



Supplement of

Bottom RedOx Model (BROM v.1.1): a coupled benthic–pelagic model for simulation of water and sediment biogeochemistry

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Section S1: run-time input file for BROM-transport (brom.yaml)

```
# IMPORTANT!!!! _ <TAB> is NOT allowed here, used <Space> only !!!!  
# Each entry must have 6 spaces before the parameter name  
instances:  
brom:  
initialization:  
##--Paramters for grid-----(see io_ascii.f90/make_vert_grid for a grid diagram)-----  
water_layer_thickness: 95. # Thickness of the water column [m] (may overriden by netCDF input, see below)  
k_wat_bbl: 18 # Number of levels above the water/BBL boundary (may be overriden by netCDF input, see below)  
bbl_thickness: 0.5 # Thickness of the high-resolution layer overlying the sediments (model "benthic boundary layer") [m] (default = 0.5 m)  
# This should be thinner than the full viscous+logarithmic layer, but thicker than the viscous layer  
# Typical thicknesses for full viscous+logarithmic layer are 1 m and 10 m for deep sea and shelf respectively (Wimbush 2012)  
hz_bbl_min: 0.02 # Minimum allowed layer thickness in the BBL near the SWI [m] (default = 0.02 m)  
hz_sed_min: 0.0005 # Minimum layer thickness in the sediments near the SWI [m] (default = 0.0005 m)  
hz_sed_max: 0.01 # Maximum layer thickness deeper in the sediments [m] (default = 0.01 m)  
k_min: 1 # Minimum k number defining the layer that is in contact with the atmosphere (default = 1)  
k_points_below_water: 17 # Number of levels below the water/BBL boundary (default = 20)  
i_min: 1 # Minimum i number (default = 1)  
i_water: 1 # Number of i for water column (default = 1)  
i_max: 1 # Maximum i number (default = 1)  
#Note: (i_min,i_water,i_max) should be (1,1,1) for 1D applications  
#  
#  
##--Boundary conditions-----  
#  
#Here we set the type of boundary condition using bctype_top_<variable name> and bctype_bottom_<variable name>  
# 0 to use surface fluxes from FABM where parameterized, otherwise no flux (default, does not need to be explicitly set)  
# 1 for constant Dirichlet, specified by bc_top_<variable name> or bc_bottom_<variable name>  
# E.g. bctype_bottom_niva_brom_bio_O2: 1  
# bc_bottom_niva_brom_bio_O2: 0.  
# 2 for sinusoidal Dirichlet, specified by bcpars_top_<variable name> or bcpars_bottom_<variable name>  
# The model is: phi(t) = a1 + a2*sin(omega*(day-a3)) where omega = 2*pi/365  
# => max(phi(t)) = a1+a2, min(phi(t)) = a1-a2, mean(phi(t)) = a1, peak at 91.25+a3 days  
# Model parameters are specified by a1top_<variable name> etc.  
# E.g. bctype_top_niva_brom_bio_NO3: 2  
# a1top_niva_brom_bio_NO3: 3.0  
# a2top_niva_brom_bio_NO3: 3.0  
# a3top_niva_brom_bio_NO3: 60.  
# 3 for arbitrary Dirichlet, read from netCDF file (see I/O options to specify netCDF variable names)  
#  
# bctype_bottom_niva_brom_bio_O2: 1  
# bc_bottom_niva_brom_bio_O2: 0.  
#  
bctype_top_niva_brom_redox_SO4: 1  
bc_top_niva_brom_redox_SO4: 25000.  
bctype_bottom_niva_brom_redox_SO4: 1  
bc_bottom_niva_brom_redox_SO4: 25000.  
#  
bctype_top_niva_brom_redox_Mn4: 1  
bc_top_niva_brom_redox_Mn4: 20.E-4  
#  
bctype_top_niva_brom_redox_Fe3: 1  
bc_top_niva_brom_redox_Fe3: 5.E-4  
#  
bctype_top_niva_brom_carb_Alk: 1  
bc_top_niva_brom_carb_Alk: 2200.  
# bctype_bottom_niva_brom_carb_Alk: 1  
# bc_bottom_niva_brom_carb_Alk: 3200.  
#  
# bctype_bottom_niva_brom_carb_DIC: 1  
# bc_bottom_niva_brom_carb_DIC: 2850.  
#  
# bctype_bottom_niva_brom_bio_NH4: 1  
# bc_bottom_niva_brom_bio_NH4: 10.  
#  
bctype_top_niva_brom_bio_NO3: 2  
a1top_niva_brom_bio_NO3: 1. # 3  
a2top_niva_brom_bio_NO3: 1.  
a3top_niva_brom_bio_NO3: 320.  
bctype_bottom_niva_brom_bio_NO3: 1
```

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bc_bottom_niva_brom_bio_NO3: 0.
#
bctype_top_niva_brom_bio_PO4: 2
a1top_niva_brom_bio_PO4: 0.7 #0.8
a2top_niva_brom_bio_PO4: 0.7
a3top_niva_brom_bio_PO4: 320. #60.
# bctype_bottom_niva_brom_bio_PO4: 1
# bc_bottom_niva_brom_bio_PO4: 10.
#
bctype_top_niva_brom_redox_Si: 2
a1top_niva_brom_redox_Si: 1.5
a2top_niva_brom_redox_Si: 1.5
a3top_niva_brom_redox_Si: 320.
# bctype_bottom_niva_brom_redox_Si: 1
# bc_bottom_niva_brom_redox_Si: 100.
#
#
##--Horizontal mixing parameters-----
#
#Here we specify horizontal mixing model using hmix_<variable name>
# 0 to assume no horizontal mixing (default, does not need to be explicitly set)
# 1 for "box model" mixing model: hmix = hmix_rate*(X_0 - X) with X_0 specified by netCDF input file and hmix_rate specified here
#
hmix_niva_brom_bio_NO3: 0
hmix_niva_brom_bio_NH4: 0
hmix_niva_brom_bio_PO4: 0
hmix_niva_brom_redox_Si: 0
hmix_niva_brom_bio_O2: 0
#
#
##--Ice model parameters-----
use_hice: 0      # 1 to use ice thickness forcing "hice" from netCDF input
#
#
##--Constant forcings-----
density: 1000.
wind_speed: 8.   # Wind speed 10 m above sea surface [m/s] (default = 8 m/s)
pco2_atm: 380.  # Atmospheric partial pressure of CO2 [ppm] (default = 380 ppm)
#
#
##--Surface irradiance model parameters-----
use_Eair: 0      # 1 to use 24-hr average surface downwelling shortwave irradiance in air from netCDF input
lat_light: 50     # Latitude of modelled site [degrees north], e.g. Hardangerfjord station H6 is at 60.228N; Sleipner=50N; Saelen=60.33N
lo: 80.          # Theoretical maximum 24-hr average surface downwelling shortwave irradiance in air [W/m2] (default = 80 W/m2)
# This should include that effect of average cloud cover (local)
light_model: 0    # Specify light model: 0 for simple model based on ersem/light.f90
#                 1 for extended model accounting for other particulates in BROM
#
#
##--Light absorption model parameters -----
Eair_to_PAR0: 0.5 # Factor to convert input or calculated surface downward irradiance Eair to surface PAR in water (default = 0.5, units dependent on Eair)
# Factor of ~0.48 to convert shortwave (0.3-4 um) to PAR-band (0.4-0.7 um) in [W/m2]
# Further factor of 0.8-0.95 to convert downward-in-air to net-in-water (Mobley and Boss, 2012, Figs. 2c, 4b, 8a)
# Latter factor becomes 0.45-0.55 if modelling PAR in terms of photon flux (Mobley and Boss, 2012, Figs. 5b, 8b)
k0r: 0.04        # Background PAR attenuation [m^-1] (default = 0.04 m^-1, from ERSEM shortwave attenuation default)
kESS: 4e-05       # Specific PAR attenuation by silt [m^2/mg] (default = 4e-05 m^2/mg, from ERSEM shortwave attenuation default)
ESS: 0.           # Assumed (constant) concentration of silt [mg/m^3] (default = 0. mg/m^3, from ERSEM shortwave attenuation default)
kPhy: 0.00023    # Specific PAR attenuation by phytoplankton [m^2/mg N] (default = 0.0023 m^2/mg N, from ERSEM shortwave attenuation default)
# From ERSEM Blackford (P1-P4), default = 0.0004 m^2/mg C * 5.68 mg C/mg N (Redfield ratio 106/16 mol/mol)
# Note misprint "e-3" instead of "e-4" in Blackford et al. (2004) Table 1
kPON: 0.          # Specific PAR attenuation due to PON [m^2/mg N] (default = 0. m^2/mg N)
#
# The following are only used if light_model = 1
kHet: 0.          # Specific PAR attenuation due to zooplankton [m^2/mg N] (default = 0. m^2/mg N)
kDON: 0.          # Specific PAR attenuation due to DON [m^2/mg N] (default = 0. m^2/mg N)
kB: 0.            # Specific PAR attenuation due to bacteria [m^2/mg N] (default = 0. m^2/mg N)
kPIV: 0.          # Specific PAR attenuation due to total particulate inorganic volume fraction (default = 0. m^-1)
#
#
##--Assumed densities for particles in the model (may be used in light/sedimentation models)-----
#
# Densities are specified by rho_<full variable name> and in same units as the model concentration
# Any missing values will use the default density rho_def
rho_def: 3.0E7      # Default density of solid particles [mmol/m3]
rho_niva_brom_bio_Phys: 1.5E7    # Density of (living) phytoplankton [mmolN/m3] (default = 1.4E6 mmolN/m3 from PON default)

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rho_niva_brom_bio_PON: 1.5E7      # Density of (dead) particulate organic matter [mmolN/m3] (default = 1.4E6 mmolN/m3, from: 1.23 g WW/cm3
(Alldredge, Gotschalk, 1988), mg DW/mg WW=0.18 and mg DW /mg C=2 (Link et al.,2006))
rho_niva_brom_bio_Het: 1.5E7      # Density of (living) non-bacterial heterotrophs [mmolN/m3] (default = 1.4E6 mmolN/m3 from PON default)
rho_niva_brom_redox_Baae: 1.5E7   # Density of (living) aerobic autotrophic bacteria [mmolN/m3] (default = 1.4E6 mmolN/m3 from PON default)
rho_niva_brom_redox_Bhae: 1.5E7   # Density of (living) aerobic heterotrophic bacteria [mmolN/m3] (default = 1.4E6 mmolN/m3 from PON default)
rho_niva_brom_redox_Baan: 1.5E7   # Density of (living) anaerobic autotrophic bacteria [mmolN/m3] (default = 1.4E6 mmolN/m3 from PON default)
rho_niva_brom_redox_Bhan: 1.5E7   # Density of (living) anaerobic heterotrophic bacteria [mmolN/m3] (default = 1.4E6 mmolN/m3 from PON default)
rho_niva_brom_redox_CaCO3: 2.80E7 # Density of calcium carbonate [mmolCa/m3] (default = 2.80E7 mmolCa/m3)
rho_niva_brom_redox_Fe3: 3.27E7   # Density of Fe3 [mmolFe/m3] (default = 3.27E7 mmolFe/m3)
rho_niva_brom_redox_FeCO3: 2.93E7 # Density of FeCO3 [mmolFe/m3] (default = 2.93E7 mmolFe/m3)
rho_niva_brom_redox_FeS: 5.90E7   # Density of FeS [mmolFe/m3] (default = 5.90E7 mmolFe/m3)
rho_niva_brom_redox_FeS2: 4.17E7  # Density of FeS2 [mmolFe/m3] (default = 4.17E7 mmolFe/m3)
rho_niva_brom_redox_Mn4: 5.78E7   # Density of Mn4 [mmolMn/m3] (default = 5.78E7 mmolMn/m3)
rho_niva_brom_redox_MnCO3: 3.20E7 # Density of MnCO3 [mmolMn/m3] (default = 3.20E7 mmolMn/m3)
rho_niva_brom_redox_MnS: 4.60E7   # Density of MnS [mmolMn/m3] (default = 4.60E7 mmolMn/m3)
rho_niva_brom_redox_S0: 6.56E7   # Density of S0 [mmolS/m3] (default = 6.56E7 mmolS/m3)
rho_niva_brom_redox_Sipart: 4.40E7 # Density of particulate silicate [mmolSi/m3] (default = 4.40E7 mmolSi/m3)

#
#
##--Time stepping parameters-----
dt: 0.0025 # Time step in [days] (default = 0.0025 days)
freq_turb: 1 # Physical mixing time step = dt/freq_turb (default = 1)
freq_sed: 1 # Sinking / bhc frequency (default = 1)
year: 1998 # Selected year (for reading netCDF inputs) WARNING: This must be a year present in the netCDF file, and nc_year0 must be correctly specified below
days_in_yr: 365 # Number of days in repeated period (typically 365 or 366, default = 365)
last_day: 3650 # Last day in simulation (~ days_in_yr * no. repeated years, default = 365)
cc0: 1.0E-11 # Resilient (minimum) concentration for all variables [mmol/m3] (default = 1.0E-11 mmol/m3)
surf_flux_with_diff: 0 # 1 to include surface fluxes in diffusion update, 0 to include in biogeochemical update (default = 0)

#
#
##--Vertical diffusivity parameters-----
diff_method: 1 # Numerical method to treat vertical diffusion (default = 1):
# 0 for FTCS approach (Forward-Time Central-Space scheme)
# 1 for GOTM approach (semi-implicit in time) using diff_center from GOTM lake (converting input/output units)
# 2 for GOTM approach (semi-implicit in time) using modified version of original GOTM diff_center (no units conversion required, should give very similar results to diff_method = 1)
# Note: If diff_method>0 and bioturb_across_SWI = 1 below, only one modified GOTM subroutine can be used (diff_center2)
cnpar: 0.6 # "Implicitness" parameter for GOTM vertical diffusion (default = 0.6):
# 0 => Forward Euler (fully explicit, first-order accurate)
# 1 => Backward Euler (fully implicit, first-order accurate)
# 0.5 => Crank-Nicolson (semi-implicit, second-order accurate)
dynamic_kz_bbl: 0 # 1 for dynamic (time-dependent) kz_bbl, 0 for static kz_bbl (default = 0)
# For deep water (e.g. >500 m) a static kz_bbl may be a reasonable approximation.
# For shallower water, probably better to set dynamic_kz_bbl = 1; kz in the BBL is then determined by linearly interpolating between zero at the SWI and the value at the bottom of the hydrodynamic model input water column
kz_bbl_type: 1 # Type of variation of eddy diffusion kz(z) assumed over the benthic boundary layer:
# 0 => constant = kz_bbl_max, 1 => linear (~=> log-layer for velocity, Holtappels & Lorké, 2011)
# This is only used if assuming a static kz_bbl (dynamic_kz_bbl = 0)
kz_bbl_max: 5.E-6 # Maximum eddy diffusivity in the benthic boundary layer [m2/s] (default = 1.0E-5 m2/s)
# This is only used if assuming a static kz_bbl (dynamic_kz_bbl = 0)
dbl_thickness: 0.0005 # Thickness of the diffusive boundary layer [m] (default = 0.0005 m = 0.5 mm)
# Jorgensen and Revsbech (1985) quote a range 1-2 mm over the deep sea floor (Boudreau and Guinasso, 1982, Wimbush 1976)
# and down to 0.1-0.2 mm over more exposed sediments (Santschi et al., 1983)
# All layers within the DBL (midpoint height above SWI < dbl_thickness) have kz = kz_mol0 (no eddy diffusivity)
kz_mol0: 1.0E-9 # Molecular diffusivity at infinite dilution [m2/s] (default = 1.0E-9 m2/s)
# Cf. range (0.5-2.7)E-9 m2/s in Boudreau 1997, Table 4.8
# This sets a single constant value for all variables that is subsequently corrected for viscosity and tortuosity
mu0_musw: 0.94 # Inverse relative viscosity of saline pore water (default = 0.94 from Boudreau 1997 Table 4.10)
# This relates the diffusivity in saline pore water to the infinite-dilution diffusivity
# assuming the approximation from Li and Gregory (1974), see Boudreau (1997) equation 4.107
kz_bioturb_max: 1.0E-11 # Maximum diffusivity due to bioturbation in the sediments [m2/s] (default = 1.0E-11 m2/s)
# Cf. range (1-100) cm2/yr = (0.3-30)E-11 m2/s cited in Soetaert and Middelburg (2009), citing Middelburg et al. (1997)
# This sets value for upper z_const_bioturb metres, then bioturbation diffusivity decays with scale z_decay_bioturb.
z_const_bioturb: 0.01 # "Mixed layer depth" in sediments over which bioturbation diffusivity = kz_bioturb_max [m] (default = 0.02 m)
# Cf. values 0.05 m and 0.01 m used by Soetaert and Middelburg (2009) for well-mixed and anoxic conditions respectively
# Meire et al. (2013) use 0.05 m as a constant value
z_decay_bioturb: 0.01 # Decay scale of bioturbation diffusivity below z_const_bioturb [m] (default = 0.01 m, following Soetaert and Middelburg, 2009)
K_O2s: 5.0 # Half-saturation constant for the effect of oxygen on bioturbation and bioirrigation [uM] (default = 5.0 uM)
# Bioturbation diffusivity and bioirrigation rate are modulated by a Michaelis-Menten function with parameter K_O2s
bioturb_across_SWI: 1 # 1 to allow (interphase) bioturbation diffusion across the SWI (default = 1)
# Bioturbation across the SWI must be interphase mixing rather than the intraphase mixing assumed within the sediments

#
#

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##---Bioirrigation parameters-----
#
# Bioirrigation rate alpha = a1_bioirr*exp(-a2_bioirr*z_s), where z_s is depth below the SWI [m]
#
a1_bioirr: 0.0 # Maximum rate of bioirrigation in the sediments [s^-1] (default = 0.E-5)
    # Schluter et al. (2000) infer a range (0-5) d^-1 = (0-6)E-5 s^-1 for a1
    # This range is also broadly consistent with the profiles of alpha inferred by Miele et al. (2001)
a2_bioirr: 50. # Decay rate with depth of bioirrigation rate [m^-1] (default = 50)
    # Schluter et al. (2000) infer a range (0-1) cm^1 = (0-100) m^-1 for a2
    # This range is also broadly consistent with the profiles of alpha inferred by Miele et al. (2001)
#
#
##---Sedimentation parameters-----
w_binf: 1.0E-10 # Particulate background burial velocity deep in the sediments where phi = phi_inf [m/s] (default = 1.0E-10 m/s = 0.3 cm/year, but note that true values are highly variable)
    # Soetaert et al. (1996) propose a regression model as a function of water depth:
    # w = 982*D^-1.548, where D is water depth in [m] and w is in cm/year, e.g. for D = 100 m, w = 0.8 cm/year = 2.5E-10 m/s
    # Note: Shallow particulate and solute burial velocities are inferred by assuming steady state compaction (Boudreau, 1997)
dynamic_w_sed: 1 # 1 to enable time-dependent advective velocities in the sediments (default = 0)
    # This uses the modelled (reactive) particulate variables to correct the advective velocities in the sediments (see calculate_sed)
    # w_binf and phi_inf then define constant background components of these velocities
#
#
##---Porosity parameters-----
#
# Porosity phi = phi_inf + (phi_0-phi_inf)*exp(-z_s/z_decay_phi), where z_s is depth below the SWI [m]
#
phi_0: 0.95 # Maximum porosity at the SWI (default = 0.95, following Soetaert et al., 1996)
phi_inf: 0.80 # Minimum porosity deep in the sediments (default = 0.80, following Soetaert et al., 1996)
z_decay_phi: 0.04 # Exponential decay scale for excess porosity in the upper sediments [m] (default = 0.04, following Soetaert et al., 1996)
#
#
##---I/O options-----
input_type: 2 # input forcing type: 0 for sinusoidal changes, 1 to read from ascii, 2 to read from netCDF (default)
ncoutfile_name: BROM_Sleipner_out20.nc # netCDF output file name
outfile_name: finish.dat # ascii output file name
port_initial_state: 1 # 0 to use FABM default (default), 1 to read from ascii file (icfile_name)
icfile_name: start19.dat # ascii initial condition file name (needed if port_initial_state = 1)
#The following are only used if reading input from netCDF (input_type = 2)
#Note: NetCDF variables (temperature, salinity, diffusivity) must have either two dimensions (depth, time) or four dimensions ((latitude, longitude, depth , time) or (longitude, latitude, depth, time))
nc_set_k_wat_bbl: 1 # 1 (default) to set the no. water column layers to agree with netCDF input
                    # 0 to use the value k_wat_bbl set above by subsampling the netCDF input
                    # Note that in both cases the water layer thickness is determined by the netCDF input, overriding water_layer_thickness above
nc_staggered_grid: 1 # 1 (default) to assume a staggered input grid, (t,s) at layer midpoints, kz on layer interfaces (e.g. ROMS, GOTM)
nc_bottom_to_top: 1 # 1 (default) if netCDF variables are stored with vertical index increasing from bottom to top (e.g. ROMS, GOTM)
nc_z_increasing_upward: 1 # 1 if netCDF depth variables are increasing upward (e.g. if "depth" is negative) (default = 0)
ncinfile_name: nns_annual.nc # netCDF input file name
ncintime_name: time # netCDF time dimension name [units since nc_year0-01-01 00:00:00]
nc_year0: 1998 # reference year for netCDF time variable (default = 1970) WARNING: This MUST be correctly specified
ncinz_name: z # netCDF depth dimension name for layer midpoints (rho points) [m]
ncinz2_name: z1 # netCDF depth dimension name for layer interfaces (w points) [m]
ncinlat_name: lat # netCDF latitude dimension name (needed if reading 4D variables)
ncinlon_name: lon # netCDF longitude dimension name (needed if reading 4D variables)
ncinlat_sel: 1 # Chosen latitude index (1,2,...,nlat) (needed if reading from 4D variables with nlat > 1)
ncinlon_sel: 1 # Chosen longitude index (1,2,...,nlon) (needed if reading from 4D variables with nlon > 1)
#
#Below we specify the names of variables in netCDF input files
#Format is <ROMS internal name>: <netCDF input name>
#Can also specify a constant scale factor "fac", e.g. to convert units, or correct bias.
#ROMS internal variable = fac * netCDF input variable (ROMS assumes fac = 1 if not specified here)
#This factor can also be used to apply a simple stoichiometric assumption in lieu of nutrient variable data
#E.g. ncinsis_name: NO3s # netCDF input surface silicate variable name [uM] - here using nitrate
#    ncinsis_fac: 1.5 # scale factor for netCDF input surface silicate - here assuming "extended Redfield ratio" Si:N = 1.5 mol Si / mol N
#
#2D physical variables used for setting ROMS forcings
#These must be arrays of size [no. water column layers (= k_wat_bbl) * no. of days for all available years]
ncint_name: temp # netCDF input temperature variable name [degC]
ncins_name: salt # netCDF input salinity variable name [psu]
ncinkz_name: nus # netCDF input vertical diffusivity variable name [m2/s]
ncinkz_fac: 1.0 # scale factor for netCDF input vertical diffusivity (default = 1.0)
#
#1D physical variables used for setting ROMS forcings
#These must be arrays of size [no. of days for all available years]

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ncinEair_name: Eair          # netCDF input shortwave irradiance in air at water surface [W/m2] (only used if use_Eair = 1)
ncinEair_fac: 1.0           # scale factor for netCDF input shortwave irradiance (default = 1.0) (only used if use_Eair = 1)
ncinhice_name: hice         # netCDF input ice thickness variable name [m] (only used if use_hice = 1)
ncinhice_fac: 1.0           # scale factor for netCDF input ice thickness (default = 1.0) (only used if use_hice = 1)
#
#Biogeochemical variables used for setting Dirichlet BCs at surface or bottom (bctype = 3)
#These must be arrays of size [1 * no. of days in repeated period (= days_in_yr)]
ncinNH4s_name: NH4s        # netCDF input surface ammonium variable name [uM]
ncinNH4s_fac: 1.0           # scale factor for netCDF input surface ammonium (default = 1.0)
ncinNO3s_name: NO3s         # netCDF input surface nitrate variable name [uM]
ncinNO3s_fac: 1.0           # scale factor for netCDF input surface nitrate (default = 1.0)
ncinPO4s_name: PO4s         # netCDF input surface phosphate variable name [uM]
ncinPO4s_fac: 1.0           # scale factor for netCDF input surface phosphate (default = 1.0)
ncinSis_name: Sis           # netCDF input surface silicate variable name [uM]
ncinSis_fac: 1.0             # scale factor for netCDF input surface silicate (default = 1.0)
ncinAlks_name: ATs          # netCDF input surface alkalinity variable name [uM]
ncinAlks_fac: 1.0            # scale factor for netCDF input surface alkalinity (default = 1.0)
#
#Biogeochemical variables used for setting horizontal mixing fluxes
#NOTE: These must be arrays of size [no. water column layers (= k_wat_bbl) * no. of days in repeated period (= days_in_yr)]
#NOTE: The depth indexing must agree with temperature and salinity inputs
#NOTE: The layer index of the mixing variable is the layer with which it mixes in the internal BROM grid
# This is does not necessarily reflect the actual depth of the mixing variable in its external location
#NOTE: This information is only used if hmix_<variable name> is > 0, see above
ncinNH4hmix_name: NH4_N    # netCDF input horizontal mixing ammonium variable name [uM]
ncinNH4hmix_fac: 1.0        # scale factor for netCDF input horizontal mixing ammonium (default = 1.0)
ncinNO3hmix_name: NO3_N    # netCDF input horizontal mixing nitrate variable name [uM]
ncinNO3hmix_fac: 1.0        # scale factor for netCDF input horizontal mixing nitrate (default = 1.0)
ncinPO4hmix_name: PO4_N    # netCDF input horizontal mixing phosphate variable name [uM]
ncinPO4s_fac: 1.0            # scale factor for netCDF input horizontal mixing phosphate (default = 1.0)
ncinSihmix_name: NO3_N      # netCDF input horizontal mixing silicate variable name [uM]
ncinSihmix_fac: 1.5          # scale factor for netCDF input horizontal mixing silicate (default = 1.0)
ncinO2hmix_name: O2_N       # netCDF input horizontal mixing oxygen variable name [uM]
ncinO2hmix_fac: 1.0          # scale factor for netCDF input horizontal mixing oxygen (default = 1.0)
#
#Horizontal mixing rates
#NOTE: This must be an array of size [no. water column layers (= k_wat_bbl) * no. of days in repeated period (= days_in_yr)]
#NOTE: The depth indexing must agree with temperature and salinity inputs
#NOTE: This information is only used if hmix_<variable name> is > 0, see above
ncinhmix_rate_name: hmix_rate # netCDF input horizontal mixing rates [day^-1]
ncinhmix_rate_fac: 1.0        # scale factor for netCDF input horizontal mixing rate (default = 1.0)
#
#
##--Options for run-time output to screen-----
show_maxmin: 0               # 1 to show the profile maximum and minimum of each variable at the end of each day (default = 0)
show_kztCFL: 0                # 1/2 to show the max/profile of total vertical diffusivity and associated Courant-Friedrichs-Lowy number at the end of
each day (default = 0)
show_wCFL: 0                  # 1/2 to show the max/profile of vertical advection and associated Courant-Friedrichs-Lowy number at the end of each day
(default = 0)
show_nan: 0                   # 1 to show the profile concentration output on NaN-termination for the offending variable (default = 1)
show_nan_kztCFL: 2            # 1/2 to show the max/profile of total vertical diffusivity and associated Courant-Friedrichs-Lowy number on NaN-
termination (default = 1)
show_nan_wCFL: 1              # 1/2 to show the max/profile of vertical advection and associated Courant-Friedrichs-Lowy number on NaN-termination
(default = 1)
#
#
## References
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```

Section S2: run-time input file for BROM-biogeochemistry (fabm.yaml)

```
# IMPORTANT!!!! _ <TAB> is NOT allowed here, used <Space> only !!!!  
# Each entry must have 6 spaces before the parameter name  
require_INITIALIZATION: true  
instances:  
#-----  
niva_brom_eqconst:  
#-----  
niva_brom_carb:  
initialization:  
Alk: 2200.  
DIC: 2100.  
coupling:  
Kc0: niva_brom_eqconst/Kc0  
Kc1: niva_brom_eqconst/Kc1  
Kc2: niva_brom_eqconst/Kc2  
Kw: niva_brom_eqconst/Kw  
Kb: niva_brom_eqconst/Kb  
Kp1: niva_brom_eqconst/Kp1  
Kp2: niva_brom_eqconst/Kp2  
Kp3: niva_brom_eqconst/Kp3  
Knh4: niva_brom_eqconst/Knh4  
Kh2s: niva_brom_eqconst/Kh2s  
# Kh2s2: niva_brom_eqconst/Kh2s2  
KSi: niva_brom_eqconst/KSi  
ks04: niva_brom_eqconst/ks04  
kflu: niva_brom_eqconst/kflu  
tot_free: niva_brom_eqconst/tot_free  
# Constants calculated: Kc0 (Weiss, 1974), Kc1, Kc2 (Roy et al., 1993), Kw, Kp1,Kp2,Kp3 (DOE, 2004),  
# Kb (Dickson,1990), KSi(Millero,1995), Knh4, Kh2s1(Luff et al, 2001), Kh2s2(Volkov 1984)  
# dissociation for B, F according to (Dickson et al., 2007), more references in the code.  
PO4: niva_brom_bio/PO4  
NH4: niva_brom_bio/NH4  
DON: niva_brom_bio/DON  
Si: niva_brom_redox/Si  
H2S: niva_brom_redox/H2S  
Mn3: niva_brom_redox/Mn3  
Mn4: niva_brom_redox/Mn4  
Fe3: niva_brom_redox/Fe3  
SO4: niva_brom_redox/SO4  
#-----  
niva_brom_bio:  
initialization:  
O2: 200.  
Phy: 0.01  
Het: 0.01  
PON: 0.01  
DON: 0.0  
NO3: 5.  
PO4: 1.  
NH4: 0.0  
parameters:  
# --- Phy -----  
K_phy_gro: 4.7    # Maximum specific growth rate (1/d) =0.9-1.3 (Savchuk, 2002), =3.(Gregoire, Lacroix, 2001) >!0.5 worked for Berre!<  
lopt: 25.        # Optimal irradiance (W/m2) =50 (Savchuk, 2002)  
bm: 0.12        # Coefficient for growth dependence on t  
cm: 1.4         # Coefficient for growth dependence on t  
K_phy_mrt: 0.20   # Specific rate of mortality, (1/d) =0.3-0.6 (Savchuk, 2002), =0.05 (Gregoire, Lacroix, 2001)  
K_phy_exc: 0.10    # Specific rate of excretion, (1/d) =0.01 (Burchard et al., 2006)  
# --- Het -----  
K_het_phy_gro: 1.1  #! Max.spec. rate of grazing of Zoo on Phy, (1/d), =0.9 (Gregoire, Lacroix, 2001), =1.5 (Burchard et al., 2006)  
K_het_phy_lim: 0.5   #! Half-sat.const.for grazing of Zoo on Phy for Phy/Zoo ratio  
K_het_pom_gro: 0.50  #! Max.spec.rate of grazing of Zoo on POP and bacteria, (1/d), =1.2 (Burchard et al., 2006)  
K_het_pom_lim: 0.05  #! Half-sat.const.for grazing of Zoo on POP for POP/Zoo ratio  
K_het_res: 0.02     #! Specific respiration rate =0.02 (Yakushev et al., 2007)  
K_het_mrt: 0.05     #! Maximum specific rate of mortality of Zoo (1/d) =0.05 (Gregoire, Lacroix, 2001)  
Uz: 0.5            #! Food absorbency for Zoo (nd) =0.5-0.7 (Savchuk, 2002)  
Hz: 0.5            #! Ratio betw. diss. and part. excretes of Zoo (nd), =0.5 (Gregoire, Lacroix, 2001)  
limGrazBac: 2.      #! Limiting parameter for bacteria grazing by Zoo, =2. (Yakushev et al., 2007)  
# --- N -----  
K_nox_lim: 0.1     #! Half-sat.const.for uptake of NO3+NO2 (uM) =0.5 (Gregoire, Lacroix, 2001)  
K_nh4_lim: 0.02    #! Half-sat.const.for uptake of NH4 (uM) =0.2 (Gregoire, Lacroix, 2001)  
K_psi: 1.46        #! Strength of NH4 inhibition of NO3 uptake constant (uM-1) =1.46_rk (Gregoire, Lacroix, 2001)
```

```

K_nfix: 0.4      #! Maximum specific rate of N-fixation (1/d) =0.5 (Savchuk, 2002)
# ----P -----
K_po4_lim: 0.012  #! Half-sat. constant for uptake of PO4 by Phy
# ----Si-----
K_si_lim: 0.1     #! Half-sat. constant for uptake of Si_lim by Phy
# ----Sinking-----
Wsed: 5.0        #! Rate of sinking of detritus (m/d), =0.4 (Savchuk, 2002), =5. (Gregoire, Lacroix, 2001), =1-370 (Allredge, Gotschalk, 1988)
Wphy: 0.2         #! Rate of sinking of Phy (m/d), =0.1-0.5 (Savchuk, 2002)
Whet: 1.          #! Rate of sinking of Het (m/d), =1. (Yakushev et al., 2007)
# ---- Stoichiometric coefficients ----
r_n_p: 16.0      #! N[μM]/P[μM]
r_o_n: 6.625     #! O2[μM]/N[μM]
r_c_n: 8.0        #! C[μM]/N[μM]
r_si_n: 1.0       #! Si[μM]/N[μM]
coupling:
NO2: niva_brom_redox/NO2
H2S: niva_brom_redox/H2S
Baan: niva_brom_redox/Baan
Baae: niva_brom_redox/Baae
Bhae: niva_brom_redox/Bhae
Bhan: niva_brom_redox/Bhan
Si: niva_brom_redox/Si
Sipart: niva_brom_redox/Sipart
DIC: niva_brom_carb/DIC
Alk: niva_brom_carb/Alk
Hplus: niva_brom_carb/Hplus
Kp1: niva_brom_eqconst/Kp1
Kp2: niva_brom_eqconst/Kp2
Kp3: niva_brom_eqconst/Kp3
Knh4: niva_brom_eqconst/Knh4
KSi: niva_brom_eqconst/KSi
# -----
niva_brom_redox:
initialization:
Mn2: 0.0
Mn3: 0.0
Mn4: 0.0
MnS: 0.0
MnCO3: 0.0
Fe2: 0.0
Fe3: 0.0
FeS: 0.0
FeCO3: 0.0
NO2: 0.0
Si: 0.0
Sipart: 0.0
H2S: 0.0
S0: 0.0
S2O3: 0.0
SO4: 25000.
Baae: 0.01
Bhae: 0.01
Baan: 0.01
Bhan: 0.01
CaCO3: 5.0
CH4: 0.001
FeS2: 0.0
parameters:
# ---- Model parameters -----
Wbact: 0.4      #! Rate of sinking of bacteria (Bhae,Baae,Bhan,Baan) (1/d), (Yakushev et al.,2007)
Wm: 7.0          #! Rate of accelerated sinking of particles with settled metal hydroxides (1/d), (Yakushev et al.,2007)
# specific rates of biogeochemical processes
#---- Mn-----
K_mn_ox1: 0.1    #! Specific rate of oxidation of Mn2 to Mn3 with O2 (1/d).
K_mn_ox2: 0.2    #! Specific rate of oxidation of Mn3 to Mn4 with O2 (1/d)
K_mn_rd1: 0.5    #! Specific rate of reduction of Mn4 to Mn3 with H2S (1/d)
K_mn_rd2: 1.0    #! Specific rate of reduction of Mn3 to Mn2 with H2S (1/d)
K_mns: 1500.     #! Conditional equilibrium constant for MnS from Mn2 with H2S (M)
K_mns_diss: 0.0005 #! Specific rate of dissolution of MnS to Mn2 and H2S (1/d)
K_mns_form: 0.00001 #! Specific rate of formation of MnS from Mn2 with H2S (1/d)
K_mnco3: 1.       #! Conditional equilibrium constant % 1.8e-11 (M) (Internet) 1 uM2 for Mn2+CO3->MnCO3 (Meysman,2003)
K_mnco3_diss: 7.e-7 #! Specific rate of dissolution of MnCO3 (1/d) =6.8e-7 (2.5 X 10-1 yr-1 (Van Cappellen, Wang, 1996) !1x10-4 yr-1) (Hunter et al, 98)
K_mnco3_form: 0.1e-4 #! Specific rate of formation of MnCO3 (1/d) =2.7e-7 (1. X 10-4 yr-1 (Van Cappellen, Wang, 1996)!1x10-4 yr-1) (Hunter et al, 98)
K_mnco3_ox: 0.0027 #! Specific rate of oxidation of MnCO3 with O2 (1/d)=0.0027 ( 1x10^(-6) M/yr (Van Cappellen, Wang, 1996).

```

K_DON_mn: 0.001 #! Specific rate of oxidation of DON with Mn4 (1/d)
 K_PON_mn: 0.001 #! Specific rate of oxidation of PON with Mn4 (1/d)
 s_mnox_mn2: 0.01 #! threshold of Mn2 oxidation (uM Mn) (Yakushev et al.,2007)
 s_mnox_mn3: 0.01 #! threshold of Mn3 oxidation (uM Mn) (Yakushev et al.,2007)
 s_mnrd_mn4: 0.01 #! threshold of Mn4 reduciton (uM Mn) (Yakushev et al.,2007)
 s_mnrd_mn3: 0.01 #! threshold of Mn3 reduciton (uM Mn) (Yakushev et al.,2007)
----- Fe-----
 K_fe_ox1: 0.5 #! Specific rate of oxidation of Fe2 to Fe3 with O2 (1/d), =4. (Konovalov et al., 2006)
 K_fe_ox2: 0.001 #! 0.1! Specific rate of oxidation of Fe2 to Fe3 with MnO2 (1/d) =0.74 (Konovalov et al., 2006); 3×10^{-6} 1/(M yr) is estimated in Van Cappellen-Wang-96
 K_fe_rd: 1.2 #!0.5! Specific rate of reduction of Fe3 to Fe2 with H2S (1/day) *=0.05 (Konovalov et al., 2006)
 K_fes: 2510.0 #!FeS equilibrium constant (Solubility Product Constant) (uM)=2510 (2.51×10^{-6} mol cm⁻³, Bektursuniva,11)
 K_fes_form: 5.e-4 #!Specific rate of precipitation of FeS from Fe2 with H2S (1/day)=1.e-5 (4×10^{-3} 1/yr, Bektursunova,11)
 K_fes_diss: 1.e-6 #!Specific rate of dissolution of FeS to Fe2 and H2S (1/day)=3.e-6 (1×10^{-3} 1/yr, Bektursunova,11)
 K_fes_ox: 0.001 #!Specific rate of oxidation of FeS with O2 (1/day)=0.001(3×10^{-5} 1/(M yr),(Van Cappellen, Wang, 1996)
 K_DON_fe: 0.00005 #!-0.0003 ! % Specific rate of oxidation of DON with Fe3 (1/day)
 K_PON_fe: 0.00001 #!-0.0001 ! % Specific rate of oxidation of PON with Fe3 (1/day)
 K_fes2_form: 1.e-6 #!specific rate of FeS2 formation by FeS oxidation by H2S (1/day)=0.000009 (10^{-4}) L/mol/s (Rickard-97)
 K_fes2_ox: 4.38e-4 #!specific rate of pyrite oxidation by O2 (1/uM/d)= 4.38×10^{-4} 1/micromolar/day (Wijsman et al -2002).
 s_feox_fe2: 0.001 #!threshold of Fe2 reduciton
 s_ferd_fe3: 0.01 #!threshold of Fe3 reduciton (uM Fe)
 K_feco3: 15. #!10. !2.e-2 ! Conditional equilibrium constant % 1.8×10^{-11} (M) (Internet) 1 uM2 for Mn2+CO3->FeCO3 (Meysman,2003)
 K_feco3_diss: 7.e-4 #!Specific rate of dissolution of FeCO3 (1/day)= 6.8×10^{-7} 1.25×10^{-1} yr-1 (Van Cappellen, Wang, 1996) ! 1×10^{-4} yr-1 (Hunter et al, 98)
 K_feco3_form: 3.e-4 #!Specific rate of formation of FeCO3 (1/day)= 2.7×10^{-7} !! 1×10^{-4} yr-1(Van Cappellen, Wang, 1996)! 1×10^{-4} yr-1 (Hunter et al, 98)
 K_feco3_ox: 0.0027 #!Specific rate of oxidation of FeCO3 with O2 (1/day)=0.0027 (1×10^{-6}) M/yr (Van Cappellen, Wang, 1996).
----- S-----
 K_hs_ox: 0.5 #! Specific rate of oxidation of H2S to S0 with O2 (1/d), =0.1 (Gregoire, Lacroix, 2001)
 K_s0_ox: 0.02 #! 0.02 Specific rate of oxidation of S0 with O2 (1/d), (Yakushev, Neretin,1997)
 K_s2o3_ox: 0.01 #! Specific rate of oxidation of S2O3 with O2 (1/d), (Yakushev, Neretin,1997)
 K_so4_rd: 5.e-6 #! Specific rate of OM sulfate reduction with sulfate (1/d), (Yakushev, Neretin,1997)
 K_s2o3_rd: 0.001 #! Specific rate of OM sulfate reduction with thiosulfate (1/d) (Yakushev, Neretin,1997)
 K_s0_disp: 0.001 #! Specific rate of S0 disproportionation (1/d) (Yakushev,2013)
 K_s0_no3: 0.9 #! Specific rate of oxidation of S0 with NO3 (1/d) (Yakushev,2013)
 K_s2o3_no3: 0.01 #! Specific rate of oxidation of S2O3 with NO3 (1/d) (Yakushev,2013)
 K_mnrd_hs: 1.0 #! half sat. of Mn reduction (uM S) (Yakushev,2013)
 K_ferd_hs: 1.0 #! half sat. of Fe reduction (uM S) (Yakushev,2013)
----- N-----!
 K_DON_ox: 0.05 #! Specific rate of oxidation of DON with O2 (1/d) = 0.1(Savchuk, 2002)
 K_PON_ox: 0.002 #! Specific rate of oxidation of PON with O2 (1/d) =0.002 (Savchuk, 2002), =0.07 (Gregoire, Lacroix, 2001)
 Tda: 13.0 #! Temperature control coefficient for OM decay (Burchard et al., 2006)
 beta_da: 20.0 #! Temperature control coefficient for OM decay (Burchard et al., 2006)
 K_omox_o2: 1.0 #! Half sat. of o2 for OM mineralization (uM) (Yakushev,2013)
 K_PON_DON: 0.1 #! Specific rate of Autolysis of PON to DON (1/d), =0.02 (Burchard et al., 2006)
 K_nitrif1: 0.01 #! Spec.rate of 1st st. of nitrification, (1/d), =0.01 (Yakushev,2013) =0.1(Savchuk, 2002) =0.1 (Gregoire, Lacroix, 2001)
 K_nitrif2: 0.1 #! Spec.rate of 2d st. of nitrification, (1/d), =0.1 (Yakushev,2013)
 K_denitr1: 0.16 #! Spec.rate of 1 stage of denitrif =0.16 (Yakushev, Neretin,1997),= 0.5(Savchuk, 2002),= 0.015(Gregoire, Lacroix, 2001)
 K_denitr2: 0.25 #! Spec.rate of 2 stage of denitrif =0.22 (Yakushev, Neretin,1997)
 K_omno_no3: 0.001 #! Half sat. of no3 for OM denitr. (uM N) (Yakushev,2013)
 K_omno_no2: 0.001 #! Half sat. of no2 for OM denitr. (uM N) (Yakushev,2013)
 K_hs_no3: 0.8 #! Spec.rate of thiodenitrification (1/d), =.015 (Gregoire, Lacroix, 2001)
 K_anammox: 0.8 #! Spec.rate of Anammox (1/d), (Gregoire, Lacroix, 2001)
----- O2-----!
 O2s_nf: 5. #! threshold of O2 saturation for nitrification, (uM), =10. (Gregoire, Lacroix, 2001)
 O2s_dn: 10.0 #! threshold of O2 for denitrification, anammox, Mn reduction (uM O2), =40 (0.72 mgO2/l) (Savchuk, 2002)
 s_omox_o2: 0.01 #! threshold of o2 for OM mineralization (uM O2) (Yakushev,2013)
 s_omno_o2: 25.0 #! threshold of o2 for OM denitrification (uM O2) (Yakushev,2013)
 s_omso_o2: 25.0 #! threshold of o2 for OM sulfate reduction (uM O2) (Yakushev,2013)
 s_omso_no3: 5.0 #! threshold of noX for OM sulfate reduction (uM O2) (Yakushev,2013)
 K_mnox_o2: 2.0 #! half sat. of Mn oxidation (uM O2) (Yakushev,2013)
----- C-----!
 K_caco3_diss: 3.0 #! CaCO3 dissolution rate constant (1/d) (wide ranges are given in (Luff et al., 2001))
 K_caco3_form: 0.0002 #! CaCO3 precipitation rate constant (1/d) (wide ranges are given in (Luff et al., 2001))
 K_DON_ch4: 0.00014 #! Specific rate of methane production from DON (1/d) (Lopes et al., 2011)
 K_PON_ch4: 0.00014 #! Specific rate of methane production from PON (1/d) (Lopes et al., 2011)
 K_ch4_o2: 0.14 #! Specific rate of oxidation of CH4 with O2 (1/d) =0.14 (Lopes et al., 2011)
 K_ch4_so4: 0.0000274 #! Specific rate of oxidation of CH4 with SO4 (1/uM/day) (0.0274 m3 /mol-1 day-1 Lopes et al., 2011)
 s_omch_so4: 30. #! threshold of of SO4 for methane production from OM (uM) (Lopes et al., 2011)
----- Si-----!
 K_sipart_diss: 0.080 #! Si dissolution rate constant (1/d), =0.008 (Popova, Srokosz, 2009)
----- Bacteria!
 K_Baae_gro: 0.1 #! Baae maximum specific growth rate (1/d) (Yakushev, 2013)
 K_Baae_mrt: 0.005 #! Baae specific rate of mortality (1/d) (Yakushev et al., 2013)
 K_Baae_mrt_h2s: 0.899 #! Baae increased specific rate of mortality due to H2S (1/d) (Yakushev et al., 2013)
 limBaae: 2.0 #! Limiting parameter for nutrient consumprion by Baae (nd) (Yakushev, 2013)

K_Bhae_gro: 0.5 #! Bhae maximum specific growth rate (1/d) (Yakushev, 2013)
 K_Bhae_mrt: 0.01 #! Bhae specific rate of mortality (1/d) (Yakushev, 2013)
 K_Bhae_mrt_h2s: 0.799 #! Bhae increased specific rate of mortality due to H2S (1/d) (Yakushev, 2013)
 limBhae: 5.0 #! Limiting parameter for OM consumprion by Bhae (nd) (Yakushev, 2013)
 K_Baan_gro: 0.2 #! Baan maximum specific growth rate (1/d) (Yakushev, 2013)
 K_Baan_mrt: 0.005 #! Baan specific rate of mortality (1/d) (Yakushev, 2013)
 limBaan: 2.0 #! Limiting parameter for nutrient consumprion by Baan (nd) (Yakushev, 2013)
 K_Bhan_gro: 0.15 #! Bhan maximum specific growth rate (1/d) (Yakushev, 2013)
 K_Bhan_mrt: 0.01 #! Bhan specific rate of mortality (1/d) (Yakushev, 2013)
 K_Bhan_mrt_o2: 0.899 #! Bhan increased specific rate of mortality due to O2 (1/d) (Yakushev, 2013)
 limBhan: 2.0 #! Limiting parameter for OM consumprion by Bhan (nd) (Yakushev, 2013)
 #---- Stoichiometric coefficients ----!
 r_fe_n: 26.5 #! Fe[uM]/N[uM] (Boudreau, 1996)
 r_mn_n: 13.25 #! Mn[uM]/Ni[uM] (Boudreau, 1996)
 f: 0.66 #! conversion factor relating solid and dissolved species concentrations
 r_fe3_p: 2.7 #! Fe[uM]/P[uM] partitioning coeff. for Fe oxide (Yakushev et al., 2007)
 r_mn3_p: 0.67 #! Mn[uM]/P[uM] complex stoichiometric coeff. for Mn(III) (Yakushev et al., 2007)
 r_fe3_si: 3. #! Fe[uM]/Si[uM] partitioning coeff. for Fe oxide
 coupling:
 O2: niva_brom_bio/O2 # O2: niva_oxydep/oxy
 NH4: niva_brom_bio/NH4
 NO3: niva_brom_bio/NO3
 PO4: niva_brom_bio/PO4
 PON: niva_brom_bio/PON
 DON: niva_brom_bio/DON
 Wsed: niva_brom_bio/Wsed
 Kp1: niva_brom_eqconst/Kp1
 Kp2: niva_brom_eqconst/Kp2
 Kp3: niva_brom_eqconst/Kp3
 Knh4: niva_brom_eqconst/Knh4
 Kh2s: niva_brom_eqconst/Kh2s
 KSi: niva_brom_eqconst/KSi
 Kc0: niva_brom_eqconst/Kc0
 Alk: niva_brom_carb/Alk
 DIC: niva_brom_carb/DIC
 Hplus: niva_brom_carb/Hplus
 Om_Ca: niva_brom_carb/Om_Ca
 Om_Ar: niva_brom_carb/Om_Ar
 CO3: niva_brom_carb/CO3
 pCO2: niva_brom_carb/pCO2
 Ca: niva_brom_carb/Ca
 # REFERENCES:
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