COPSE model description

As published in Tostevin and Mills (2020), Royal Society Interface Focus. This version combines various extensions of the most recent major COPSE model version (Lenton et al. 2018). Full list of additions:

- Extension of forcings into Neoproterozoic and improved weathering-climate relationships (Mills et al., 2019).
- Introduction of reduced gas flux as a sink for O_2 and parallel Monte-Carlo ensemble computation (Williams et al. 2019).
- Added bioturbation effects on C burial and P recycling (van de Velde et al. 2018).
- Added marine DOC reservoir, DOC oxidation flux and input of sulfur in the Ediacaran (Shields et al. 2019)

1. Model structure

The model uses a single box to represent the atmosphere and ocean, and boxes to represent the sedimentary inventories of the different chemical species. There are no spatial dimensions.

2. Model species

Model species are shown in table 1 below. Each inventory is allowed to evolve during the model run. A schematic representation of the model is shown in Figure 1.

Description	Name	Exists in box	Size at present
Atmospheric CO_2	A	Hydrosphere	3.193×10^{18} mol C
Buried organic C	G	Crust	1.25×10^{21} mol C
Buried carbonate C	C	Crust	5.0×10^{21} mol C
Ocean sulfate	S	Hydrosphere	4×10^{19} mol S
Buried pyrite sulfur	PYR	Crust	1.8×10^{20} mol S
Buried gypsum sulfur	GYP	Crust	2.0×10^{20} mol S
Ocean phosphate	P	Hydrosphere	3.1×10^{15} mol P
Ocean nitrate	N	Hydrosphere	4.35×10^{16} mol N
Atmospheric oxygen	O	Hydrosphere	3.7×10^{19} mol O
Marine dissolved organic carbon	DOC	Hydrosphere	1.5×10^{20} mol C

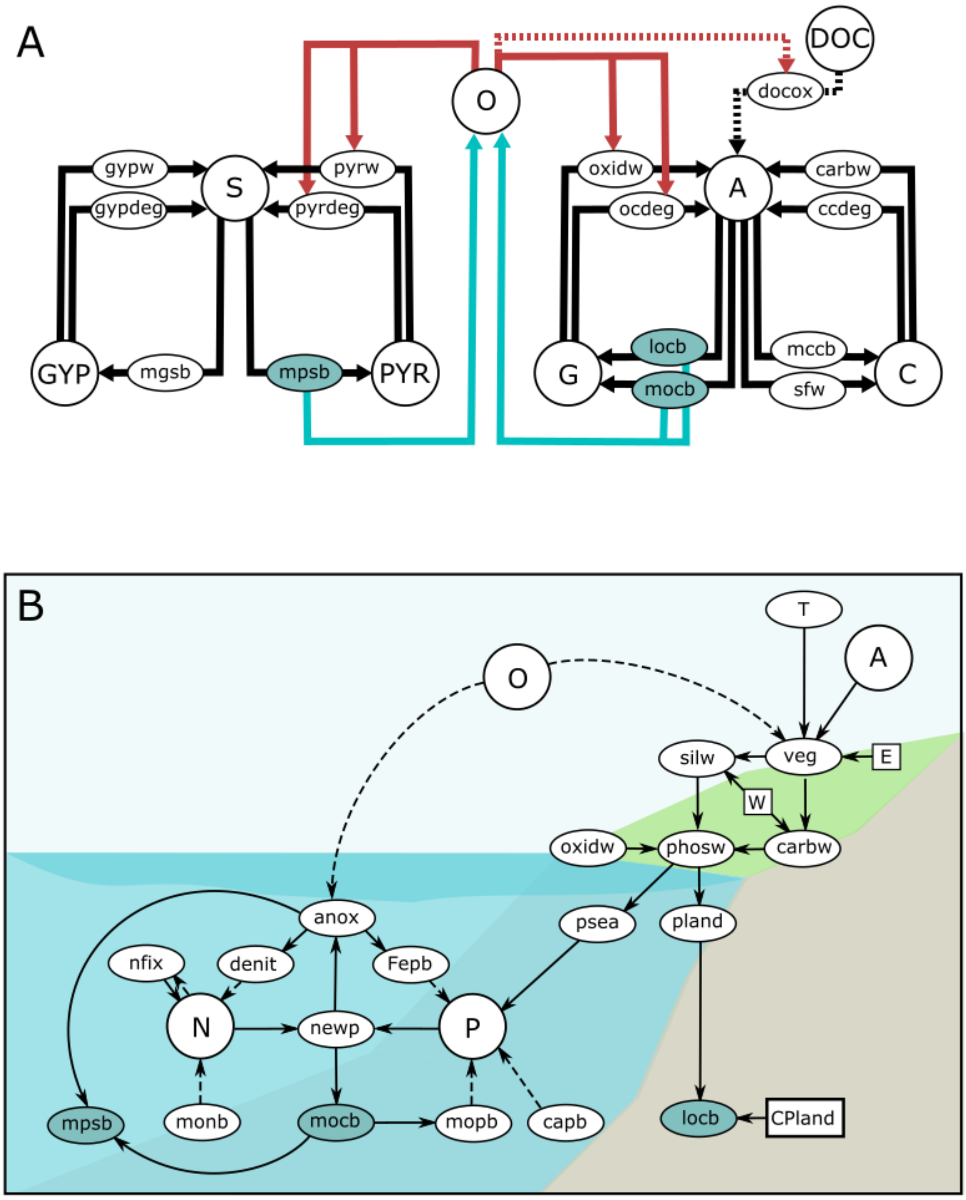

***Figure 1. COPSE model schematic: a**. Carbon, Sulphur and Oxygen cycle fluxes. Here arrows show mass fluxes, blue arrows show oxygen sources and red arrows show oxygen sinks. Dashed lines show DOC reservoir fluxes. **B**. Dynamic nutrient and biosphere system. Here arrows show positive/direct (solid) or negative/inverse (dashed) relationships between major model processes. In both diagrams blue ovals show burial fluxes of organic carbon and pyrite sulphur, which are the long-term sources of free oxygen.*

3. Differential equations

The following equations dictate the inputs and outputs of each of the model reservoirs.

Marine phosphate:

$$\frac{dP}{dx} = psea - f_{mopb} - f_{capb} - f_{fepb}$$

Atmosphere and ocean oxygen:

$$\frac{dO}{dx} = f_{locb} + f_{mocb} - f_{oxidw} - f_{ocdeg} + 2\left(f_{mpsb} - f_{pyrw} - f_{pyrdeg} - PYR_{input}\right) - f_{DOC_{ox}} - f_{reduct}$$

Hydrosphere carbon:

$$\frac{dA}{dx} = f_{oxidw} + f_{carbw} + f_{ocdeg} + f_{ccdeg} - f_{locb} - f_{mocb} - f_{mccb} - f_{sfw} + DOC_{ox} + f_{reduct}$$

Marine sulfate:

$$\frac{dS}{dx} = f_{gypw} + f_{pyrw} + f_{gypdeg} + f_{pyrdeg} - f_{mpsb} - f_{mgsb} + PYR_{input} + GYP_{input}$$

Buried organic carbon: $\frac{dG}{dx} = f_{locb} + f_{mocb} - f_{oxidw} - f_{ocdeg}$

Buried carbonate carbon: $\frac{dC}{dx} = f_{mccb} + f_{sfw} - f_{carbw} - f_{ccdeg}$

Buried pyrite S: $\frac{dPYR}{dx} = f_{mpsb} - f_{pyrw} - f_{pyrdeg} - PYR_{input}$

Buried gypsum S: $\frac{dGYP}{dx} = f_{mgsb} - f_{gypw} - f_{gypdeg} - GYP_{input}$

Marine nitrate: $\frac{dN}{dx} = f_{nfix} - f_{denit} - f_{monb}$

Marine DOC: $\frac{dDOC}{dx} = -DOC_{ox}$

4. Model fluxes

Model fluxes are described below. They generally take the form of a present day rate multiplied by a series of scalings, which include the size of the parent reservoir, forcing factors, and non-flux calculations such as temperature or the degree of marine anoxia.

Degassing: sediment to hydrosphere

Carbonate C degassing: $f_{ccdeg} = k_{ccdeg} \cdot D \cdot B \cdot \left(\frac{C}{C_0}\right)$

Organic C degassing: $f_{ccdeg} = k_{ocdeg} \cdot D \cdot \left(\frac{G}{G_0}\right)$

Pyrite S degassing: $f_{pyrdeg} = k_{pyrdeg} \cdot D \cdot \left(\frac{PYR}{PYR_0}\right)$

Gypsum S degassing: $f_{gypdeg} = k_{gypdeg} \cdot D \cdot \left(\frac{GYP}{GYP_0}\right)$

Weathering: sediment to hydrosphere

Oxidative C weathering: $f_{oxidw} = k_{oxidw} \cdot U^{Usil} \cdot \left(\frac{G}{G_0}\right) \cdot \left(\frac{O}{O_0}\right)^{0.5}$

Carbonate C weathering: $f_{carbw} = k_{carbw} \cdot U^{Ucarb} \cdot \left(\frac{C}{C_0}\right) \cdot CA \cdot PG \cdot f_{biota} \cdot g_T$

Pyrite S weathering: $f_{pyrw} = k_{pyrw} \cdot U^{Usil} \cdot \left(\frac{PYR}{PYR_0}\right)$

Gypsum S weathering: $f_{gypw} = k_{gypw} \cdot \frac{f_{carbw}}{k_{carbw}} \cdot \left(\frac{GYP}{GYP_0}\right)$

Pyrite S additional input: $PYR_{input} = k_{pyrw} \cdot EVAP$

Gypsum S additional input: $GYP_{input} = k_{gypw} \cdot EVAP$

Phosphorus weathering:

$$f_{phosw} = k_{phosw} \cdot EP \cdot \left\{kp_{sil}\left(\frac{f_{silw}}{k_{silw}}\right) + kp_{carb}\left(\frac{f_{carbw}}{k_{carbw}}\right) + kp_{ox}\left(\frac{f_{oxidw}}{k_{oxidw}}\right)\right\}$$

Burial: hydrosphere to sediment

Marine organic C burial: $f_{mocb} = k_{mocb} \cdot \left(\frac{newp}{newp_0}\right)^2 \cdot CB$

Land organic C burial: $f_{locb} = k_{locb} \cdot \left(\frac{p_{land}}{p_{land_0}}\right) \cdot CP_{land}$

Marine carbonate burial: $f_{mccb} = f_{silw} + f_{carbw}$

Seafloor weathering: $f_{sfw} = k_{sfw} \cdot f_{T_{sfw}} \cdot D$

Marine pyrite S burial:

$$f_{mpsb} = k_{mpsb} \cdot \left(\frac{S}{S_0}\right) \cdot \left(\frac{O_0}{O}\right) \cdot \left(\frac{f_{mocb}}{k_{mocb}}\right) + \frac{4}{5}(PYR_{input} + GYP_{input})$$

Marine gypsum S burial:

$$f_{mgsb} = k_{mgsb} \cdot \left(\frac{S}{S_0}\right) + \frac{1}{5}(PYR_{input} + GYP_{input})$$

Fe-phosphate burial: $f_{fepb} = k_{fepb} \cdot \left(\frac{1-ANOX}{k_{oxfrac}}\right) \cdot \left(\frac{P}{P_0}\right)$

Ca-phosphate burial: $f_{capb} = k_{capb} \cdot \left(\frac{f_{mocb}}{k_{mocb}}\right)$

Organic P burial: $f_{mopb} = f_{mocb}\left(\left(\frac{f_{biot}}{CP_{biot}}\right) + \left(\frac{1-f_{biot}}{CP_{lam}}\right)\right)$

Organic N burial: $f_{monb} = \left(\frac{f_{mocb}}{CN_{sea}}\right)$

Internal fluxes:

Granite weathering: $f_{granw} = k_{granw} \cdot U^{kw_{sil}} \cdot GA \cdot PG \cdot f_{biota} \cdot f_{T_{gran}}$

Basalt weathering: $f_{basw} = k_{basw} \cdot BA \cdot PG \cdot f_{biota} \cdot f_{T_{bas}}$

Silicate weathering: $f_{silw} = f_{granw} + f_{basw}$

Denitrification: $f_{denit} = k_{denit} \cdot \left(1 + \left(\frac{ANOX}{1-k_{oxfrac}}\right)\right) \cdot \left(\frac{N}{N_0}\right)$

Nitrogen fixation:

$$f_{nfix} = \begin{cases} k_{nfix} \cdot \left(\frac{P-\frac{N}{16}}{P_0-\frac{N_0}{16}}\right)^2 & , \quad \frac{N}{16} < P \\ 0 & , \quad \frac{N}{16} \geq P \end{cases}$$

Marine new production: $newp = 117 \cdot \min\left(\frac{[N]}{16}, [P]\right)$

P flux to land: $p_{land} = k_{landfrac} \cdot VEG \cdot f_{phosw} \cdot \left(k_{aq} + \left(1 - k_{aq}\right) \cdot COALF\right)$

P flux to sea: $p_{sea} = f_{phosw} - p_{land}$

5. Non-flux calculations

Carbon atmospheric fraction $atfrac = atfrac_0 \cdot \left(\frac{A}{A_0}\right)$

Relative atmospheric CO_2: $RCO_2 = (\frac{A}{A_0}) \cdot \left(\frac{atfrac}{atfrac_0}\right)$

Atmospheric O_2 mixing ratio: $O_{2_{mr}} = \frac{\frac{O}{O_0}}{\frac{O}{O_0} + k_{mr}}$

Global average surface temperature: $T_{gast} = 15 + climsens \cdot \frac{\log RCO_2}{\log(2)} - k_l \cdot \left(\frac{t}{570}\right)$

Average temperature for weathering: $T_{surf} = T_{gast} \cdot k_{Tgradm} + k_{Tgradc}$

Granite weathering T effect:

$$f_{T_{gran}} = e^{0.0724\left(T_{surf}-15\right)} \cdot \left(1 + 0.038 \cdot \left(T_{surf} - 15\right)\right)^{0.65}$$

Basalt weathering T effect:

$$f_{T_{bas}} = e^{0.0608\left(T_{surf}-15\right)} \cdot \left(1 + 0.038 \cdot \left(T_{surf} - 15\right)\right)^{0.65}$$

Carbonate weathering T effect: $g_T = 1 + 0.087\left(T_{surf} - 15\right)$

Seafloor weathering T effect: $f_{T_{sfw}} = e^{0.0608\left(T_{surf}-15\right)}$

Temperature effect on vegetation: $V_T = 1 - \left(\frac{T_{surf}-25}{25}\right)^2$

CO_2 effect on vegetation: $V_{CO_2} = \frac{CO_2ppm - p_{minim}}{p_{half} + p_{atm} - p_{minim}}$

Oxygen effect on vegetation: $V_{O_2} = 1.5 - 0.5\left(\frac{O}{O_0}\right)$

Overall limitation of terrestrial NPP: $V_{NPP} = 2 \cdot EVO \cdot V_T \cdot V_{CO_2} \cdot V_{O_2}$

Fire ignition probability scaling: $ignit = \min\left(max\left(48 \cdot O_{2_{mr}} - 9.08,\ 0\right)\right)$

Fire effect on terrestrial biomass: $firef = \frac{k_{fire}}{k_{fire} - 1 + ignit}$

Mass of terrestrial biota: $VEG = V_{NPP} \cdot firef$

Terrestrial biota weathering effect:

$$f_{biota} = \{1 - \min(V \cdot W, 1)\} \cdot k_{plantenhance} \cdot RCO_2{}^{0.5} + V \cdot W$$

Marine P concentration: $[P] = 2.2\left(\frac{P}{P_0}\right)$

Marine N concentration: $[N] = 30.9\left(\frac{N}{N_0}\right)$

Marine anoxic fraction: $ANOX = \frac{1}{1+e^{-k_{anox}\cdot\left(k_u\left(\frac{newp}{newp_0}\right)-\left(\frac{O}{O_0}\right)\right)}}$

Hydrothermal reductant input: $f_{reduct} = k_{reduct} \cdot D$

Marine DOC oxidation:

$$f_{DOC_{ox}} = \begin{cases} 0 & , \quad DOC < 1 \times 10^{12}\ mol \\ -\dfrac{k_{DOC}}{1 + e^{-a_{DOC}(1-ANOX-c_{DOC})}}\left(\dfrac{DOC}{DOC_0}\right) & , \quad DOC \geq 1 \times 10^{12}\ mol \end{cases}$$

6. Forcing factors

All model forcing factors are detailed below. All have the value of 1 at the present day and are nondimensional.

Description	**Name**	**Based on**
Tectonic degassing	D	Reconstructed subduction zone and rift lengths
Continental uplift	U	Sediment abundance
Carbonate burial depth	B	Fossil record
Basalt silicate exposed area	BA	Degassing and flood basalt emplacements
Granite silicate exposed area	GA	Paleogeographic reconstruction
Land plant evolution	EVO	Fossil record
Land plant weathering effect	W	Experimental and field studies
Land plant C:P ratio	CP_{land}	Sedimentary coal deposition record
Selective P weathering	EP	Experimental studies
Paleogeog. weathering effect	PG	Climate modelling
Coal basin depositional fraction	$COALF$	Coal basin depositional area
Evaporite weathering spike	$EVAP$	Evidence for evaporite exposure
Bioturbation	f_{biot}	Burrowing depth reconstruction
Bioturbation effect on C burial	CB	Field studies

7. Fixed parameters

Fixed parameters are shown in the table below.

Description	Name	Value
Present day marine organic carbon burial	k_{mocb}	2.5×10^{12} mol C yr^{-1}
Present day land organic carbon burial	k_{locb}	2.5×10^{12} mol C yr^{-1}
Present day organic carbon degassing	k_{ogdeg}	1.25×10^{12} mol C yr^{-1}
Present day organic carbon weathering	k_{oxidw}	3.35×10^{12} mol C yr^{-1}
Present day carbonate burial	k_{mccb}	2.125×10^{13} mol C yr^{-1}
Present day carbonate degassing	k_{ccdeg}	1.5×10^{13} mol C yr^{-1}
Present day carbonate weathering	k_{carbw}	8×10^{12} mol C yr^{-1}
Present day seafloor weathering	k_{sfw}	1.75×10^{12} mol C yr^{-1}
Present day basalt weathering	k_{basw}	3.975×10^{12} mol C yr^{-1}
Present day granite weathering	k_{granw}	9.275×10^{12} mol C yr^{-1}
Present day silicate weathering	k_{sil}	1.325×10^{13} mol C yr^{-1}
Present day phosphorus weathering	k_{phosw}	4.25×10^{10} mol P yr^{-1}
Present day pyrite burial	k_{mpsb}	7×10^{11} mol S yr^{-1}
Present day gypsum burial	k_{mgsb}	1.5×10^{12} mol S yr^{-1}
Present day pyrite weathering	k_{pyrw}	4.5×10^{11} mol S yr^{-1}
Present day gypsum weathering	k_{gypw}	1×10^{12} mol S yr^{-1}
Present day pyrite degassing	k_{pyrdeg}	2.5×10^{11} mol S yr^{-1}
Present day gypsum degassing	k_{gypdeg}	5×10^{11} mol S yr^{-1}
Present day Ca-P burial	k_{capb}	2×10^{10} mol P yr^{-1}
Present day Fe-P burial	k_{fepb}	1×10^{10} mol P yr^{-1}
Present day nitrogen fixation	k_{nfix}	8.67×10^{12} mol N yr^{-1}
Present day denitrification	k_{denit}	4.3×10^{12} mol N yr^{-1}
Present day hydrothermal reductant input	$k_{reductant}$	4×10^{11} mol O_2 eq. yr^{-1}
Present day ocean oxic fraction	k_{oxfrac}	0.9975
Atmospheric O_2 mixing ratio conversion	k_{mr}	3.762
Pre-plant weathering enhancement factor	$k_{preplant}$	0.25
Uplift effect on carbonate weathering	kw_{carb}	0.9
Uplift effect on silicate weathering	kw_{sil}	0.33

Phosphorus input from silicate weathering	kp_{sil}	0.8
Phosphorus input from carbonate weathering	kp_{carb}	0.14
Phosphorus input from organic carbon oxidation	kp_{ox}	0.06
Fraction of phosphorus buried on land	$k_{landfrac}$	0.0588
C:P ratio of buried marine organics	CP_{sea}	250
C:N ratio of buried marine organics	CN_{sea}	37.5
Present day atmospheric fraction of CO_2	$atfrac_0$	0.01614
Long-term climate sensitivity	$climsens$	5 K
Solar luminosity difference at 570 Ma	k_l	7.4 W m^{-2}
Latitudinal temperature gradient slope	k_{Tgradm}	0.66
Latitudinal temperature gradient constant	k_{Tgradc}	4.95
Vegetation CO_2 minimum	$p_{minimum}$	10 ppm
Vegetation CO_2 half saturation	p_{half}	183.6 ppm
Fire effect on vegetation biomass	k_{fire}	3
Terrestrial-aquatic organic matter burial fraction	k_{aq}	0.8
Steepness of anoxia transition	k_{anox}	10
Marine oxygen utilization parameter	k_u	0.4
DOC oxidation slope parameter	a_{DOC}	300
DOC oxidation threshold parameter	c_{DOC}	0.5
DOC oxidation rate parameter	k_{DOC}	1×10^{14} mol C yr^{-1}
C:P burial ratio bioturbated sediment	CP_{biot}	250
C:P burial ratio laminated sediment	CP_{lam}	1000

8. References

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