Parameter and variable	Unit	Value	Description
Stoichiometric factors and molecular ratios			
NC_i	$mol\,mol^{-1}$	$\frac{y}{x} = \frac{16}{106}$	Nitrogen to carbon ratio
PC_i	$mol\,mol^{-1}$	$\frac{z}{x} = \frac{1}{106}$	Phosphorus to carbon ratio
MC	$mol\,mol^{-1}$	0.5	Methane to carbon ratio produced during methanogenesis
$DICC^I$	$mol\,mol^{-1}$	1.0	DIC to carbon ratio until z_{SO_4}
$DICC^{II}$	$mol\,mol^{-1}$	0.5	DIC to carbon ratio below z_{SO_4}
O_2C	$mol\,mol^{-1}$	$\frac{x+2y}{x} = \frac{138}{106}$	Oxygen to carbon ratio
NO_3C	$mol\,mol^{-1}$	$\frac{4x+3y}{5x} = \frac{94.4}{106}$	Nitrate to carbon ratio
SO_4C	$mol\,mol^{-1}$	$\frac{106}{212}$	Sulfate to carbon ratio
ALK^{OX}	$mol\,mol^{-1}$	$\frac{y-2z}{x} = \frac{14}{106}$	ALK from aerobic degradation
ALK^{NIT}	$mol\,mol^{-1}$	-2	ALK from nitrification
ALK^{DEN}	$mol\,mol^{-1}$	$\frac{4x+3y-10z}{5x} = \frac{92.4}{106}$	ALK from denitrification
ALK^{SUL}	$mol\,mol^{-1}$	$\frac{x+y-2z}{x} = \frac{120}{106}$	ALK from sulfate reduction
ALK^{MET}	$mol\,mol^{-1}$	$\frac{y-2z}{x} = \frac{14}{106}$	ALK from methanogenesis
ALK^{H_2S}	$mol\,mol^{-1}$	-2	ALK from H_2S oxidation
ALK^{FeS}	$mol\,mol^{-1}$	-2	ALK from pyrite precipitation
ALK^{AOM}	$mol\,mol^{-1}$	2	ALK from AOM
Secondary reaction parameters			
γ_{NH_4}	–	0.9	Fraction of NH_4 that is nitrified
γ_{H_2S}	–	1.0	Fraction of H_2S that is oxidised (oxic bottom waters)
	–	0.95	Fraction of H_2S that is oxidised (anoxic bottom waters)
γ_{FeS}	–	0.0	Fraction of H_2S that is precipitated as pyrite
γ_{CH_4}	–	0.99	Fraction of CH_4 that is oxidised
Adsorption coefficients (Wang and Van Cappellen, 1996; Slomp et al., 1998)			
K_{NH_4}	–	1.4	NH_4 adsorption coefficient
$K_{PO_4}^{ox}$, $\quad K_{PO_4}^{anox}$	–	200.0, 2.0	PO_4 adsorption coefficient (oxic, anoxic)
P-related parameters (Slomp et al., 1996)			
k_s	yr^{-1}	94.9	Rate constant for PO_4 sorption
k_m	yr^{-1}	0.193	Rate constant for Fe-bound P release
k_a	yr^{-1}	0.365	Rate constant for authigenic CFA precipitation
PO_4^s	$mol\,cm^{-3}$	1×10^{-9}	Equilibrium conc. for P sorption
FeP^∞	$mol\,cm^{-3}$	1.99×10^{-10}	Asymptotic concentration for Fe-bound P
PO_4^a	$mol\,cm^{-3}$	3.7×10^{-9}	Equilibrium conc. for authigenic P precipitation