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Supplement of

A global scavenging and circulation ocean model of thorium-230 and protactinium-231 with improved particle dynamics (NEMO–ProThorP 0.1)

Marco van Hulten et al.

Correspondence to: Marco van Hulten (marco.hulten@uib.no)

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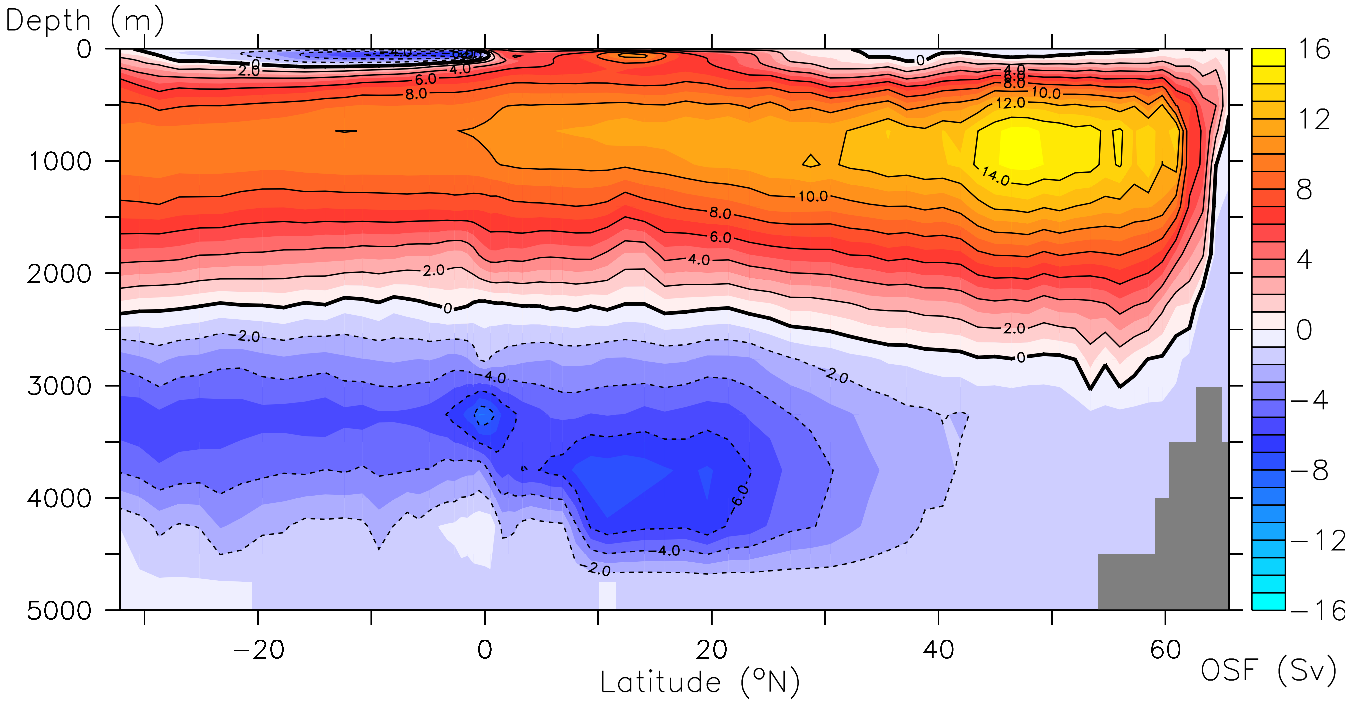

Figure S1. The Atlantic Overturning Stream Function (OSF), a measure for the AMOC in Sv (1 Sv = 10^6 $m^3 s^{-1}$; clockwise is positive).

Symbol	Description	Value	Unit	Code
$\mathcal{A}$	Horizontal eddy diffusion	2000	$m^2 s^{-1}$	`aht0`
$\mathcal{B}$	Vertical eddy diffusion	$1.2 \cdot 10^{-5}$	$m^2 s^{-1}$	`avt0`
Δz_1	Thickness of top layer	10	m	`fse3t(:,:,1)`
Φ_{dust}	Dust flux	Variable	$g\,m^{-2} s^{-1}$	`dust(:,:)`
f	Fraction of dust → small|big particles	0.2|0.8	–	`fdust1, fdust2`
w_s	Slow sinking speed	2	$m\,d^{-1}$	`wsbio3`
w_b	Fast sinking speed	50	$m\,d^{-1}$	`wsbio4`
k	$CaCO_3$ dissolution rate constant	2.5	mo^{-1}	`kdca`
n	$CaCO_3$ dissolution order	3.9	–	`nca`
–	Any biogeochemical PISCES tracer	Variable	$mol\,dm^{-3}$	`trn(jp_pisces0:jp_pisces1,:,:,:)`
P^{Lith}	Lithogenic particle concentration	Variable	$g\,L^{-1}$	`trn(jp_lith0:jp_lith1,:,:,:)`
A_{ij}	Activity of nuclide i on particle j	Variable	$Bq\,m^{-3}$	`trn(jp_protac0:jp_protac1,:,:,:)`
K_{ij}	Partition coefficient	See Table 2	$Mg\,g^{-1}$	`k_pa_poc, k_th_poc, k_pa_goc, ...`
β_{Pa}	Production rate of ^{231}Pa	$2.33 \cdot 10^{-3}$	$dpm\,m^{-3}\,yr^{-1}$	`beta_pa231`
β_{Th}	Production rate of ^{230}Th	$2.52 \cdot 10^{-2}$	$dpm\,m^{-3}\,yr^{-1}$	`beta_th230`
λ_{Pa}	Decay rate of ^{231}Pa	$2.116 \cdot 10^{-5}$	yr^{-1}	`lambda_pa231`
λ_{Th}	Decay rate of ^{230}Th	$9.195 \cdot 10^{-6}$	yr^{-1}	`lambda_th230`

Table S1. Parameters and variables with values, associated units, and variable names in the Fortran code of NEMO–ProThorP 0.1.

Simulation	Spin-up time	Characteristic
Dynamics	200 yr	climatological conditions
Standard/spin-up	300 yr	–
Standard	+200 yr	$bSiO_2$ same
Th-$bSiO_2$	+200 yr	more Th affinity

Table S2. Simulations for each component.

Radionuclide	Particle	Equilibrium partition coefficient K_d ($\mathrm{Mg\,g^{-1}}$)				
		This study	Dutay et al. (2009)	Hayes et al. (2015)	Geibert and Usbeck (2004)	Range
^{231}Pa	POC	2.0	10–1000	0.6 ± 0.2	-	0.4–1.0
^{230}Th	POC	5.0	10–1000	3 ± 2	-	1–5
^{231}Pa	GOC	0.4	1–10	0.6 ± 0.2	-	0.4–0.8
^{230}Th	GOC	1.0	1–10	3 ± 2	-	1–5
^{231}Pa	$bSiO_2$	0.5 (0.4)	1.7	–	0.4–1.0	0.4–1.7
^{230}Th	$bSiO_2$	0.5 (1.0)	0.05–0.5	–	<0.8–2.0	0.5–2.0
^{231}Pa	$CaCO_3$	0.12	0.25	0.9 ± 0.4	0.03–0.34	0.03–0.34
^{230}Th	$CaCO_3$	5.0	10	30 ± 4	0.5–7.9	0.5–7.9
^{231}Pa	Litho small	10.0	–	2.3 ± 0.2	1.2–1.9	1.2–1.9
^{230}Th	Litho small	50.0	–	23 ± 2	4.6–10.2	4.6–10.2
^{231}Pa	Litho big	1.0	–	2.3 ± 0.2	1.2–1.9	1.2–1.9
^{230}Th	Litho big	5.0	–	23 ± 2	4.6–10.2	4.6–10.2

Table S3. Equilibrium partition coefficients used in this study, and other studies. The value between braces are used for the sensitivity study in the paper. Units are in millions of gram of seawater per gram of particle.

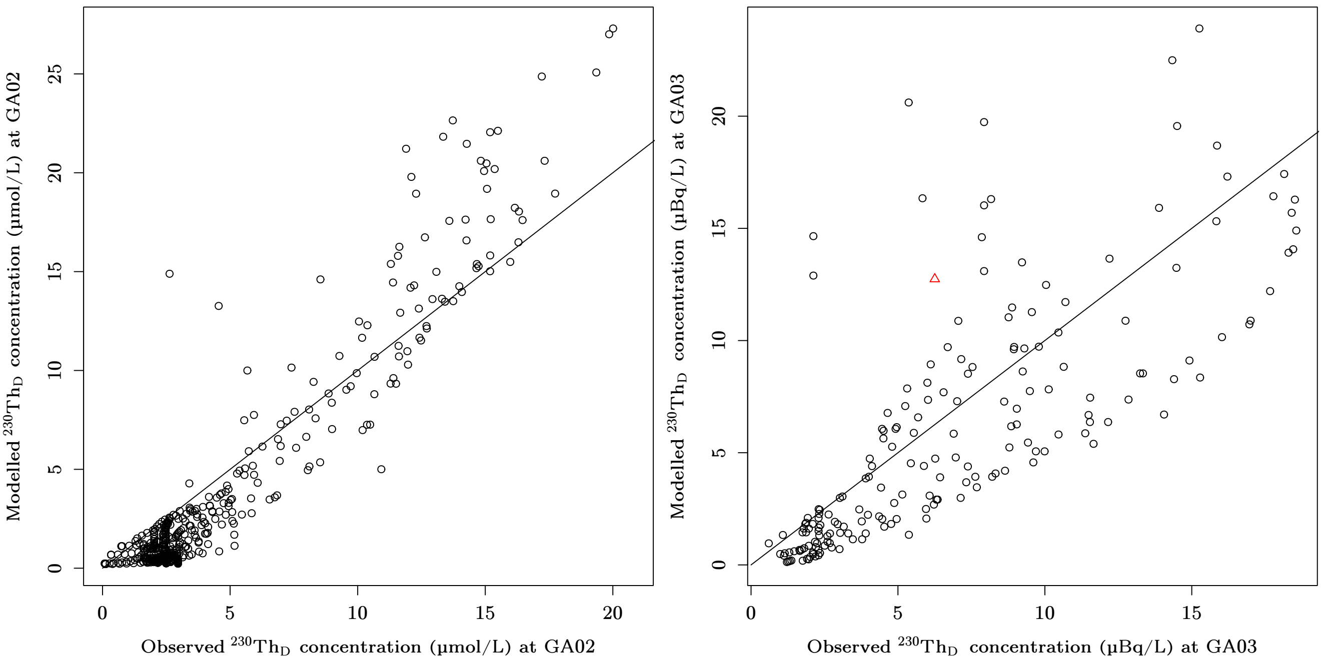

Figure S2. Modelled (y-axis) versus observed (x-axis) dissolved ^{230}Th concentration for the West Atlantic GA02 transect, $r = 0.80$ (left panel), and the North Atlantic GA03 transect, $r = 0.78$ (right panel). The units are $\mathrm{mBq\,m^{-3}}$. The red triangle corresponds with the grid box just above the hydrothermal vent «TAG» at 44.83° W. We presume that the much higher modelled version is because we did not include scavengers from hydrothermal origin (most notably manganese oxide). The line is $y = x$.

Julia code

The statistics on the GEOTRACES GA02 and GA03 transects are performed with Julia 1.0, using the below scripts. This code is tested for Julia 1.0 (see Discussion Paper for Julia 0.6 specific code, which yields the same coefficients). Please, contact the first author if there are issues.

Prepare data

```
# protac.jl - Read model and observations, and then interpolate on ORCA2 grid.

# Set your tracer and transect
tracer   = "Th230d"
transect = "GA02_merid"
sim_num  = 7

# Model
using NCDatasets
using Missings      # coalesce()
tracer_transect = string(tracer, "_", transect)
model = Dataset(string(tracer_transect, "_", sim_num, ".nc"), "r")
c_mod = zeros(size(model[uppercase(tracer_transect)]))
c_mod .= coalesce.(model[uppercase(tracer_transect)][:,:], NaN)
bnds = model["DEPTHT_bnds"]

# Observations
using CSV
observations = CSV.read("HayesThPa_hack.csv"; datarow=3, types=[Int,Int,Int,Float64,Float64,
Float64,Float64,Float64,Float64,Float64])

if !(size(unique(observations[:STNNBR]))[1] == size(c_mod)[1])
    error("Number of stations in model does not match that in observations!")
end
nstations = size(c_mod)[1]
nsamples = sum(observations[:STNNBR] .== collect(1:nstations)', dims=1)
profiles = Array{Float64}(undef, nstations, max(nsamples...))
profiles .= NaN
depths = copy(profiles)

for i = 1:nstations
    profiles[i,1:nsamples[i]] .= observations[:Th_230_D_CONC][observations[:STNNBR].==i]
    depths[i,1:nsamples[i]] .= observations[:Depth][observations[:STNNBR].==i]
end

c_obs = Array{Float64}(undef, size(c_mod))
c_obs .= NaN

using Statistics
for i = 1:nstations
    for k = 1:size(c_mod)[2]
        c_obs[i,k] = mean(profiles[i, bnds[1,k].<=depths[i,:].<bnds[2,k]])
    end
end
```

Pearson correlation coefficient

```
# stats.jl - Calculate goodness-of-fit coefficients
# https://discourse.julialang.org/t/reducing-verbosity-in-array-calculations/8778

function r(obs, mod)
    bis = .!isnan.(obs) .& .!isnan.(mod)
    dobs = obs[bis] .- mean(obs[bis])
    dmod = mod[bis] .- mean(mod[bis])
    sum((dobs .* dmod)) / sqrt( sum((dobs .^ 2)) * sum((dmod .^ 2)) )
end
```

Tracer		Standard simulation		Decreased $K_{\mathrm{Pa,bSiO_2}}$	
↓	Transect →	GA02	GA03	GA02	GA03
Dissolved ^{230}Th		0.80	0.78	0.83	0.76
Dissolved ^{231}Pa		0.73	n/a	0.73	n/a
Small particulate ^{230}Th		0.66	n/a	0.66	n/a
Small particulate ^{231}Pa		0.54	n/a	0.49	n/a

Table S4. Pearson correlation coefficients r for different radionuclide isotopes and phases at the GEOTRACES GA02 and GA03 transects.

References

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