(k_boron+h3o)+alk_h2s/(k1_h2s+
h3o)+k_water/(h3o*h3o)+1-dalkp_dh3o-dalkc_dh3o)

calculated iteratively, 10 iterations, initial value = 0.0

newly determined pH value [1]

temp1 = alk_residual/dalkresidual_dpH

ph = ph_temp - temp1 + theta(abs(temp1) - 1)*0.5*temp1

calculated iteratively, 10 iterations, initial value = 0.0

h3o ion concentration [mol/kg]

h3o = power(10.0,0.0-max(1.0,min(13.0,ph)))

calculated iteratively, 10 iterations, initial value = 1.0e-8

h3o ion concentration [mol/kg]

oh = power(10.0,log(k_water)/log(10.0)+max(1.0,min(13.0,ph)))

ionic strength of the solution [mol/kg]

ionic_strength = 0.02*cgt_sali

continued on next page...

Auxiliary variables, continued from previous page

rate constant iron-II oxidation by o2 [kg3/mol3/d]

```
k_feo2 = power(10.0,21.56-1545.0/temp_k-3.29*
              power(ionic_strength,0.5)+1.52*ionic_strength)
```

Constants

oxygen half-saturation constant for nitrification [mol/kg]

```
o2_min_nit = 1.0E-6
```

q10 rule factor for nitrification [1/K]

```
q10_nit = 0.11
```

nitrification rate at 0°C [1/day]

```
r_nh4_nitrif = 0.1
```

nitrification rate for ammonium in the sediment at 0°C [1/d]

```
k_nh4_o2 = 274000.0
```

Process limitation factors

```
lim_t_o2_0 = 1.0-exp(-t_o2/o2_min_nit)
```

```
lim_t_o2_1 = t_o2/(t_o2+o2_min_nit)
```

```
lim_t_o2_12 = theta(t_o2-0.0)
```

```
lim_t_nh4_16 = theta(t_nh4-0.0)
```

```
lim_t_fe2_55 = theta(t_fe2-0.0)
```

```
lim_t_aim_67 = theta(t_aim-0.0)
```

3.8 Process type BGC/pelagic/zooplankton

Processes	
grazing of zooplankton eating large-cell phytoplankton [mol/kg/day]	
t_lpp -> t_zoo	
p_lpp_graz_zoo =	$((t_{\text{zoo}} + \text{zoo0}) * \text{lr_graz_zoo} * t_{\text{lpp}} / \max(\text{food_zoo}, \text{epsilon})) * \text{lim_t_lpp_17}$
grazing of zooplankton eating small-cell phytoplankton [mol/kg/day]	
t_spp -> t_zoo	
p_spp_graz_zoo =	$((t_{\text{zoo}} + \text{zoo0}) * \text{lr_graz_zoo} * t_{\text{spp}} / \max(\text{food_zoo}, \text{epsilon})) * \text{lim_t_spp_18}$
grazing of zooplankton eating diazotroph cyanobacteria [mol/kg/day]	
t_cya -> t_zoo	
p_cya_graz_zoo =	$((t_{\text{zoo}} + \text{zoo0}) * \text{lr_graz_zoo} * (0.5 * t_{\text{cya}}) / \max(\text{food_zoo}, \text{epsilon})) * \text{lim_t_cya_19}$
respiration of zooplankton [mol/kg/day]	
0.8125*h3oplus + 6.625*t_o2 + t_zoo -> 7.4375*h2o + rfr_c*t_dic + rfr_p*t_po4 + (1-don_fraction)*t_nh4 + don_fraction*t_don	
p_zoo_resp_nh4 =	$(\text{zoo_eff} * r_{\text{zoo_resp}} * (1.0 - \text{cgt_in_sediment})) * \text{lim_t_o2_12} * \text{lim_t_zoo_20}$
mortality of zooplankton (index 1 to 6) [mol/kg/day]	
(1.0-(1.0/rfr_pc_enrichment_det))*h3oplus + t_zoo -> (1.0-(1.0/rfr_pc_enrichment_det))*h2o + (1.0-(1.0/rfr_pc_enrichment_det))*t_nh4 + (1.0/rfr_pc_enrichment_det)*t_det_1 + (1.0/rfr_pc_enrichment_det)*t_detp_1	
p_zoo_mort_det_1 =	$(\text{frac_det_1} * \text{zoo_eff} * r_{\text{zoo_mort}} * (1 + 9 * \theta(5.0e-6 - t_{\text{o2}}))) * \text{lim_t_zoo_20}$
Auxiliary variables	
square of positive temperature [°C * °C]	
temp_sq =	$\max(0.0, \text{cgt_temp}) * \max(0.0, \text{cgt_temp})$
effectice zooplankton concentration assumed for mortality and respiration process [mol/kg]	
zoo_eff =	$t_{\text{zoo}} * t_{\text{zoo}} / \text{zoo_cl}$
suitable food for zooplankton (weighted with food preferences) [mol/kg]	
food_zoo =	$t_{\text{lpp}} + t_{\text{spp}} + 0.5 * t_{\text{cya}}$
growth rate of zooplankton, limited by food, oxygen and temperature [1/day]	
lr_graz_zoo =	$r_{\text{zoo_graz}} * (1 - \exp(-\text{food_zoo} * \text{food_zoo} / (\text{food_min_zoo} * \text{food_min_zoo}))) * \theta(t_{\text{o2}} - 2 * t_{\text{h2s}}) * (1.0 + \text{temp_sq} / (\text{temp_opt_zoo} * \text{temp_opt_zoo}) * \exp(2.0 - \text{cgt_temp} * 2.0 / \text{temp_opt_zoo}))$
continued on next page...	

Auxiliary variables, continued from previous page

Constants	
no division by 0	
epsilon =	4.5E-17
Ivlev phytoplankton concentration for zooplankton grazing [mol/kg]	
food_min_zoo =	4.108E-6
maximum zooplankton grazing rate [1/day]	
r_zoo_graz =	0.5
mortality rate of zooplankton [1/day]	
r_zoo_mort =	0.03
respiration rate of zooplankton [1/day]	
r_zoo_resp =	0.01
redfield ratio C/N	
rfr_c =	6.625
redfield ratio P/N	
rfr_p =	0.0625
enrichment factor for P and C in detritus [1]	
rfr_pc_enrichment_de	1.5
=	
optimal temperature for zooplankton grazing [°C]	
temp_opt_zoo =	20.0
seed concentration for zooplankton [mol/kg]	
zoo0 =	4.5E-9
zooplankton closure parameter [mol/kg]	
zoo_cl =	9.0E-8
fraction of DON in respiration products	
don_fraction =	0.1
fraction of this detritus class in total detritus production [1]	
frac_det_1 =	0.26
fraction of this detritus class in total detritus production [1]	
continued on next page...	

Constants, continued from previous page	
frac_det_2 =	0.16
fraction of this detritus class in total detritus production [1]	
frac_det_3 =	0.16
fraction of this detritus class in total detritus production [1]	
frac_det_4 =	0.16
fraction of this detritus class in total detritus production [1]	
frac_det_5 =	0.08
fraction of this detritus class in total detritus production [1]	
frac_det_6 =	0.18
Process limitation factors	
lim_t_o2_12 =	theta(t_o2-0.0)
lim_t_spp_18 =	theta(t_spp-0.0)
lim_t_zoo_20 =	theta(t_zoo-0.0)
lim_t_lpp_17 =	theta(t_lpp-0.0)
lim_t_cya_19 =	theta(t_cya-0.0)

3.9 Process type gas_exchange

Processes	
downward nitrogen flux through the surface (surface only) [mol/m ² /day]	
-> t_n2	
p_n2_stf_down =	w_n2_stf*(n2_sat-t_n2)*theta(n2_sat-t_n2)*cgt_density
upward nitrogen flux through the surface (surface only) [mol/m ² /day]	
t_n2 ->	
p_n2_stf_up =	(w_n2_stf*(t_n2-n2_sat)*theta(t_n2-n2_sat)*cgt_density)* lim_t_n2_11
downward oxygen flux through the surface (surface only) [mol/m ² /day]	
-> t_o2	
p_o2_stf_down =	w_o2_stf*(o2_sat-t_o2)*theta(o2_sat-t_o2)*cgt_density
upward oxygen flux through the surface (surface only) [mol/m ² /day]	
t_o2 ->	
p_o2_stf_up =	(w_o2_stf*(t_o2-o2_sat)*theta(t_o2-o2_sat)*cgt_density)* lim_t_o2_12
downward co2 flux through the surface (surface only) [mol/m ² /day]	
-> t_dic	
p_co2_stf_down =	w_co2_stf*(patm_co2-pco2)*k0_co2*theta(patm_co2-pco2)* cgt_density
upward co2 flux through the surface (surface only) [mol/m ² /day]	
t_dic ->	
p_co2_stf_up =	(w_co2_stf*(pco2-patm_co2)*k0_co2*theta(pco2-patm_co2)* cgt_density)*lim_t_dic_13
Auxiliary variables	
absolute temperature [K]	
temp_k =	cgt_temp + 273.15
temporary value assumed for pH [1]	
ph_temp =	0.0-log(min(max(h3o,1.0e-12),1.0e-2))/log(10.0)
calculated iteratively, 10 iterations, initial value = 0.0	
self-ionization constant of Water [mol ² /kg ²]	
k_water =	exp(-13847.26 / temp_k + 148.96502 - 23.6521 * log(temp_k) + (118.67/temp_k - 5.977 + 1.0495 * log(temp_k)) * sqrt(cgt_sali) - 0.01615 * cgt_sali)
Solubility of CO2 [mol/kg/Pa]	
k0_co2 =	exp(9345.17 / temp_k - 60.2409 + 23.3585 * (log(temp_k) - 4.605170186) + cgt_sali*(0.023517 - 0.00023656 * temp_k + 0.00000047036 *temp_k*temp_k))/101325.0
continued on next page...	

Auxiliary variables, continued from previous page

Acid dissociation constant $\text{CO}_2 + 2 \text{H}_2\text{O} \rightleftharpoons \text{HCO}_3^- + \text{H}_3\text{O}^+$ [mol/kg]

```
k1_co2 = power(10.0, ( -3633.86 / temp_k + 61.2172 - 9.6777 *
log(temp_k) + 0.011555 * cgt_sali - 0.0001152 * cgt_sali *
cgt_sali))
```

Acid dissociation constant $\text{HCO}_3^- + \text{H}_2\text{O} \rightleftharpoons [\text{CO}_3^{2-}] + \text{H}_3\text{O}^+$ [mol/kg]

```
k2_co2 = power(10.0, ( -471.78 / temp_k - 25.929 + 3.16967 *
log(temp_k) + 0.01781 * cgt_sali - 0.0001122 * cgt_sali *
cgt_sali))
```

Acid dissociation constant of boric acid [mol/kg]

```
k_boron = exp(( -8966.9 - 2890.53*sqrt(cgt_sali) - 77.942*cgt_sali +
1.728*cgt_sali*sqrt(cgt_sali) - 0.0996*cgt_sali*cgt_sali) /
temp_k + 148.0248 + 137.1942*sqrt(cgt_sali) + 1.62142*
cgt_sali + (-24.4344 - 25.085*sqrt(cgt_sali) - 0.2474*
cgt_sali)*log(temp_k) + 0.053105*sqrt(cgt_sali)*temp_k )
```

Acid dissociation constant $\text{H}_3\text{PO}_4 + \text{H}_2\text{O} \rightleftharpoons [\text{H}_2\text{PO}_4^-] + \text{H}_3\text{O}^+$ [mol/kg]

```
k1_po4 = exp( -4576.752/temp_k + 115.525 - 18.453*log(temp_k) +
(0.69171 - 106.736/temp_k)*sqrt(cgt_sali) - (0.01844 +
0.65643/temp_k)*cgt_sali )
```

Acid dissociation constant $[\text{H}_2\text{PO}_4^-] + \text{H}_2\text{O} \rightleftharpoons [\text{HPO}_4^{2-}] + \text{H}_3\text{O}^+$ [mol/kg]

```
k2_po4 = exp( -8814.715/temp_k + 172.0883 - 27.927*log(temp_k) +
(1.35660 - 160.340/temp_k)*sqrt(cgt_sali) - (0.05778 -
0.37335/temp_k)*cgt_sali )
```

Acid dissociation constant $[\text{HPO}_4^{2-}] + \text{H}_2\text{O} \rightleftharpoons [\text{PO}_4^{3-}] + \text{H}_3\text{O}^+$ [mol/kg]

```
k3_po4 = exp( -3070.75/temp_k - 18.141 + (2.81197 + 17.27039/temp_k)
*sqrt(cgt_sali) - (0.09984 + 44.99486/temp_k)*cgt_sali )
```

Acid dissociation constant $\text{H}_2\text{S} + \text{H}_2\text{O} \rightleftharpoons \text{HS}^- + \text{H}_3\text{O}^+$ [mol/kg]

```
k1_h2s = exp( -3131.42/temp_k - 5.818 + 0.368*
(power(max(0.0, cgt_sali), (1.0/3.0))))
```

total concentration of boron [mol/kg]

```
boron_total = 0.000416 * cgt_sali/35.0
```

boron alkalinity [mol/kg]

```
alk_boron = boron_total * k_boron / (k_boron + h3o)
calculated iteratively, 10 iterations, initial value = 0.0
```

hydrogen sulfide alkalinity [mol/kg]

continued on next page...

Auxiliary variables, continued from previous page

$\text{alk_h2s} = \text{t_h2s} * \text{k1_h2s} / (\text{k1_h2s} + \text{h3o})$

calculated iteratively, 10 iterations, initial value = 0.0

water alkalinity [mol/kg]

$\text{alk_water} = \text{k_water} / \text{h3o} - \text{h3o}$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in phosphate alkalinity formula [mol3/kg3]

$\text{alk_po4_denominator} (\text{h3o} * \text{h3o} * \text{h3o} + \text{k1_po4} * \text{h3o} * \text{h3o} + \text{k1_po4} * \text{k2_po4} * \text{h3o} + \text{k1_po4} * \text{k2_po4} * \text{k3_po4})$

calculated iteratively, 10 iterations, initial value = 0.0

phosphate alkalinity [mol/kg]

$\text{alk_po4} = \text{t_po4} * (\text{k1_po4} * \text{k2_po4} * \text{h3o} + 2.0 * \text{k1_po4} * \text{k2_po4} * \text{k3_po4} - \text{h3o} * \text{h3o} * \text{h3o}) / \text{alk_po4_denominator}$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in carbonate alkalinity formula [mol2/kg2]

$\text{alk_co2_denominator} (\text{h3o} * \text{h3o} + \text{k1_co2} * \text{h3o} + \text{k1_co2} * \text{k2_co2})$

=

calculated iteratively, 10 iterations, initial value = 0.0

carbonate alkalinity [mol/kg]

$\text{alk_co2} = \text{t_dic} * \text{k1_co2} * (\text{h3o} + 2 * \text{k2_co2}) / \text{alk_co2_denominator}$

calculated iteratively, 10 iterations, initial value = 0.0

error in total alkalinity calculation at the assumed pH [mol/kg]

$\text{alk_residual} = \text{t_alk} - \text{alk_co2} - \text{alk_po4} - \text{alk_boron} - \text{alk_h2s} - \text{alk_water}$

calculated iteratively, 10 iterations, initial value = 0.0

derivative of phosphate alkalinity with respect to h3o [1]

$\text{dalkp_dh3o} = \text{t_po4} * (0.0 - \text{k1_po4} * \text{h3o} * \text{h3o} * \text{h3o} * \text{h3o} - 4 * \text{k1_po4} * \text{k2_po4} * \text{h3o} * \text{h3o} - \text{h3o} - (\text{k1_po4} * \text{k1_po4} * \text{k2_po4} + 9 * \text{k1_po4} * \text{k2_po4} * \text{k3_po4}) * \text{h3o} * \text{h3o} - 4 * \text{k1_po4} * \text{k1_po4} * \text{k2_po4} * \text{k3_po4} * \text{h3o} - \text{k1_po4} * \text{k1_po4} * \text{k2_po4} * \text{k2_po4} * \text{k3_po4}) / (\text{alk_po4_denominator} * \text{alk_po4_denominator})$

calculated iteratively, 10 iterations, initial value = 0.0

derivative of carbonate alkalinity with respect to h3o [1]

$\text{dalkc_dh3o} = \text{t_dic} * (0.0 - \text{k1_co2} * \text{h3o} * \text{h3o} - \text{k1_co2} * \text{k1_co2} * \text{k2_co2} - 4 * \text{k1_co2} * \text{k2_co2} * \text{h3o}) / (\text{alk_co2_denominator} * \text{alk_co2_denominator})$

calculated iteratively, 10 iterations, initial value = 0.0

derivative of residual_alk with respect to pH [mol/kg]

$\text{dalkresidual_dpH} = 0.0 - \log(10.0) * \text{h3o} * (\text{alk_boron} / (\text{k_boron} + \text{h3o}) + \text{alk_h2s} / (\text{k1_h2s} + \text{h3o}) + \text{k_water} / (\text{h3o} * \text{h3o}) + 1 - \text{dalkp_dh3o} - \text{dalkc_dh3o})$

continued on next page...

Auxiliary variables, continued from previous page

calculated iteratively, 10 iterations, initial value = 0.0

newly determined pH value [1]

```
temp1 =      alk_residual/dalkresidual_dpH
ph =      ph_temp - temp1 + theta(abs(temp1) - 1)*0.5*temp1
calculated iteratively, 10 iterations, initial value = 0.0
```

h3o ion concentration [mol/kg]

```
h3o =      power(10.0,0.0-max(1.0,min(13.0,ph)))
calculated iteratively, 10 iterations, initial value = 1.0e-8
```

co2 partial pressure [Pa]

```
pco2 =      t_dic / k0_co2 / (1 + k1_co2/h3o + k1_co2*k2_co2/h3o/h3o)
```

oxygen saturation concentration [mol/kg]

```
o2_sat =      (10.18e0+((5.306e-3-4.8725e-5*cgt_temp)*cgt_temp-0.2785e0)*
cgt_temp+cgt_sali*((2.2258e-3+(4.39e-7*cgt_temp-4.645e-5)*
cgt_temp)*cgt_temp-6.33e-2))*44.66e0*1e-6
```

dissolved molecular nitrogen saturation concentration [mol/kg]

```
temp1 =      log((298.15-cgt_temp)/(273.15+cgt_temp))
temp2 =      temp1*temp1
temp3 =      temp2*temp1
n2_sat =      1e-6*exp(6.42931 + 2.92704*temp1 + 4.32531*temp2 + 4.69149*
temp3 + cgt_sali*(0.0 -7.44129e-3 - 8.02566e-3*temp1 -
1.46775e-2*temp2))
```

Constants

atmospheric partial pressure of CO2 [Pa]

```
patm_co2 =      35.8
```

piston velocity for co2 surface flux [m/d]

```
w_co2_stf =      0.5
```

piston velocity for n2 surface flux [m/d]

```
w_n2_stf =      5.0
```

piston velocity for oxygen surface flux [m/d]

```
w_o2_stf =      5.0
```

Process limitation factors

```
lim_t_n2_11 =      theta(t_n2-0.0)
```

```
lim_t_o2_12 =      theta(t_o2-0.0)
```

```
lim_t_dic_13 =      theta(t_dic-0.0)
```

continued on next page...

Process limitation factors, continued from previous page
--

3.10 Process type only1d

Processes
transport from fluffy layer to deep basins (sediment only) [mol/m²/day] t_ihs -> p_ihs_removal = (r_fluffy_moveaway*t_ihs*(1.0-cgt_in_sediment))* lim_t_ihs_53
transport from fluffy layer to deep basins (sediment only) [mol/m²/day] t_ips -> p_ips_removal = (r_fluffy_moveaway*t_ips*(1.0-cgt_in_sediment))* lim_t_ips_52
transport from fluffy layer to deep basins (sediment only) [mol/m²/day] t_ims -> p_ims_removal = (r_fluffy_moveaway*t_ims*(1.0-cgt_in_sediment))* lim_t_ims_57
transport from fluffy layer to deep basins (sediment only) [mol/m²/day] t_pyr -> p_pyr_removal = (r_fluffy_moveaway*t_pyr*(1.0-cgt_in_sediment))* lim_t_pyr_58
transport from fluffy layer to deep basins (sediment only) [mol/m²/day] t_mos -> p_mos_removal = (r_fluffy_moveaway*t_mos*(1.0-cgt_in_sediment))* lim_t_mos_59
transport from fluffy layer to deep basins (sediment only) [mol/m²/day] t_rho -> t_rho_removal = (r_fluffy_moveaway*t_rho*(1.0-cgt_in_sediment))* lim_t_rho_60
transport from fluffy layer to deep basins (sediment only) [mol/m²/day] t_iim -> p_iim_removal = (r_fluffy_moveaway*t_iim*(1.0-cgt_in_sediment))* lim_t_iim_61
transport from fluffy layer to deep basins (sediment only) [mol/m²/day] t_ihc -> p_ihc_removal = (r_fluffy_moveaway*t_ihc*(1.0-cgt_in_sediment))* lim_t_ihc_54
transport from fluffy layer to deep basins (index 1 to 6) (sediment only) [mol/m²/day]
continued on next page...

Processes, continued from previous page

t_sed_1 ->

p_sed_1_removal = (r_fluffy_moveaway*t_sed_1*(1.0-cgt_in_sediment))*
lim_t_sed_1_22

transport from fluffy layer to deep basins (index 1 to 6) (sediment only)
[mol/m²/day]

t_sedp_1 ->

p_sedp_1_removal = (r_fluffy_moveaway*t_sedp_1*(1.0-cgt_in_sediment))*
lim_t_sedp_1_46

relax alkalinity to default value to compensate for detritus removal [mol/kg/day]

-> ohminus

p_stf_alk = theta(0.0024-t_alk)*0.01*(0.0024-t_alk)*(1.0-
cgt_in_sediment)*theta(20.0-cgt_bottomdepth)

relax alkalinity to default value to compensate for detritus removal [mol/kg/day]

ohminus ->

p_stf_alk_up = theta(t_alk-0.0024)*0.01*(t_alk-0.0024)*(1.0-
cgt_in_sediment)*theta(20.0-cgt_bottomdepth)

Auxiliary variables

Constants

rate with which fluffy layer is transported to deeper areas [1/d]

r_fluffy_moveaway = 0.0

Process limitation factors

lim_t_ips_52 = theta(t_ips-0.0)

lim_t_sed_1_22 = theta(t_sed_1-0.0)

lim_t_sed_2_23 = theta(t_sed_2-0.0)

lim_t_sed_3_24 = theta(t_sed_3-0.0)

lim_t_sed_4_25 = theta(t_sed_4-0.0)

lim_t_sed_5_26 = theta(t_sed_5-0.0)

lim_t_sed_6_27 = theta(t_sed_6-0.0)

lim_t_ihs_53 = theta(t_ihs-0.0)

lim_t_pyr_58 = theta(t_pyr-0.0)

continued on next page...

Process limitation factors, continued from previous page	
lim_t_ims_57 =	theta(t_ims-0.0)
lim_t_mos_59 =	theta(t_mos-0.0)
lim_t_rho_60 =	theta(t_rho-0.0)
lim_t_iim_61 =	theta(t_iim-0.0)
lim_t_ihc_54 =	theta(t_ihc-0.0)
lim_t_sedp_1_46 =	theta(t_sedp_1-0.0)
lim_t_sedp_2_47 =	theta(t_sedp_2-0.0)
lim_t_sedp_3_48 =	theta(t_sedp_3-0.0)
lim_t_sedp_4_49 =	theta(t_sedp_4-0.0)
lim_t_sedp_5_50 =	theta(t_sedp_5-0.0)
lim_t_sedp_6_51 =	theta(t_sedp_6-0.0)

3.11 Process type physics/adsorption

Processes
adsorption of phosphate to iron hydroxide particles (sediment only) [mol/m²/day] $t_{po4} + t_{ihs} \rightarrow 3*ohminus + t_{ips}$ $p_{po4_ads_ips} = (k_{ips_dissolution} * (t_{po4} - po4_eq_ips) * theta(t_{po4} - po4_eq_ips) * cgt_cellheight * cgt_density) * lim_t_{po4_15} * lim_t_{ihs_53}$
dissolution of iron phosphate (sediment only) [mol/m²/day] $3*ohminus + t_{ips} \rightarrow t_{po4} + t_{ihs}$ $p_{ips_diss_po4} = (k_{ips_dissolution} * (po4_eq_ips - t_{po4}) * theta(po4_eq_ips - t_{po4}) * cgt_cellheight * cgt_density) * lim_t_{ips_52}$
adsorption of phosphate to iron hydroxide particles [mol/kg/day] $t_{ihw} + t_{po4} \rightarrow t_{ipw} + 3*ohminus$ $p_{po4_ads_ipw} = (k_{ips_dissolution} * (t_{po4} - po4_eq_ipw) * theta(t_{po4} - po4_eq_ipw) * (1.0 - cgt_in_sediment)) * lim_t_{ihw_44} * lim_t_{po4_15}$
dissolution of iron phosphate [mol/kg/day] $3*ohminus + t_{ipw} \rightarrow t_{po4} + t_{ihw}$ $p_{ipw_diss_po4} = (k_{ips_dissolution} * (po4_eq_ipw - t_{po4}) * theta(po4_eq_ipw - t_{po4}) * (1.0 - cgt_in_sediment)) * lim_t_{ipw_43}$
phosphate adsorption to illite-montmorillonite mixed layer minerals (sediment only) [mol/m²/day] $t_{po4} + 3*h3oplus \rightarrow t_{pim} + 3*h2o$ $p_{po4_ads_pim} = (cgt_in_sediment * min(t_{po4} * cgt_cellheight * cgt_density, max(0.0, pim_eq - t_{pim})) * r_{po4_ads_pim}) * lim_t_{po4_15}$
phosphate liberation from illite-montmorillonite mixed layer minerals (sediment only) [mol/m²/day] $t_{pim} + 3*h2o \rightarrow t_{po4} + 3*h3oplus$ $p_{pim_lib_po4} = (cgt_in_sediment * min(po4_ads_pim * cgt_cellheight * cgt_density, max(0.0, t_{pim} - pim_eq)) * r_{po4_ads_pim} + (1.0 - cgt_in_sediment) * t_{pim} * r_{po4_ads_pim}) * lim_t_{pim_66}$
ammonium adsorption to illite-montmorillonite mixed layer minerals (sediment only) [mol/m²/day] $ohminus + t_{nh4} \rightarrow h2o + t_{aim}$ $p_{nh4_ads_aim} = (cgt_in_sediment * min(t_{nh4} * cgt_cellheight * cgt_density, max(0.0, aim_eq - t_{aim})) * r_{nh4_ads_aim}) * lim_t_{nh4_16}$
continued on next page...

Processes, continued from previous page

ammonium liberation from illite-montmorillonite mixed layer minerals (sediment only) [mol/m²/day]

$\text{h2o} + \text{t_aim} \rightarrow \text{ohminus} + \text{t_nh4}$

$\text{p_aim_lib_nh4} = (\text{cgt_in_sediment} * \min(\text{nh4_ads_aim} * \text{cgt_cellheight} * \text{cgt_density}, \max(0.0, \text{t_aim} - \text{aim_eq})) * \text{r_nh4_ads_aim} + (1.0 - \text{cgt_in_sediment}) * \text{t_aim} * \text{r_nh4_ads_aim}) * \text{lim_t_aim_67}$

Auxiliary variables

absolute temperature [K]

$\text{temp_k} = \text{cgt_temp} + 273.15$

temporary value assumed for pH [1]

$\text{ph_temp} = 0.0 - \log(\min(\max(\text{h3o}, 1.0\text{e-}12), 1.0\text{e-}2)) / \log(10.0)$

calculated iteratively, 10 iterations, initial value = 0.0

self-ionization constant of Water [mol²/kg²]

$\text{k_water} = \exp(-13847.26 / \text{temp_k} + 148.96502 - 23.6521 * \log(\text{temp_k}) + (118.67 / \text{temp_k} - 5.977 + 1.0495 * \log(\text{temp_k})) * \sqrt{\text{cgt_sali}} - 0.01615 * \text{cgt_sali})$

Acid dissociation constant $\text{CO}_2 + 2 \text{H}_2\text{O} \leftrightarrow \text{HCO}_3^- + \text{H}_3\text{O}^+$ [mol/kg]

$\text{k1_co2} = \text{power}(10.0, (-3633.86 / \text{temp_k} + 61.2172 - 9.6777 * \log(\text{temp_k}) + 0.011555 * \text{cgt_sali} - 0.0001152 * \text{cgt_sali} * \sqrt{\text{cgt_sali}}))$

Acid dissociation constant $\text{HCO}_3^- + \text{H}_2\text{O} \leftrightarrow [\text{CO}_3^{2-}] + \text{H}_3\text{O}^+$ [mol/kg]

$\text{k2_co2} = \text{power}(10.0, (-471.78 / \text{temp_k} - 25.929 + 3.16967 * \log(\text{temp_k}) + 0.01781 * \text{cgt_sali} - 0.0001122 * \text{cgt_sali} * \sqrt{\text{cgt_sali}}))$

Acid dissociation constant of boric acid [mol/kg]

$\text{k_boron} = \exp((-8966.9 - 2890.53 * \sqrt{\text{cgt_sali}} - 77.942 * \text{cgt_sali} + 1.728 * \text{cgt_sali} * \sqrt{\text{cgt_sali}} - 0.0996 * \text{cgt_sali} * \text{cgt_sali}) / \text{temp_k} + 148.0248 + 137.1942 * \sqrt{\text{cgt_sali}} + 1.62142 * \text{cgt_sali} + (-24.4344 - 25.085 * \sqrt{\text{cgt_sali}} - 0.2474 * \text{cgt_sali}) * \log(\text{temp_k}) + 0.053105 * \sqrt{\text{cgt_sali}} * \text{temp_k})$

Acid dissociation constant $\text{H}_3\text{PO}_4 + \text{H}_2\text{O} \leftrightarrow [\text{H}_2\text{PO}_4^-] + \text{H}_3\text{O}^+$ [mol/kg]

$\text{k1_po4} = \exp(-4576.752 / \text{temp_k} + 115.525 - 18.453 * \log(\text{temp_k}) + (0.69171 - 106.736 / \text{temp_k}) * \sqrt{\text{cgt_sali}} - (0.01844 + 0.65643 / \text{temp_k}) * \text{cgt_sali})$

continued on next page...

Auxiliary variables, continued from previous page

Acid dissociation constant $[H_2PO_4^-] + H_2O \rightleftharpoons [HPO_4^{2-}] + H_3O^+$ [mol/kg]

$$k2_po4 = \exp(-8814.715/temp_k + 172.0883 - 27.927*\log(temp_k) + (1.35660 - 160.340/temp_k)*\sqrt{cgt_sali} - (0.05778 - 0.37335/temp_k)*cgt_sali)$$

Acid dissociation constant $[HPO_4^{2-}] + H_2O \rightleftharpoons [PO_4^{3-}] + H_3O^+$ [mol/kg]

$$k3_po4 = \exp(-3070.75/temp_k - 18.141 + (2.81197 + 17.27039/temp_k)*\sqrt{cgt_sali} - (0.09984 + 44.99486/temp_k)*cgt_sali)$$

Acid dissociation constant $H_2S + H_2O \rightleftharpoons HS^- + H_3O^+$ [mol/kg]

$$k1_h2s = \exp(-3131.42/temp_k - 5.818 + 0.368*(\text{power}(\max(0.0, cgt_sali), (1.0/3.0))))$$

total concentration of boron [mol/kg]

$$boron_total = 0.000416 * cgt_sali / 35.0$$

boron alkalinity [mol/kg]

$$alk_boron = boron_total * k_boron / (k_boron + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

hydrogen sulfide alkalinity [mol/kg]

$$alk_h2s = t_h2s * k1_h2s / (k1_h2s + h3o)$$

calculated iteratively, 10 iterations, initial value = 0.0

water alkalinity [mol/kg]

$$alk_water = k_water / h3o - h3o$$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in phosphate alkalinity formula [mol³/kg³]

$$alk_po4_denominator = (h3o*h3o*h3o + k1_po4*h3o*h3o + k1_po4*k2_po4*h3o + k1_po4*k2_po4*k3_po4)$$

calculated iteratively, 10 iterations, initial value = 0.0

phosphate alkalinity [mol/kg]

$$alk_po4 = (t_po4*(k1_po4*k2_po4*h3o + 2.0*k1_po4*k2_po4*k3_po4 - h3o*h3o) / alk_po4_denominator)$$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in carbonate alkalinity formula [mol²/kg²]

$$alk_co2_denominator = (h3o*h3o + k1_co2*h3o + k1_co2*k2_co2)$$

calculated iteratively, 10 iterations, initial value = 0.0

continued on next page...

Auxiliary variables, continued from previous page

carbonate alkalinity [mol/kg]

$\text{alk_co2} = \text{t_dic} * \text{k1_co2} * (\text{h3o} + 2 * \text{k2_co2}) / \text{alk_co2_denominator}$

calculated iteratively, 10 iterations, initial value = 0.0

error in total alkalinity calculation at the assumed pH [mol/kg]

$\text{alk_residual} = \text{t_alk} - \text{alk_co2} - \text{alk_po4} - \text{alk_boron} - \text{alk_h2s} - \text{alk_water}$

calculated iteratively, 10 iterations, initial value = 0.0

derivative of phosphate alkalinity with respect to h3o [1]

$\text{dalkp_dh3o} = \frac{\text{t_po4} * (0.0 - \text{k1_po4} * \text{h3o} * \text{h3o} * \text{h3o} * \text{h3o} - 4 * \text{k1_po4} * \text{k2_po4} * \text{h3o} * \text{h3o} * \text{h3o} - (\text{k1_po4} * \text{k1_po4} * \text{k2_po4} + 9 * \text{k1_po4} * \text{k2_po4} * \text{k3_po4}) * \text{h3o} * \text{h3o} - 4 * \text{k1_po4} * \text{k1_po4} * \text{k2_po4} * \text{k3_po4} * \text{h3o} - \text{k1_po4} * \text{k1_po4} * \text{k2_po4} * \text{k2_po4} * \text{k3_po4})}{(\text{alk_po4_denominator} * \text{alk_po4_denominator})}$

calculated iteratively, 10 iterations, initial value = 0.0

derivative of carbonate alkalinity with respect to h3o [1]

$\text{dalkc_dh3o} = \frac{\text{t_dic} * (0.0 - \text{k1_co2} * \text{h3o} * \text{h3o} - \text{k1_co2} * \text{k1_co2} * \text{k2_co2} - 4 * \text{k1_co2} * \text{k2_co2} * \text{h3o})}{(\text{alk_co2_denominator} * \text{alk_co2_denominator})}$

calculated iteratively, 10 iterations, initial value = 0.0

derivative of residual_alk with respect to pH [mol/kg]

$\text{dalkresidual_dpH} = 0.0 - \log(10.0) * \text{h3o} * (\text{alk_boron} / (\text{k_boron} + \text{h3o}) + \text{alk_h2s} / (\text{k1_h2s} + \text{h3o}) + \text{k_water} / (\text{h3o} * \text{h3o}) + 1 - \text{dalkp_dh3o} - \text{dalkc_dh3o})$

calculated iteratively, 10 iterations, initial value = 0.0

newly determined pH value [1]

$\text{temp1} = \text{alk_residual} / \text{dalkresidual_dpH}$

$\text{ph} = \text{ph_temp} - \text{temp1} + \text{theta}(\text{abs}(\text{temp1}) - 1) * 0.5 * \text{temp1}$

calculated iteratively, 10 iterations, initial value = 0.0

h3o ion concentration [mol/kg]

$\text{h3o} = \text{power}(10.0, 0.0 - \max(1.0, \min(13.0, \text{ph})))$

calculated iteratively, 10 iterations, initial value = 1.0e-8

theoretical phosphate concentration in equilibrium with iron phosphate in the sediments [mol/kg]

$\text{po4_eq_ips} = \text{power}(\max(\text{t_ips} / \max(\text{t_ips} + \text{t_ihs}, \text{epsilon}) / 0.201 - 1.483 + 0.157 * \text{pH}, 0.0), 2.0) / 1000.0$

theoretical phosphate concentration in equilibrium with iron phosphate in the water [mol/kg]

$\text{po4_eq_ipw} = \text{power}(\max(\text{t_ipw} / \max(\text{t_ipw} + \text{t_ihw}, \text{epsilon}) / 0.201 - 1.483 + 0.157 * \text{pH}, 0.0), 2.0) / 1000.0$

continued on next page...

Auxiliary variables, continued from previous page

amount of phosphate that can be maximally adsorbed to illite-montmorillonite mixed-layer minerals [mol/m²]

```
temp1 = 2.7 * max(vol_fraction_im*(1.0-POR),epsilon)
temp2 = temp1*p_content_im
temp3 = temp2/55.0
pim_max = temp3 * 1000 * cgt_cellheight*cgt_density
```

pim in equilibrium with po4 concentration

```
pim_eq = pim_max*min(1.0,t_po4/max(po4_ads_pim,epsilon))
```

amount of phosphate that can be maximally adsorbed to illite-montmorillonite mixed-layer minerals [mol/m²]

```
temp1 = 2.7 * max(vol_fraction_im*(1.0-POR),epsilon)
temp2 = temp1*n_content_im
temp3 = temp2/18.0
aim_max = temp3 * 1000 * cgt_cellheight*cgt_density
```

aim in equilibrium with po4 concentration

```
aim_eq = aim_max*min(1.0,t_nh4/max(nh4_ads_aim,epsilon))
```

Constants

no division by 0

```
epsilon = 4.5E-17
```

inverse timescale for dissolution of iron phosphate [1/d]

```
k_ips_dissolution = 0.1
```

porosity

```
por = 0.77
```

fraction of illite-montmorillonite mixed layer minerals on volume of all minerals [1]

```
vol_fraction_im = 0.5
```

mass fraction of phosphate that can be adsorbed/desorbed to illite-montmorillonite mixed layer minerals [1]

```
p_content_im = 0.0002
```

mass fraction of ammonium that can be adsorbed/desorbed to illite-montmorillonite mixed layer minerals [1]

```
n_content_im = 0.0
```

phosphate concentration when phosphate in illite-montmorillonite mixed layer minerals is fully adsorbed [mol/kg]

```
po4_ads_pim = 3.0E-5
```

continued on next page...

Constants, continued from previous page	
---	--

ammonium concentration when ammonium in illite-montmorillonite mixed layer minerals is fully adsorbed [mol/kg]	
--	--

nh4_ads_aim =	4.0E-5
---------------	--------

rate of phosphate adsorption/desorption to illite-montmorillonite [1/d]	
---	--

r_po4_ads_pim =	0.1
-----------------	-----

rate of ammonium adsorption/desorption to illite-montmorillonite mixed-layer minerals [1/d]	
---	--

r_nh4_ads_aim =	0.1
-----------------	-----

Process limitation factors	
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lim_t_nh4_16 =	theta(t_nh4-0.0)
----------------	------------------

lim_t_po4_15 =	theta(t_po4-0.0)
----------------	------------------

lim_t_ips_52 =	theta(t_ips-0.0)
----------------	------------------

lim_t_ipw_43 =	theta(t_ipw-0.0)
----------------	------------------

lim_t_ihs_53 =	theta(t_ihs-0.0)
----------------	------------------

lim_t_ihw_44 =	theta(t_ihw-0.0)
----------------	------------------

lim_t_pim_66 =	theta(t_pim-0.0)
----------------	------------------

lim_t_aim_67 =	theta(t_aim-0.0)
----------------	------------------

3.12 Process type physics/erosion

Processes
sedimentary detritus erosion (index 1 to 6) (sediment only) [mol/m ² /day] t_sed_1 -> t_det_1 p_sed_1_ero_det = (erosion_is_active*r_sed_ero*t_sed_1*(1.0-cgt_in_sediment)) *lim_t_sed_1_22
sedimentary detritus erosion (index 1 to 6) (sediment only) [mol/m ² /day] t_sedp_1 -> t_detp_1 p_sedp_1_ero_detp = (erosion_is_active*r_sed_ero*t_sedp_1*(1.0-cgt_in_sediment)))*lim_t_sedp_1_46
erosion of iron PO4 (sediment only) [mol/m ² /day] t_ips -> t_ipw p_ips_ero_ipw = (erosion_is_active*r_ips_ero*t_ips*(1.0-cgt_in_sediment))* lim_t_ips_52
erosion of iron PO4 (sediment only) [mol/m ² /day] t_ihs -> t_ihw p_ihs_ero_ihw = (erosion_is_active*r_ips_ero*t_ihs*(1.0-cgt_in_sediment))* lim_t_ihs_53
erosion of larger-crystalline iron PO4 (sediment only) [mol/m ² /day] t_ihc -> t_ihw p_ihc_ero_ihw = (erosion_is_active*r_ips_ero*t_ihc*(1.0-cgt_in_sediment))* lim_t_ihc_54
resuspension of iron monosulfide (sediment only) [mol/m ² /day] t_ims + 2.25*h2o + 0.25*h3oplus + 0.125*t_so4 -> 1.125*t_h2s + t_ihw p_ims_ero_ihw = (erosion_is_active*r_ips_ero*t_ihw*(1.0-cgt_in_sediment))* lim_t_ims_57*lim_t_so4_28
resuspension of pyrite (sediment only) [mol/m ² /day] t_pyr + 3.75*h2o -> 0.25*h3oplus + 1.875*t_h2s + 0.125*t_so4 + t_ihw p_pyr_ero_ihw = (erosion_is_active*r_ips_ero*t_pyr*(1.0-cgt_in_sediment))* lim_t_pyr_58
bio resuspension of manganese oxide (sediment only) [mol/m ² /day] t_mos -> t_mow p_mos_ero_mow = (erosion_is_active*r_ips_ero*t_mos*(1.0-cgt_in_sediment))* lim_t_mos_59
bio resuspension of rhodochrosite (sediment only) [mol/m ² /day] 0.25*t_so4 + 1.7*h3oplus + t_rho -> t_mow + 0.25*t_h2s + 2.3*h2o + 0.6*t_ca2 + 1.6*t_dic
continued on next page...

Processes, continued from previous page

```
p_rho_ero_mow = (erosion_is_active*r_ips_ero*t_rho*(1.0-cgt_in_sediment))*
lim_t_so4_28*lim_t_rho_60
```

bio resuspension of iron in clay minerals (sediment only) [mol/m²/day]

```
0.125*t_so4 + 0.25*h2o + 0.25*h3oplus + t_iim -> t_ihw + 0.125*t_h2s
p_iim_ero_ihw = (erosion_is_active*r_ips_ero*t_iim*(1.0-cgt_in_sediment))*
lim_t_so4_28*lim_t_iim_61
```

Auxiliary variables

switch (1=erosion, 0=no erosion) which depends on the combined bottom stress of currents and waves

```
erosion_is_active = theta(cgt_current_wave_stress - critical_stress)
```

Constants

critical shear stress for sediment erosion [N/m²]

```
critical_stress = 0.016
```

erosion rate for iron PO₄ [1/day]

```
r_ips_ero = 6.0
```

maximum sediment detritus erosion rate [1/day]

```
r_sed_ero = 6.0
```

Process limitation factors

```
lim_t_ips_52 = theta(t_ips-0.0)
```

```
lim_t_so4_28 = theta(t_so4-0.0)
```

```
lim_t_sed_1_22 = theta(t_sed_1-0.0)
```

```
lim_t_sed_2_23 = theta(t_sed_2-0.0)
```

```
lim_t_sed_3_24 = theta(t_sed_3-0.0)
```

```
lim_t_sed_4_25 = theta(t_sed_4-0.0)
```

```
lim_t_sed_5_26 = theta(t_sed_5-0.0)
```

```
lim_t_sed_6_27 = theta(t_sed_6-0.0)
```

```
lim_t_ihs_53 = theta(t_ihs-0.0)
```

```
lim_t_pyr_58 = theta(t_pyr-0.0)
```

continued on next page...

Process limitation factors, continued from previous page	
lim_t_ims_57 =	theta(t_ims-0.0)
lim_t_mos_59 =	theta(t_mos-0.0)
lim_t_rho_60 =	theta(t_rho-0.0)
lim_t_iim_61 =	theta(t_iim-0.0)
lim_t_ihc_54 =	theta(t_ihc-0.0)
lim_t_sedp_1_46 =	theta(t_sedp_1-0.0)
lim_t_sedp_2_47 =	theta(t_sedp_2-0.0)
lim_t_sedp_3_48 =	theta(t_sedp_3-0.0)
lim_t_sedp_4_49 =	theta(t_sedp_4-0.0)
lim_t_sedp_5_50 =	theta(t_sedp_5-0.0)
lim_t_sedp_6_51 =	theta(t_sedp_6-0.0)

3.13 Process type physics/parameterization_deep_burial

Processes	
<p>parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (index 1 to 6) (sediment only) [mol/m²/day]</p> <pre> t_sed_1 + rfr_pc_enrichment_det*3.3125*t_so4 + (1.0+rfr_pc_enrichment_det* 6.625)*h3oplus -> rfr_si*t_sil + t_nh4 + rfr_pc_enrichment_det*rfr_c*t_dic + rfr_pc_enrichment_det*3.3125*t_h2s + (1.0+rfr_pc_enrichment_det*13.25)*h2o (t_sed_1*vel_remin_deep*24.0*3600.0/0.02*theta(k-21.0))* p_sed_1_sulfdeep_nh4lim_t_sed_1_22*lim_t_so4_28 = </pre>	
<p>parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (index 1 to 6) (sediment only) [mol/m²/day]</p> <pre> t_sedp_1 + 3*rfr_pc_enrichment_det*rfr_p*h2o -> 3*rfr_pc_enrichment_det*rfr_p* h3oplus + rfr_pc_enrichment_det*rfr_p*t_po4 (t_sedp_1*vel_remin_deep*24.0*3600.0/0.02*theta(k-21.0))* p_sedp_1_sulfdeep_polim_t_sedp_1_46 = </pre>	
Auxiliary variables	
Constants	
redfield ratio C/N	
rfr_c =	6.625
redfield ratio P/N	
rfr_p =	0.0625
enrichment factor for P and C in detritus [1]	
rfr_pc_enrichment_de	1.5
average ratio Si/N [1]	
rfr_si =	0.9375
effective velocity of detritus mineralization in the deepest layer [m/s]	
vel_remin_deep =	0.0
Process limitation factors	
lim_t_so4_28 =	theta(t_so4-0.0)
lim_t_sed_1_22 =	theta(t_sed_1-0.0)
continued on next page...	

Process limitation factors, continued from previous page	
lim_t_sed_2_23 =	theta(t_sed_2-0.0)
lim_t_sed_3_24 =	theta(t_sed_3-0.0)
lim_t_sed_4_25 =	theta(t_sed_4-0.0)
lim_t_sed_5_26 =	theta(t_sed_5-0.0)
lim_t_sed_6_27 =	theta(t_sed_6-0.0)
lim_t_sedp_1_46 =	theta(t_sedp_1-0.0)
lim_t_sedp_2_47 =	theta(t_sedp_2-0.0)
lim_t_sedp_3_48 =	theta(t_sedp_3-0.0)
lim_t_sedp_4_49 =	theta(t_sedp_4-0.0)
lim_t_sedp_5_50 =	theta(t_sedp_5-0.0)
lim_t_sedp_6_51 =	theta(t_sedp_6-0.0)

3.14 Process type physics/parameterization_diffusion

Processes	
relax_ohm_quickdiff	tracer against actual OH- concentration [mol/kg/day] -> t_ohm_quickdiff $\text{theta}(\text{oh}-\text{t_ohm_quickdiff}) * (\text{oh}-\text{t_ohm_quickdiff}) / \text{cgt_timestep}$ relax_ohm_quickdiff_ =
relax_ohm_quickdiff	tracer against actual OH- concentration [mol/kg/day] t_ohm_quickdiff -> $(\text{theta}(\text{t_ohm_quickdiff}-\text{oh}) * (\text{t_ohm_quickdiff}-\text{oh}) / \text{cgt_timestep}) * \text{lim_t_ohm_quickdiff_63}$ relax_ohm_quickdiff_ =
relax_ohm_slowdiff	tracer against actual OH- concentration [mol/kg/day] -> t_ohm_slowdiff $\text{theta}(\text{oh}-\text{t_ohm_slowdiff}) * (\text{oh}-\text{t_ohm_slowdiff}) / \text{cgt_timestep}$ relax_ohm_slowdiff_u =
relax_ohm_slowdiff	tracer against actual OH- concentration [mol/kg/day] t_ohm_slowdiff -> $(\text{theta}(\text{t_ohm_slowdiff}-\text{oh}) * (\text{t_ohm_slowdiff}-\text{oh}) / \text{cgt_timestep}) * \text{lim_t_ohm_slowdiff_64}$ relax_ohm_slowdiff_d =
p_alk_rise_ohmdiff	rise of total alkalinity by quicker-than-assumed diffusion of OH- [mol/kg/day] -> ohminus $\text{theta}(\text{t_ohm_quickdiff}-\text{t_ohm_slowdiff}) * (\text{t_ohm_quickdiff}-\text{t_ohm_slowdiff}) / \text{cgt_timestep}$ =
p_alk_fall_ohmdiff	falling of total alkalinity by quicker-than-assumed diffusion of OH- [mol/kg/day] -> h3oplus $\text{theta}(\text{t_ohm_slowdiff}-\text{t_ohm_quickdiff}) * (\text{t_ohm_slowdiff}-\text{t_ohm_quickdiff}) / \text{cgt_timestep}$ =

Auxiliary variables	
absolute temperature [K]	
temp_k =	cgt_temp + 273.15
temporary value assumed for pH [1]	
ph_temp =	0.0-log(min(max(h3o,1.0e-12),1.0e-2))/log(10.0)
calculated iteratively, 10 iterations, initial value = 0.0	
self-ionization constant of Water [mol2/kg2]	
k_water =	exp(-13847.26 / temp_k + 148.96502 - 23.6521 * log(temp_k) + (118.67/temp_k - 5.977 + 1.0495 * log(temp_k)) * sqrt(cgt_sali) - 0.01615 * cgt_sali)
continued on next page...	

Auxiliary variables, continued from previous page

Acid dissociation constant $\text{CO}_2 + 2 \text{H}_2\text{O} \rightleftharpoons \text{HCO}_3^- + \text{H}_3\text{O}^+$ [mol/kg]

```
k1_co2 = power(10.0, ( -3633.86 / temp_k + 61.2172 - 9.6777 *
log(temp_k) + 0.011555 * cgt_sali - 0.0001152 * cgt_sali *
cgt_sali))
```

Acid dissociation constant $\text{HCO}_3^- + \text{H}_2\text{O} \rightleftharpoons [\text{CO}_3^{2-}] + \text{H}_3\text{O}^+$ [mol/kg]

```
k2_co2 = power(10.0, ( -471.78 / temp_k - 25.929 + 3.16967 *
log(temp_k) + 0.01781 * cgt_sali - 0.0001122 * cgt_sali *
cgt_sali))
```

Acid dissociation constant of boric acid [mol/kg]

```
k_boron = exp(( -8966.9 - 2890.53*sqrt(cgt_sali) - 77.942*cgt_sali +
1.728*cgt_sali*sqrt(cgt_sali) - 0.0996*cgt_sali*cgt_sali) /
temp_k + 148.0248 + 137.1942*sqrt(cgt_sali) + 1.62142*
cgt_sali + (-24.4344 - 25.085*sqrt(cgt_sali) - 0.2474*
cgt_sali)*log(temp_k) + 0.053105*sqrt(cgt_sali)*temp_k )
```

Acid dissociation constant $\text{H}_3\text{PO}_4 + \text{H}_2\text{O} \rightleftharpoons [\text{H}_2\text{PO}_4^-] + \text{H}_3\text{O}^+$ [mol/kg]

```
k1_po4 = exp( -4576.752/temp_k + 115.525 - 18.453*log(temp_k) +
(0.69171 - 106.736/temp_k)*sqrt(cgt_sali) - (0.01844 +
0.65643/temp_k)*cgt_sali )
```

Acid dissociation constant $[\text{H}_2\text{PO}_4^-] + \text{H}_2\text{O} \rightleftharpoons [\text{HPO}_4^{2-}] + \text{H}_3\text{O}^+$ [mol/kg]

```
k2_po4 = exp( -8814.715/temp_k + 172.0883 - 27.927*log(temp_k) +
(1.35660 - 160.340/temp_k)*sqrt(cgt_sali) - (0.05778 -
0.37335/temp_k)*cgt_sali )
```

Acid dissociation constant $[\text{HPO}_4^{2-}] + \text{H}_2\text{O} \rightleftharpoons [\text{PO}_4^{3-}] + \text{H}_3\text{O}^+$ [mol/kg]

```
k3_po4 = exp( -3070.75/temp_k - 18.141 + (2.81197 + 17.27039/temp_k)
*sqrt(cgt_sali) - (0.09984 + 44.99486/temp_k)*cgt_sali )
```

Acid dissociation constant $\text{H}_2\text{S} + \text{H}_2\text{O} \rightleftharpoons \text{HS}^- + \text{H}_3\text{O}^+$ [mol/kg]

```
k1_h2s = exp( -3131.42/temp_k - 5.818 + 0.368*
(power(max(0.0, cgt_sali), (1.0/3.0))))
```

total concentration of boron [mol/kg]

```
boron_total = 0.000416 * cgt_sali/35.0
```

boron alkalinity [mol/kg]

```
alk_boron = boron_total * k_boron / (k_boron + h3o)
calculated iteratively, 10 iterations, initial value = 0.0
```

hydrogen sulfide alkalinity [mol/kg]

continued on next page...

Auxiliary variables, continued from previous page

$\text{alk_h2s} = \text{t_h2s} * \text{k1_h2s} / (\text{k1_h2s} + \text{h3o})$
 calculated iteratively, 10 iterations, initial value = 0.0

water alkalinity [mol/kg]

$\text{alk_water} = \text{k_water} / \text{h3o} - \text{h3o}$
 calculated iteratively, 10 iterations, initial value = 0.0

denominator in phosphate alkalinity formula [mol3/kg3]

$\text{alk_po4_denominator} (\text{h3o} * \text{h3o} * \text{h3o} + \text{k1_po4} * \text{h3o} * \text{h3o} + \text{k1_po4} * \text{k2_po4} * \text{h3o} + \text{k1_po4} * \text{k2_po4} * \text{k3_po4})$
 calculated iteratively, 10 iterations, initial value = 0.0

phosphate alkalinity [mol/kg]

$\text{alk_po4} = \text{t_po4} * (\text{k1_po4} * \text{k2_po4} * \text{h3o} + 2.0 * \text{k1_po4} * \text{k2_po4} * \text{k3_po4} - \text{h3o} * \text{h3o} * \text{h3o}) / \text{alk_po4_denominator}$
 calculated iteratively, 10 iterations, initial value = 0.0

denominator in carbonate alkalinity formula [mol2/kg2]

$\text{alk_co2_denominator} (\text{h3o} * \text{h3o} + \text{k1_co2} * \text{h3o} + \text{k1_co2} * \text{k2_co2})$
 calculated iteratively, 10 iterations, initial value = 0.0

carbonate alkalinity [mol/kg]

$\text{alk_co2} = \text{t_dic} * \text{k1_co2} * (\text{h3o} + 2 * \text{k2_co2}) / \text{alk_co2_denominator}$
 calculated iteratively, 10 iterations, initial value = 0.0

error in total alkalinity calculation at the assumed pH [mol/kg]

$\text{alk_residual} = \text{t_alk} - \text{alk_co2} - \text{alk_po4} - \text{alk_boron} - \text{alk_h2s} - \text{alk_water}$
 calculated iteratively, 10 iterations, initial value = 0.0

derivative of phosphate alkalinity with respect to h3o [1]

$\text{dalkp_dh3o} = \text{t_po4} * (0.0 - \text{k1_po4} * \text{h3o} * \text{h3o} * \text{h3o} * \text{h3o} - 4 * \text{k1_po4} * \text{k2_po4} * \text{h3o} * \text{h3o} - \text{h3o} - (\text{k1_po4} * \text{k1_po4} * \text{k2_po4} + 9 * \text{k1_po4} * \text{k2_po4} * \text{k3_po4}) * \text{h3o} * \text{h3o} - 4 * \text{k1_po4} * \text{k1_po4} * \text{k2_po4} * \text{k3_po4} * \text{h3o} - \text{k1_po4} * \text{k1_po4} * \text{k2_po4} * \text{k2_po4} * \text{k3_po4}) / (\text{alk_po4_denominator} * \text{alk_po4_denominator})$
 calculated iteratively, 10 iterations, initial value = 0.0

derivative of carbonate alkalinity with respect to h3o [1]

$\text{dalkc_dh3o} = \text{t_dic} * (0.0 - \text{k1_co2} * \text{h3o} * \text{h3o} - \text{k1_co2} * \text{k1_co2} * \text{k2_co2} - 4 * \text{k1_co2} * \text{k2_co2} * \text{h3o}) / (\text{alk_co2_denominator} * \text{alk_co2_denominator})$
 calculated iteratively, 10 iterations, initial value = 0.0

derivative of residual_alk with respect to pH [mol/kg]

$\text{dalkresidual_dpH} = 0.0 - \log(10.0) * \text{h3o} * (\text{alk_boron} / (\text{k_boron} + \text{h3o}) + \text{alk_h2s} / (\text{k1_h2s} + \text{h3o}) + \text{k_water} / (\text{h3o} * \text{h3o}) + 1 - \text{dalkp_dh3o} - \text{dalkc_dh3o})$

continued on next page...

Auxiliary variables, continued from previous page

calculated iteratively, 10 iterations, initial value = 0.0
--

newly determined pH value [1]

temp1 =	alk_residual/dalkresidual_dpH
---------	-------------------------------

ph =	ph_temp - temp1 + theta(abs(temp1) - 1)*0.5*temp1
------	---

calculated iteratively, 10 iterations, initial value = 0.0
--

h3o ion concentration [mol/kg]

h3o =	power(10.0,0.0-max(1.0,min(13.0,ph)))
-------	---------------------------------------

calculated iteratively, 10 iterations, initial value = 1.0e-8

h3o ion concentration [mol/kg]

oh =	power(10.0,log(k_water)/log(10.0)+max(1.0,min(13.0,ph)))
------	--

Constants

Process limitation factors

	theta(t_ohm_quickdiff-0.0)
--	----------------------------

lim_t_ohm_quickdiff_	
----------------------	--

=	
---	--

	theta(t_ohm_slowdiff-0.0)
--	---------------------------

lim_t_ohm_slowdiff_6	
----------------------	--

=	
---	--

3.15 Process type physics/parameterization_lateral

Processes
<p>surface flux of detritus (index 1 to 6) (sediment only) [mol/m²/day]</p> <p>-> t_detp_1 + t_det_1</p> <p>p_stf_det_1 = $\text{frac_det_1} * \text{accrate_det_1} * 2.47\text{e-}4 * (1.0 - \text{cgt_in_sediment})$</p>
<p>raise SO4 concentration in the water column to salinity-determined default value [mol/kg/day]</p> <p>-> t_so4</p> <p>p_so4_relax_upwards $(0.077 * \text{sal_for_so4} / (32 + 4 * 16) - t_{\text{so4}}) * \text{theta}(0.077 * \text{sal_for_so4} / (32 + 4 * 16) - t_{\text{so4}}) * (1.0 - \text{cgt_in_sediment})$</p>
<p>lower SO4 concentration in the water column to salinity-determined default value [mol/kg/day]</p> <p>t_so4 -></p> <p>$((t_{\text{so4}} - 0.077 * \text{sal_for_so4} / (32 + 4 * 16)) * \text{theta}(t_{\text{so4}} - 0.077 * \text{sal_for_so4} / (32 + 4 * 16)) * (1.0 - \text{cgt_in_sediment})) * \text{lim_t_so4_28}$</p>
<p>raise Ca2+ concentration in the water column to salinity-determined default value [mol/kg/day]</p> <p>-> t_ca2</p> <p>p_ca2_relax_upwards $(0.0118 * \text{sal_for_so4} / (40.1) - t_{\text{ca2}}) * \text{theta}(0.0118 * \text{sal_for_so4} / (40.0) - t_{\text{ca2}}) * (1.0 - \text{cgt_in_sediment})$</p>
<p>lower Ca2+ concentration in the water column to salinity-determined default value [mol/kg/day]</p> <p>t_ca2 -></p> <p>$((t_{\text{ca2}} - 0.0118 * \text{sal_for_so4} / (40.1)) * \text{theta}(t_{\text{ca2}} - 0.0118 * \text{sal_for_so4} / (40.0)) * (1.0 - \text{cgt_in_sediment})) * \text{lim_t_ca2_56}$</p>
<p>remove silicate in water column as it gets too much [mol/kg/day]</p> <p>t_sil -></p> <p>p_remove_silicate = $((t_{\text{sil}} - 1.0\text{e-}5) * 0.1 * (1.0 - \text{cgt_in_sediment}) * (20.0 - \text{cgt_bottomdepth})) * \text{lim_t_sil_65}$</p>
<p>iron hydroxide generation by internal sources (surface only) [mol/m²/day]</p> <p>-> t_ihw</p> <p>p_stf_ihw_3d = $9.42\text{e-}5$</p>
Auxiliary variables
<p>salinity used for so4 calculation</p> <p>sal_for_so4 = cgt_sali</p>
<p>accumulation ratio of detritus [1]</p>
continued on next page...

Auxiliary variables, continued from previous page	
accrate_det_1 =	0.0
accumulation ratio of detritus [1]	
accrate_det_2 =	0.0
accumulation ratio of detritus [1]	
accrate_det_3 =	accratedet
accumulation ratio of detritus [1]	
accrate_det_4 =	accratedet
accumulation ratio of detritus [1]	
accrate_det_5 =	accratedet
accumulation ratio of detritus [1]	
accrate_det_6 =	accratedet
Constants	
fraction of this detritus class in total detritus production [1]	
frac_det_1 =	0.26
fraction of this detritus class in total detritus production [1]	
frac_det_2 =	0.16
fraction of this detritus class in total detritus production [1]	
frac_det_3 =	0.16
fraction of this detritus class in total detritus production [1]	
frac_det_4 =	0.16
fraction of this detritus class in total detritus production [1]	
frac_det_5 =	0.08
fraction of this detritus class in total detritus production [1]	
frac_det_6 =	0.18
accumulation ratio of detritus (import vs. local production) [1]	
accratedet =	0.0
Process limitation factors	
lim_t_so4_28 =	theta(t_so4-0.0)
lim_t_ca2_56 =	theta(t_ca2-0.0)
lim_t_sil_65 =	theta(t_sil-0.0)
continued on next page...	

Process limitation factors, continued from previous page
--

3.16 Process type physics/precipitation

Processes
<p>precipitation of iron II as siderite (sediment only) [mol/m²/day]</p> <p>$t_{\text{fe2}} + t_{\text{h2s}} + 2.0 \cdot \text{ohminus} \rightarrow t_{\text{ims}} + 2.0 \cdot \text{h2o}$</p> <p>$p_{\text{fe2_prec_ims}} = (\text{fe2_ims_is_smallest} \cdot \text{cgt_in_sediment} \cdot \text{theta}(t_{\text{fe2}} - \text{fe2_smooth})) \cdot (t_{\text{fe2}} - \text{fe2_smooth}) / \text{cgt_timestep} \cdot \text{cgt_cellheight} \cdot \text{cgt_density} \cdot \text{lim_t_fe2_55} \cdot \text{lim_t_h2s_29}$</p>
<p>dissolution of magnetite to iron II (precipitating iron hydroxides) (sediment only) [mol/m²/day]</p> <p>$2.0 \cdot \text{h3opplus} + t_{\text{ims}} \rightarrow 2.0 \cdot \text{h2o} + t_{\text{h2s}} + t_{\text{fe2}}$</p> <p>$p_{\text{ims_diss_fe2}} = (\text{fe2_ims_is_smallest} \cdot \text{cgt_in_sediment} \cdot \text{theta}(\text{fe2_smooth} - t_{\text{fe2}})) \cdot (\text{fe2_smooth} - t_{\text{fe2}}) / \text{cgt_timestep} \cdot \text{cgt_cellheight} \cdot \text{cgt_density} \cdot \text{lim_t_ims_57}$</p>
<p>precipitation of iron II as minnesotaite (sediment only) [mol/m²/day]</p> <p>$2 \cdot \text{ohminus} + t_{\text{fe2}} \rightarrow t_{\text{iim}}$</p> <p>$p_{\text{fe2_prec_iim}} = (\text{fe2_iim_is_smallest} \cdot \text{cgt_in_sediment} \cdot \text{theta}(t_{\text{fe2}} - \text{fe2_smooth})) \cdot (t_{\text{fe2}} - \text{fe2_smooth}) / \text{cgt_timestep} \cdot \text{cgt_cellheight} \cdot \text{cgt_density} \cdot \text{lim_t_fe2_55}$</p>
<p>dissolution minnesotaite to of iron-II (sediment only) [mol/m²/day]</p> <p>$t_{\text{iim}} \rightarrow t_{\text{fe2}} + 2 \cdot \text{ohminus}$</p> <p>$p_{\text{iim_diss_fe2}} = (\text{fe2_iim_is_smallest} \cdot \text{cgt_in_sediment} \cdot \text{theta}(\text{fe2_smooth} - t_{\text{fe2}})) \cdot (\text{fe2_smooth} - t_{\text{fe2}}) / \text{cgt_timestep} \cdot \text{cgt_cellheight} \cdot \text{cgt_density} \cdot \text{lim_t_iim_61}$</p>
<p>iron monosulfide transformation to minnesotaite (sediment only) [mol/m²/day]</p> <p>$t_{\text{ims}} + 2 \cdot \text{h2o} \rightarrow t_{\text{iim}} + t_{\text{h2s}}$</p> <p>$p_{\text{ims_trans_iim}} = (\text{fe2_iim_is_smallest} \cdot \text{theta}(\text{ims_dissolution_rate})) \cdot \text{ims_dissolution_rate} \cdot \text{lim_t_ims_57}$</p>
<p>minnesotaite transformation to iron monosulfide (sediment only) [mol/m²/day]</p> <p>$t_{\text{iim}} + t_{\text{h2s}} \rightarrow t_{\text{ims}} + 2 \cdot \text{h2o}$</p> <p>$p_{\text{iim_trans_ims}} = (\text{fe2_ims_is_smallest} \cdot \text{theta}(\text{iim_dissolution_rate})) \cdot \text{iim_dissolution_rate} \cdot \text{lim_t_iim_61} \cdot \text{lim_t_h2s_29}$</p>
<p>rhodochrosite dissolution to manganese-II (sediment only) [mol/m²/day]</p> <p>$t_{\text{rho}} + 3.2 \cdot \text{h3opplus} \rightarrow 4.8 \cdot \text{h2o} + 0.6 \cdot t_{\text{ca2}} + t_{\text{mn2}} + 1.6 \cdot t_{\text{dic}}$</p> <p>$p_{\text{rho_diss_mn2}} = (0.1 \cdot 1.0 \cdot 10^{-5} \cdot \text{theta}(1.0 - \text{saturation_rhodochrosite})) \cdot \text{cgt_in_sediment} \cdot \text{cgt_cellheight} \cdot \text{cgt_density} \cdot \text{lim_t_rho_60}$</p>
<p>pyrite formation from iron monosulfide (sediment only) [mol/m²/day]</p> <p>$0.5 \cdot \text{h3opplus} + 0.25 \cdot t_{\text{so4}} + 0.75 \cdot t_{\text{h2s}} + t_{\text{ims}} \rightarrow t_{\text{pyr}} + 1.5 \cdot \text{h2o}$</p>
continued on next page...

Processes, continued from previous page	
p_ims_form2_pyr =	(t_ims*t_h2s*k_pyrite)*lim_t_so4_28*lim_t_h2s_29* lim_t_ims_57
Auxiliary variables	
absolute temperature [K]	
temp_k =	cgt_temp + 273.15
temporary value assumed for pH [1]	
ph_temp =	0.0-log(min(max(h3o,1.0e-12),1.0e-2))/log(10.0)
calculated iteratively, 10 iterations, initial value = 0.0	
self-ionization constant of Water [mol²/kg²]	
k_water =	exp(-13847.26 / temp_k + 148.96502 - 23.6521 * log(temp_k) + (118.67/temp_k - 5.977 + 1.0495 * log(temp_k)) * sqrt(cgt_sali) - 0.01615 * cgt_sali)
Solubility of CO₂ [mol/kg/Pa]	
k0_co2 =	exp(9345.17 / temp_k - 60.2409 + 23.3585 * (log(temp_k) - 4.605170186) + cgt_sali*(0.023517 - 0.00023656 * temp_k + 0.00000047036 *temp_k*temp_k))/101325.0
Acid dissociation constant CO₂ + 2 H₂O <-> HCO₃⁻ + H₃O⁺ [mol/kg]	
k1_co2 =	power(10.0,(-3633.86 / temp_k + 61.2172 - 9.6777 * log(temp_k) + 0.011555 * cgt_sali - 0.0001152 * cgt_sali * cgt_sali))
Acid dissociation constant HCO₃⁻ + H₂O <-> [CO₃²⁻] + H₃O⁺ [mol/kg]	
k2_co2 =	power(10.0,(-471.78 / temp_k - 25.929 + 3.16967 * log(temp_k) + 0.01781 * cgt_sali - 0.0001122 * cgt_sali * cgt_sali))
Acid dissociation constant of boric acid [mol/kg]	
k_boron =	exp((-8966.9 - 2890.53*sqrt(cgt_sali) - 77.942*cgt_sali + 1.728*cgt_sali*sqrt(cgt_sali) - 0.0996*cgt_sali*cgt_sali) / temp_k + 148.0248 + 137.1942*sqrt(cgt_sali) + 1.62142* cgt_sali + (-24.4344 - 25.085*sqrt(cgt_sali) - 0.2474* cgt_sali)*log(temp_k) + 0.053105*sqrt(cgt_sali)*temp_k)
Acid dissociation constant H₃PO₄ + H₂O <-> [H₂PO₄⁻] + H₃O⁺ [mol/kg]	
k1_po4 =	exp(-4576.752/temp_k + 115.525 - 18.453*log(temp_k) + (0.69171 - 106.736/temp_k)*sqrt(cgt_sali) - (0.01844 + 0.65643/temp_k)*cgt_sali)
continued on next page...	

Auxiliary variables, continued from previous page

Acid dissociation constant $[H_2PO_4^-] + H_2O \rightleftharpoons [HPO_4^{2-}] + H_3O^+$ [mol/kg]

$k2_{po4} = \exp(-8814.715/temp_k + 172.0883 - 27.927*\log(temp_k) + (1.35660 - 160.340/temp_k)*\sqrt{cgt_sali} - (0.05778 - 0.37335/temp_k)*cgt_sali)$

Acid dissociation constant $[HPO_4^{2-}] + H_2O \rightleftharpoons [PO_4^{3-}] + H_3O^+$ [mol/kg]

$k3_{po4} = \exp(-3070.75/temp_k - 18.141 + (2.81197 + 17.27039/temp_k)*\sqrt{cgt_sali} - (0.09984 + 44.99486/temp_k)*cgt_sali)$

Acid dissociation constant $H_2S + H_2O \rightleftharpoons HS^- + H_3O^+$ [mol/kg]

$k1_{h2s} = \exp(-3131.42/temp_k - 5.818 + 0.368*(power(max(0.0, cgt_sali), (1.0/3.0))))$

total concentration of boron [mol/kg]

$boron_total = 0.000416 * cgt_sali / 35.0$

boron alkalinity [mol/kg]

$alk_boron = boron_total * k_boron / (k_boron + h3o)$

calculated iteratively, 10 iterations, initial value = 0.0

hydrogen sulfide alkalinity [mol/kg]

$alk_h2s = t_h2s * k1_{h2s} / (k1_{h2s} + h3o)$

calculated iteratively, 10 iterations, initial value = 0.0

water alkalinity [mol/kg]

$alk_water = k_water / h3o - h3o$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in phosphate alkalinity formula [mol³/kg³]

$alk_po4_denominator = (h3o*h3o*h3o + k1_{po4}*h3o*h3o + k1_{po4}*k2_{po4}*h3o + k1_{po4}*k2_{po4}*k3_{po4})$

calculated iteratively, 10 iterations, initial value = 0.0

phosphate alkalinity [mol/kg]

$alk_po4 = (t_{po4}*(k1_{po4}*k2_{po4}*h3o + 2.0*k1_{po4}*k2_{po4}*k3_{po4} - h3o*h3o) / alk_po4_denominator)$

calculated iteratively, 10 iterations, initial value = 0.0

denominator in carbonate alkalinity formula [mol²/kg²]

$alk_co2_denominator = (h3o*h3o + k1_{co2}*h3o + k1_{co2}*k2_{co2})$

calculated iteratively, 10 iterations, initial value = 0.0

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Auxiliary variables, continued from previous page

carbonate alkalinity [mol/kg]

$\text{alk_co2} = \text{t_dic} * \text{k1_co2} * (\text{h3o} + 2 * \text{k2_co2}) / \text{alk_co2_denominator}$

calculated iteratively, 10 iterations, initial value = 0.0

error in total alkalinity calculation at the assumed pH [mol/kg]

$\text{alk_residual} = \text{t_alk} - \text{alk_co2} - \text{alk_po4} - \text{alk_boron} - \text{alk_h2s} - \text{alk_water}$

calculated iteratively, 10 iterations, initial value = 0.0

derivative of phosphate alkalinity with respect to h3o [1]

$\text{dalkp_dh3o} = \frac{\text{t_po4} * (0.0 - \text{k1_po4} * \text{h3o} * \text{h3o} * \text{h3o} * \text{h3o} - 4 * \text{k1_po4} * \text{k2_po4} * \text{h3o} * \text{h3o} * \text{h3o} - (\text{k1_po4} * \text{k1_po4} * \text{k2_po4} + 9 * \text{k1_po4} * \text{k2_po4} * \text{k3_po4}) * \text{h3o} * \text{h3o} - 4 * \text{k1_po4} * \text{k1_po4} * \text{k2_po4} * \text{k3_po4} * \text{h3o} - \text{k1_po4} * \text{k1_po4} * \text{k2_po4} * \text{k2_po4} * \text{k3_po4})}{(\text{alk_po4_denominator} * \text{alk_po4_denominator})}$

calculated iteratively, 10 iterations, initial value = 0.0

derivative of carbonate alkalinity with respect to h3o [1]

$\text{dalkc_dh3o} = \frac{\text{t_dic} * (0.0 - \text{k1_co2} * \text{h3o} * \text{h3o} - \text{k1_co2} * \text{k1_co2} * \text{k2_co2} - 4 * \text{k1_co2} * \text{k2_co2} * \text{h3o})}{(\text{alk_co2_denominator} * \text{alk_co2_denominator})}$

calculated iteratively, 10 iterations, initial value = 0.0

derivative of residual_alk with respect to pH [mol/kg]

$\text{dalkresidual_dpH} = 0.0 - \log(10.0) * \text{h3o} * (\text{alk_boron} / (\text{k_boron} + \text{h3o}) + \text{alk_h2s} / (\text{k1_h2s} + \text{h3o}) + \text{k_water} / (\text{h3o} * \text{h3o}) + 1 - \text{dalkp_dh3o} - \text{dalkc_dh3o})$

calculated iteratively, 10 iterations, initial value = 0.0

newly determined pH value [1]

$\text{temp1} = \text{alk_residual} / \text{dalkresidual_dpH}$

$\text{ph} = \text{ph_temp} - \text{temp1} + \text{theta}(\text{abs}(\text{temp1}) - 1) * 0.5 * \text{temp1}$

calculated iteratively, 10 iterations, initial value = 0.0

h3o ion concentration [mol/kg]

$\text{h3o} = \text{power}(10.0, 0.0 - \max(1.0, \min(13.0, \text{ph})))$

calculated iteratively, 10 iterations, initial value = 1.0e-8

co2 partial pressure [Pa]

$\text{pco2} = \text{t_dic} / \text{k0_co2} / (1 + \text{k1_co2} / \text{h3o} + \text{k1_co2} * \text{k2_co2} / \text{h3o} / \text{h3o})$

Acid dissociation constant $\text{H2S} + \text{H2O} \rightleftharpoons \text{HS}^- + \text{H3O}^+$ [mol/kg]

$\text{k1_h2s_sed} = \exp(-3131.42 / \text{temp_k} - 5.818 + 0.368 * (\text{power}(\max(0.0, \text{cgt_sali}), (1.0 / 3.0))))$

ionic strength of the solution [mol/kg]

$\text{ionic_strength} = 0.02 * \text{cgt_sali}$

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Auxiliary variables, continued from previous page

dielectric constant of seawater [F/m]

```
temp1 = cgt_sali*(1.707e-2+1.205e-5*cgt_sali+4.058e-9*
power(cgt_sali,2.0))
temp2 = 1.0-0.2551*temp1+5.151e-2*temp1*temp1-6.889e-3*temp1*temp1*
temp1
temp3 = 87.74-0.40008*temp_k+9.398e-4*temp_k*temp_k+1.401e-6*
temp_k*temp_k*temp_k
dielectric_constant temp2*temp3
=
```

CO2 concentration in the surface layer [mol/kg]

```
co2 = pco2*k0_co2
```

concentration of HS- ions [mol/kg]

```
hsminus = t_h2s * k1_h2s_sed / (k1_h2s_sed + h3o)
```

parameter A for the Davies formula [mol^{0.5} l^{-0.5}]

```
davies_parameter_a 1.82e6*power(dielectric_constant*temp_k,-1.5)
=
```

concentration of HCO3- ions

```
hco3minus = co2*k1_co2/h3o
```

activity to concentration ratio of ions with a charge of +1/-1 [1]

```
power(10.0,0.0-davies_parameter_a*1*(sqrt(ionic_strength)
activity_coefficient/(1+sqrt(ionic_strength))-0.3*ionic_strength))
=
```

activity to concentration ratio of ions with a charge of +2/-2 [1]

```
power(10.0,0.0-davies_parameter_a*2*(sqrt(ionic_strength)
activity_coefficient/(1+sqrt(ionic_strength))-0.3*ionic_strength))
=
```

concentration of CO3-- ions

```
co32minus = hco3minus*k2_co2/h3o
```

activity of H3O+ ions (concentration corrected by ionic strength) [mol/kg]

```
activity_h3oplus = h3o*activity_coefficient_1
```

activity of CO3-- ions (concentration corrected by ionic strength) [mol/kg]

```
activity_co32minus co32minus*activity_coefficient_2
=
```

relative saturation of iron monosulfide [1]

```
saturation_ims = t_fe2*activity_coefficient_2*hsminus*
activity_coefficient_1/activity_h3oplus/power(10.0,-2.95)
```

continued on next page...

Auxiliary variables, continued from previous page

relative saturation of rhodochrosite [1]

```

      t_mn2*activity_coefficient_2*
saturation_rhodochroactivity_co32minus/power(10.0,-9.5)
=

```

relative saturation of iron-II to be adsorbed on illite-montmorillonite mixed-layer minerals [1]

```

temp1 =      2.7 * max(vol_fraction_im*(1.0-POR),epsilon)
saturation_iim = t_fe2/((max(t_iim,epsilon)/cgt_cellheight/cgt_density)
                    /(100*temp1))

```

dissolution rate of iron monosulfide [mol/m2/d]

```

      r_ims_diss*theta(1.0-saturation_ims)*(1.0-saturation_ims)*
ims_dissolution_ratecgt_cellheight*cgt_density
=

```

desorption rate of iron adsorbed to illite-minnesotaite mixed-layer minerals [mol/m2/d]

```

      r_iim_diss*theta(1.0-saturation_iim)*(1.0-saturation_iim)*
iim_dissolution_ratecgt_cellheight*cgt_density
=

```

Fe-II concentration in equilibrium with iron monosulfide precipitation [mol/kg]

```

fe2_eq_ims =      power(10.0,-2.95)*activity_h3oplus/max(hsminus*
                    activity_coefficient_1,1.0e-3*epsilon)
                    /activity_coefficient_2

```

Fe-II concentration in equilibrium with iron adsorbed to illite-montmorillonite mixed layer minerals [mol/kg]

```

temp1 =      2.7 * max(vol_fraction_im*(1.0-POR),epsilon)
fe2_eq_iim =      (max(t_iim,epsilon)/cgt_cellheight/cgt_density)/(100*temp1)
                    +1000*(1.0-cgt_in_sediment)

```

siderite is the favoured species for precipitation (0 or 1) [1]

```

fe2_ims_is_smallest theta(fe2_eq_iim-fe2_eq_ims)
=

```

minnesotaite is the favoured species for precipitation (0 or 1) [1]

```

fe2_iim_is_smallest theta(fe2_eq_ims-fe2_eq_iim)
=

```

Fe-II concentration in equilibrium with the fastest precipitating Fe species

```

fe2_eq =      fe2_ims_is_smallest*fe2_eq_ims+fe2_iim_is_smallest*
                    fe2_eq_iim

```

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Auxiliary variables, continued from previous page	
smoother value for fe2_eq [mol/kg]	
temp1 =	3.0e-6
fe2_smooth =	fe2_eq
Constants	
no division by 0	
epsilon =	4.5E-17
rate constant for formation of pyrite [kg/mol/d]	
k_pyrite =	8.9
porosity	
por =	0.77
fraction of illite-montmorillonite mixed layer minerals on volume of all minerals [1]	
vol_fraction_im =	0.5
rate of iron monosulfide dissolution [1/d]	
r_ims_diss =	0.001
dissolution rate of iron adsorbed to illite-montmorillonite mixed-layer minerals [1/d]	
r_iim_diss =	0.001
Process limitation factors	
lim_t_h2s_29 =	theta(t_h2s-0.0)
lim_t_so4_28 =	theta(t_so4-0.0)
lim_t_fe2_55 =	theta(t_fe2-0.0)
lim_t_ims_57 =	theta(t_ims-0.0)
lim_t_rho_60 =	theta(t_rho-0.0)
lim_t_iim_61 =	theta(t_iim-0.0)

Processes	
detritus sedimentation (index 1 to 6) (sediment only) [mol/m ² /day]	
t_det_1 -> t_sed_1	
p_det_1_sedi_sed =	((1.0-erosion_is_active)*(0.0-w_det_sedi)*t_det_1* cgt_density*(1.0-cgt_in_sediment) + cgt_in_sediment* (t_det_1*cgt_density*cgt_cellheight*0.1))*lim_t_det_1_31
detritus sedimentation (index 1 to 6) (sediment only) [mol/m ² /day]	
t_detp_1 -> t_sedp_1	
p_detp_1_sedi_sedp =	((1.0-erosion_is_active)*(0.0-w_det_sedi)*t_detp_1* cgt_density*(1.0-cgt_in_sediment) + cgt_in_sediment* (t_detp_1*cgt_density*cgt_cellheight*0.1))*lim_t_detp_1_37
sedimentation of iron PO4 (sediment only) [mol/m ² /day]	
t_ipw -> t_ips	
p_ipw_sedi_ips =	((1.0-erosion_is_active)*(0.0-w_ipw_sedi)*t_ipw* cgt_density*(1.0-cgt_in_sediment))*lim_t_ipw_43
sedimentation of iron hydroxide (sediment only) [mol/m ² /day]	
t_ihw -> t_ihs	
p_ihw_sedi_ihs =	((1.0-erosion_is_active)*(0.0-w_ipw_sedi)*t_ihw* cgt_density*(1.0-cgt_in_sediment))*lim_t_ihw_44
sedimentation of iron hydroxide (sediment only) [mol/m ² /day]	
t_mow -> t_mos	
p_mow_sedi_mos =	((1.0-erosion_is_active)*(0.0-w_ipw_sedi)*t_mow* cgt_density*(1.0-cgt_in_sediment))*lim_t_mow_45
Auxiliary variables	
switch (1=erosion, 0=no erosion) which depends on the combined bottom stress of currents and waves	
erosion_is_active = theta(cgt_current_wave_stress - critical_stress)	
Constants	
critical shear stress for sediment erosion [N/m ²]	
critical_stress =	0.016
sedimentation velocity (negative for downward) [m/day]	
w_det_sedi =	-0.5
sedimentation velocity for iron PO4 [m/day]	
w_ipw_sedi =	-0.5

Process limitation factors	
lim_t_ipw_43 =	theta(t_ipw-0.0)
lim_t_det_1_31 =	theta(t_det_1-0.0)
lim_t_det_2_32 =	theta(t_det_2-0.0)
lim_t_det_3_33 =	theta(t_det_3-0.0)
lim_t_det_4_34 =	theta(t_det_4-0.0)
lim_t_det_5_35 =	theta(t_det_5-0.0)
lim_t_det_6_36 =	theta(t_det_6-0.0)
lim_t_ihw_44 =	theta(t_ihw-0.0)
lim_t_mow_45 =	theta(t_mow-0.0)
lim_t_detp_1_37 =	theta(t_detp_1-0.0)
lim_t_detp_2_38 =	theta(t_detp_2-0.0)
lim_t_detp_3_39 =	theta(t_detp_3-0.0)
lim_t_detp_4_40 =	theta(t_detp_4-0.0)
lim_t_detp_5_41 =	theta(t_detp_5-0.0)
lim_t_detp_6_42 =	theta(t_detp_6-0.0)

3.18 Process type standard

Processes
Auxiliary variables
Constants
Process limitation factors

4 Tracer equations

Tracer equations

Change of: autochthonous dissolved organic nitrogen

$$\begin{aligned} \frac{d}{dt} t_{\text{don}} = & \\ & + (p_{\text{lpp_resp_nh4}}) * \text{respiration of large-cell phytoplankton} \\ & \quad (\text{don_fraction}) \\ & + (p_{\text{spp_resp_nh4}}) * \text{respiration of small-cell phytoplankton} \\ & \quad (\text{don_fraction}) \\ & + (p_{\text{cya_resp_nh4}}) * \text{respiration of diazotroph cyanobacteria} \\ & \quad (\text{don_fraction}) \\ & + (p_{\text{zoo_resp_nh4}}) * \text{respiration of zooplankton} \\ & \quad (\text{don_fraction}) \\ & - p_{\text{don_rec_nh4}} \quad \text{mineralization of DON} \end{aligned}$$

Change of: dissolved molecular nitrogen

$$\begin{aligned} \frac{d}{dt} t_{\text{n2}} = & \\ & + \text{downward nitrogen flux through the surface} \\ & \quad p_{\text{n2_stf_down}} / (\text{cgt_cellheight} * \\ & \quad \text{cgt_density}) \\ & + (p_{\text{sed_1_denit_nh4}}) * \text{recycling of sedimentary detritus to ammonium} \\ & \quad (\text{rfr_pc_enrichment_det} * 2.65) \text{ using nitrate (denitrification)} \\ & \quad / (\text{cgt_cellheight} * \text{cgt_density}) \\ & + (p_{\text{sed_2_denit_nh4}}) * \text{recycling of sedimentary detritus to ammonium} \\ & \quad (\text{rfr_pc_enrichment_det} * 2.65) \text{ using nitrate (denitrification)} \\ & \quad / (\text{cgt_cellheight} * \text{cgt_density}) \\ & + (p_{\text{sed_3_denit_nh4}}) * \text{recycling of sedimentary detritus to ammonium} \\ & \quad (\text{rfr_pc_enrichment_det} * 2.65) \text{ using nitrate (denitrification)} \\ & \quad / (\text{cgt_cellheight} * \text{cgt_density}) \\ & + (p_{\text{sed_4_denit_nh4}}) * \text{recycling of sedimentary detritus to ammonium} \\ & \quad (\text{rfr_pc_enrichment_det} * 2.65) \text{ using nitrate (denitrification)} \\ & \quad / (\text{cgt_cellheight} * \text{cgt_density}) \end{aligned}$$

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Tracer equations, continued from previous page

+ (p_sed_5_denit_nh4)* (rfr_pc_enrichment_det*2.65) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
+ (p_sed_6_denit_nh4)* (rfr_pc_enrichment_det*2.65) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
+ (p_h2s_oxno3_sul)*(0.2)	oxidation of hydrogen sulfide with nitrate
+ (p_sul_oxno3_so4)*(0.6)	oxidation of elemental sulfur with nitrate
+ (p_det_1_denit_nh4)* (rfr_pc_enrichment_det*2.65)	recycling of detritus to ammonium using nitrate (denitrification)
+ (p_det_2_denit_nh4)* (rfr_pc_enrichment_det*2.65)	recycling of detritus to ammonium using nitrate (denitrification)
+ (p_det_3_denit_nh4)* (rfr_pc_enrichment_det*2.65)	recycling of detritus to ammonium using nitrate (denitrification)
+ (p_det_4_denit_nh4)* (rfr_pc_enrichment_det*2.65)	recycling of detritus to ammonium using nitrate (denitrification)
+ (p_det_5_denit_nh4)* (rfr_pc_enrichment_det*2.65)	recycling of detritus to ammonium using nitrate (denitrification)
+ (p_det_6_denit_nh4)* (rfr_pc_enrichment_det*2.65)	recycling of detritus to ammonium using nitrate (denitrification)
+ (p_poc_denit)*(0.4)	recycling of POC using nitrate (denitrification)
- p_n2_stf_up/(cgt_cellheight* cgt_density)	upward nitrogen flux through the surface
- (p_n2_assim_cya)*(0.5)	fixation of dinitrogen by diazotroph cyanobacteria

Change of: dissolved molecular oxygen

$$\frac{d}{dt} t_{o2} =$$

+	downward oxygen flux through the surface
p_o2_stf_down/(cgt_cellheight* cgt_density)	

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Tracer equations, continued from previous page

+ (p_no3_assim_lpp)*(8.625)	assimilation of nitrate by large-cell phytoplankton
+ (p_nh4_assim_lpp)*(6.625)	assimilation of ammonium by large-cell phytoplankton
+ (p_no3_assim_spp)*(8.625)	assimilation of nitrate by small-cell phytoplankton
+ (p_nh4_assim_spp)*(6.625)	assimilation of ammonium by small-cell phytoplankton
+ (p_n2_assim_cya)*(7.375)	fixation of dinitrogen by diazotroph cyanobacteria
+ p_assim_lpp_poc	Production of POC by LPP
+ p_assim_spp_poc	Production of POC by SPP
+ p_assim_cya_poc	Production of POC by CYA
- p_o2_stf_up/(cgt_cellheight* cgt_density)	upward oxygen flux through the surface
- (p_lpp_resp_nh4)*(6.625)	respiration of large-cell phytoplankton
- (p_spp_resp_nh4)*(6.625)	respiration of small-cell phytoplankton
- (p_cya_resp_nh4)*(6.625)	respiration of diazotroph cyanobacteria
- (p_zoo_resp_nh4)*(6.625)	respiration of zooplankton
- (p_nh4_nit_no3)*(2)	nitrification
- (p_nh4_nit_no3_sed)*(2)	nitrification in the sediment
- (p_sed_1_resp_nh4)* (rfr_pc_enrichment_det*6.625) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using oxygen (respiration)
- (p_sed_2_resp_nh4)* (rfr_pc_enrichment_det*6.625) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using oxygen (respiration)

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Tracer equations, continued from previous page

- (p_sed_3_resp_nh4)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*6.625) using oxygen (respiration)
/(cgt_cellheight*cgt_density)
- (p_sed_4_resp_nh4)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*6.625) using oxygen (respiration)
/(cgt_cellheight*cgt_density)
- (p_sed_5_resp_nh4)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*6.625) using oxygen (respiration)
/(cgt_cellheight*cgt_density)
- (p_sed_6_resp_nh4)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*6.625) using oxygen (respiration)
/(cgt_cellheight*cgt_density)
- (p_h2s_oxo2_sul)*(0.5) oxidation of hydrogen sulfide with oxygen
- (p_sul_oxo2_so4)*(1.5) oxidation of elemental sulfur with oxygen
- (p_det_1_resp_nh4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*6.625) oxygen (respiration)
- (p_det_2_resp_nh4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*6.625) oxygen (respiration)
- (p_det_3_resp_nh4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*6.625) oxygen (respiration)
- (p_det_4_resp_nh4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*6.625) oxygen (respiration)
- (p_det_5_resp_nh4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*6.625) oxygen (respiration)
- (p_det_6_resp_nh4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*6.625) oxygen (respiration)
- (p_fe2_ox_ihs)*(0.25) oxidation of Fe2+ to iron hydroxide in the
/(cgt_cellheight*cgt_density) sediment
- (p_fe2_ox_ihw)*(0.25) oxidation of Fe2+ to iron hydroxide in the
sediment

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Tracer equations, continued from previous page

- $(p_mn2_ox_mos)*(0.5) / (cgt_cellheight*cgt_density)$ oxidation of Mn²⁺ to manganese oxide in the sediment
- $(p_pyr_oxo2_ihs)*(0.25) / (cgt_cellheight*cgt_density)$ oxidation of pyrite by manganese oxide to iron oxyhydroxide
- $(p_imm_oxo2_ihs)*(0.25) / (cgt_cellheight*cgt_density)$ oxidation of minnesotaite by oxygen to iron oxyhydroxide
- $(p_i2i_oxo2_i3i)*(0.25) / (cgt_cellheight*cgt_density)$ oxidation of iron-II in illite-montmorillonite mixed layer minerals to iron-III
- $(p_aim_nit_no3_sed)*(2) / (cgt_cellheight*cgt_density)$ nitrification in the sediment
- $(p_ims_oxo2_ihs)*(2.25) / (cgt_cellheight*cgt_density)$ iron monosulfide oxidation to iron oxihydroxides
- p_poc_resp respiration of POC

Change of: dissolved inorganic carbon

$$\frac{d}{dt} t_dic =$$

- + $p_co2_stf_down / (cgt_cellheight * cgt_density)$ downward co₂ flux through the surface
- + $(p_lpp_resp_nh4)*(rfr_c)$ respiration of large-cell phytoplankton
- + $(p_spp_resp_nh4)*(rfr_c)$ respiration of small-cell phytoplankton
- + $(p_cya_resp_nh4)*(rfr_c)$ respiration of diazotroph cyanobacteria
- + $(p_zoo_resp_nh4)*(rfr_c)$ respiration of zooplankton
- + $(p_sed_1_resp_nh4)*(rfr_pc_enrichment_det*rfr_c) / (cgt_cellheight*cgt_density)$ recycling of sedimentary detritus to ammonium using oxygen (respiration)
- + $(p_sed_2_resp_nh4)*(rfr_pc_enrichment_det*rfr_c) / (cgt_cellheight*cgt_density)$ recycling of sedimentary detritus to ammonium using oxygen (respiration)

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Tracer equations, continued from previous page

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+ (p_sed_3_resp_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using oxygen (respiration)
/(cgt_cellheight*cgt_density)

+ (p_sed_4_resp_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using oxygen (respiration)
/(cgt_cellheight*cgt_density)

+ (p_sed_5_resp_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using oxygen (respiration)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_resp_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using oxygen (respiration)
/(cgt_cellheight*cgt_density)

+ (p_sed_1_denit_nh4)*     recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using nitrate (denitrification)
/(cgt_cellheight*cgt_density)

+ (p_sed_2_denit_nh4)*     recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using nitrate (denitrification)
/(cgt_cellheight*cgt_density)

+ (p_sed_3_denit_nh4)*     recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using nitrate (denitrification)
/(cgt_cellheight*cgt_density)

+ (p_sed_4_denit_nh4)*     recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using nitrate (denitrification)
/(cgt_cellheight*cgt_density)

+ (p_sed_5_denit_nh4)*     recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using nitrate (denitrification)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_denit_nh4)*     recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using nitrate (denitrification)
/(cgt_cellheight*cgt_density)

+ (p_sed_1_sulf_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)
/(cgt_cellheight*cgt_density)

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Tracer equations, continued from previous page

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+ (p_sed_2_sulf_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_3_sulf_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_4_sulf_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_5_sulf_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_sulf_nh4)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)
/(cgt_cellheight*cgt_density)

+ (p_det_1_resp_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) oxygen (respiration)

+ (p_det_2_resp_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) oxygen (respiration)

+ (p_det_3_resp_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) oxygen (respiration)

+ (p_det_4_resp_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) oxygen (respiration)

+ (p_det_5_resp_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) oxygen (respiration)

+ (p_det_6_resp_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) oxygen (respiration)

+ (p_det_1_denit_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) nitrate (denitrification)

+ (p_det_2_denit_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) nitrate (denitrification)

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Tracer equations, continued from previous page

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+ (p_det_3_denit_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) nitrate (denitrification)

+ (p_det_4_denit_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) nitrate (denitrification)

+ (p_det_5_denit_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) nitrate (denitrification)

+ (p_det_6_denit_nh4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_c) nitrate (denitrification)

+ (p_det_1_sulf_nh4)*       recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)

+ (p_det_2_sulf_nh4)*       recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)

+ (p_det_3_sulf_nh4)*       recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)

+ (p_det_4_sulf_nh4)*       recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)

+ (p_det_5_sulf_nh4)*       recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)

+ (p_det_6_sulf_nh4)*       recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using sulfate (sulfate reduction)

+ (p_sed_1_mnred_mn2)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using manganese oxide (manganese reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_2_mnred_mn2)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using manganese oxide (manganese reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_3_mnred_mn2)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using manganese oxide (manganese reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_4_mnred_mn2)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using manganese oxide (manganese reduction)
/(cgt_cellheight*cgt_density)

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Tracer equations, continued from previous page

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+ (p_sed_5_mnred_mn2)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using manganese oxide (manganese reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_mnred_mn2)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using manganese oxide (manganese reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_1_irred_ims)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_2_irred_ims)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_3_irred_ims)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_4_irred_ims)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_5_irred_ims)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_irred_ims)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_1_irredips_ims)*   recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron phosphate (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_2_irredips_ims)*   recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron phosphate (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_3_irredips_ims)*   recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron phosphate (iron reduction)
/(cgt_cellheight*cgt_density)

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Tracer equations, continued from previous page

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+ (p_sed_4_irredips_ims)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron phosphate (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_5_irredips_ims)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron phosphate (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_irredips_ims)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron phosphate (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_1_irred_iim)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_2_irred_iim)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_3_irred_iim)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_4_irred_iim)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_5_irred_iim)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_irred_iim)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_1_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_2_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

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Tracer equations, continued from previous page

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+ (p_sed_3_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_4_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_5_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_i3i_1_irred_i2i)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron-III in clay minerals (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_i3i_2_irred_i2i)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron-III in clay minerals (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_i3i_3_irred_i2i)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron-III in clay minerals (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_i3i_4_irred_i2i)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron-III in clay minerals (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_i3i_5_irred_i2i)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron-III in clay minerals (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_i3i_6_irred_i2i)*         recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*rfr_c) using iron-III in clay minerals (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_rho_diss_mn2)*(1.6)       rhodochrosite dissolution to manganese-II
/(cgt_cellheight*cgt_density)

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Tracer equations, continued from previous page	
+ (p_sed_1_sulfdeep_nh4)* (rfr_pc_enrichment_det*rfr_c) /(cgt_cellheight*cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_2_sulfdeep_nh4)* (rfr_pc_enrichment_det*rfr_c) /(cgt_cellheight*cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_3_sulfdeep_nh4)* (rfr_pc_enrichment_det*rfr_c) /(cgt_cellheight*cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_4_sulfdeep_nh4)* (rfr_pc_enrichment_det*rfr_c) /(cgt_cellheight*cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_5_sulfdeep_nh4)* (rfr_pc_enrichment_det*rfr_c) /(cgt_cellheight*cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_6_sulfdeep_nh4)* (rfr_pc_enrichment_det*rfr_c) /(cgt_cellheight*cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_rho_biores_mow)*(1.6) /(cgt_cellheight*cgt_density)	bio resuspension of rhodochrosite
+ (p_rho_ero_mow)*(1.6) /(cgt_cellheight*cgt_density)	bio resuspension of rhodochrosite
+ p_poc_resp	respiration of POC
+ p_poc_denit	recycling of POC using nitrate (denitrification)
+ p_poc_sulf	Mineralization of POC, e-acceptor sulfate (sulfate reduction)
- p_co2_stf_up/(cgt_cellheight* cgt_density)	upward co2 flux through the surface
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Tracer equations, continued from previous page

- (p_no3_assim_lpp)*(rfr_c)	assimilation of nitrate by large-cell phytoplankton
- (p_nh4_assim_lpp)*(rfr_c)	assimilation of ammonium by large-cell phytoplankton
- (p_no3_assim_spp)*(rfr_c)	assimilation of nitrate by small-cell phytoplankton
- (p_nh4_assim_spp)*(rfr_c)	assimilation of ammonium by small-cell phytoplankton
- (p_n2_assim_cya)*(rfr_c)	fixation of dinitrogen by diazotroph cyanobacteria
- (p_mn2_prec_rho)*(1.6)/(cgt_cellheight*cgt_density)	manganese-II precipitation to rhodochrosite
- p_assim_lpp_poc	Production of POC by LPP
- p_assim_spp_poc	Production of POC by SPP
- p_assim_cya_poc	Production of POC by CYA

Change of: ammonium

$\frac{d}{dt} t_nh4 =$	
+ (p_lpp_resp_nh4)*((1-don_fraction))	respiration of large-cell phytoplankton
+ (p_spp_resp_nh4)*((1-don_fraction))	respiration of small-cell phytoplankton
+ (p_cya_resp_nh4)*((1-don_fraction))	respiration of diazotroph cyanobacteria
+ (p_zoo_resp_nh4)*((1-don_fraction))	respiration of zooplankton
+ p_don_rec_nh4	mineralization of DON
+ (p_lpp_mort_det_1)*((1.0-(1.0/rfr_pc_enrichment_det)))	mortality of large-cell phytoplankton

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Tracer equations, continued from previous page

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+ (p_lpp_mort_det_2)*((1.0- mortality of large-cell phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_lpp_mort_det_3)*((1.0- mortality of large-cell phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_lpp_mort_det_4)*((1.0- mortality of large-cell phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_lpp_mort_det_5)*((1.0- mortality of large-cell phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_lpp_mort_det_6)*((1.0- mortality of large-cell phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_spp_mort_det_1)*((1.0- mortality of small-scale phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_spp_mort_det_2)*((1.0- mortality of small-scale phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_spp_mort_det_3)*((1.0- mortality of small-scale phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_spp_mort_det_4)*((1.0- mortality of small-scale phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_spp_mort_det_5)*((1.0- mortality of small-scale phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_spp_mort_det_6)*((1.0- mortality of small-scale phytoplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_cya_mort_det_1)*((1.0- mortality of diazotroph cyanobacteria
(1.0/rfr_pc_enrichment_det)))

+ (p_cya_mort_det_2)*((1.0- mortality of diazotroph cyanobacteria
(1.0/rfr_pc_enrichment_det)))

+ (p_cya_mort_det_3)*((1.0- mortality of diazotroph cyanobacteria
(1.0/rfr_pc_enrichment_det)))

+ (p_cya_mort_det_4)*((1.0- mortality of diazotroph cyanobacteria
(1.0/rfr_pc_enrichment_det)))

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Tracer equations, continued from previous page

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+ (p_cya_mort_det_5)*((1.0- mortality of diazotroph cyanobacteria
(1.0/rfr_pc_enrichment_det)))

+ (p_cya_mort_det_6)*((1.0- mortality of diazotroph cyanobacteria
(1.0/rfr_pc_enrichment_det)))

+ (p_zoo_mort_det_1)*((1.0- mortality of zooplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_zoo_mort_det_2)*((1.0- mortality of zooplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_zoo_mort_det_3)*((1.0- mortality of zooplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_zoo_mort_det_4)*((1.0- mortality of zooplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_zoo_mort_det_5)*((1.0- mortality of zooplankton
(1.0/rfr_pc_enrichment_det)))

+ (p_zoo_mort_det_6)*((1.0- mortality of zooplankton
(1.0/rfr_pc_enrichment_det)))

+
recycling of sedimentary detritus to ammonium
p_sed_1_resp_nh4/(cgt_cellheigusing oxygen (respiration)
cgt_density)

+
recycling of sedimentary detritus to ammonium
p_sed_2_resp_nh4/(cgt_cellheigusing oxygen (respiration)
cgt_density)

+
recycling of sedimentary detritus to ammonium
p_sed_3_resp_nh4/(cgt_cellheigusing oxygen (respiration)
cgt_density)

+
recycling of sedimentary detritus to ammonium
p_sed_4_resp_nh4/(cgt_cellheigusing oxygen (respiration)
cgt_density)

+
recycling of sedimentary detritus to ammonium
p_sed_5_resp_nh4/(cgt_cellheigusing oxygen (respiration)
cgt_density)

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Tracer equations, continued from previous page

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+                                recycling of sedimentary detritus to ammonium
p_sed_6_resp_nh4/(cgt_cellheigusing oxygen (respiration)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_1_denit_nh4/(cgt_cellheigusing nitrate (denitrification)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_2_denit_nh4/(cgt_cellheigusing nitrate (denitrification)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_3_denit_nh4/(cgt_cellheigusing nitrate (denitrification)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_4_denit_nh4/(cgt_cellheigusing nitrate (denitrification)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_5_denit_nh4/(cgt_cellheigusing nitrate (denitrification)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_6_denit_nh4/(cgt_cellheigusing nitrate (denitrification)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_1_sulf_nh4/(cgt_cellheigusing sulfate (sulfate reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_2_sulf_nh4/(cgt_cellheigusing sulfate (sulfate reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_3_sulf_nh4/(cgt_cellheigusing sulfate (sulfate reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_4_sulf_nh4/(cgt_cellheigusing sulfate (sulfate reduction)
cgt_density)

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Tracer equations, continued from previous page

+ p_sed_5_sulf_nh4/(cgt_cellheig cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ p_sed_6_sulf_nh4/(cgt_cellheig cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ p_det_1_resp_nh4	recycling of detritus to ammonium using oxygen (respiration)
+ p_det_2_resp_nh4	recycling of detritus to ammonium using oxygen (respiration)
+ p_det_3_resp_nh4	recycling of detritus to ammonium using oxygen (respiration)
+ p_det_4_resp_nh4	recycling of detritus to ammonium using oxygen (respiration)
+ p_det_5_resp_nh4	recycling of detritus to ammonium using oxygen (respiration)
+ p_det_6_resp_nh4	recycling of detritus to ammonium using oxygen (respiration)
+ p_det_1_denit_nh4	recycling of detritus to ammonium using nitrate (denitrification)
+ p_det_2_denit_nh4	recycling of detritus to ammonium using nitrate (denitrification)
+ p_det_3_denit_nh4	recycling of detritus to ammonium using nitrate (denitrification)
+ p_det_4_denit_nh4	recycling of detritus to ammonium using nitrate (denitrification)
+ p_det_5_denit_nh4	recycling of detritus to ammonium using nitrate (denitrification)
+ p_det_6_denit_nh4	recycling of detritus to ammonium using nitrate (denitrification)

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Tracer equations, continued from previous page

+ p_det_1_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ p_det_2_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ p_det_3_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ p_det_4_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ p_det_5_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ p_det_6_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ p_sed_1_mnred_mn2/(cgt_cellhei cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ p_sed_2_mnred_mn2/(cgt_cellhei cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ p_sed_3_mnred_mn2/(cgt_cellhei cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ p_sed_4_mnred_mn2/(cgt_cellhei cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ p_sed_5_mnred_mn2/(cgt_cellhei cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ p_sed_6_mnred_mn2/(cgt_cellhei cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ p_sed_1_irred_ims/(cgt_cellhei cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)

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Tracer equations, continued from previous page

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+                                recycling of sedimentary detritus to ammonium
p_sed_2_irred_ims/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_3_irred_ims/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_4_irred_ims/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_5_irred_ims/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_6_irred_ims/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_1_irredips_ims/(cgt_cellusing iron phosphate (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_2_irredips_ims/(cgt_cellusing iron phosphate (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_3_irredips_ims/(cgt_cellusing iron phosphate (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_4_irredips_ims/(cgt_cellusing iron phosphate (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_5_irredips_ims/(cgt_cellusing iron phosphate (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_6_irredips_ims/(cgt_cellusing iron phosphate (iron reduction)
cgt_density)

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Tracer equations, continued from previous page

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+                                recycling of sedimentary detritus to ammonium
p_sed_1_irred_iim/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_2_irred_iim/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_3_irred_iim/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_4_irred_iim/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_5_irred_iim/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_6_irred_iim/(cgt_cellheusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_1_irredips_iim/(cgt_cellusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_2_irredips_iim/(cgt_cellusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_3_irredips_iim/(cgt_cellusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_4_irredips_iim/(cgt_cellusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_sed_5_irredips_iim/(cgt_cellusing iron hydroxide (iron reduction)
cgt_density)

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Tracer equations, continued from previous page

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+                                recycling of sedimentary detritus to ammonium
p_sed_6_irredips_iim/(cgt_cellusing iron hydroxide (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_i3i_1_irred_i2i/(cgt_cellheiusing iron-III in clay minerals (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_i3i_2_irred_i2i/(cgt_cellheiusing iron-III in clay minerals (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_i3i_3_irred_i2i/(cgt_cellheiusing iron-III in clay minerals (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_i3i_4_irred_i2i/(cgt_cellheiusing iron-III in clay minerals (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_i3i_5_irred_i2i/(cgt_cellheiusing iron-III in clay minerals (iron reduction)
cgt_density)

+                                recycling of sedimentary detritus to ammonium
p_i3i_6_irred_i2i/(cgt_cellheiusing iron-III in clay minerals (iron reduction)
cgt_density)

+                                ammonium liberation from illite-
p_aim_lib_nh4/(cgt_cellheight*montmorillonite mixed layer minerals
cgt_density)

+                                parameterization for recycling of sedimentary
p_sed_1_sulfdeep_nh4/(cgt_celldetritus to ammonium below the deepest
cgt_density)                                sediment layer (sulfate reduction / methane
                                                formation)

+                                parameterization for recycling of sedimentary
p_sed_2_sulfdeep_nh4/(cgt_celldetritus to ammonium below the deepest
cgt_density)                                sediment layer (sulfate reduction / methane
                                                formation)

+                                parameterization for recycling of sedimentary
p_sed_3_sulfdeep_nh4/(cgt_celldetritus to ammonium below the deepest
cgt_density)                                sediment layer (sulfate reduction / methane
                                                formation)

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Tracer equations, continued from previous page

+	$p_sed_4_sulfdeep_nh4 / (cgt_cellheight \cdot detritus_to_ammonium_below_the_deepest_sediment_layer)$	parameterization for recycling of sedimentary ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+	$p_sed_5_sulfdeep_nh4 / (cgt_cellheight \cdot detritus_to_ammonium_below_the_deepest_sediment_layer)$	parameterization for recycling of sedimentary ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+	$p_sed_6_sulfdeep_nh4 / (cgt_cellheight \cdot detritus_to_ammonium_below_the_deepest_sediment_layer)$	parameterization for recycling of sedimentary ammonium below the deepest sediment layer (sulfate reduction / methane formation)
-	$p_nh4_assim_lpp$	assimilation of ammonium by large-cell phytoplankton
-	$p_nh4_assim_spp$	assimilation of ammonium by small-cell phytoplankton
-	$p_nh4_nit_no3$	nitrification
-	$p_nh4_nit_no3_sed$	nitrification in the sediment
-	$p_nh4_ads_aim / (cgt_cellheight \cdot mixed_layer_minerals)$	ammonium adsorption to illite-montmorillonite

Change of: nitrate

$$\frac{d}{dt} t_no3 =$$

+	$p_nh4_nit_no3$	nitrification
+	$p_nh4_nit_no3_sed$	nitrification in the sediment
+	$p_aim_nit_no3_sed / (cgt_cellheight \cdot detritus_to_ammonium_below_the_deepest_sediment_layer)$	nitrification in the sediment
-	$p_no3_assim_lpp$	assimilation of nitrate by large-cell phytoplankton
-	$p_no3_assim_spp$	assimilation of nitrate by small-cell phytoplankton

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Tracer equations, continued from previous page

- (p_sed_1_denit_nh4)* (rfr_pc_enrichment_det*5.3) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- (p_sed_2_denit_nh4)* (rfr_pc_enrichment_det*5.3) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- (p_sed_3_denit_nh4)* (rfr_pc_enrichment_det*5.3) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- (p_sed_4_denit_nh4)* (rfr_pc_enrichment_det*5.3) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- (p_sed_5_denit_nh4)* (rfr_pc_enrichment_det*5.3) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- (p_sed_6_denit_nh4)* (rfr_pc_enrichment_det*5.3) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- (p_h2s_oxno3_sul)*(0.4)	oxidation of hydrogen sulfide with nitrate
- (p_sul_oxno3_so4)*(1.2)	oxidation of elemental sulfur with nitrate
- (p_det_1_denit_nh4)* (rfr_pc_enrichment_det*5.3)	recycling of detritus to ammonium using nitrate (denitrification)
- (p_det_2_denit_nh4)* (rfr_pc_enrichment_det*5.3)	recycling of detritus to ammonium using nitrate (denitrification)
- (p_det_3_denit_nh4)* (rfr_pc_enrichment_det*5.3)	recycling of detritus to ammonium using nitrate (denitrification)
- (p_det_4_denit_nh4)* (rfr_pc_enrichment_det*5.3)	recycling of detritus to ammonium using nitrate (denitrification)
- (p_det_5_denit_nh4)* (rfr_pc_enrichment_det*5.3)	recycling of detritus to ammonium using nitrate (denitrification)

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Tracer equations, continued from previous page

- (p_det_6_denit_nh4)* (rfr_pc_enrichment_det*5.3)	recycling of detritus to ammonium using nitrate (denitrification)
- (p_poc_denit)*(0.8)	recycling of POC using nitrate (denitrification)

Change of: phosphate

$\frac{d}{dt} t_{po4} =$	
+ (p_lpp_resp_nh4)*(rfr_p)	respiration of large-cell phytoplankton
+ (p_spp_resp_nh4)*(rfr_p)	respiration of small-cell phytoplankton
+ (p_cya_resp_nh4)*(rfr_p)	respiration of diazotroph cyanobacteria
+ (p_zoo_resp_nh4)*(rfr_p)	respiration of zooplankton
+ (p_sed_1_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_2_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_3_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_4_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_5_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_6_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_1_irredips_iim)* (rfr_pc_enrichment_det*26.5) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)

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Tracer equations, continued from previous page

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+ (p_sed_2_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_3_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_4_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_5_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_irredips_iim)*      recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density)

+                               dissolution of iron phosphate
p_ips_diss_po4/(cgt_cellheight
cgt_density)

+ p_ipw_diss_po4                dissolution of iron phosphate

+                               phosphate liberation from illite-
p_pim_lib_po4/(cgt_cellheight*montmorillonite mixed layer minerals
cgt_density)

+ (p_detp_1_remin_po4)*        recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration)

+ (p_detp_2_remin_po4)*        recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration)

+ (p_detp_3_remin_po4)*        recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration)

+ (p_detp_4_remin_po4)*        recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration)

+ (p_detp_5_remin_po4)*        recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration)

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Tracer equations, continued from previous page

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+ (p_detp_6_remin_po4)*      recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration)

+ (p_sedp_1_remin_po4)*      recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p)
/(cgt_cellheight*cgt_density)

+ (p_sedp_2_remin_po4)*      recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p)
/(cgt_cellheight*cgt_density)

+ (p_sedp_3_remin_po4)*      recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p)
/(cgt_cellheight*cgt_density)

+ (p_sedp_4_remin_po4)*      recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p)
/(cgt_cellheight*cgt_density)

+ (p_sedp_5_remin_po4)*      recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p)
/(cgt_cellheight*cgt_density)

+ (p_sedp_6_remin_po4)*      recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p)
/(cgt_cellheight*cgt_density)

+ (p_sedp_1_sulfdeep_po4)*    parameterization for recycling of sedimentary
(rfr_pc_enrichment_det*rfr_p) detritus to ammonium below the deepest
/(cgt_cellheight*cgt_density) sediment layer (sulfate reduction / methane
formation)

+ (p_sedp_2_sulfdeep_po4)*    parameterization for recycling of sedimentary
(rfr_pc_enrichment_det*rfr_p) detritus to ammonium below the deepest
/(cgt_cellheight*cgt_density) sediment layer (sulfate reduction / methane
formation)

+ (p_sedp_3_sulfdeep_po4)*    parameterization for recycling of sedimentary
(rfr_pc_enrichment_det*rfr_p) detritus to ammonium below the deepest
/(cgt_cellheight*cgt_density) sediment layer (sulfate reduction / methane
formation)

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Tracer equations, continued from previous page

+ (p_sedp_4_sulfdeep_po4)* (rfr_pc_enrichment_det*rfr_p) /(cgt_cellheight*cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sedp_5_sulfdeep_po4)* (rfr_pc_enrichment_det*rfr_p) /(cgt_cellheight*cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sedp_6_sulfdeep_po4)* (rfr_pc_enrichment_det*rfr_p) /(cgt_cellheight*cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
- (p_no3_assim_lpp)*(rfr_p)	assimilation of nitrate by large-cell phytoplankton
- (p_nh4_assim_lpp)*(rfr_p)	assimilation of ammonium by large-cell phytoplankton
- (p_no3_assim_spp)*(rfr_p)	assimilation of nitrate by small-cell phytoplankton
- (p_nh4_assim_spp)*(rfr_p)	assimilation of ammonium by small-cell phytoplankton
- (p_n2_assim_cya)*(rfr_p)	fixation of dinitrogen by diazotroph cyanobacteria
- p_po4_ads_ips/(cgt_cellheight*particles cgt_density)	adsorption of phosphate to iron hydroxide particles
- p_po4_ads_ipw	adsorption of phosphate to iron hydroxide particles
- p_po4_ads_pim/(cgt_cellheight*mixed layer minerals cgt_density)	phosphate adsorption to illite-montmorillonite mixed layer minerals

Change of: small-cell phytoplankton

 $\frac{d}{dt} t_{spp} =$

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Tracer equations, continued from previous page

+ p_no3_assim_spp	assimilation of nitrate by small-cell phytoplankton
+ p_nh4_assim_spp	assimilation of ammonium by small-cell phytoplankton
- p_spp_graz_zoo	grazing of zooplankton eating small-cell phytoplankton
- p_spp_resp_nh4	respiration of small-cell phytoplankton
- p_spp_mort_det_1	mortality of small-scale phytoplankton
- p_spp_mort_det_2	mortality of small-scale phytoplankton
- p_spp_mort_det_3	mortality of small-scale phytoplankton
- p_spp_mort_det_4	mortality of small-scale phytoplankton
- p_spp_mort_det_5	mortality of small-scale phytoplankton
- p_spp_mort_det_6	mortality of small-scale phytoplankton

Change of: zooplankton

$$\frac{d}{dt} t_{\text{zoo}} =$$

+ p_lpp_graz_zoo	grazing of zooplankton eating large-cell phytoplankton
+ p_spp_graz_zoo	grazing of zooplankton eating small-cell phytoplankton
+ p_cya_graz_zoo	grazing of zooplankton eating diazotroph cyanobacteria
- p_zoo_resp_nh4	respiration of zooplankton
- p_zoo_mort_det_1	mortality of zooplankton
- p_zoo_mort_det_2	mortality of zooplankton
- p_zoo_mort_det_3	mortality of zooplankton
- p_zoo_mort_det_4	mortality of zooplankton

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Tracer equations, continued from previous page

- p_zoo_mort_det_5	mortality of zooplankton
- p_zoo_mort_det_6	mortality of zooplankton

Change of: hydrogen sulfide

$\frac{d}{dt} t_{h2s} =$	
+ (p_sed_1_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_2_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_3_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_4_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_5_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_6_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_det_1_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_det_2_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)

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Tracer equations, continued from previous page

+ (p_det_3_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_det_4_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_det_5_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_det_6_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ p_ims_diss_fe2/(cgt_cellheight cgt_density)	dissolution of magnetite to iron II (precipitating iron hydroxides)
+ p_ims_trans_iim/(cgt_cellheight cgt_density)	iron monosulfide transformation to minnesotaite
+ (p_pyr_oxmos_ihs)*(1.625) /(cgt_cellheight*cgt_density)	oxidation of pyrite by manganese oxide to iron oxyhydroxide
+ (p_pyr_oxo2_ihs)*(1.75) /(cgt_cellheight*cgt_density)	oxidation of pyrite by manganese oxide to iron oxyhydroxide
+ (p_sed_1_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_2_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_3_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

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Tracer equations, continued from previous page

+ (p_sed_4_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_5_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_6_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_ims_biores_ihw)*(1.125) /(cgt_cellheight*cgt_density)	bio resuspension of iron monosulfide
+ (p_pyr_biores_ihw)*(1.875) /(cgt_cellheight*cgt_density)	bio resuspension of pyrite
+ (p_rho_biores_mow)*(0.25) /(cgt_cellheight*cgt_density)	bio resuspension of rhodochrosite
+ (p_iim_biores_ihw)*(0.125) /(cgt_cellheight*cgt_density)	bio resuspension of iron in clay minerals
+ (p_ims_ero_ihw)*(1.125) /(cgt_cellheight*cgt_density)	resuspension of iron monosulfide
+ (p_pyr_ero_ihw)*(1.875) /(cgt_cellheight*cgt_density)	resuspension of pyrite
+ (p_rho_ero_mow)*(0.25) /(cgt_cellheight*cgt_density)	bio resuspension of rhodochrosite
+ (p_iim_ero_ihw)*(0.125) /(cgt_cellheight*cgt_density)	bio resuspension of iron in clay minerals
+ (p_poc_sulf)*(0.5)	Mineralization of POC, e-acceptor sulfate (sulfate reduction)
- p_h2s_oxo2_sul	oxidation of hydrogen sulfide with oxygen

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Tracer equations, continued from previous page

- p_h2s_oxno3_sul	oxidation of hydrogen sulfide with nitrate
- (p_sed_1_irred_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_2_irred_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_3_irred_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_4_irred_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_5_irred_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_6_irred_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_1_irredips_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_2_irredips_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_3_irredips_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_4_irredips_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_5_irredips_ims)*(26.5*rfr_pc_enrichment_det)/(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)

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Tracer equations, continued from previous page

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- (p_sed_6_irredips_ims)*      recycling of sedimentary detritus to ammonium
(26.5*rfr_pc_enrichment_det)  using iron phosphate (iron reduction)
/(cgt_cellheight*cgt_density)

-                               reduction of sedimentary iron hydroxide to
p_ihs_red_iim/(cgt_cellheight*iron-II
cgt_density)

- (p_ihs_red_ims)*(9.0)        reduction of sedimentary iron hydroxide to
/(cgt_cellheight*cgt_density) iron-II

-                               precipitation of iron II as siderite
p_fe2_prec_ims/(cgt_cellheight
cgt_density)

-                               minnesotaite transformation to iron
p_iim_trans_ims/(cgt_cellheightmonosulfide
cgt_density)

- (p_ims_form2_pyr)*(0.75)     pyrite formation from iron monosulfide
/(cgt_cellheight*cgt_density)

-                               reduction of iron-III in clay minerals to iron-II
p_i3i_redh2s_i2i/(cgt_cellheightconsuming h2s
cgt_density)

-                               reduction of sedimentary iron hydroxide to
p_ihc_red_iim/(cgt_cellheight*iron-II
cgt_density)

- (p_ihc_red_ims)*(9.0)        reduction of sedimentary iron hydroxide to
/(cgt_cellheight*cgt_density) iron-II

- (p_h2s_mnox_so4)*(0.25)      oxidation of h2s by reduction of MnO2
/(cgt_cellheight*cgt_density)

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Change of: sulfur

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 $\frac{d}{dt} t_{sul} =$ 
+ p_h2s_oxo2_sul              oxidation of hydrogen sulfide with oxygen
+ p_h2s_oxno3_sul             oxidation of hydrogen sulfide with nitrate
- p_sul_oxo2_so4              oxidation of elemental sulfur with oxygen

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Tracer equations, continued from previous page

- p_sul_oxno3_so4	oxidation of elemental sulfur with nitrate
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Change of: total alkalinity

$$\frac{d}{dt} t_{\text{alk}} =$$

+ (1)*(p_po4_ads_ips)*(3) /(cgt_cellheight*cgt_density)	adsorption of phosphate to iron hydroxide particles (produces ohminus)
+ (1)*(p_po4_ads_ipw)*(3)	adsorption of phosphate to iron hydroxide particles (produces ohminus)
+ (1)*(p_iim_diss_fe2)*(2) /(cgt_cellheight*cgt_density)	dissolution minnesotaite to of iron-II (produces ohminus)
+ (1)*(p_stf_alk)	relax alkalinity to default value to compensate for detritus removal (produces ohminus)
+ (1)*(p_alk_rise_ohmdiff)	rise of total alkalinity by quicker-than-assumed diffusion of OH- (produces ohminus)
+ (1)*(p_aim_lib_nh4) /(cgt_cellheight*cgt_density)	ammonium liberation from illite-montmorillonite mixed layer minerals (produces ohminus)
- (1)*(p_sed_1_irred_iim)* (53*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (consumes ohminus)
- (1)*(p_sed_2_irred_iim)* (53*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (consumes ohminus)
- (1)*(p_sed_3_irred_iim)* (53*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (consumes ohminus)
- (1)*(p_sed_4_irred_iim)* (53*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (consumes ohminus)
- (1)*(p_sed_5_irred_iim)* (53*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (consumes ohminus)

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Tracer equations, continued from previous page

- (1)*(p_sed_6_irred_iim)* recycling of sedimentary detritus to ammonium
(53*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes ohminus)
- (1)*(p_sed_1_irredips_iim)* recycling of sedimentary detritus to ammonium
(53*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes ohminus)
- (1)*(p_sed_2_irredips_iim)* recycling of sedimentary detritus to ammonium
(53*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes ohminus)
- (1)*(p_sed_3_irredips_iim)* recycling of sedimentary detritus to ammonium
(53*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes ohminus)
- (1)*(p_sed_4_irredips_iim)* recycling of sedimentary detritus to ammonium
(53*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes ohminus)
- (1)*(p_sed_5_irredips_iim)* recycling of sedimentary detritus to ammonium
(53*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes ohminus)
- (1)*(p_sed_6_irredips_iim)* recycling of sedimentary detritus to ammonium
(53*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes ohminus)
- (1)*(p_ips_diss_po4)*(3) dissolution of iron phosphate (consumes
/(cgt_cellheight*cgt_density) ohminus)
- (1)*(p_ipw_diss_po4)*(3) dissolution of iron phosphate (consumes
ohminus)
- (1)*(p_fe2_prec_ims)*(2.0) precipitation of iron II as siderite (consumes
/(cgt_cellheight*cgt_density) ohminus)
- (1)*(p_fe2_prec_iim)*(2) precipitation of iron II as minnesotaite
/(cgt_cellheight*cgt_density) (consumes ohminus)
- (1)*(p_stf_alk_up) relax alkalinity to default value to compensate
for detritus removal (consumes ohminus)

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Tracer equations, continued from previous page	
$-(1)*(p_nh4_ads_aim) / (cgt_cellheight*cgt_density)$	ammonium adsorption to illite-montmorillonite mixed layer minerals (consumes ohminus)
$+(-1)*(p_nh4_assim_lpp)*(0.8125)$	assimilation of ammonium by large-cell phytoplankton (produces h3oplus)
$+(-1)*(p_nh4_assim_spp)*(0.8125)$	assimilation of ammonium by small-cell phytoplankton (produces h3oplus)
$+(-1)*(p_nh4_nit_no3)*(2)$	nitrification (produces h3oplus)
$+(-1)*(p_nh4_nit_no3_sed)*(2)$	nitrification in the sediment (produces h3oplus)
$+(-1)*(p_sul_oxo2_so4)*(2)$	oxidation of elemental sulfur with oxygen (produces h3oplus)
$+(-1)*(p_sul_oxno3_so4)*(0.8)$	oxidation of elemental sulfur with nitrate (produces h3oplus)
$+(-1)*(p_det_1_resp_nh4)*(0)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+(-1)*(p_det_2_resp_nh4)*(0)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+(-1)*(p_det_3_resp_nh4)*(0)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+(-1)*(p_det_4_resp_nh4)*(0)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+(-1)*(p_det_5_resp_nh4)*(0)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+(-1)*(p_det_6_resp_nh4)*(0)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+(-1)*(p_fe2_ox_ihs)*(2) / (cgt_cellheight*cgt_density)$	oxidation of Fe ²⁺ to iron hydroxide in the sediment (produces h3oplus)
$+(-1)*(p_fe2_ox_ihw)*(2)$	oxidation of Fe ²⁺ to iron hydroxide in the sediment (produces h3oplus)
$+(-1)*(p_sed_1_irredips_ims)*(238.6875*rfr_pc_enrichment_det) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction) (produces h3oplus)
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Tracer equations, continued from previous page

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+ (-1)*(p_sed_2_irredips_ims) recycling of sedimentary detritus to ammonium
*(238.6875* using iron phosphate (iron reduction)
rfr_pc_enrichment_det) (produces h3oplus)
/(cgt_cellheight*cgt_density)

+ (-1)*(p_sed_3_irredips_ims) recycling of sedimentary detritus to ammonium
*(238.6875* using iron phosphate (iron reduction)
rfr_pc_enrichment_det) (produces h3oplus)
/(cgt_cellheight*cgt_density)

+ (-1)*(p_sed_4_irredips_ims) recycling of sedimentary detritus to ammonium
*(238.6875* using iron phosphate (iron reduction)
rfr_pc_enrichment_det) (produces h3oplus)
/(cgt_cellheight*cgt_density)

+ (-1)*(p_sed_5_irredips_ims) recycling of sedimentary detritus to ammonium
*(238.6875* using iron phosphate (iron reduction)
rfr_pc_enrichment_det) (produces h3oplus)
/(cgt_cellheight*cgt_density)

+ (-1)*(p_sed_6_irredips_ims) recycling of sedimentary detritus to ammonium
*(238.6875* using iron phosphate (iron reduction)
rfr_pc_enrichment_det) (produces h3oplus)
/(cgt_cellheight*cgt_density)

+ (-1)*(p_sed_1_irredips_iim) recycling of sedimentary detritus to ammonium
*(79.5*rfr_pc_enrichment_det) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) h3oplus)

+ (-1)*(p_sed_2_irredips_iim) recycling of sedimentary detritus to ammonium
*(79.5*rfr_pc_enrichment_det) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) h3oplus)

+ (-1)*(p_sed_3_irredips_iim) recycling of sedimentary detritus to ammonium
*(79.5*rfr_pc_enrichment_det) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) h3oplus)

+ (-1)*(p_sed_4_irredips_iim) recycling of sedimentary detritus to ammonium
*(79.5*rfr_pc_enrichment_det) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) h3oplus)

+ (-1)*(p_sed_5_irredips_iim) recycling of sedimentary detritus to ammonium
*(79.5*rfr_pc_enrichment_det) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) h3oplus)

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Tracer equations, continued from previous page

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+ (-1)*(p_sed_6_irredips_iim) recycling of sedimentary detritus to ammonium
*(79.5*rfr_pc_enrichment_det) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) h3oplus)

+ (-1)*(p_ihs_red_iim)*(2.0) reduction of sedimentary iron hydroxide to
/(cgt_cellheight*cgt_density) iron-II (produces h3oplus)

+ (-1)*(p_ihs_red_ims)*(2.0) reduction of sedimentary iron hydroxide to
/(cgt_cellheight*cgt_density) iron-II (produces h3oplus)

+ (-1)*(p_mn2_ox_mos)*(2) oxidation of Mn2+ to manganese oxide in the
/(cgt_cellheight*cgt_density) sediment (produces h3oplus)

+ (-1)*(p_alk_fall_ohmdiff) falling of total alkalinity by quicker-than-
assumed diffusion of OH- (produces h3oplus)

+ (-1)*(p_pyr_oxo2_ihs)*(0.5) oxidation of pyrite by manganese oxide to iron
/(cgt_cellheight*cgt_density) oxyhydroxide (produces h3oplus)

+ (-1)*(p_i3i_redh2s_i2i)*(2) reduction of iron-III in clay minerals to iron-II
/(cgt_cellheight*cgt_density) consuming h2s (produces h3oplus)

+ (-1)*(p_ihc_red_iim)*(2.0) reduction of sedimentary iron hydroxide to
/(cgt_cellheight*cgt_density) iron-II (produces h3oplus)

+ (-1)*(p_ihc_red_ims)*(2.0) reduction of sedimentary iron hydroxide to
/(cgt_cellheight*cgt_density) iron-II (produces h3oplus)

+ (-1)*(p_pim_lib_po4)*(3) phosphate liberation from illite-
/(cgt_cellheight*cgt_density) montmorillonite mixed layer minerals
(produces h3oplus)

+ (-1)*(p_aim_nit_no3_sed) nitrification in the sediment (produces h3oplus)
/(cgt_cellheight*cgt_density)

+ (-1)*(p_fe2_mnox_ihs)*(2.0) oxidation of Fe2+ by reduction of MnO2
/(cgt_cellheight*cgt_density) (produces h3oplus)

+ (-1)*(p_ims_oxo2_ihs)*(2) iron monosulfide oxidation to iron
/(cgt_cellheight*cgt_density) oxihydroxides (produces h3oplus)

+ (-1)*(p_detp_1_remin_po4)* recycling of detritus to ammonium using
(3*rfr_pc_enrichment_det* oxygen (respiration) (produces h3oplus)
rfr_p)

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Tracer equations, continued from previous page

$+ (-1)*(p_detp_2_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+ (-1)*(p_detp_3_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+ (-1)*(p_detp_4_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+ (-1)*(p_detp_5_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+ (-1)*(p_detp_6_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)$	recycling of detritus to ammonium using oxygen (respiration) (produces h3oplus)
$+ (-1)*(p_sedp_1_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)/(cgt_cellheight*$ $cgt_density)$	recycling of sediment detrital phosphate (produces h3oplus)
$+ (-1)*(p_sedp_2_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)/(cgt_cellheight*$ $cgt_density)$	recycling of sediment detrital phosphate (produces h3oplus)
$+ (-1)*(p_sedp_3_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)/(cgt_cellheight*$ $cgt_density)$	recycling of sediment detrital phosphate (produces h3oplus)
$+ (-1)*(p_sedp_4_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)/(cgt_cellheight*$ $cgt_density)$	recycling of sediment detrital phosphate (produces h3oplus)
$+ (-1)*(p_sedp_5_remin_po4)*$ $(3*rfr_pc_enrichment_det*$ $rfr_p)/(cgt_cellheight*$ $cgt_density)$	recycling of sediment detrital phosphate (produces h3oplus)

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Tracer equations, continued from previous page

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+ (-1)*(p_sedp_6_remin_po4)* recycling of sediment detrital phosphate
(3*rfr_pc_enrichment_det* (produces h3oplus)
rfr_p)/(cgt_cellheight*
cgt_density)

+ (-1)*(p_mn2_prec_rho)*(3.2) manganese-II precipitation to rhodochrosite
/(cgt_cellheight*cgt_density) (produces h3oplus)

+ (-1)* parameterization for recycling of sedimentary
(p_sedp_1_sulfdeep_po4)*(3* detritus to ammonium below the deepest
rfr_pc_enrichment_det*rfr_p) sediment layer (sulfate reduction / methane
/(cgt_cellheight*cgt_density) formation) (produces h3oplus)

+ (-1)* parameterization for recycling of sedimentary
(p_sedp_2_sulfdeep_po4)*(3* detritus to ammonium below the deepest
rfr_pc_enrichment_det*rfr_p) sediment layer (sulfate reduction / methane
/(cgt_cellheight*cgt_density) formation) (produces h3oplus)

+ (-1)* parameterization for recycling of sedimentary
(p_sedp_3_sulfdeep_po4)*(3* detritus to ammonium below the deepest
rfr_pc_enrichment_det*rfr_p) sediment layer (sulfate reduction / methane
/(cgt_cellheight*cgt_density) formation) (produces h3oplus)

+ (-1)* parameterization for recycling of sedimentary
(p_sedp_4_sulfdeep_po4)*(3* detritus to ammonium below the deepest
rfr_pc_enrichment_det*rfr_p) sediment layer (sulfate reduction / methane
/(cgt_cellheight*cgt_density) formation) (produces h3oplus)

+ (-1)* parameterization for recycling of sedimentary
(p_sedp_5_sulfdeep_po4)*(3* detritus to ammonium below the deepest
rfr_pc_enrichment_det*rfr_p) sediment layer (sulfate reduction / methane
/(cgt_cellheight*cgt_density) formation) (produces h3oplus)

+ (-1)* parameterization for recycling of sedimentary
(p_sedp_6_sulfdeep_po4)*(3* detritus to ammonium below the deepest
rfr_pc_enrichment_det*rfr_p) sediment layer (sulfate reduction / methane
/(cgt_cellheight*cgt_density) formation) (produces h3oplus)

+ (-1)*(p_pyr_biores_ihw)* bio resuspension of pyrite (produces h3oplus)
(0.25)/(cgt_cellheight*
cgt_density)

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Tracer equations, continued from previous page

$+ (-1) * (p_pyr_ero_ihw) * (0.25) / (cgt_cellheight * cgt_density)$	resuspension of pyrite (produces h3oplus)
$- (-1) * (p_no3_assim_lpp) * (1.1875)$	assimilation of nitrate by large-cell phytoplankton (consumes h3oplus)
$- (-1) * (p_no3_assim_spp) * (1.1875)$	assimilation of nitrate by small-cell phytoplankton (consumes h3oplus)
$- (-1) * (p_n2_assim_cya) * (0.1875)$	fixation of dinitrogen by diazotroph cyanobacteria (consumes h3oplus)
$- (-1) * (p_lpp_resp_nh4) * (0.8125)$	respiration of large-cell phytoplankton (consumes h3oplus)
$- (-1) * (p_spp_resp_nh4) * (0.8125)$	respiration of small-cell phytoplankton (consumes h3oplus)
$- (-1) * (p_cya_resp_nh4) * (0.8125)$	respiration of diazotroph cyanobacteria (consumes h3oplus)
$- (-1) * (p_zoo_resp_nh4) * (0.8125)$	respiration of zooplankton (consumes h3oplus)
$- (-1) * (p_lpp_mort_det_1) * ((1.0 - (1.0 / rfr_pc_enrichment_det)))$	mortality of large-cell phytoplankton (consumes h3oplus)
$- (-1) * (p_lpp_mort_det_2) * ((1.0 - (1.0 / rfr_pc_enrichment_det)))$	mortality of large-cell phytoplankton (consumes h3oplus)
$- (-1) * (p_lpp_mort_det_3) * ((1.0 - (1.0 / rfr_pc_enrichment_det)))$	mortality of large-cell phytoplankton (consumes h3oplus)
$- (-1) * (p_lpp_mort_det_4) * ((1.0 - (1.0 / rfr_pc_enrichment_det)))$	mortality of large-cell phytoplankton (consumes h3oplus)
$- (-1) * (p_lpp_mort_det_5) * ((1.0 - (1.0 / rfr_pc_enrichment_det)))$	mortality of large-cell phytoplankton (consumes h3oplus)

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Tracer equations, continued from previous page

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- (-1)*(p_lpp_mort_det_6)*      mortality of large-cell phytoplankton
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_spp_mort_det_1)*      mortality of small-scale phytoplankton
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_spp_mort_det_2)*      mortality of small-scale phytoplankton
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_spp_mort_det_3)*      mortality of small-scale phytoplankton
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_spp_mort_det_4)*      mortality of small-scale phytoplankton
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_spp_mort_det_5)*      mortality of small-scale phytoplankton
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_spp_mort_det_6)*      mortality of small-scale phytoplankton
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_cya_mort_det_1)*      mortality of diazotroph cyanobacteria
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_cya_mort_det_2)*      mortality of diazotroph cyanobacteria
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_cya_mort_det_3)*      mortality of diazotroph cyanobacteria
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

- (-1)*(p_cya_mort_det_4)*      mortality of diazotroph cyanobacteria
((1.0-                           (consumes h3oplus)
(1.0/rfr_pc_enrichment_det)))

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Tracer equations, continued from previous page

- $(-1) \cdot (p_cya_mort_det_5) \cdot ((1.0 - (1.0/rfr_pc_enrichment_det)))$ mortality of diazotroph cyanobacteria (consumes h3oplus)
- $(-1) \cdot (p_cya_mort_det_6) \cdot ((1.0 - (1.0/rfr_pc_enrichment_det)))$ mortality of diazotroph cyanobacteria (consumes h3oplus)
- $(-1) \cdot (p_zoo_mort_det_1) \cdot ((1.0 - (1.0/rfr_pc_enrichment_det)))$ mortality of zooplankton (consumes h3oplus)
- $(-1) \cdot (p_zoo_mort_det_2) \cdot ((1.0 - (1.0/rfr_pc_enrichment_det)))$ mortality of zooplankton (consumes h3oplus)
- $(-1) \cdot (p_zoo_mort_det_3) \cdot ((1.0 - (1.0/rfr_pc_enrichment_det)))$ mortality of zooplankton (consumes h3oplus)
- $(-1) \cdot (p_zoo_mort_det_4) \cdot ((1.0 - (1.0/rfr_pc_enrichment_det)))$ mortality of zooplankton (consumes h3oplus)
- $(-1) \cdot (p_zoo_mort_det_5) \cdot ((1.0 - (1.0/rfr_pc_enrichment_det)))$ mortality of zooplankton (consumes h3oplus)
- $(-1) \cdot (p_zoo_mort_det_6) \cdot ((1.0 - (1.0/rfr_pc_enrichment_det)))$ mortality of zooplankton (consumes h3oplus)
- $(-1) \cdot (p_sed_1_resp_nh4) / (cgt_cellheight \cdot cgt_density)$ recycling of sedimentary detritus to ammonium using oxygen (respiration) (consumes h3oplus)
- $(-1) \cdot (p_sed_2_resp_nh4) / (cgt_cellheight \cdot cgt_density)$ recycling of sedimentary detritus to ammonium using oxygen (respiration) (consumes h3oplus)
- $(-1) \cdot (p_sed_3_resp_nh4) / (cgt_cellheight \cdot cgt_density)$ recycling of sedimentary detritus to ammonium using oxygen (respiration) (consumes h3oplus)
- $(-1) \cdot (p_sed_4_resp_nh4) / (cgt_cellheight \cdot cgt_density)$ recycling of sedimentary detritus to ammonium using oxygen (respiration) (consumes h3oplus)

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Tracer equations, continued from previous page

$- (-1)*(p_sed_5_resp_nh4) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using oxygen (respiration) (consumes h3oplus)
$- (-1)*(p_sed_6_resp_nh4) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using oxygen (respiration) (consumes h3oplus)
$- (-1)*(p_sed_1_denit_nh4)* ((1.0+5.3*rfr_pc_enrichment_det)) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
$- (-1)*(p_sed_2_denit_nh4)* ((1.0+5.3*rfr_pc_enrichment_det)) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
$- (-1)*(p_sed_3_denit_nh4)* ((1.0+5.3*rfr_pc_enrichment_det)) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
$- (-1)*(p_sed_4_denit_nh4)* ((1.0+5.3*rfr_pc_enrichment_det)) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
$- (-1)*(p_sed_5_denit_nh4)* ((1.0+5.3*rfr_pc_enrichment_det)) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
$- (-1)*(p_sed_6_denit_nh4)* ((1.0+5.3*rfr_pc_enrichment_det)) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
$- (-1)*(p_sed_1_sulf_nh4)* ((1.0+rfr_pc_enrichment_det*6.625)) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
$- (-1)*(p_sed_2_sulf_nh4)* ((1.0+rfr_pc_enrichment_det*6.625)) / (cgt_cellheight*cgt_density)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)

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Tracer equations, continued from previous page

- (-1)*(p_sed_3_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
- (-1)*(p_sed_4_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
- (-1)*(p_sed_5_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
- (-1)*(p_sed_6_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
- (-1)*(p_h2s_oxno3_sul)* (0.4)	oxidation of hydrogen sulfide with nitrate (consumes h3oplus)
- (-1)*(p_det_1_resp_nh4)	recycling of detritus to ammonium using oxygen (respiration) (consumes h3oplus)
- (-1)*(p_det_2_resp_nh4)	recycling of detritus to ammonium using oxygen (respiration) (consumes h3oplus)
- (-1)*(p_det_3_resp_nh4)	recycling of detritus to ammonium using oxygen (respiration) (consumes h3oplus)
- (-1)*(p_det_4_resp_nh4)	recycling of detritus to ammonium using oxygen (respiration) (consumes h3oplus)
- (-1)*(p_det_5_resp_nh4)	recycling of detritus to ammonium using oxygen (respiration) (consumes h3oplus)
- (-1)*(p_det_6_resp_nh4)	recycling of detritus to ammonium using oxygen (respiration) (consumes h3oplus)
- (-1)*(p_det_1_denit_nh4)* ((1.0+5.3* rfr_pc_enrichment_det))	recycling of detritus to ammonium using nitrate (denitrification) (consumes h3oplus)

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Tracer equations, continued from previous page

- (-1)*(p_det_2_denit_nh4)* ((1.0+5.3* rfr_pc_enrichment_det))	recycling of detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
- (-1)*(p_det_3_denit_nh4)* ((1.0+5.3* rfr_pc_enrichment_det))	recycling of detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
- (-1)*(p_det_4_denit_nh4)* ((1.0+5.3* rfr_pc_enrichment_det))	recycling of detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
- (-1)*(p_det_5_denit_nh4)* ((1.0+5.3* rfr_pc_enrichment_det))	recycling of detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
- (-1)*(p_det_6_denit_nh4)* ((1.0+5.3* rfr_pc_enrichment_det))	recycling of detritus to ammonium using nitrate (denitrification) (consumes h3oplus)
- (-1)*(p_det_1_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
- (-1)*(p_det_2_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
- (-1)*(p_det_3_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
- (-1)*(p_det_4_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
- (-1)*(p_det_5_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)
- (-1)*(p_det_6_sulf_nh4)* ((1.0+rfr_pc_enrichment_det* 6.625))	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction) (consumes h3oplus)

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Tracer equations, continued from previous page

$- (-1) * (p_sed_1_mnred_mn2) * ((1.0 + 26.5 * rfr_pc_enrichment_det)) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction) (consumes h3oplus)
$- (-1) * (p_sed_2_mnred_mn2) * ((1.0 + 26.5 * rfr_pc_enrichment_det)) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction) (consumes h3oplus)
$- (-1) * (p_sed_3_mnred_mn2) * ((1.0 + 26.5 * rfr_pc_enrichment_det)) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction) (consumes h3oplus)
$- (-1) * (p_sed_4_mnred_mn2) * ((1.0 + 26.5 * rfr_pc_enrichment_det)) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction) (consumes h3oplus)
$- (-1) * (p_sed_5_mnred_mn2) * ((1.0 + 26.5 * rfr_pc_enrichment_det)) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction) (consumes h3oplus)
$- (-1) * (p_sed_6_mnred_mn2) * ((1.0 + 26.5 * rfr_pc_enrichment_det)) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction) (consumes h3oplus)
$- (-1) * (p_sed_1_irred_ims) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (consumes h3oplus)
$- (-1) * (p_sed_2_irred_ims) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (consumes h3oplus)
$- (-1) * (p_sed_3_irred_ims) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction) (consumes h3oplus)

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Tracer equations, continued from previous page

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- (-1)*(p_sed_4_irred_ims) recycling of sedimentary detritus to ammonium
/(cgt_cellheight*cgt_density) using iron hydroxide (iron reduction)
                               (consumes h3oplus)

- (-1)*(p_sed_5_irred_ims) recycling of sedimentary detritus to ammonium
/(cgt_cellheight*cgt_density) using iron hydroxide (iron reduction)
                               (consumes h3oplus)

- (-1)*(p_sed_6_irred_ims) recycling of sedimentary detritus to ammonium
/(cgt_cellheight*cgt_density) using iron hydroxide (iron reduction)
                               (consumes h3oplus)

- (-1)*(p_sed_1_irredips_ims) recycling of sedimentary detritus to ammonium
*((1.0+159.1875*          using iron phosphate (iron reduction)
rfr_pc_enrichment_det)) (consumes h3oplus)
/(cgt_cellheight*cgt_density)

- (-1)*(p_sed_2_irredips_ims) recycling of sedimentary detritus to ammonium
*((1.0+159.1875*          using iron phosphate (iron reduction)
rfr_pc_enrichment_det)) (consumes h3oplus)
/(cgt_cellheight*cgt_density)

- (-1)*(p_sed_3_irredips_ims) recycling of sedimentary detritus to ammonium
*((1.0+159.1875*          using iron phosphate (iron reduction)
rfr_pc_enrichment_det)) (consumes h3oplus)
/(cgt_cellheight*cgt_density)

- (-1)*(p_sed_4_irredips_ims) recycling of sedimentary detritus to ammonium
*((1.0+159.1875*          using iron phosphate (iron reduction)
rfr_pc_enrichment_det)) (consumes h3oplus)
/(cgt_cellheight*cgt_density)

- (-1)*(p_sed_5_irredips_ims) recycling of sedimentary detritus to ammonium
*((1.0+159.1875*          using iron phosphate (iron reduction)
rfr_pc_enrichment_det)) (consumes h3oplus)
/(cgt_cellheight*cgt_density)

- (-1)*(p_sed_6_irredips_ims) recycling of sedimentary detritus to ammonium
*((1.0+159.1875*          using iron phosphate (iron reduction)
rfr_pc_enrichment_det)) (consumes h3oplus)
/(cgt_cellheight*cgt_density)

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Tracer equations, continued from previous page

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- (-1)*(p_sed_1_irred_iim)*  recycling of sedimentary detritus to ammonium
(53.0*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes h3oplus)

- (-1)*(p_sed_1_irred_iim)    recycling of sedimentary detritus to ammonium
/(cgt_cellheight*cgt_density) using iron hydroxide (iron reduction)
                                (consumes h3oplus)

- (-1)*(p_sed_2_irred_iim)*  recycling of sedimentary detritus to ammonium
(53.0*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes h3oplus)

- (-1)*(p_sed_2_irred_iim)    recycling of sedimentary detritus to ammonium
/(cgt_cellheight*cgt_density) using iron hydroxide (iron reduction)
                                (consumes h3oplus)

- (-1)*(p_sed_3_irred_iim)*  recycling of sedimentary detritus to ammonium
(53.0*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes h3oplus)

- (-1)*(p_sed_3_irred_iim)    recycling of sedimentary detritus to ammonium
/(cgt_cellheight*cgt_density) using iron hydroxide (iron reduction)
                                (consumes h3oplus)

- (-1)*(p_sed_4_irred_iim)*  recycling of sedimentary detritus to ammonium
(53.0*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes h3oplus)

- (-1)*(p_sed_4_irred_iim)    recycling of sedimentary detritus to ammonium
/(cgt_cellheight*cgt_density) using iron hydroxide (iron reduction)
                                (consumes h3oplus)

- (-1)*(p_sed_5_irred_iim)*  recycling of sedimentary detritus to ammonium
(53.0*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes h3oplus)

- (-1)*(p_sed_5_irred_iim)    recycling of sedimentary detritus to ammonium
/(cgt_cellheight*cgt_density) using iron hydroxide (iron reduction)
                                (consumes h3oplus)

- (-1)*(p_sed_6_irred_iim)*  recycling of sedimentary detritus to ammonium
(53.0*rfr_pc_enrichment_det) using iron hydroxide (iron reduction)
/(cgt_cellheight*cgt_density) (consumes h3oplus)

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Tracer equations, continued from previous page

- $(-1) \cdot (p_{\text{sed}_6\text{irred_iim}})$ recycling of sedimentary detritus to ammonium
 $/(\text{cgt_cellheight} \cdot \text{cgt_density})$ using iron hydroxide (iron reduction)
 (consumes h3oplus)

- $(-1) \cdot (p_{\text{sed}_1\text{irredips_iim}})$ recycling of sedimentary detritus to ammonium
 $\cdot ((1+53.0 \cdot \text{rfr_pc_enrichment_det}))$ using iron hydroxide (iron reduction)
 $/(\text{cgt_cellheight} \cdot \text{cgt_density})$ (consumes h3oplus)

- $(-1) \cdot (p_{\text{sed}_2\text{irredips_iim}})$ recycling of sedimentary detritus to ammonium
 $\cdot ((1+53.0 \cdot \text{rfr_pc_enrichment_det}))$ using iron hydroxide (iron reduction)
 $/(\text{cgt_cellheight} \cdot \text{cgt_density})$ (consumes h3oplus)

- $(-1) \cdot (p_{\text{sed}_3\text{irredips_iim}})$ recycling of sedimentary detritus to ammonium
 $\cdot ((1+53.0 \cdot \text{rfr_pc_enrichment_det}))$ using iron hydroxide (iron reduction)
 $/(\text{cgt_cellheight} \cdot \text{cgt_density})$ (consumes h3oplus)

- $(-1) \cdot (p_{\text{sed}_4\text{irredips_iim}})$ recycling of sedimentary detritus to ammonium
 $\cdot ((1+53.0 \cdot \text{rfr_pc_enrichment_det}))$ using iron hydroxide (iron reduction)
 $/(\text{cgt_cellheight} \cdot \text{cgt_density})$ (consumes h3oplus)

- $(-1) \cdot (p_{\text{sed}_5\text{irredips_iim}})$ recycling of sedimentary detritus to ammonium
 $\cdot ((1+53.0 \cdot \text{rfr_pc_enrichment_det}))$ using iron hydroxide (iron reduction)
 $/(\text{cgt_cellheight} \cdot \text{cgt_density})$ (consumes h3oplus)

- $(-1) \cdot (p_{\text{sed}_6\text{irredips_iim}})$ recycling of sedimentary detritus to ammonium
 $\cdot ((1+53.0 \cdot \text{rfr_pc_enrichment_det}))$ using iron hydroxide (iron reduction)
 $/(\text{cgt_cellheight} \cdot \text{cgt_density})$ (consumes h3oplus)

- $(-1) \cdot (p_{\text{i3i}_1\text{irred_i2i}})$ recycling of sedimentary detritus to ammonium
 $/(\text{cgt_cellheight} \cdot \text{cgt_density})$ using iron-III in clay minerals (iron reduction)
 (consumes h3oplus)

- $(-1) \cdot (p_{\text{i3i}_2\text{irred_i2i}})$ recycling of sedimentary detritus to ammonium
 $/(\text{cgt_cellheight} \cdot \text{cgt_density})$ using iron-III in clay minerals (iron reduction)
 (consumes h3oplus)

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Tracer equations, continued from previous page

- $(-1) \cdot (p_{i3i_3_irred_i2i}) / (cgt_cellheight \cdot cgt_density)$ recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction) (consumes h3oplus)
- $(-1) \cdot (p_{i3i_4_irred_i2i}) / (cgt_cellheight \cdot cgt_density)$ recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction) (consumes h3oplus)
- $(-1) \cdot (p_{i3i_5_irred_i2i}) / (cgt_cellheight \cdot cgt_density)$ recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction) (consumes h3oplus)
- $(-1) \cdot (p_{i3i_6_irred_i2i}) / (cgt_cellheight \cdot cgt_density)$ recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction) (consumes h3oplus)
- $(-1) \cdot (p_{ims_diss_fe2}) \cdot (2.0) / (cgt_cellheight \cdot cgt_density)$ dissolution of magnetite to iron II (precipitating iron hydroxides) (consumes h3oplus)
- $(-1) \cdot (p_{rho_diss_mn2}) \cdot (3.2) / (cgt_cellheight \cdot cgt_density)$ rhodochrosite dissolution to manganese-II (consumes h3oplus)
- $(-1) \cdot (p_{ims_form2_pyr}) \cdot (0.5) / (cgt_cellheight \cdot cgt_density)$ pyrite formation from iron monosulfide (consumes h3oplus)
- $(-1) \cdot (p_{pyr_oxmos_ihs}) \cdot (1.25) / (cgt_cellheight \cdot cgt_density)$ oxidation of pyrite by manganese oxide to iron oxyhydroxide (consumes h3oplus)
- $(-1) \cdot (p_{po4_ads_pim}) \cdot (3) / (cgt_cellheight \cdot cgt_density)$ phosphate adsorption to illite-montmorillonite mixed layer minerals (consumes h3oplus)
- $(-1) \cdot (p_{h2s_mnox_so4}) \cdot (1.5) / (cgt_cellheight \cdot cgt_density)$ oxidation of h2s by reduction of MnO2 (consumes h3oplus)
- $(-1) \cdot (p_{sed_1_sulfdeep_nh4}) \cdot ((1.0 + rfr_pc_enrichment_det \cdot 6.625)) / (cgt_cellheight \cdot cgt_density)$ parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (consumes h3oplus)

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Tracer equations, continued from previous page

- $(-1) \cdot (p_sed_2_sulfdeep_nh4) \cdot ((1.0 + rfr_pc_enrichment_det \cdot 6.625) / (cgt_cellheight \cdot cgt_density))$ parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (consumes h3oplus)
- $(-1) \cdot (p_sed_3_sulfdeep_nh4) \cdot ((1.0 + rfr_pc_enrichment_det \cdot 6.625) / (cgt_cellheight \cdot cgt_density))$ parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (consumes h3oplus)
- $(-1) \cdot (p_sed_4_sulfdeep_nh4) \cdot ((1.0 + rfr_pc_enrichment_det \cdot 6.625) / (cgt_cellheight \cdot cgt_density))$ parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (consumes h3oplus)
- $(-1) \cdot (p_sed_5_sulfdeep_nh4) \cdot ((1.0 + rfr_pc_enrichment_det \cdot 6.625) / (cgt_cellheight \cdot cgt_density))$ parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (consumes h3oplus)
- $(-1) \cdot (p_sed_6_sulfdeep_nh4) \cdot ((1.0 + rfr_pc_enrichment_det \cdot 6.625) / (cgt_cellheight \cdot cgt_density))$ parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (consumes h3oplus)
- $(-1) \cdot (p_ims_biores_ihw) \cdot (0.25) / (cgt_cellheight \cdot cgt_density)$ bio resuspension of iron monosulfide (consumes h3oplus)
- $(-1) \cdot (p_rho_biores_mow) \cdot (1.7) / (cgt_cellheight \cdot cgt_density)$ bio resuspension of rhodochrosite (consumes h3oplus)
- $(-1) \cdot (p_iim_biores_ihw) \cdot (0.25) / (cgt_cellheight \cdot cgt_density)$ bio resuspension of iron in clay minerals (consumes h3oplus)
- $(-1) \cdot (p_ims_ero_ihw) \cdot (0.25) / (cgt_cellheight \cdot cgt_density)$ resuspension of iron monosulfide (consumes h3oplus)
- $(-1) \cdot (p_rho_ero_mow) \cdot (1.7) / (cgt_cellheight \cdot cgt_density)$ bio resuspension of rhodochrosite (consumes h3oplus)

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Tracer equations, continued from previous page

- (-1)*(p_iim_ero_ihw)*(0.25) /(cgt_cellheight*cgt_density)	bio resuspension of iron in clay minerals (consumes h3oplus)
- (-1)*(p_poc_denit)*(0.8)	recycling of POC using nitrate (denitrification) (consumes h3oplus)
- (-1)*(p_poc_sulf)	Mineralization of POC, e-acceptor sulfate (sulfate reduction) (consumes h3oplus)
+ (2)*(p_lpp_resp_nh4)* (rfr_p)	respiration of large-cell phytoplankton (produces t_po4)
+ (2)*(p_spp_resp_nh4)* (rfr_p)	respiration of small-cell phytoplankton (produces t_po4)
+ (2)*(p_cya_resp_nh4)* (rfr_p)	respiration of diazotroph cyanobacteria (produces t_po4)
+ (2)*(p_zoo_resp_nh4)* (rfr_p)	respiration of zooplankton (produces t_po4)
+ (2)*(p_sed_1_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction) (produces t_po4)
+ (2)*(p_sed_2_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction) (produces t_po4)
+ (2)*(p_sed_3_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction) (produces t_po4)
+ (2)*(p_sed_4_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction) (produces t_po4)
+ (2)*(p_sed_5_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction) (produces t_po4)
+ (2)*(p_sed_6_irredips_ims)* (26.5*rfr_pc_enrichment_det) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction) (produces t_po4)

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Tracer equations, continued from previous page

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+ (2)*(p_sed_1_irredips_iim)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) t_po4)

+ (2)*(p_sed_2_irredips_iim)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) t_po4)

+ (2)*(p_sed_3_irredips_iim)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) t_po4)

+ (2)*(p_sed_4_irredips_iim)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) t_po4)

+ (2)*(p_sed_5_irredips_iim)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) t_po4)

+ (2)*(p_sed_6_irredips_iim)* recycling of sedimentary detritus to ammonium
(rfr_pc_enrichment_det*26.5) using iron hydroxide (iron reduction) (produces
/(cgt_cellheight*cgt_density) t_po4)

+ (2)*(p_ips_diss_po4)          dissolution of iron phosphate (produces t_po4)
/(cgt_cellheight*cgt_density)

+ (2)*(p_ipw_diss_po4)          dissolution of iron phosphate (produces t_po4)

+ (2)*(p_pim_lib_po4)          phosphate liberation from illite-
/(cgt_cellheight*cgt_density) montmorillonite mixed layer minerals
(produces t_po4)

+ (2)*(p_detp_1_remin_po4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration) (produces t_po4)

+ (2)*(p_detp_2_remin_po4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration) (produces t_po4)

+ (2)*(p_detp_3_remin_po4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration) (produces t_po4)

+ (2)*(p_detp_4_remin_po4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration) (produces t_po4)

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Tracer equations, continued from previous page

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+ (2)*(p_detp_5_remin_po4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration) (produces t_po4)

+ (2)*(p_detp_6_remin_po4)* recycling of detritus to ammonium using
(rfr_pc_enrichment_det*rfr_p) oxygen (respiration) (produces t_po4)

+ (2)*(p_sedp_1_remin_po4)* recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p) (produces t_po4)
/(cgt_cellheight*cgt_density)

+ (2)*(p_sedp_2_remin_po4)* recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p) (produces t_po4)
/(cgt_cellheight*cgt_density)

+ (2)*(p_sedp_3_remin_po4)* recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p) (produces t_po4)
/(cgt_cellheight*cgt_density)

+ (2)*(p_sedp_4_remin_po4)* recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p) (produces t_po4)
/(cgt_cellheight*cgt_density)

+ (2)*(p_sedp_5_remin_po4)* recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p) (produces t_po4)
/(cgt_cellheight*cgt_density)

+ (2)*(p_sedp_6_remin_po4)* recycling of sediment detrital phosphate
(rfr_pc_enrichment_det*rfr_p) (produces t_po4)
/(cgt_cellheight*cgt_density)

+ (2)*(p_sedp_1_sulfdeep_po4) parameterization for recycling of sedimentary
*(rfr_pc_enrichment_det* detritus to ammonium below the deepest
rfr_p)/(cgt_cellheight* sediment layer (sulfate reduction / methane
cgt_density) formation) (produces t_po4)

+ (2)*(p_sedp_2_sulfdeep_po4) parameterization for recycling of sedimentary
*(rfr_pc_enrichment_det* detritus to ammonium below the deepest
rfr_p)/(cgt_cellheight* sediment layer (sulfate reduction / methane
cgt_density) formation) (produces t_po4)

+ (2)*(p_sedp_3_sulfdeep_po4) parameterization for recycling of sedimentary
*(rfr_pc_enrichment_det* detritus to ammonium below the deepest
rfr_p)/(cgt_cellheight* sediment layer (sulfate reduction / methane
cgt_density) formation) (produces t_po4)

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Tracer equations, continued from previous page

$+(2)*(p_sedp_4_sulfdeep_po4)*$ $(rfr_pc_enrichment_det*$ $rfr_p)/(cgt_cellheight*$ $cgt_density)$	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (produces t_po4)
$+(2)*(p_sedp_5_sulfdeep_po4)*$ $(rfr_pc_enrichment_det*$ $rfr_p)/(cgt_cellheight*$ $cgt_density)$	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (produces t_po4)
$+(2)*(p_sedp_6_sulfdeep_po4)*$ $(rfr_pc_enrichment_det*$ $rfr_p)/(cgt_cellheight*$ $cgt_density)$	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation) (produces t_po4)
$-(2)*(p_no3_assim_lpp)*$ (rfr_p)	assimilation of nitrate by large-cell phytoplankton (consumes t_po4)
$-(2)*(p_nh4_assim_lpp)*$ (rfr_p)	assimilation of ammonium by large-cell phytoplankton (consumes t_po4)
$-(2)*(p_no3_assim_spp)*$ (rfr_p)	assimilation of nitrate by small-cell phytoplankton (consumes t_po4)
$-(2)*(p_nh4_assim_spp)*$ (rfr_p)	assimilation of ammonium by small-cell phytoplankton (consumes t_po4)
$-(2)*(p_n2_assim_cya)*$ (rfr_p)	fixation of dinitrogen by diazotroph cyanobacteria (consumes t_po4)
$-(2)*(p_po4_ads_ips)$ $/(cgt_cellheight*cgt_density)$	adsorption of phosphate to iron hydroxide particles (consumes t_po4)
$-(2)*(p_po4_ads_ipw)$	adsorption of phosphate to iron hydroxide particles (consumes t_po4)
$-(2)*(p_po4_ads_pim)$ $/(cgt_cellheight*cgt_density)$	phosphate adsorption to illite-montmorillonite mixed layer minerals (consumes t_po4)

Change of: iron-bound phosphate in the sediment

$$\frac{d}{dt} t_ips =$$

$$+ p_ipw_sedi_ips \quad \text{sedimentation of iron PO4}$$

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Tracer equations, continued from previous page

+ p_po4_ads_ips	adsorption of phosphate to iron hydroxide particles
- p_ips_ero_ipw	erosion of iron PO4
- p_ips_biores_ipw	bio resuspension of iron PO4
- (p_sed_1_irredips_ims)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_2_irredips_ims)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_3_irredips_ims)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_4_irredips_ims)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_5_irredips_ims)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_6_irredips_ims)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- (p_sed_1_irredips_iim)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_2_irredips_iim)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_3_irredips_iim)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_4_irredips_iim)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_5_irredips_iim)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_6_irredips_iim)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_ips_diss_po4	dissolution of iron phosphate

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Tracer equations, continued from previous page

- p_ips_removal transport from fluffy layer to deep basins

Change of: sulfate

$\frac{d}{dt} t_{so4} =$

+ p_sul_oxo2_so4 oxidation of elemental sulfur with oxygen

+ p_sul_oxno3_so4 oxidation of elemental sulfur with nitrate

+ reduction of sedimentary iron hydroxide to
p_ihs_red_iim/(cgt_cellheight*iron-II
cgt_density)

+ reduction of sedimentary iron hydroxide to
p_ihs_red_ims/(cgt_cellheight*iron-II
cgt_density)

+ p_so4_relax_upwards raise SO4 concentration in the water column to
salinity-determined default value

+ (p_pyr_oxmos_ihs)*(0.375) oxidation of pyrite by manganese oxide to iron
/(cgt_cellheight*cgt_density) oxyhydroxide

+ (p_pyr_oxo2_ihs)*(0.25) oxidation of pyrite by manganese oxide to iron
/(cgt_cellheight*cgt_density) oxyhydroxide

+ reduction of iron-III in clay minerals to iron-II
p_i3i_redh2s_i2i/(cgt_cellheight*cgt_density) consuming h2s

+ reduction of sedimentary iron hydroxide to
p_ihc_red_iim/(cgt_cellheight*iron-II
cgt_density)

+ reduction of sedimentary iron hydroxide to
p_ihc_red_ims/(cgt_cellheight*iron-II
cgt_density)

+ (p_h2s_mnox_so4)*(0.25) oxidation of h2s by reduction of MnO2
/(cgt_cellheight*cgt_density)

+ iron monosulfide oxidation to iron
p_ims_oxo2_ihs/(cgt_cellheight*cgt_density) toxihydroxides

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Tracer equations, continued from previous page

$+ (p_pyr_biores_ihw) * (0.125)$ $/(cgt_cellheight * cgt_density)$	bio resuspension of pyrite
$+ (p_pyr_ero_ihw) * (0.125)$ $/(cgt_cellheight * cgt_density)$	resuspension of pyrite
$- (p_sed_1_sulf_nh4) * (rfr_pc_enrichment_det * 3.3125) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
$- (p_sed_2_sulf_nh4) * (rfr_pc_enrichment_det * 3.3125) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
$- (p_sed_3_sulf_nh4) * (rfr_pc_enrichment_det * 3.3125) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
$- (p_sed_4_sulf_nh4) * (rfr_pc_enrichment_det * 3.3125) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
$- (p_sed_5_sulf_nh4) * (rfr_pc_enrichment_det * 3.3125) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
$- (p_sed_6_sulf_nh4) * (rfr_pc_enrichment_det * 3.3125) / (cgt_cellheight * cgt_density)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
$- (p_det_1_sulf_nh4) * (rfr_pc_enrichment_det * 3.3125)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
$- (p_det_2_sulf_nh4) * (rfr_pc_enrichment_det * 3.3125)$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)

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Tracer equations, continued from previous page

- (p_det_3_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
- (p_det_4_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
- (p_det_5_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
- (p_det_6_sulf_nh4)* (rfr_pc_enrichment_det* 3.3125)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
- p_so4_relax_downwards	lower SO4 concentration in the water column to salinity-determined default value
- (p_ims_form2_pyr)*(0.25) /(cgt_cellheight*cgt_density)	pyrite formation from iron monosulfide
- (p_sed_1_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
- (p_sed_2_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
- (p_sed_3_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
- (p_sed_4_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

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Tracer equations, continued from previous page

- (p_sed_5_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
- (p_sed_6_sulfdeep_nh4)* (rfr_pc_enrichment_det* 3.3125)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
- (p_ims_biores_ihw)*(0.125) /(cgt_cellheight*cgt_density)	bio resuspension of iron monosulfide
- (p_rho_biores_mow)*(0.25) /(cgt_cellheight*cgt_density)	bio resuspension of rhodochrosite
- (p_iim_biores_ihw)*(0.125) /(cgt_cellheight*cgt_density)	bio resuspension of iron in clay minerals
- (p_ims_ero_ihw)*(0.125) /(cgt_cellheight*cgt_density)	resuspension of iron monosulfide
- (p_rho_ero_mow)*(0.25) /(cgt_cellheight*cgt_density)	bio resuspension of rhodochrosite
- (p_iim_ero_ihw)*(0.125) /(cgt_cellheight*cgt_density)	bio resuspension of iron in clay minerals
- (p_poc_sulf)*(0.5)	Mineralization of POC, e-acceptor sulfate (sulfate reduction)

Change of: suspended iron phosphate

$$\frac{d}{dt} t_{ipw} =$$

+	erosion of iron PO4
p_ips_ero_ipw/(cgt_cellheight* cgt_density)	
+	bio resuspension of iron PO4
p_ips_biores_ipw/(cgt_cellheight* cgt_density)	
+ p_po4_ads_ipw	adsorption of phosphate to iron hydroxide particles

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Tracer equations, continued from previous page

- sedimentation of iron PO4
p_ipw_sedi_ips/(cgt_cellheight
cgt_density)
- p_ipw_diss_po4 dissolution of iron phosphate

Change of: large-cell phytoplankton

$$\frac{d}{dt} t_{lpp} =$$

- + p_no3_assim_lpp assimilation of nitrate by large-cell phytoplankton
- + p_nh4_assim_lpp assimilation of ammonium by large-cell phytoplankton
- p_lpp_graz_zoo grazing of zooplankton eating large-cell phytoplankton
- p_lpp_resp_nh4 respiration of large-cell phytoplankton
- p_lpp_mort_det_1 mortality of large-cell phytoplankton
- p_lpp_mort_det_2 mortality of large-cell phytoplankton
- p_lpp_mort_det_3 mortality of large-cell phytoplankton
- p_lpp_mort_det_4 mortality of large-cell phytoplankton
- p_lpp_mort_det_5 mortality of large-cell phytoplankton
- p_lpp_mort_det_6 mortality of large-cell phytoplankton

Change of: diazotroph cyanobacteria

$$\frac{d}{dt} t_{cya} =$$

- + p_n2_assim_cya fixation of dinitrogen by diazotroph cyanobacteria
- p_cya_graz_zoo grazing of zooplankton eating diazotroph cyanobacteria
- p_cya_resp_nh4 respiration of diazotroph cyanobacteria
- p_cya_mort_det_1 mortality of diazotroph cyanobacteria

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Tracer equations, continued from previous page

- p_cya_mort_det_2	mortality of diazotroph cyanobacteria
- p_cya_mort_det_3	mortality of diazotroph cyanobacteria
- p_cya_mort_det_4	mortality of diazotroph cyanobacteria
- p_cya_mort_det_5	mortality of diazotroph cyanobacteria
- p_cya_mort_det_6	mortality of diazotroph cyanobacteria

Change of: detritus fractions_1

$$\begin{aligned}
 \frac{d}{dt} t_det_1 = & \\
 & + (p_lpp_mort_det_1)* \quad \text{mortality of large-cell phytoplankton} \\
 & ((1.0/rfr_pc_enrichment_det)) \\
 & + (p_spp_mort_det_1)* \quad \text{mortality of small-scale phytoplankton} \\
 & ((1.0/rfr_pc_enrichment_det)) \\
 & + (p_cya_mort_det_1)* \quad \text{mortality of diazotroph cyanobacteria} \\
 & ((1.0/rfr_pc_enrichment_det)) \\
 & + (p_zoo_mort_det_1)* \quad \text{mortality of zooplankton} \\
 & ((1.0/rfr_pc_enrichment_det)) \\
 & + \quad \text{sedimentary detritus erosion} \\
 & p_sed_1_ero_det/(cgt_cellheight \\
 & cgt_density) \\
 & + \quad \text{bio resuspension of sedimentary detritus} \\
 & p_sed_1_biores_det/(cgt_cellheight \\
 & cgt_density) \\
 & + \quad \text{surface flux of detritus} \\
 & p_stf_det_1/(cgt_cellheight* \\
 & cgt_density) \\
 & - \quad \text{detritus sedimentation} \\
 & p_det_1_sedi_sed/(cgt_cellheight \\
 & cgt_density) \\
 & - p_det_1_resp_nh4 \quad \text{recycling of detritus to ammonium using} \\
 & \quad \text{oxygen (respiration)}
 \end{aligned}$$

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Tracer equations, continued from previous page

- p_det_1_denit_nh4 recycling of detritus to ammonium using
nitrate (denitrification)
- p_det_1_sulf_nh4 recycling of sedimentary detritus to ammonium
using sulfate (sulfate reduction)

Change of: detritus fractions_2

$$\begin{aligned} \frac{d}{dt} t_det_2 = & \\ & + (p_lpp_mort_det_2)* \quad \text{mortality of large-cell phytoplankton} \\ & ((1.0/rfr_pc_enrichment_det)) \\ & + (p_spp_mort_det_2)* \quad \text{mortality of small-scale phytoplankton} \\ & ((1.0/rfr_pc_enrichment_det)) \\ & + (p_cya_mort_det_2)* \quad \text{mortality of diazotroph cyanobacteria} \\ & ((1.0/rfr_pc_enrichment_det)) \\ & + (p_zoo_mort_det_2)* \quad \text{mortality of zooplankton} \\ & ((1.0/rfr_pc_enrichment_det)) \\ & + \quad \text{sedimentary detritus erosion} \\ & p_sed_2_ero_det/(cgt_cellheight \\ & cgt_density) \\ & + \quad \text{bio resuspension of sedimentary detritus} \\ & p_sed_2_biores_det/(cgt_cellheight \\ & cgt_density) \\ & + \quad \text{surface flux of detritus} \\ & p_stf_det_2/(cgt_cellheight* \\ & cgt_density) \\ & - \quad \text{detritus sedimentation} \\ & p_det_2_sedi_sed/(cgt_cellheight \\ & cgt_density) \\ & - p_det_2_resp_nh4 \quad \text{recycling of detritus to ammonium using} \\ & \text{oxygen (respiration)} \\ & - p_det_2_denit_nh4 \quad \text{recycling of detritus to ammonium using} \\ & \text{nitrate (denitrification)} \\ & - p_det_2_sulf_nh4 \quad \text{recycling of sedimentary detritus to ammonium} \\ & \text{using sulfate (sulfate reduction)} \end{aligned}$$

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Tracer equations, continued from previous page

Change of: detritus fractions_3

$$\begin{aligned}
\frac{d}{dt} t_det_3 = & \\
& + (p_lpp_mort_det_3)* \quad \text{mortality of large-cell phytoplankton} \\
& \quad ((1.0/rfr_pc_enrichment_det)) \\
& + (p_spp_mort_det_3)* \quad \text{mortality of small-scale phytoplankton} \\
& \quad ((1.0/rfr_pc_enrichment_det)) \\
& + (p_cya_mort_det_3)* \quad \text{mortality of diazotroph cyanobacteria} \\
& \quad ((1.0/rfr_pc_enrichment_det)) \\
& + (p_zoo_mort_det_3)* \quad \text{mortality of zooplankton} \\
& \quad ((1.0/rfr_pc_enrichment_det)) \\
& + \quad \text{sedimentary detritus erosion} \\
& \quad p_sed_3_ero_det/(cgt_cellheight \\
& \quad \quad cgt_density) \\
& + \quad \text{bio resuspension of sedimentary detritus} \\
& \quad p_sed_3_biores_det/(cgt_cellheight \\
& \quad \quad cgt_density) \\
& + \quad \text{surface flux of detritus} \\
& \quad p_stf_det_3/(cgt_cellheight* \\
& \quad \quad cgt_density) \\
& - \quad \text{detritus sedimentation} \\
& \quad p_det_3_sedi_sed/(cgt_cellheight \\
& \quad \quad cgt_density) \\
& - p_det_3_resp_nh4 \quad \text{recycling of detritus to ammonium using} \\
& \quad \quad \text{oxygen (respiration)} \\
& - p_det_3_denit_nh4 \quad \text{recycling of detritus to ammonium using} \\
& \quad \quad \text{nitrate (denitrification)} \\
& - p_det_3_sulf_nh4 \quad \text{recycling of sedimentary detritus to ammonium} \\
& \quad \quad \text{using sulfate (sulfate reduction)}
\end{aligned}$$

Change of: detritus fractions_4

$$\begin{aligned}
\frac{d}{dt} t_det_4 = & \\
& + (p_lpp_mort_det_4)* \quad \text{mortality of large-cell phytoplankton} \\
& \quad ((1.0/rfr_pc_enrichment_det))
\end{aligned}$$

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Tracer equations, continued from previous page

$$\begin{aligned}
& + (p_spp_mort_det_4)* \quad \text{mortality of small-scale phytoplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_cya_mort_det_4)* \quad \text{mortality of diazotroph cyanobacteria} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_zoo_mort_det_4)* \quad \text{mortality of zooplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + \quad \text{sedimentary detritus erosion} \\
& p_sed_4_ero_det/(cgt_cellheigh \\
& cgt_density) \\
& + \quad \text{bio resuspension of sedimentary detritus} \\
& p_sed_4_biores_det/(cgt_cellhe \\
& cgt_density) \\
& + \quad \text{surface flux of detritus} \\
& p_stf_det_4/(cgt_cellheight* \\
& cgt_density) \\
& - \quad \text{detritus sedimentation} \\
& p_det_4_sedi_sed/(cgt_cellheig \\
& cgt_density) \\
& - p_det_4_resp_nh4 \quad \text{recycling of detritus to ammonium using} \\
& \quad \text{oxygen (respiration)} \\
& - p_det_4_denit_nh4 \quad \text{recycling of detritus to ammonium using} \\
& \quad \text{nitrate (denitrification)} \\
& - p_det_4_sulf_nh4 \quad \text{recycling of sedimentary detritus to ammonium} \\
& \quad \text{using sulfate (sulfate reduction)}
\end{aligned}$$

Change of: detritus fractions_5

$$\frac{d}{dt} t_det_5 =$$

$$\begin{aligned}
& + (p_lpp_mort_det_5)* \quad \text{mortality of large-cell phytoplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_spp_mort_det_5)* \quad \text{mortality of small-scale phytoplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_cya_mort_det_5)* \quad \text{mortality of diazotroph cyanobacteria} \\
& ((1.0/rfr_pc_enrichment_det))
\end{aligned}$$

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Tracer equations, continued from previous page

$$\begin{aligned}
& + (p_zoo_mort_det_5) * \text{mortality of zooplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + \text{sedimentary detritus erosion} \\
& p_sed_5_ero_det / (cgt_cellheight \\
& cgt_density) \\
& + \text{bio resuspension of sedimentary detritus} \\
& p_sed_5_biores_det / (cgt_cellheight \\
& cgt_density) \\
& + \text{surface flux of detritus} \\
& p_stf_det_5 / (cgt_cellheight * \\
& cgt_density) \\
& - \text{detritus sedimentation} \\
& p_det_5_sedi_sed / (cgt_cellheight \\
& cgt_density) \\
& - p_det_5_resp_nh4 \quad \text{recycling of detritus to ammonium using} \\
& \quad \text{oxygen (respiration)} \\
& - p_det_5_denit_nh4 \quad \text{recycling of detritus to ammonium using} \\
& \quad \text{nitrate (denitrification)} \\
& - p_det_5_sulf_nh4 \quad \text{recycling of sedimentary detritus to ammonium} \\
& \quad \text{using sulfate (sulfate reduction)}
\end{aligned}$$

Change of: detritus fractions_6

$$\frac{d}{dt} t_det_6 =$$

$$\begin{aligned}
& + (p_lpp_mort_det_6) * \text{mortality of large-cell phytoplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_spp_mort_det_6) * \text{mortality of small-scale phytoplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_cya_mort_det_6) * \text{mortality of diazotroph cyanobacteria} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_zoo_mort_det_6) * \text{mortality of zooplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + \text{sedimentary detritus erosion} \\
& p_sed_6_ero_det / (cgt_cellheight \\
& cgt_density)
\end{aligned}$$

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Tracer equations, continued from previous page

+	bio resuspension of sedimentary detritus
$p_sed_6_biores_det/(cgt_cellhe$	
$cgt_density)$	
+	surface flux of detritus
$p_stf_det_6/(cgt_cellheight*$	
$cgt_density)$	
-	detritus sedimentation
$p_det_6_sedi_sed/(cgt_cellheig$	
$cgt_density)$	
- $p_det_6_resp_nh4$	recycling of detritus to ammonium using oxygen (respiration)
- $p_det_6_denit_nh4$	recycling of detritus to ammonium using nitrate (denitrification)
- $p_det_6_sulf_nh4$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)

Change of: sedimentary detritus fractions_1

$$\frac{d}{dt} t_sed_1 =$$

+	$p_det_1_sedi_sed$	detritus sedimentation
-	$p_sed_1_resp_nh4$	recycling of sedimentary detritus to ammonium using oxygen (respiration)
-	$p_sed_1_denit_nh4$	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
-	$p_sed_1_sulf_nh4$	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
-	$p_sed_1_ero_det$	sedimentary detritus erosion
-	$p_sed_1_biores_det$	bio resuspension of sedimentary detritus
-	$p_sed_1_mnred_mn2$	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
-	$p_sed_1_irred_ims$	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)

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Tracer equations, continued from previous page

- p_sed_1_irredips_ims	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- p_sed_1_irred_iim	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_sed_1_irredips_iim	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_i3i_1_irred_i2i	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- p_sed_1_removal	transport from fluffy layer to deep basins
- p_sed_1_sulfdeep_nh4	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: sedimentary detritus fractions_2

$$\frac{d}{dt} t_{sed_2} =$$

+ p_det_2_sedi_sed	detritus sedimentation
- p_sed_2_resp_nh4	recycling of sedimentary detritus to ammonium using oxygen (respiration)
- p_sed_2_denit_nh4	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- p_sed_2_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
- p_sed_2_ero_det	sedimentary detritus erosion
- p_sed_2_biores_det	bio resuspension of sedimentary detritus
- p_sed_2_mnred_mn2	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- p_sed_2_irred_ims	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)

continued on next page...

Tracer equations, continued from previous page

- p_sed_2_irredips_ims	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- p_sed_2_irred_iim	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_sed_2_irredips_iim	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_i3i_2_irred_i2i	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- p_sed_2_removal	transport from fluffy layer to deep basins
- p_sed_2_sulfdeep_nh4	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: sedimentary detritus fractions_3

$\frac{d}{dt} t_{sed_3} =$	
+ p_det_3_sedi_sed	detritus sedimentation
- p_sed_3_resp_nh4	recycling of sedimentary detritus to ammonium using oxygen (respiration)
- p_sed_3_denit_nh4	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- p_sed_3_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
- p_sed_3_ero_det	sedimentary detritus erosion
- p_sed_3_biores_det	bio resuspension of sedimentary detritus
- p_sed_3_mnred_mn2	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- p_sed_3_irred_ims	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_sed_3_irredips_ims	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)

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Tracer equations, continued from previous page

- p_sed_3_irred_iim	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_sed_3_irredips_iim	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_i3i_3_irred_i2i	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- p_sed_3_removal	transport from fluffy layer to deep basins
- p_sed_3_sulfdeep_nh4	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: sedimentary detritus fractions_4

$\frac{d}{dt} t_sed_4 =$	
+ p_det_4_sedi_sed	detritus sedimentation
- p_sed_4_resp_nh4	recycling of sedimentary detritus to ammonium using oxygen (respiration)
- p_sed_4_denit_nh4	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- p_sed_4_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
- p_sed_4_ero_det	sedimentary detritus erosion
- p_sed_4_biores_det	bio resuspension of sedimentary detritus
- p_sed_4_mnred_mn2	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- p_sed_4_irred_ims	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_sed_4_irredips_ims	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)

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Tracer equations, continued from previous page		
- p_sed_4_irred_iim		recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_sed_4_irredips_iim		recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_i3i_4_irred_i2i		recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- p_sed_4_removal		transport from fluffy layer to deep basins
- p_sed_4_sulfdeep_nh4		parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: sedimentary detritus fractions_5

$\frac{d}{dt} t_{sed_5} =$		
+ p_det_5_sedi_sed		detritus sedimentation
- p_sed_5_resp_nh4		recycling of sedimentary detritus to ammonium using oxygen (respiration)
- p_sed_5_denit_nh4		recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- p_sed_5_sulf_nh4		recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
- p_sed_5_ero_det		sedimentary detritus erosion
- p_sed_5_biores_det		bio resuspension of sedimentary detritus
- p_sed_5_mnred_mn2		recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- p_sed_5_irred_ims		recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_sed_5_irredips_ims		recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- p_sed_5_irred_iim		recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)

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Tracer equations, continued from previous page

- p_sed_5_irredips_iim	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_i3i_5_irred_i2i	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- p_sed_5_removal	transport from fluffy layer to deep basins
- p_sed_5_sulfdeep_nh4	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: sedimentary detritus fractions_6

$\frac{d}{dt} t_{sed_6} =$	
+ p_det_6_sedi_sed	detritus sedimentation
- p_sed_6_resp_nh4	recycling of sedimentary detritus to ammonium using oxygen (respiration)
- p_sed_6_denit_nh4	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
- p_sed_6_sulf_nh4	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
- p_sed_6_ero_det	sedimentary detritus erosion
- p_sed_6_biores_det	bio resuspension of sedimentary detritus
- p_sed_6_mnred_mn2	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- p_sed_6_irred_ims	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_sed_6_irredips_ims	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
- p_sed_6_irred_iim	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)

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Tracer equations, continued from previous page

- p_sed_6_irredips_iim	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- p_i3i_6_irred_i2i	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- p_sed_6_removal	transport from fluffy layer to deep basins
- p_sed_6_sulfdeep_nh4	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: iron hydroxide in the sediment

$\frac{d}{dt} t_{ihs} =$	
+ p_ihw_sedi_ihs	sedimentation of iron hydroxide
+ p_fe2_ox_ihs	oxidation of Fe ²⁺ to iron hydroxide in the sediment
+ p_ips_diss_po4	dissolution of iron phosphate
+ p_pyr_oxmos_ihs	oxidation of pyrite by manganese oxide to iron oxyhydroxide
+ p_pyr_oxo2_ihs	oxidation of pyrite by manganese oxide to iron oxyhydroxide
+ p_imm_oxo2_ihs	oxidation of minnesotaite by oxygen to iron oxyhydroxide
+ (p_fe2_mnox_ihs)*(2.0)	oxidation of Fe ²⁺ by reduction of MnO ₂
+ p_ims_oxo2_ihs	iron monosulfide oxidation to iron oxihydroxides
- p_ihs_ero_ihw	erosion of iron PO ₄
- p_ihs_biores_ihw	bio resuspension of iron hydroxyde
- (p_sed_1_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)

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Tracer equations, continued from previous page	
- (p_sed_2_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_3_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_4_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_5_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_6_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_1_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_2_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_3_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_4_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_5_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_sed_6_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
- (p_ihs_red_iim)*(8.0)	reduction of sedimentary iron hydroxide to iron-II
- (p_ihs_red_ims)*(8.0)	reduction of sedimentary iron hydroxide to iron-II
- p_po4_ads_ips	adsorption of phosphate to iron hydroxide particles
- p_ihs_removal	transport from fluffy layer to deep basins
- p_ihs_trans_ihc	transformation of amorphous iron oxyhydroxides to crystalline phase
continued on next page...	

Tracer equations, continued from previous page

Change of: suspended iron hydroxide

$$\begin{aligned}
\frac{d}{dt} t_{ihw} = & \\
& + \text{erosion of iron PO4} \\
& p_{ihs_ero_ihw}/(cgt_cellheight* \\
& cgt_density) \\
& + \text{erosion of larger-crystalline iron PO4} \\
& p_{ihc_ero_ihw}/(cgt_cellheight* \\
& cgt_density) \\
& + \text{bio resuspension of iron hydroxyde} \\
& p_{ihs_biores_ihw}/(cgt_cellheig \\
& cgt_density) \\
& + \text{bio resuspension of iron hydroxyde} \\
& p_{ihc_biores_ihw}/(cgt_cellheig \\
& cgt_density) \\
& + p_{fe2_ox_ihw} \quad \text{oxidation of Fe2+ to iron hydroxide in the} \\
& \quad \text{sediment} \\
& + p_{ipw_diss_po4} \quad \text{dissolution of iron phosphate} \\
& + \text{bio resuspension of iron monosulfide} \\
& p_{ims_biores_ihw}/(cgt_cellheig \\
& cgt_density) \\
& + \text{bio resuspension of pyrite} \\
& p_{pyr_biores_ihw}/(cgt_cellheig \\
& cgt_density) \\
& + \text{bio resuspension of iron in clay minerals} \\
& p_{iim_biores_ihw}/(cgt_cellheig \\
& cgt_density) \\
& + \text{resuspension of iron monosulfide} \\
& p_{ims_ero_ihw}/(cgt_cellheight* \\
& cgt_density) \\
& + \text{resuspension of pyrite} \\
& p_{pyr_ero_ihw}/(cgt_cellheight* \\
& cgt_density)
\end{aligned}$$

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Tracer equations, continued from previous page

$$\begin{aligned}
& + \text{bio resuspension of iron in clay minerals} \\
& p_{iim_ero_ihw}/(cgt_cellheight* \\
& cgt_density) \\
& + \text{iron hydroxide generation by internal sources} \\
& p_{stf_ihw_3d}/(cgt_cellheight* \\
& cgt_density) \\
& - \text{sedimentation of iron hydroxide} \\
& p_{ihw_sedi_ihs}/(cgt_cellheight \\
& cgt_density) \\
& - p_{po4_ads_ipw} \quad \text{adsorption of phosphate to iron hydroxide} \\
& \quad \quad \quad \text{particles}
\end{aligned}$$

Change of: ferrous iron

$$\begin{aligned}
\frac{d}{dt} t_{fe2} = & \\
& + \text{dissolution of magnetite to iron II} \\
& p_{ims_diss_fe2}/(cgt_cellheight(precipitating iron hydroxides) \\
& cgt_density) \\
& + \text{dissolution minnesotaite to of iron-II} \\
& p_{iim_diss_fe2}/(cgt_cellheight \\
& cgt_density) \\
& - \text{oxidation of Fe2+ to iron hydroxide in the} \\
& p_{fe2_ox_ihs}/(cgt_cellheight* sediment \\
& cgt_density) \\
& - p_{fe2_ox_ihw} \quad \text{oxidation of Fe2+ to iron hydroxide in the} \\
& \quad \quad \quad \text{sediment} \\
& - \text{precipitation of iron II as siderite} \\
& p_{fe2_prec_ims}/(cgt_cellheight \\
& cgt_density) \\
& - \text{precipitation of iron II as minnesotaite} \\
& p_{fe2_prec_iim}/(cgt_cellheight \\
& cgt_density) \\
& - (p_{fe2_mnox_ihs})*(2.0) \quad \text{oxidation of Fe2+ by reduction of MnO2} \\
& /(cgt_cellheight*cgt_density)
\end{aligned}$$

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Tracer equations, continued from previous page

Change of: pyrite

$\frac{d}{dt} t_{\text{pyr}} =$	
+ p_ims_form2_pyr	pyrite formation from iron monosulfide
- p_pyr_removal	transport from fluffy layer to deep basins
- p_pyr_oxmos_ihs	oxidation of pyrite by manganese oxide to iron oxyhydroxide
- p_pyr_oxo2_ihs	oxidation of pyrite by manganese oxide to iron oxyhydroxide
- p_pyr_biores_ihw	bio resuspension of pyrite
- p_pyr_ero_ihw	resuspension of pyrite

Change of: iron monosulphide

$\frac{d}{dt} t_{\text{ims}} =$	
+ (p_sed_1_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_2_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_3_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_4_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_5_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_6_irred_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_1_irredips_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_2_irredips_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_3_irredips_ims)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)

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Tracer equations, continued from previous page

+ (p_sed_4_irredips_ims)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_5_irredips_ims)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_6_irredips_ims)* (26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_ihs_red_ims)*(8.0)	reduction of sedimentary iron hydroxide to iron-II
+ p_fe2_prec_ims	precipitation of iron II as siderite
+ p_iim_trans_ims	minnesotaite transformation to iron monosulfide
+ (p_ihc_red_ims)*(8.0)	reduction of sedimentary iron hydroxide to iron-II
- p_ims_removal	transport from fluffy layer to deep basins
- p_ims_diss_fe2	dissolution of magnetite to iron II (precipitating iron hydroxides)
- p_ims_trans_iim	iron monosulfide transformation to minnesotaite
- p_ims_form2_pyr	pyrite formation from iron monosulfide
- p_ims_oxo2_ihs	iron monosulfide oxidation to iron oxihydroxides
- p_ims_biores_ihw	bio resuspension of iron monosulfide
- p_ims_ero_ihw	resuspension of iron monosulfide

Change of: dissolved calcium

$\frac{d}{dt} t_{ca2} =$	
+ p_ca2_relax_upwards	raise Ca ²⁺ concentration in the water column to salinity-determined default value
+ (p_rho_diss_mn2)*(0.6) /(cgt_cellheight*cgt_density)	rhodochrosite dissolution to manganese-II

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Tracer equations, continued from previous page

+ (p_rho_biores_mow)*(0.6) /(cgt_cellheight*cgt_density)	bio resuspension of rhodochrosite
+ (p_rho_ero_mow)*(0.6) /(cgt_cellheight*cgt_density)	bio resuspension of rhodochrosite
- p_ca2_relax_downwards	lower Ca ²⁺ concentration in the water column to salinity-determined default value
- (p_mn2_prec_rho)*(0.6) /(cgt_cellheight*cgt_density)	manganese-II precipitation to rhodochrosite

Change of: manganese oxide in the sediments

$\frac{d}{dt} t_{mos} =$	
+ p_mow_sedi_mos	sedimentation of iron hydroxide
+ p_mn2_ox_mos	oxidation of Mn ²⁺ to manganese oxide in the sediment
- (p_sed_1_mnred_mn2)*(13.25* rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- (p_sed_2_mnred_mn2)*(13.25* rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- (p_sed_3_mnred_mn2)*(13.25* rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- (p_sed_4_mnred_mn2)*(13.25* rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- (p_sed_5_mnred_mn2)*(13.25* rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- (p_sed_6_mnred_mn2)*(13.25* rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
- p_mos_removal	transport from fluffy layer to deep basins
- p_pyr_oxmos_ihs	oxidation of pyrite by manganese oxide to iron oxyhydroxide
- p_fe2_mnox_ihs	oxidation of Fe ²⁺ by reduction of MnO ₂

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Tracer equations, continued from previous page

- p_h2s_mnox_so4 oxidation of h2s by reduction of MnO2
- p_mos_biores_mow bio resuspension of manganese oxide
- p_mos_ero_mow bio resuspension of manganese oxide

Change of: suspended manganese oxide

$$\begin{aligned} \frac{d}{dt} t_{\text{mow}} = & \\ & + \text{bio resuspension of manganese oxide} \\ & p_{\text{mos_biores_mow}} / (cgt_cellheight \\ & cgt_density) \\ & + \text{bio resuspension of rhodochrosite} \\ & p_{\text{rho_biores_mow}} / (cgt_cellheight \\ & cgt_density) \\ & + \text{bio resuspension of manganese oxide} \\ & p_{\text{mos_ero_mow}} / (cgt_cellheight * \\ & cgt_density) \\ & + \text{bio resuspension of rhodochrosite} \\ & p_{\text{rho_ero_mow}} / (cgt_cellheight * \\ & cgt_density) \\ & - \text{sedimentation of iron hydroxide} \\ & p_{\text{mow_sedi_mos}} / (cgt_cellheight \\ & cgt_density) \end{aligned}$$

Change of: dissolved manganese-II

$$\begin{aligned} \frac{d}{dt} t_{\text{mn2}} = & \\ & + (p_{\text{sed_1_mnred_mn2}}) * (13.25 * \text{recycling of sedimentary detritus to ammonium} \\ & rfr_pc_enrichment_det) \text{ using manganese oxide (manganese reduction)} \\ & / (cgt_cellheight * cgt_density) \\ & + (p_{\text{sed_2_mnred_mn2}}) * (13.25 * \text{recycling of sedimentary detritus to ammonium} \\ & rfr_pc_enrichment_det) \text{ using manganese oxide (manganese reduction)} \\ & / (cgt_cellheight * cgt_density) \\ & + (p_{\text{sed_3_mnred_mn2}}) * (13.25 * \text{recycling of sedimentary detritus to ammonium} \\ & rfr_pc_enrichment_det) \text{ using manganese oxide (manganese reduction)} \\ & / (cgt_cellheight * cgt_density) \end{aligned}$$

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Tracer equations, continued from previous page

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+ (p_sed_4_mnred_mn2)*(13.25* recycling of sedimentary detritus to ammonium
rfr_pc_enrichment_det)          using manganese oxide (manganese reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_5_mnred_mn2)*(13.25* recycling of sedimentary detritus to ammonium
rfr_pc_enrichment_det)          using manganese oxide (manganese reduction)
/(cgt_cellheight*cgt_density)

+ (p_sed_6_mnred_mn2)*(13.25* recycling of sedimentary detritus to ammonium
rfr_pc_enrichment_det)          using manganese oxide (manganese reduction)
/(cgt_cellheight*cgt_density)

+                                rhodochrosite dissolution to manganese-II
p_rho_diss_mn2/(cgt_cellheight
cgt_density)

+                                oxidation of pyrite by manganese oxide to iron
p_pyr_oxmos_ihs/(cgt_cellheightoxyhydroxide
cgt_density)

+                                oxidation of Fe2+ by reduction of MnO2
p_fe2_mnox_ihs/(cgt_cellheight
cgt_density)

+                                oxidation of h2s by reduction of MnO2
p_h2s_mnox_so4/(cgt_cellheight
cgt_density)

-                                oxidation of Mn2+ to manganese oxide in the
p_mn2_ox_mos/(cgt_cellheight* sediment
cgt_density)

-                                manganese-II precipitation to rhodochrosite
p_mn2_prec_rho/(cgt_cellheight
cgt_density)

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Change of: rhodochrosite

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 $\frac{d}{dt} t\_rho =$ 
+ p_mn2_prec_rho          manganese-II precipitation to rhodochrosite

- t_rho_removal          transport from fluffy layer to deep basins

- p_rho_diss_mn2          rhodochrosite dissolution to manganese-II

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Tracer equations, continued from previous page

- p_rho_biores_mow bio resuspension of rhodochrosite
- p_rho_ero_mow bio resuspension of rhodochrosite

Change of: OH- ions with realistically quick diffusion

$$\frac{d}{dt} t_{ohm_quickdiff} =$$

- + relax_ohm_quickdiff_up relax ohm_quickdiff tracer against actual OH-concentration
- relax_ohm_quickdiff_down relax ohm_quickdiff tracer against actual OH-concentration

Change of: OH- ions which move unrealistically slow with alkalinity

$$\frac{d}{dt} t_{ohm_slowdiff} =$$

- + relax_ohm_slowdiff_up relax ohm_slowdiff tracer against actual OH-concentration
- relax_ohm_slowdiff_down relax ohm_slowdiff tracer against actual OH-concentration

Change of: silicate

$$\frac{d}{dt} t_{sil} =$$

- + (p_sed_1_resp_nh4)*(rfr_si) recycling of sedimentary detritus to ammonium / (cgt_cellheight*cgt_density) using oxygen (respiration)
- + (p_sed_2_resp_nh4)*(rfr_si) recycling of sedimentary detritus to ammonium / (cgt_cellheight*cgt_density) using oxygen (respiration)
- + (p_sed_3_resp_nh4)*(rfr_si) recycling of sedimentary detritus to ammonium / (cgt_cellheight*cgt_density) using oxygen (respiration)
- + (p_sed_4_resp_nh4)*(rfr_si) recycling of sedimentary detritus to ammonium / (cgt_cellheight*cgt_density) using oxygen (respiration)
- + (p_sed_5_resp_nh4)*(rfr_si) recycling of sedimentary detritus to ammonium / (cgt_cellheight*cgt_density) using oxygen (respiration)
- + (p_sed_6_resp_nh4)*(rfr_si) recycling of sedimentary detritus to ammonium / (cgt_cellheight*cgt_density) using oxygen (respiration)
- + (p_sed_1_denit_nh4)* recycling of sedimentary detritus to ammonium
(rfr_si)/(cgt_cellheight* using nitrate (denitrification)
cgt_density)

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Tracer equations, continued from previous page

+ (p_sed_2_denit_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
+ (p_sed_3_denit_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
+ (p_sed_4_denit_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
+ (p_sed_5_denit_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
+ (p_sed_6_denit_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using nitrate (denitrification)
+ (p_sed_1_sulf_nh4)*(rfr_si) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_2_sulf_nh4)*(rfr_si) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_3_sulf_nh4)*(rfr_si) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_4_sulf_nh4)*(rfr_si) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_5_sulf_nh4)*(rfr_si) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_6_sulf_nh4)*(rfr_si) /(cgt_cellheight*cgt_density)	recycling of sedimentary detritus to ammonium using sulfate (sulfate reduction)
+ (p_sed_1_mnred_mn2)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ (p_sed_2_mnred_mn2)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)

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Tracer equations, continued from previous page

+ (p_sed_3_mnred_mn2)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ (p_sed_4_mnred_mn2)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ (p_sed_5_mnred_mn2)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ (p_sed_6_mnred_mn2)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using manganese oxide (manganese reduction)
+ (p_sed_1_irred_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_2_irred_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_3_irred_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_4_irred_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_5_irred_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_6_irred_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_1_irredips_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)

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Tracer equations, continued from previous page

+ (p_sed_2_irredips_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_3_irredips_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_4_irredips_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_5_irredips_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_6_irredips_ims)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron phosphate (iron reduction)
+ (p_sed_1_irred_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_2_irred_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_3_irred_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_4_irred_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_5_irred_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_6_irred_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)

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Tracer equations, continued from previous page

+ (p_sed_1_irredips_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_2_irredips_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_3_irredips_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_4_irredips_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_5_irredips_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_6_irredips_iim)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_i3i_1_irred_i2i)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
+ (p_i3i_2_irred_i2i)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
+ (p_i3i_3_irred_i2i)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
+ (p_i3i_4_irred_i2i)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
+ (p_i3i_5_irred_i2i)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)

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Tracer equations, continued from previous page

+ (p_i3i_6_irred_i2i)* (rfr_si)/(cgt_cellheight* cgt_density)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
+ (p_sed_1_sulfdeep_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_2_sulfdeep_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_3_sulfdeep_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_4_sulfdeep_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_5_sulfdeep_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
+ (p_sed_6_sulfdeep_nh4)* (rfr_si)/(cgt_cellheight* cgt_density)	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)
- p_remove_silicate	remove silicate in water column as it gets too much

Change of: iron-II adsorbed to illite-montmorillonite mixed layer minerals

$\frac{d}{dt} t_{iim} =$	
+ (p_sed_1_irred_iim)*(26.5* rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)

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Tracer equations, continued from previous page

+ (p_sed_2_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_3_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_4_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_5_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_6_irred_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_1_irredips_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_2_irredips_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_3_irredips_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_4_irredips_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_5_irredips_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_sed_6_irredips_iim)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron hydroxide (iron reduction)
+ (p_ihs_red_iim)*(8.0)	reduction of sedimentary iron hydroxide to iron-II
+ p_fe2_prec_iim	precipitation of iron II as minnesotaite
+ p_ims_trans_iim	iron monosulfide transformation to minnesotaite
+ (p_ihc_red_iim)*(8.0)	reduction of sedimentary iron hydroxide to iron-II

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Tracer equations, continued from previous page

- p_iim_removal	transport from fluffy layer to deep basins
- p_iim_diss_fe2	dissolution minnesotaite to of iron-II
- p_iim_trans_ims	minnesotaite transformation to iron monosulfide
- p_imm_oxo2_ihs	oxidation of minnesotaite by oxygen to iron oxyhydroxide
- p_iim_biores_ihw	bio resuspension of iron in clay minerals
- p_iim_ero_ihw	bio resuspension of iron in clay minerals

Change of: potentially reducible iron-III in illite-montmorillonite mixed layer minerals

$\frac{d}{dt} t_{i3i} =$	
+ p_i2i_oxo2_i3i	oxidation of iron-II in illite-montmorillonite mixed layer minerals to iron-III
- (p_i3i_1_irred_i2i)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- (p_i3i_2_irred_i2i)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- (p_i3i_3_irred_i2i)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- (p_i3i_4_irred_i2i)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- (p_i3i_5_irred_i2i)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- (p_i3i_6_irred_i2i)*(26.5*rfr_pc_enrichment_det)	recycling of sedimentary detritus to ammonium using iron-III in clay minerals (iron reduction)
- (p_i3i_redh2s_i2i)*(8)	reduction of iron-III in clay minerals to iron-II consuming h2s

Change of: iron hydroxide in the sediment - crystalline phase

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Tracer equations, continued from previous page

$\frac{d}{dt} t_{ihc} =$	
+ p_ihs_trans_ihc	transformation of amorphous iron oxyhydroxides to crystalline phase
- p_ihc_ero_ihw	erosion of larger-crystalline iron PO4
- p_ihc_biores_ihw	bio resuspension of iron hydroxyde
- p_ihc_removal	transport from fluffy layer to deep basins
- (p_ihc_red_iim)*(8.0)	reduction of sedimentary iron hydroxide to iron-II
- (p_ihc_red_ims)*(8.0)	reduction of sedimentary iron hydroxide to iron-II

Change of: phosphate adsorbed to illite-montmorillonite

$\frac{d}{dt} t_{pim} =$	
+ p_po4_ads_pim	phosphate adsorption to illite-montmorillonite mixed layer minerals
- p_pim_lib_po4	phosphate liberation from illite-montmorillonite mixed layer minerals

Change of: ammonium adsorbed to illite-montmorillonite

$\frac{d}{dt} t_{aim} =$	
+ p_nh4_ads_aim	ammonium adsorption to illite-montmorillonite mixed layer minerals
- p_aim_lib_nh4	ammonium liberation from illite-montmorillonite mixed layer minerals
- p_aim_nit_no3_sed	nitrification in the sediment

Change of: phosphate in detritus fractions_1

$\frac{d}{dt} t_{detp_1} =$	
+ (p_lpp_mort_det_1)* ((1.0/rfr_pc_enrichment_det))	mortality of large-cell phytoplankton
+ (p_spp_mort_det_1)* ((1.0/rfr_pc_enrichment_det))	mortality of small-scale phytoplankton

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Tracer equations, continued from previous page

$$\begin{aligned}
& + (p_cya_mort_det_1) * \quad \text{mortality of diazotroph cyanobacteria} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_zoo_mort_det_1) * \quad \text{mortality of zooplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + \quad \text{sedimentary detritus erosion} \\
& p_sedp_1_ero_detp / (cgt_cellhei \\
& cgt_density) \\
& + \quad \text{bio resuspension of sedimentary detritus} \\
& p_sedp_1_biores_detp / (cgt_cell \\
& cgt_density) \\
& + \quad \text{surface flux of detritus} \\
& p_stf_det_1 / (cgt_cellheight * \\
& cgt_density) \\
& - \quad \text{detritus sedimentation} \\
& p_detp_1_sedi_sedp / (cgt_cellhe \\
& cgt_density) \\
& - p_detp_1_remin_po4 \quad \text{recycling of detritus to ammonium using} \\
& \quad \text{oxygen (respiration)}
\end{aligned}$$

Change of: phosphate in detritus fractions__2

$$\frac{d}{dt} t_detp_2 =$$

$$\begin{aligned}
& + (p_lpp_mort_det_2) * \quad \text{mortality of large-cell phytoplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_spp_mort_det_2) * \quad \text{mortality of small-scale phytoplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_cya_mort_det_2) * \quad \text{mortality of diazotroph cyanobacteria} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_zoo_mort_det_2) * \quad \text{mortality of zooplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + \quad \text{sedimentary detritus erosion} \\
& p_sedp_2_ero_detp / (cgt_cellhei \\
& cgt_density)
\end{aligned}$$

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Tracer equations, continued from previous page

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+                                bio resuspension of sedimentary detritus
p_sedp_2_biores_detp/(cgt_cell
cgt_density)

+                                surface flux of detritus
p_stf_det_2/(cgt_cellheight*
cgt_density)

-                                detritus sedimentation
p_detp_2_sedi_sedp/(cgt_cellhe
cgt_density)

- p_detp_2_remin_po4            recycling of detritus to ammonium using
                                oxygen (respiration)

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Change of: phosphate in detritus fractions_3

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 $\frac{d}{dt}$  t_detp_3 =
+ (p_lpp_mort_det_3)*          mortality of large-cell phytoplankton
((1.0/rfr_pc_enrichment_det))

+ (p_spp_mort_det_3)*          mortality of small-scale phytoplankton
((1.0/rfr_pc_enrichment_det))

+ (p_cya_mort_det_3)*          mortality of diazotroph cyanobacteria
((1.0/rfr_pc_enrichment_det))

+ (p_zoo_mort_det_3)*          mortality of zooplankton
((1.0/rfr_pc_enrichment_det))

+                                sedimentary detritus erosion
p_sedp_3_ero_detp/(cgt_cellhei
cgt_density)

+                                bio resuspension of sedimentary detritus
p_sedp_3_biores_detp/(cgt_cell
cgt_density)

+                                surface flux of detritus
p_stf_det_3/(cgt_cellheight*
cgt_density)

-                                detritus sedimentation
p_detp_3_sedi_sedp/(cgt_cellhe
cgt_density)

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Tracer equations, continued from previous page

- p_detp_3_remin_po4 recycling of detritus to ammonium using
oxygen (respiration)

Change of: phosphate in detritus fractions_4

$$\frac{d}{dt} t_detp_4 =$$

+ (p_lpp_mort_det_4)* mortality of large-cell phytoplankton
((1.0/rfr_pc_enrichment_det))

+ (p_spp_mort_det_4)* mortality of small-scale phytoplankton
((1.0/rfr_pc_enrichment_det))

+ (p_cya_mort_det_4)* mortality of diazotroph cyanobacteria
((1.0/rfr_pc_enrichment_det))

+ (p_zoo_mort_det_4)* mortality of zooplankton
((1.0/rfr_pc_enrichment_det))

+ sedimentary detritus erosion
p_sedp_4_ero_detp/(cgt_cellhei
cgt_density)

+ bio resuspension of sedimentary detritus
p_sedp_4_biores_detp/(cgt_cell
cgt_density)

+ surface flux of detritus
p_stf_det_4/(cgt_cellheight*
cgt_density)

- detritus sedimentation
p_detp_4_sedi_sedp/(cgt_cellhe
cgt_density)

- p_detp_4_remin_po4 recycling of detritus to ammonium using
oxygen (respiration)

Change of: phosphate in detritus fractions_5

$$\frac{d}{dt} t_detp_5 =$$

+ (p_lpp_mort_det_5)* mortality of large-cell phytoplankton
((1.0/rfr_pc_enrichment_det))

+ (p_spp_mort_det_5)* mortality of small-scale phytoplankton
((1.0/rfr_pc_enrichment_det))

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Tracer equations, continued from previous page

$$\begin{aligned}
& + (p_cya_mort_det_5) * \quad \text{mortality of diazotroph cyanobacteria} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_zoo_mort_det_5) * \quad \text{mortality of zooplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + \quad \text{sedimentary detritus erosion} \\
& p_sedp_5_ero_detp / (cgt_cellhei \\
& cgt_density) \\
& + \quad \text{bio resuspension of sedimentary detritus} \\
& p_sedp_5_biores_detp / (cgt_cell \\
& cgt_density) \\
& + \quad \text{surface flux of detritus} \\
& p_stf_det_5 / (cgt_cellheight * \\
& cgt_density) \\
& - \quad \text{detritus sedimentation} \\
& p_detp_5_sedi_sedp / (cgt_cellhe \\
& cgt_density) \\
& - p_detp_5_remin_po4 \quad \text{recycling of detritus to ammonium using} \\
& \quad \text{oxygen (respiration)}
\end{aligned}$$

Change of: phosphate in detritus fractions_6

$$\frac{d}{dt} t_detp_6 =$$

$$\begin{aligned}
& + (p_lpp_mort_det_6) * \quad \text{mortality of large-cell phytoplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_spp_mort_det_6) * \quad \text{mortality of small-scale phytoplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_cya_mort_det_6) * \quad \text{mortality of diazotroph cyanobacteria} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + (p_zoo_mort_det_6) * \quad \text{mortality of zooplankton} \\
& ((1.0/rfr_pc_enrichment_det)) \\
& + \quad \text{sedimentary detritus erosion} \\
& p_sedp_6_ero_detp / (cgt_cellhei \\
& cgt_density)
\end{aligned}$$

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Tracer equations, continued from previous page

$$\begin{aligned}
& + \text{p_sedp_6_biores_detp} / (\text{cgt_cell} \\
& \text{cgt_density}) \quad \text{bio resuspension of sedimentary detritus} \\
& + \text{p_stf_det_6} / (\text{cgt_cellheight} * \\
& \text{cgt_density}) \quad \text{surface flux of detritus} \\
& - \text{p_detp_6_sedi_sedp} / (\text{cgt_cellhe} \\
& \text{cgt_density}) \quad \text{detritus sedimentation} \\
& - \text{p_detp_6_remin_po4} \quad \text{recycling of detritus to ammonium using} \\
& \quad \text{oxygen (respiration)}
\end{aligned}$$

Change of: phosphate in sedimentary detritus fractions__1

$$\begin{aligned}
\frac{d}{dt} \text{t_sedp_1} = & \\
& + \text{p_detp_1_sedi_sedp} \quad \text{detritus sedimentation} \\
& - \text{p_sedp_1_ero_detp} \quad \text{sedimentary detritus erosion} \\
& - \text{p_sedp_1_biores_detp} \quad \text{bio resuspension of sedimentary detritus} \\
& - \text{p_sedp_1_removal} \quad \text{transport from fluffy layer to deep basins} \\
& - \text{p_sedp_1_remin_po4} \quad \text{recycling of sediment detrital phosphate} \\
& - \text{p_sedp_1_sulfdeep_po4} \quad \text{parameterization for recycling of sedimentary} \\
& \quad \text{detritus to ammonium below the deepest} \\
& \quad \text{sediment layer (sulfate reduction / methane} \\
& \quad \text{formation)}
\end{aligned}$$

Change of: phosphate in sedimentary detritus fractions__2

$$\begin{aligned}
\frac{d}{dt} \text{t_sedp_2} = & \\
& + \text{p_detp_2_sedi_sedp} \quad \text{detritus sedimentation} \\
& - \text{p_sedp_2_ero_detp} \quad \text{sedimentary detritus erosion} \\
& - \text{p_sedp_2_biores_detp} \quad \text{bio resuspension of sedimentary detritus} \\
& - \text{p_sedp_2_removal} \quad \text{transport from fluffy layer to deep basins}
\end{aligned}$$

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Tracer equations, continued from previous page

- p_sedp_2_remin_po4 recycling of sediment detrital phosphate
- p_sedp_2_sulfdeep_po4 parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: phosphate in sedimentary detritus fractions_3

$$\frac{d}{dt} t_sedp_3 =$$

- + p_detp_3_sedi_sedp detritus sedimentation
- p_sedp_3_ero_detp sedimentary detritus erosion
- p_sedp_3_biores_detp bio resuspension of sedimentary detritus
- p_sedp_3_removal transport from fluffy layer to deep basins
- p_sedp_3_remin_po4 recycling of sediment detrital phosphate
- p_sedp_3_sulfdeep_po4 parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: phosphate in sedimentary detritus fractions_4

$$\frac{d}{dt} t_sedp_4 =$$

- + p_detp_4_sedi_sedp detritus sedimentation
- p_sedp_4_ero_detp sedimentary detritus erosion
- p_sedp_4_biores_detp bio resuspension of sedimentary detritus
- p_sedp_4_removal transport from fluffy layer to deep basins
- p_sedp_4_remin_po4 recycling of sediment detrital phosphate
- p_sedp_4_sulfdeep_po4 parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

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Tracer equations, continued from previous page

Change of: phosphate in sedimentary detritus fractions_5

$$\frac{d}{dt} t_sedp_5 =$$

+ p_detp_5_sedi_sedp	detritus sedimentation
- p_sedp_5_ero_detp	sedimentary detritus erosion
- p_sedp_5_biores_detp	bio resuspension of sedimentary detritus
- p_sedp_5_removal	transport from fluffy layer to deep basins
- p_sedp_5_remin_po4	recycling of sediment detrital phosphate
- p_sedp_5_sulfdeep_po4	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: phosphate in sedimentary detritus fractions_6

$$\frac{d}{dt} t_sedp_6 =$$

+ p_detp_6_sedi_sedp	detritus sedimentation
- p_sedp_6_ero_detp	sedimentary detritus erosion
- p_sedp_6_biores_detp	bio resuspension of sedimentary detritus
- p_sedp_6_removal	transport from fluffy layer to deep basins
- p_sedp_6_remin_po4	recycling of sediment detrital phosphate
- p_sedp_6_sulfdeep_po4	parameterization for recycling of sedimentary detritus to ammonium below the deepest sediment layer (sulfate reduction / methane formation)

Change of: particulate organic carbon

$$\frac{d}{dt} t_poc =$$

+ p_assim_lpp_poc	Production of POC by LPP
+ p_assim_spp_poc	Production of POC by SPP

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Tracer equations, continued from previous page	
+ p_assim_cya_poc	Production of POC by CYA
- p_poc_resp	respiration of POC
- p_poc_denit	recycling of POC using nitrate (denitrification)
- p_poc_sulf	Mineralization of POC, e-acceptor sulfate (sulfate reduction)