

Title: Production of Neoproterozoic banded iron formations in a partially ice-covered ocean

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Abstract:

Neoproterozoic snowball Earth events challenge our understanding of the climate system. Specifically, it is debated whether the oceans were completely ice-covered ('hard' snowball) or whether the tropical ocean was ice-free ('soft' snowball), with implications for interpretations of the geochemical record and the survival of photosynthetic life. Banded iron formations associated with the older and longer Sturtian glaciation are considered evidence for a hard snowball, in which Fe²⁺ accumulated in the anoxic ocean interior. Here, using a state-of-the-art ocean model including representation of thick sea glaciers and Neoproterozoic biogeochemistry, we find that ocean circulation in a soft snowball yields iron deposition at the interface between ferruginous and oxygenated water masses, in spatial patterns that agree with the observed distribution of Sturtian banded iron formations.

Main Text:

Banded iron formations (BIFs) are iron- and silica-rich sedimentary rocks, the genesis of which is thought to require low oceanic O₂ concentrations, in agreement with their occurrence before ~1800 million years ago (Ma), when Earth's oceans are proposed to have been anoxic^{1,2}. An exception to this pattern of occurrence, Neoproterozoic (1000–541 Ma) iron formations were deposited when atmospheric O₂ levels were 1–10% of today's³. Neoproterozoic BIFs occur in association with the earlier and longer of two low-latitude glaciations, the so-called 'snowball Earth' events^{4–7}, in which the ocean and continents are suggested to have been ice-covered for tens of millions of years^{8,9}. Widespread sedimentary and geochemical evidence supports the occurrence of the Neoproterozoic pan-glacials, though the exact nature of these events, including the meridional extent of marine ice is still debated. The Neoproterozoic BIFs have been suggested to support a 'hard' snowball^{4,5}, in which pole-to-pole ice cover renders the ocean anoxic, allowing the accumulation of ferrous iron (Fe²⁺). Although viable explanations for the survival of the photosynthesis-based marine biosphere through a hard snowball have been proposed¹⁰, such an extreme climate poses a serious challenge to life⁵. Alternatively, a 'soft' snowball⁷ with tropical swaths of open water does not pose a similar challenge to the biosphere, but O₂ input to the ocean

40 by air-sea gas exchange may have prevented the mobility of Fe^{2+} required for widespread
 41 deposition of BIFs^{10,11}.

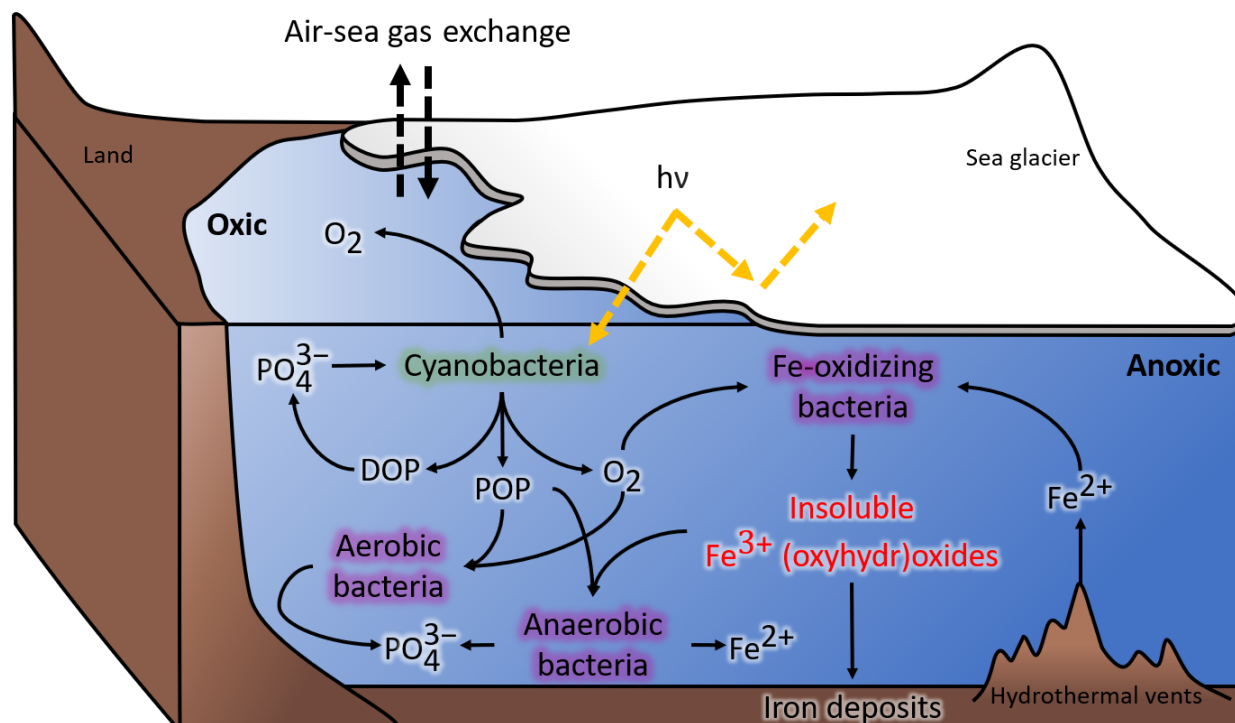


Fig. 1. Schematic representation of the biogeochemical model. Cyanobacteria, limited by low seawater $[\text{PO}_4^{3-}]$, produce organic matter (dissolved organic phosphorus, DOP and particulate organic phosphorus, POP) and O_2 in ice-free regions. Aerobic respiration of the organic matter consumes some of the O_2 , as do Fe^{2+} -oxidizing bacteria, which produce Fe^{3+} oxides. The fraction of Fe^{3+} oxides that is not used by anaerobic bacteria to remineralize organic matter settles to the seabed, forming iron deposits.

42 We revisit the notion that BIFs cannot precipitate under soft snowball conditions using a state-of-
 43 the-art ocean general circulation model (GCM), which includes the representation of thick sea
 44 glaciers that extend to a prescribed latitude and a new biogeochemical model tailored to the
 45 Neoproterozoic (Fig. 1; see Methods and Supplementary Information, SI, for details). In the model
 46 biogeochemical iron cycle, a hydrothermal source of Fe^{2+} (estimated to be 0.36 Tmol y^{-1} , SI) at
 47 mid-oceanic ridges is balanced by oxidation and deposition of ferric iron (Fe^{3+}) oxides, which
 48 occurs where Fe^{2+} -bearing waters meet oxygenated waters. The location of such reaction and
 49 deposition fronts depends on the transport of Fe^{2+} and O_2 from their hydrothermal and
 50 photosynthetic sources, respectively. Patterns of phosphate concentration ($[\text{PO}_4^{3-}]$) and $[\text{O}_2]$
 51 obtained in an idealized model configuration (SI) with a 100% modern $[\text{PO}_4^{3-}]$ and a stoichiometry
 52 of organic matter oxidation (O_2 consumed to P released) representative of modern marine organic
 53 matter are consistent with today's ocean (Fig. S1), and atmospheric O_2 stabilizes at $\sim 62\%$ present
 54 atmospheric levels.

55 Previous ocean-atmosphere-cryosphere modelling efforts have identified multiple stable climate
 56 states in which ice-free ocean exists equatorward of latitudes between 60° and 5° ^{11,12}. Accordingly,
 57 we examined a completely ice-free ocean and partially glaciated oceans in which the ice-free

region extended from 30°S to 30°N and 12°S to 12°N. The size of the marine PO_4^{3-} pool during snowball Earth episodes is unknown, though several factors lead to expectations of lower-than-present seawater $[\text{PO}_4^{3-}]$. These include low continental weathering rates, photosynthetic carbon fixation and nutrient uptake during the glacial advance and in regions of open water, limited organic matter remineralization in a partly ice-covered ocean, and PO_4^{3-} adsorption onto iron oxides in an ocean with relatively high Fe^{2+} concentrations. Hence, we examined iron deposition patterns at 100%, 10%, 3% and 1% the mean present-day seawater $[\text{PO}_4^{3-}]$ (3 μM), the lower three of which are within the proposed range required to sustain low Proterozoic atmospheric O_2 levels^{13,14}, and consistent with low Proterozoic primary productivity¹⁵. With these parameter combinations, cases in which 90% or more of the iron deposited within the model grid points corresponding to the hydrothermal Fe^{2+} sources were considered less viable for BIF deposition on multiple continental margins, as suggested by the sedimentary record¹⁰.

We first discuss the ocean's circulation at the three ice-cover extents considered here. The depth-averaged velocity field (the barotropic flow) in the ice-free ocean (Fig. S2A) indicates the presence of a strong eastward zonal jet ($\sim 10 \text{ cm s}^{-1}$) in the northern high latitudes. The flow everywhere else in the ocean is much weaker ($\sim 1 \text{ cm s}^{-1}$), especially in the young ocean basins formed during the breakup of the supercontinent Rodinia ($\sim 0.1 \text{ cm s}^{-1}$). The barotropic flow in the ocean weakens with an increase in the ice cover, particularly at the high latitudes (Fig. S2B-C). The meridional overturning circulation in the ice-free case is predominantly driven by sinking of cold water in the southern high latitudes and upwelling everywhere else (Fig. S2D). An increase in the extent of ice cover modifies the overturning patterns drastically, and in contrast to the ice-free ocean, the circulation in both the 30°S to 30°N and 12°S to 12°N ice-free region cases is most intense in the equatorial region near the ocean surface (Fig. S2E-F).

The zonally averaged $[\text{O}_2]$ distributions vary with the extent of the ice-free region (Fig. 2A-C). As an example, when the mean seawater $[\text{PO}_4^{3-}]$ is 3% present-day, the mean $[\text{O}_2]$ in the ocean is 1.6 μM , 4.7 μM and 17 μM in the 12°S to 12°N ocean, 30°S to 30°N ocean and the completely ice-free ocean, respectively, which is \sim hundred-fold lower than today, due to limitation of primary productivity by the low PO_4^{3-} levels. In an ice-free ocean, the mean $[\text{Fe}^{2+}]$ is $\sim 0.01 \text{ nM}$ and Fe^{2+} is restricted to the vicinity of the hydrothermal ridges (Fig. 2D). However, the low $[\text{O}_2]$ in the partially glaciated oceans allows Fe^{2+} build-up, with a $[\text{Fe}^{2+}]$ range of 0 to $>1000 \text{ nM}$, and a mean of 4.8 nM and 4 nM for the snowballs with an ice-free region from 12°S to 12°N and 30°S to 30°N, respectively (Fig. 2E-F). With the model $[\text{Fe}^{2+}]$ and $[\text{O}_2]$ fields, we compared model iron deposition rates and spatial patterns with estimates based on Neoproterozoic BIFs. To this end, we compiled reports of Sturtian BIFs^{16–21} and used the fractional concentration of hematite in the samples, their density, thickness and the approximate deposition duration to conservatively estimate that iron deposition rates during the Sturtian glaciation were between ~ 0.003 and $\sim 0.4 \text{ mol m}^{-2} \text{ y}^{-1}$ (SI). The distributions of model iron deposition rates show precipitation away from the hydrothermal sources that is within the range of calculated BIF deposition rates for the 12°S to 12°N ocean and 30°S to 30°N ocean, when the mean $[\text{PO}_4^{3-}]$ is 1–10% of today's (Figs. 2H-I, S3H-I and S4H-I). We note that this model consistency with the observations is achieved at $[\text{Fe}^{2+}]$ \sim two orders of magnitude lower than previously thought to be required for widespread Neoproterozoic BIF deposition^{22,23}. Thus, we suggest that Fe^{2+} supply and mobility, not concentration, are the actual requirements for widespread BIF deposition, in the Neoproterozoic and over Earth history in general. At modern mean seawater $[\text{PO}_4^{3-}]$, most of the ocean interior is

102 oxygenated, and >95% of the iron oxide precipitation occurs only in the model grid points
 103 corresponding to the hydrothermal Fe^{2+} sources (Figs. 3A and S5G-I).

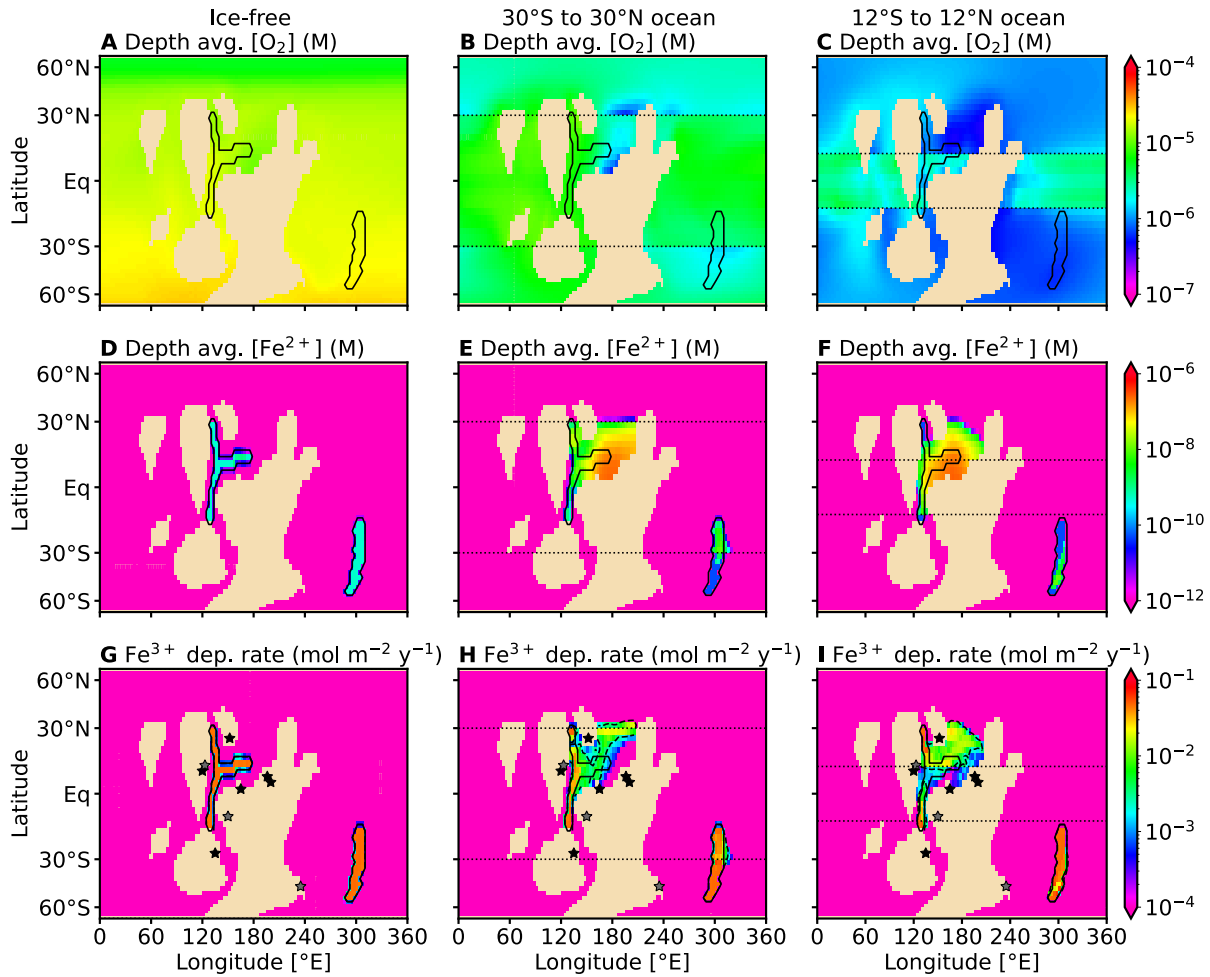


Fig. 2. Results of the 3D ocean model with a mean seawater $[\text{PO}_4^{3-}]$ of $0.1 \mu\text{M}$ (3% modern). (A)-(C) Depth-averaged distribution of $[\text{O}_2]$ and (D)-(F) $[\text{Fe}^{2+}]$ and the (G)-(I) spatial distribution of iron deposition rates in snowballs with different meridional extents of sea glaciers. Iron deposition rates are calculated by vertical integration of net Fe^{2+} oxidation profiles. The solid black contours mark the sites of hydrothermal Fe^{2+} injection, based on estimated locations of mid-oceanic ridges. The dotted black horizontal lines denote the extent of the ice-free region. The dashed black lines in (G)-(I) enclose the region where iron deposition rates are within the range estimated from Neoproterozoic BIFs. The stars indicate the approximate location of BIFs associated with the Sturtian pan-glacial. BIFs denoted by the gray stars have been excluded from the estimation of BIF deposition rate (SI).

104 Multiple BIF deposition sites emerge in the simulations with 1-10% modern $[\text{PO}_4^{3-}]$ (Figs. 2H-I,
 105 S3H-I and S4H-I), several of which are located in the deep ocean away from the continents. BIFs
 106 deposited at these deep sites are unlikely to be preserved, in contrast with the BIFs deposited on
 107 the continental margins facing the young ocean basins that formed during the breakup of Rodinia.
 108 This is consistent with the clustering of all but one of the BIFs dated to the Sturtian pan-glacial

around these young ocean basins. The paleogeographic reconstruction does not resolve inland seas, which host some of the Neoproterozoic BIFs, but we postulate that iron deposition is expected also in such seas that were connected to the basins represented in the model (e.g., apparent inland BIF locations in Fig. 2G-I). To assess the agreement between iron deposition patterns obtained in different simulations with the spatial distribution of Neoproterozoic BIFs, we calculated the fraction of the continental margin area in the vicinity of approximate BIF locations [Fig. S6, Ref. 10,24,25] where model iron deposition rates are within the range inferred from the compilation of Sturtian BIFs.

Our simulations show that the spatial pattern of iron precipitation is sensitive to both the extent of ice cover and the mean seawater $[\text{PO}_4^{3-}]$. For example, at 3% modern $[\text{PO}_4^{3-}]$ levels, reaction fronts between O_2 -bearing and Fe^{2+} -bearing water masses result in a spatial distribution of iron oxidation and deposition such that ~18% of continental margins under consideration are viable for precipitation of BIFs in the snowballs with 30°S to 30°N and 12°S to 12°N ice-free ocean, while practically none (<3%) of the margins are found to be suitable for precipitation of BIFs in the ice-free case (Fig. 3B). More generally, in simulations with mean seawater $[\text{PO}_4^{3-}]$ between 1% and 10% modern levels, O_2 -bearing and Fe^{2+} -bearing water masses meet in the vicinity of Sturtian BIFs for the two partially ice-covered oceans considered. However, neither the ice-free ocean nor the partially ice-covered oceans show an affinity for precipitation of BIFs at modern $[\text{PO}_4^{3-}]$ levels, and all of the Fe^{2+} is deposited close to the hydrothermal source (Fig. 3A and Fig. S5G-I). These results suggest that iron deposition patterns and rates consistent with the Sturtian BIFs can be obtained in partially ice-covered oceans with lower-than-present seawater $[\text{PO}_4^{3-}]$ (<~10% modern levels). Due to model uncertainties, we stop short of attempting to identify the precise $[\text{PO}_4^{3-}]$ levels and meridional ice extent that yield the most consistent iron deposition patterns.

Climate models of different degrees of complexity show that Earth's climate can exhibit both soft and hard snowball states^{11,26–28}. Perturbation of the soft snowball state in existing climate models leads to deglaciation or full glaciation (hard snowball)²⁹. Nevertheless, evidence of a productive and diverse marine ecosystem during both pan-glacials, which would be challenging to achieve under hard snowball conditions, warrants a critical examination of the soft snowball's viability¹⁰.

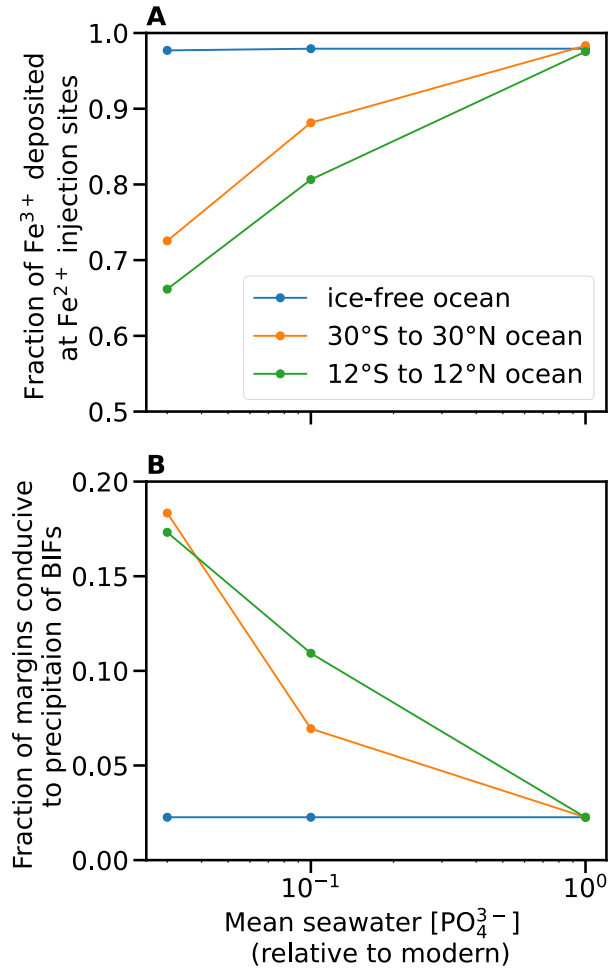


Fig. 3. (A) Fraction of Fe^{3+} deposited at the Fe^{2+} injection site. (B) Fraction of continental margins in the vicinity of Sturtian BIFs that are viable for model precipitation of BIFs.

The hard snowball state^{27,28,30,31} is suggested to have led to an anoxic ocean interior in which dissolved Fe²⁺ accumulated, to be oxidized and deposited only in spatially limited regions where O₂ was available, such as the interface between anoxic seawater and oxygenated meltwater plumes near the ice grounding line^{10,32}. Under such a scenario, precipitation of iron oxides and production of BIFs is expected on all glaciated continental margins¹⁰, in contrast with the occurrence of Neoproterozoic BIFs only on some continental margins (Fig. 2G-I). Our analysis shows that a phosphate-deficient ocean is conducive to production of BIFs for different extents of marine ice-cover, wherever Fe²⁺-bearing and oxygenated water masses meet. We find several combinations of [PO₄³⁻] and marine ice-cover that predict BIF deposition at multiple sites, including on the continental margins facing the young ocean basins that formed during the fragmentation of Rodinia, consistent with the observed distribution of Sturtian BIFs (Figs. 2H-I, S3H-I and S4H-I). Though we cannot predict the meridional extent of marine ice cover with the present model, our findings prompt investigations of the plausibility of a soft snowball state in more complete climate models, which include atmosphere-ocean-cryosphere coupling and a realistic continental configuration. Lastly, our findings highlight the role of Fe²⁺ fluxes into, and mobility within, Earth's oceans as the necessary conditions for widespread BIF deposition. In contrast with previous suggestions, a high Fe²⁺ concentration is found unnecessary.

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Methods:

Ocean

We use the Massachusetts Institute of Technology General Circulation Model (MITgcm)³³ to perform the simulations discussed in this study. The MITgcm is a free, open-source, general circulation model in which a finite volume method is implemented to solve the equations of fluid motion (i.e., momentum equations, continuity equation, and diffusion equations of temperature and salinity and equation of state). We employ the full equation of state provided in the MITgcm, MDJWF³⁴, and make the hydrostatic and Boussinesq approximations. The model uses a spherical grid spanning 72°S to 72°N with a resolution of 3° in latitude and has 37 vertical levels spanning a depth of 3000 m (height of vertical levels from the surface to the bottom: 10 m, 12 m, 16 m, 20 m, 25 m, 32 m, 40 m, 50 m, 60 m, 75 m, 80 m, 2 levels × 90 m, and 24 levels × 100 m). The longitudinal resolution is 3° as well, with 20 grid points in the idealized box configuration simulations and 120 grid points in the Neoproterozoic simulations. Unresolved eddies in the ocean are parameterized using the Gent-McWilliams/Redi (GM-Redi) scheme^{35,36}, and the background diffusion coefficient is set to 1000 m² s⁻¹. The lateral and vertical viscosities are set to 5 × 10⁵ m² s⁻¹ and 10⁻³ m² s⁻¹, and the vertical diffusivity and implicit vertical diffusivity for convection are set to 10⁻⁴ m² s⁻¹ and 10 m² s⁻¹. We also use a nondimensional grid-dependent biharmonic viscosity of 0.1 to suppress the grid-scale noise. The vertical diffusivity for biogeochemical variables is set to 3 × 10⁻⁵ m² s⁻¹. The third-order direct space-time flux limiter advection scheme (no. 33) is used for both momentum tracers and biogeochemical variables. The flat bathymetry ocean is subjected to a constant geothermal heat flux of 0.1 W m⁻²³⁷. At the surface, the ocean is forced by a zonal wind stress that changes for the different meridional extent of the sea glaciers. The wind stress field for the idealized box configuration simulations is similar to the present-day, and for ice-free Neoproterozoic simulation is the zonally averaged wind stress obtained from fully coupled ocean-atmosphere simulation of Cambrian-Precambrian boundary³⁸. The wind stress fields for our snowball simulation conditions (spatial grid and ice opening) are generated by setting the wind stress over the ice-covered region to zero and using zonally averaged wind stress profiles over the ice-free region that are based on results from simulations of partially glaciated climate states carried out on fully coupled general circulation models^{39,40}. The temperature at the surface (z = 0 m) is restored to temperature fields that are also generated on the basis of coupled model results^{11,12}. Fig. S7A-B show the zonally-averaged restoration temperature and wind stress over the ocean for different meridional extents of sea glaciers. Fig. S7C shows the evaporation minus precipitation (E-P) fields over the ocean in the box simulations and in the Neoproterozoic ice-free simulations, these idealized E-P fields are generated by introducing a small asymmetry to the E-P field described in Ref. ⁴¹. In both the snowballs, melting under the sea glaciers is balanced by evaporation in the ice-free region, which conserves the mean salinity of the ocean.

Sea glaciers

Given the uncertainties regarding the thickness of ice during the Neoproterozoic glaciations, we estimate ice thickness using a simplified energy balance. A similar calculation has been used to estimate the thickness of ice on Jupiter's moon Europa⁴². We begin by assuming that a constant geothermal flux of 0.1 W m⁻² is applied to the ocean bottom and that the component of tidal heating in both the ice and ocean is negligible. Moreover, the temperature within the ice varies linearly with depth. In this case, the thickness of ice is given by:

$$h = \rho_i c_{p,i} \kappa \frac{T_f - T_i}{Q},$$

where ρ_i is the density, $c_{p,i}$ is the heat capacity and κ is the temperature diffusion constant of ice. T_f and T_i are the freezing and surface temperature of the ice, and Q is the internal heat flux (the geothermal heat flux). T_f is a function of temperature and salinity:

$$T_f = 273.16 + 0.0901 - 0.0575 \times S - 7.61 \times 10^{-8} \times P_b,$$

where S is the salinity and $P_b = \rho_i g h$ is the pressure at the bottom of the ice. The gradient in solar insolation yields a gradient in the surface temperature of the ice, and in turn, a gradient in ice thickness. This gradient in ice thickness causes it to flow smoothly, thereby partially relaxing the gradient⁴³. Hence, we approximate the thickness of the ice as the meridional average of h calculated using the prescribed temperature field. Under these assumptions, the ice thickness can iteratively be estimated as:

$$\langle h \rangle_{j+1} = \rho_i c_{p,i} \kappa \frac{\langle T_f \rangle_j - \langle T_i \rangle}{Q}.$$

The algorithm⁴², when initialized from the typical seawater freezing temperature of 271 K and the surface temperature fields such as the ones given in Ref. ^{11,12}, predicts a certain ice thickness, which implies a certain P_b value and a modified freezing temperature. For the temperature fields shown in Fig. S7A, the ice thickness converges to 490 m and 253 m below the sea surface within a few iterations for snowballs with 12°S to 12°N ice-free ocean and 30°S to 30°N ice-free ocean, respectively. To avoid any numerical artifacts that may arise from partially filled grid-cells, we use a thickness of 510 m and 265 m below the sea surface for the snowballs with 12°S to 12°N ocean and 30°S to 30°N ocean respectively. The effect of this sea glacier is simulated using the SHELFICE package⁴⁴. Unlike the SEAICE package, the SHELFICE package in the MITgcm can handle a thick sea glacier spanning over multiple vertical levels, which makes it better suited to snowball Earth modeling.

Biogeochemical cycle

The biogeochemical model presented here is based on Refs. ^{45,46}, implemented in the MITgcm using a combination of the ‘GCHEM’ and ‘DIC’ packages. (https://mitgcm.readthedocs.io/en/latest/phys_pkgs/phys_pkgs.html#biogeochemistry-packages). MITgcm’s biogeochemical setup (GCHEM+DIC), in its default configuration, considers coupled cycles of carbon, oxygen, phosphorus and alkalinity. These cycles are expressed using five variables that do not affect the physical circulation: dissolved inorganic carbon (DIC), alkalinity (Alk), phosphate (PO_4^{3-}), dissolved organic phosphorus (DOP), and oxygen (O_2). The velocity fields and eddy diffusivities calculated by the physical model are used to transport these compounds, which are additionally produced and consumed locally by biogeochemical reactions, as described below.

For this study, we focus on the phosphorus and oxygen cycles. Additionally, we incorporate an iron (Fe^{2+}) cycle and a well-mixed atmospheric box to the pre-existing setup. The atmospheric box only keeps track of the total O_2 in the atmosphere. The values of all parameters described below are provided in Table S1. The sources and sinks for each tracer are summarized below:

$$\frac{\partial}{\partial t} [\text{PO}_4^{3-}] = -J_{\text{production}} - \frac{\partial}{\partial z} F_P + \kappa_{\text{remin}} [\text{DOP}],$$

$$\frac{\partial}{\partial t} [\text{DOP}] = f_{\text{DOP}} J_{\text{production}} - \kappa_{\text{remin}} [\text{DOP}],$$

$$\frac{\partial}{\partial t} [O_2] = \frac{k_w}{\Delta z_{\text{surf}}} \left(\frac{n_{O_2}^{\text{model atmosphere}}}{n_{O_2}^{\text{present-day}}} [O_2]_{\text{sat}} - [O_2]_{\text{surf}} \right) + f([O_2]) \times \left(r_{O_2:P} \frac{\partial}{\partial t} [PO_4^{3-}] \right) - k_{Fe} [Fe^{2+}],$$

$$\frac{\partial}{\partial t} [Fe^{2+}] = F_{Fe}^{\text{hydrothermal}} - k_{Fe} [Fe^{2+}] - \frac{\partial}{\partial z} F_{Fe}^{\text{recycle}},$$

where square brackets denote concentration, $J_{\text{production}}$ is primary production, $\frac{\partial}{\partial z} F_P$ is the partial derivative with depth of the particulate organic phosphorus sinking flux, and κ_{remin} is the rate constant of remineralization of DOP to PO_4^{3-} . The gas transfer velocity for O_2 is given by k_w and Δz_{surf} is the thickness of the surface layer. The moles of O_2 in the model atmosphere and the present-day atmosphere are given by $n_{O_2}^{\text{model atmosphere}}$ and $n_{O_2}^{\text{present-day}}$ respectively, and $[O_2]_{\text{sat}}$ and $[O_2]_{\text{surf}}$ are the saturation and surface concentration of O_2 , respectively. The function $f([O_2]) = 1$ for $[O_2] > 0$ and 0 otherwise. The number of moles of O_2 consumed to remineralize 1 mole of the typical Neoproterozoic marine biomass is given by: $-r_{O_2:P}$ (see below).

$F_{Fe}^{\text{hydrothermal}}$ is the hydrothermal influx of Fe^{2+} to the ocean, k_{Fe} is the oxidation rate of Fe^{2+} to Fe^{3+} , which accounts for both abiotic and microbial pathways (described below), and $\frac{\partial}{\partial z} F_{Fe}^{\text{recycle}}$ is the partial derivative with depth of the particulate Fe^{3+} sinking flux, which gives the rate at which particulate Fe^{3+} is recycled back to Fe^{2+} by anaerobic remineralization of organic matter. The tendency term for the number of moles of O_2 in the model atmosphere ($n_{O_2}^{\text{model atmosphere}}$) is:

$$\frac{d}{dt} n_{O_2}^{\text{model atmosphere}} = -\xi \left(k_w A_{\text{surf}} \left(\frac{n_{O_2}^{\text{model atmosphere}}}{n_{O_2}^{\text{present-day}}} [O_2]_{\text{sat}} - [O_2]_{\text{surf}} \right) - \Phi_{\text{red}} \right),$$

where, $\xi = 10^4$ is an arbitrary constant introduced to accelerate the convergence of the atmospheric box to a steady state, A_{surf} is the area of the ocean surface, Φ_{red} is the (mole equivalent) rate of consumption of O_2 required to balance the volcanic flux of reduced gases into the atmosphere (e.g., SO_2 , H_2S , CO , CH_4 , H_2). Other oxygen sinks relevant to the present-day Earth system, like oxidative weathering of the continents and respiration by the terrestrial biosphere are considered negligible during a global glaciation.

$J_{\text{production}}$, which is a function of the light (L) and $[PO_4^{3-}]$, is given by:

$$J_{\text{production}} = \alpha \frac{L}{L + \kappa_L} \frac{[PO_4^{3-}]}{[PO_4^{3-}] + \kappa_{PO_4^{3-}}},$$

where κ_L and $\kappa_{PO_4^{3-}}$ are Michaelis-Menten-type half-saturation constants typical of ocean biology, and α is the maximum community production. The expression for L is given by:

$$L = f_{\text{PAR}} Q_{\text{SW}} \times \exp(-kz),$$

where, f_{PAR} is the fraction of shortwave radiation (SW) available for photosynthesis and k is the light attenuation constant. Since the light available for photosynthesis declines exponentially with depth, most of the biological activity in the ocean is close to the surface. Primary production

converts a fraction of PO_4^{3-} to DOP (f_{DOP}), which can be advected by the physical circulation in the ocean, while the rest forms particulate organic phosphorus (POP), which sinks⁴⁷. The downward sinking flux of POP is given by:

$$F_{\text{POP}} = \begin{cases} (1 - f_{\text{DOP}}) \int_0^{z_i} J_{\text{production}} dz & \text{if } z < z_c \\ (1 - f_{\text{DOP}}) \int_0^{z_c} J_{\text{production}} dz & \text{if } z \geq z_c \end{cases},$$

where z_i is a reference depth below which the downward flux of POP is calculated and z_c is the compensation depth. In present-day ocean models, POP is remineralized according to a power law relation related almost entirely to aerobic respiration⁴⁸. Additionally, our model accounts for remineralization of POP by anaerobic microbes that reduce Fe^{3+} particles (see below).

As was previously mentioned, Fe^{2+} in the ocean can be oxidized by abiotic and microbial pathways, both O_2 -related and light driven. The Fe^{2+} oxidation rate accounting for both abiotic and microbial processes is:

$$k_{\text{Fe}} = \frac{k_{\text{Fe}}^{\text{ab}}}{1 - f_{\text{bio}}},$$

where $k_{\text{Fe}}^{\text{ab}}$ is the abiotic rate constant of oxidation and f_{bio} is the fraction of microbial Fe^{2+} oxidation out of the total oxidation as a function of available $[\text{O}_2]$ ⁴⁹; $k_{\text{Fe}}^{\text{ab}}$ is given by:

$$\log k_1 = 21.56 - \frac{1545}{T} - 3.29 \sqrt{I} + 1.52 I,$$

where T is the temperature (in Kelvins), $I = \frac{19.992 S}{10^3 - 1.005 S}$ and S is the salinity of seawater (48). The fraction of microbial Fe^{2+} oxidation is given by:

$$f_{\text{bio}} = 1.074 \times 10^{-3} \times \exp\left(\left(\frac{[\text{O}_2]}{K_H}\right)\right),$$

where K_H is Henry's Law constant for O_2 :

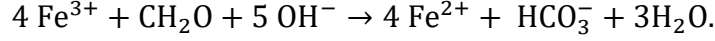
$$K_H = 1.3 \times 10^{-3} \times \exp\left(1500 \left(\frac{1}{T} - \frac{1}{298.15}\right)\right).$$

f_{bio} is capped at 0.95, an upper bound based on experimental results⁴⁹. To allow model timesteps that are long enough so that convergence is reached over reasonable runtimes, chemical rate constants could not be too large. Thus, we prescribed an upper limit on k_{Fe} of 10^{-5} s^{-1} . This upper limit was applied wherever O_2 concentrations were high enough to result in k_{Fe} that was too large to allow efficient model timesteps, typically in the well oxygenated regions in the ocean (e.g., near the surface in the snowball with 12°S to 12°N ocean). The upper limit of k_{Fe} was prescribed in $\sim 68\%$ of the ocean volume in the snowball simulation with 12°S to 12°N ocean with 1% modern $[\text{PO}_4^{3-}]$, in $>90\%$ of the ocean volume for a lower ice-cover or higher $[\text{PO}_4^{3-}]$. The model results were relatively insensitive to this choice of an upper limit on k_{Fe} (Fig. S8).

The downward flux of Fe^{3+} produced from oxidation of Fe^{2+} is given by:

$$F_{\text{Fe}}^{\text{down}} = \int_0^{z_u} k_{\text{Fe}} [\text{Fe}^{2+}] dz,$$

where z_u is the reference up to which the downward flux of Fe^{3+} is calculated. We assume that a fraction of sinking Fe^{3+} is preserved ($f_{\text{preserved}}$) while the rest is remineralized by anaerobic microbes. This process restores some Fe^{2+} and is summarized by the following reaction:



The anaerobic reduction of Fe^{3+} by bacteria follows Michaelis-Menten-type kinetics with respect to the concentrations of both organic matter and Fe^{3+} :

$$\frac{d}{dt} [\text{Fe}^{3+}] = \mu \min \left(\frac{[\text{Fe}^{3+}]}{\kappa_{\text{Fe}} + [\text{Fe}^{3+}]}, \frac{[\text{C}]}{\kappa_{\text{C}} + [\text{C}]} \right),$$

where μ is the typical respiration rate, $[\text{Fe}^{3+}]$ and $[\text{C}]$ are the concentrations of Fe^{3+} and organic matter respectively. The relevant half saturation constants for Fe^{3+} and C are κ_{Fe} and κ_{C} respectively, and the smaller of the saturation terms is considered to limit the Fe^{3+} reduction rate. Assuming a typical C:P ratio of 100:1 yields:

$$\frac{d}{dt} [\text{Fe}^{3+}] = \mu \min \left(\frac{[\text{Fe}^{3+}]}{\kappa_{\text{Fe}} + [\text{Fe}^{3+}]}, \frac{[\text{POP}]}{\kappa_{\text{C}}/100 + [\text{POP}]} \right),$$

and

$$\frac{d}{dt} [\text{POP}] = \frac{\mu}{400} \min \left(\frac{[\text{Fe}^{3+}]}{\kappa_{\text{Fe}} + [\text{Fe}^{3+}]}, \frac{[\text{POP}]}{\kappa_{\text{C}}/100 + [\text{POP}]} \right).$$

The factor of 400 comes from the Fe:C:P stoichiometry of the reaction. To calculate the flux of recycled Fe^{3+} ($F_{\text{Fe}}^{\text{recycle}}$) and the effect of Fe^{3+} reduction on the vertical POP remineralization profile, we further assume that $[\text{POP}]$ and $[\text{Fe}^{3+}]$ are proportional to F_{P} and $F_{\text{Fe}}^{\text{down}}$ respectively. If $F_{\text{Fe}}^{\text{down}} > (F_{\text{P}}/400)$, the fluxes of recycled Fe^{3+} and POP are given by:

$$F_{\text{P}}(z) = \begin{cases} F_{\text{POP}} \left(\frac{z}{z_i} \right)^{-\left(a_{\text{remin}} + \frac{\mu}{4 \kappa_{\text{C}} \times a}\right)} & \text{if } F_{\text{P}} < w(z) (\kappa_{\text{C}}/100) \\ F_{\text{POP}} \left(\frac{z}{z_i} \right)^{-a_{\text{remin}}} & \text{otherwise} \end{cases},$$

and

$$F_{\text{Fe}}^{\text{recycle}}(z) = (1 - f_{\text{preserved}}) F_{\text{Fe}}^{\text{down}} - \mu \frac{F_{\text{P}}(z)}{w(z) (\kappa_{\text{C}}/100) + F_{\text{P}}(z)}.$$

Similarly, when $F_{\text{Fe}}^{\text{down}} < (F_{\text{P}}/400)$, the fluxes of recycled Fe^{3+} and POP are given by:

$$F_{\text{P}}(z) = F_{\text{POP}} \left(\frac{z}{z_i} \right)^{-a_{\text{remin}}},$$

and

449

$$F_{\text{Fe}}^{\text{recycle}}(z) = \begin{cases} (1 - f_{\text{preserved}}) F_{\text{Fe}}^{\text{down}} \left(\frac{z}{z_i} \right)^{-\frac{\mu}{a \kappa_{\text{Fe}}}} & \text{if } F_{\text{Fe}}^{\text{down}} < w(z) \kappa_{\text{Fe}} \\ (1 - f_{\text{preserved}}) F_{\text{Fe}}^{\text{down}} & \text{otherwise} \end{cases}$$

450

451 Here, z_i is a reference depth below which the downward flux of POP is calculated (note that $z_i =$
 452 z_c when $z > z_c$), a is the vertical gradient of particle sinking velocity such that $w(z) = az$ yields
 453 the speed of the sinking particles at depth z , and a_{remin} is the exponent in Martin's curve for POP
 454 remineralization in the modern ocean.

455

456 The Fe^{2+} influx to the ocean from axial and off-axis hydrothermal circulation depends on the Fe^{2+}
 457 concentration in the fluid and the total water fluxes. The concentration of Fe^{2+} in axial and off-axis
 458 hydrothermal fluids is estimated to be in the range $(0.75 - 6.5) \times 10^{-3} \text{ mol kg}^{-1}$ and
 459 $(0.4 - 6.0) \times 10^{-6} \text{ mol kg}^{-1}$, respectively⁵¹⁻⁵³. Assuming that the Fe^{2+} concentration is uniformly
 460 distributed in these ranges and the axial and off-axis water fluxes follow the distributions shown
 461 in Ref. ⁵⁴, we generated probability distributions corresponding to the axial and off-axis influx of
 462 hydrothermal Fe^{2+} to the ocean (Fig. S9A-B). Separate from hydrothermal Fe^{2+} fluxes, weathering
 463 of seafloor basalt can deliver Fe^{2+} to the ocean^{55,56}. The Fe^{2+} flux from seafloor weathering is rather
 464 difficult to constrain in the well-oxygenated modern ocean but it is estimated to be $\sim 0.1 - 0.3 \text{ Tmol}$
 465 y^{-1} and as high as 1.0 Tmol y^{-1} ⁵⁷, though it is unclear that all the Fe^{2+} lost from the basalt actually
 466 reaches the ocean. Given the existing estimates, we adopt a weathering Fe^{2+} flux uniformly
 467 distributed between 0.1 and 0.3 Tmol y^{-1} (Fig. S9C).

468

469 Convolution of the distributions of axial and off-axis hydrothermal fluxes and seafloor weathering
 470 flux yields a range of Fe^{2+} influxes between 0.2 and 0.67 Tmol y^{-1} (95% confidence interval) with
 471 a mode of 0.36 Tmol y^{-1} (Fig. S9D). Though some have suggested higher hydrothermal fluxes in
 472 Earth's deep past due to higher radiogenic heat production in the mantle⁵⁸, it remains unclear
 473 whether the higher heat production led instead to more sluggish seafloor spreading⁵⁹ and a
 474 hydrothermal flux similar to the Phanerozoic. We do not upscale the hydrothermal water flux,
 475 leading to conservatively low Fe^{2+} influx estimates. Following the above analysis, we distribute
 476 the mode Fe^{2+} influx of 0.36 Tmol y^{-1} on the model grid points corresponding to the suggested
 477 locations of seafloor spreading centers during the Sturtian glaciation. Moreover, we do not taper
 478 the Fe^{2+} influx with increasing distance from the spreading centers, since both near-axis and off-
 479 axis hydrothermal inputs occur close to the spreading centers (considering the spatial resolution of
 480 the ocean model), and the dissolved products of seafloor weathering are expected to reach the
 481 ocean mostly where the sedimentary cover on the basaltic crust is thin to absent (i.e., near the
 482 spreading centers).

483

484 The marine phytoplankton community during the Neoproterozoic primarily comprised of
 485 cyanobacteria. Previous studies⁶⁰⁻⁶³ show that the metabolite content of typical cyanobacterial
 486 biomass is: 51% protein, 16% carbohydrates, 23% lipid and 10% nucleic acid which is slightly
 487 different from the average composition of modern phytoplankton (which includes diatoms,
 488 coccolithophores, dinoflagellates, and cyanobacteria): 54% protein, 26% carbohydrates, 16% lipid
 489 and 4% nucleic acid⁶⁴. Despite these differences in the metabolite content, the oxidation state of
 490 cyanobacterial biomass is not significantly different from the gross modern assemblage (we
 491 estimated $< 1\%$ variation in H:C_{org} and $< 10\%$ variation in O:C_{org} ratios), which suggests that the
 492 difference between the Neoproterozoic and present-day $\text{O}_2\text{:P}$ ratio is expected to arise from a
 493 difference between the C:P ratios of cyanobacteria and the modern assemblage and not from the

difference in the carbon oxidation state. Using the mean C:N:P ratio of 152:25:1 for cyanobacteria⁶⁵, we calculate the following elemental composition of typical Neoproterozoic plankton: C₁₅₂H₂₄₇O₆₁N₂₅P. As per this mean composition, the $r_{O_2:P}$ ratio is estimated to be -216, which is ~45% more negative than its present-day value of -150⁶⁴. In other words, 45% more O₂ is consumed per mole of organic phosphorus liberated during organic matter remineralization.

As mentioned above, the majority of O₂ sinks on the present-day Earth were negligible during the Neoproterozoic snowball Earth events. However, reducing volcanic emissions (SO₂, H₂S, CO, CH₄, H₂) can be an important sink for O₂ in a globally glaciated climate (Table S2). All listed fluxes are approximate but can be used to reasonably estimate the equivalent moles of O₂ consumed annually by oxidation of the reduced gases.

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586 **Data and code availability:**

587 The simulations are carried out using the MITgcm, an open-source ocean model that can be
588 downloaded from: <https://mitgcm.readthedocs.io/en/latest/overview/overview.html>. The specific
589 model configuration is available upon request.

590

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596

597 **Author contributions:**

598 Conceptualization: KG, IH, HG, YA, ET

599 Data curation: KG

600 Formal Analysis: KG

601 Funding acquisition: HG, YA

602 Investigation: KG

603 Methodology: KG, IH, HG

604 Project administration: HG, YA

605 Resources: HG, YA

606 Software: KG, YA

607 Supervision: IH, HG, YA, ET

608 Validation: KG, IH, HG

609 Visualization: KG, IH, HG

610 Writing – original draft: KG, IH, HG, YA, ET

611

612 **Competing interests:**

613 Authors declare that they have no competing interests.

614

615 **Supplementary Information:**

616

617 **Rate of Fe²⁺ oxidation during the Sturtian pan-glacial**

618 To compare our model results with observations, we estimate the rate of Fe²⁺ oxidation (and Fe³⁺
619 deposition) during the Sturtian pan-glacial from BIFs dated to the glaciation using the following
620 expression:

621
$$R_{\text{Fe}^{3+}} = n_{\text{Fe}} \times f_{\text{Fe}_2\text{O}_3} \times \rho_{\text{BIF}} \times \frac{h}{T_{\text{deposition}}},$$

where $n_{\text{Fe}} = 12.525$ is the number of moles of Fe in 1 kg of Fe_2O_3 , $f_{\text{Fe}_2\text{O}_3}$ is the fraction of Fe_2O_3 in the BIF samples, ρ_{BIF} is the density of BIF in kg m^{-3} , and h and $T_{\text{deposition}}$ are the observed thickness and the estimated depositional duration of the sampled BIF, respectively.

Iron formation and hematite mudstone samples obtained from diamond drill cores Y-5 and N-7 in the Snake River deposit indicate that $f_{\text{Fe}_2\text{O}_3}$ in the two cores is 48.5% and 41.7% and the thickness of the iron formation (estimated from the stratigraphic sections) is ~82 m and ~26 m, respectively¹⁶. The estimated ρ_{BIF} , calculated by assuming that the non-iron-bearing-component in BIFs has a density of 2,700 kg m^{-3} , for the two cores is 3,894 kg m^{-3} and 3,649 kg m^{-3} . The Snake River deposit is a part of the Rapitan Group of glacial deposits. Another glacial unit of the Rapitan Group is exposed along the Hard Luck Creek in the Tatonduk inlier. The iron formation in this region is ~3 m thick¹⁷ and the median $f_{\text{Fe}_2\text{O}_3}$ is 17.2%²⁵, which yields a ρ_{BIF} of 3,155 kg m^{-3} . The Rapitan BIFs sit in the Sayunei formation that is under the Shezal formation. The transition from the Sayunei to the Shezal formation is dated to 711.34 ± 0.25 Ma⁶⁶. Assuming that none of the iron precipitated prior to the onset of the Sturtian pan-glacial (717 ± 0.5 Ma; Ref. ¹⁰) and that deposition of other iron-poor facies in the formation (e.g., siltstone, sandstone) was rather rapid, suggests that the Rapitan BIFs were deposited in 4.9–6.4 million years. The equation above, yields $R_{\text{Fe}^{3+}}$ corresponding to the Rapitan BIFs that is between ~0.003 and ~0.4 $\text{mol m}^{-2} \text{y}^{-1}$.

The BIFs in the Kingston Peak Formation are ~28 m thick and have a median $f_{\text{Fe}_2\text{O}_3}$ of 50%¹⁸, which yields $\rho_{\text{BIF}} = 3,970 \text{ kg m}^{-3}$. The upper Kingston Peak Formation that contains the BIFs is correlated with the Wildrose submember⁶⁷, the depositional age of which has been constrained to be between 705.4 ± 0.3 and 645 Ma⁸. This suggests that the Kingston Peak Formation BIFs were deposited over ~60 million years. However, we assume that duration of iron deposition did not exceed the duration of the Sturtian pan-glacial, which yields $T_{\text{deposition}} = \sim 58$ million years¹⁰. Hence, $R_{\text{Fe}^{3+}}$ for these IFs is constrained to ~0.01 $\text{mol m}^{-2} \text{y}^{-1}$.

Samples obtained from the Zhongjiajiang and Lanyang section of the Fulu Formation have a median $f_{\text{Fe}_2\text{O}_3}$ of 19.6% and 24.2% and the maximum thickness of iron formation in the two sections is ~22 m and ~50 m, respectively¹⁹. The estimated ρ_{BIF} for the two sections is 3,196 kg m^{-3} and 3,313 kg m^{-3} . The maximum and minimum age of the Fulu formation is estimated to be 715.9 ± 2.8 Ma and 691.9 ± 8.0 Ma¹⁹, which suggests that $T_{\text{deposition}}$ could have varied between 13.2 million years and 34.8 million years. Hence, $R_{\text{Fe}^{3+}}$ for the Fulu Formation is constrained to be between ~0.005 and ~0.04 $\text{mol m}^{-2} \text{y}^{-1}$.

The Flinders Ranges in southern Australia house two more occurrences of BIFs, the Braemar and the Holowilena Ironstones. The thickness of the Braemar Ironstone varies between ~24 m and ~76 m and the $f_{\text{Fe}_2\text{O}_3}$ is 58%²⁰, which yields a ρ_{BIF} of 4,192 kg m^{-3} . In contrast, stratigraphic sections of the Holowilena Ironstone show that the thickness of banded hematite and jasper facies is negligible and the formation predominantly comprises of ferruginous shale and diamictite⁶⁸. We estimate that the $T_{\text{deposition}}$ for these correlated formations⁶⁸ is between ~13.5 million years and 58 million years, based on the age of authigenic monazite from the upper part of the interglacial succession [680 ± 23 Ma, Ref. ⁶⁹] and the onset of the glaciation. Hence, $R_{\text{Fe}^{3+}}$ for the Australian BIFs is constrained to between ~0.01 and ~0.2 $\text{mol m}^{-2} \text{y}^{-1}$.

Ironstone samples corresponding to the Chuos Formation obtained from the Mitten Fold locality in the Damara Belt have a median $f_{\text{Fe}_2\text{O}_3}$ of 88.7% and the thickness of ironstone is $\sim 25 \text{ m}^{21}$. The estimated ρ_{BIF} is $4,921 \text{ kg m}^{-3}$. Age constraints from geologic formations above and below the Chuos Formation suggest that it was deposited between $760 \pm 1 \text{ Ma}$ and $635 \pm 1 \text{ Ma}^{70,71}$, longer than the duration of the Sturtian glaciation. Since the iron formation is syn-glacial, we adopt a conservatively long $T_{\text{deposition}}$ of ~ 58 million years (the duration of the glaciation), yielding $R_{\text{Fe}^{3+}}$ of $\sim 0.02 \text{ mol m}^{-2} \text{ y}^{-1}$.

The above analysis suggests that the typical Fe^{3+} deposition rates during the Sturtian pan-glacial were between ~ 0.003 and $\sim 0.4 \text{ mol m}^{-2} \text{ y}^{-1}$. This deposition rate is conservatively low, since in all cases the BIFs deposited over a duration that is shorter than or equal to the duration of deposition estimated from radiometric ages or from the duration of the Sturtian glaciation. We have excluded the Jakkalsberg member of the Numees formation and the Tany formation from this analysis due to difficulties in evaluating the thickness and Fe content of the Fe-rich parts of these two formations.

Numerical simulations

While carrying out the simulations, we use asynchronous integration⁷² with a momentum time step of 1,800 seconds and a tracer (temperature and salinity) time step of 18,000 seconds to integrate the primitive equations, to a quasi-steady state. Subsequently, the distribution of biogeochemical variables was determined from the velocity fields and eddy diffusivities calculated from the primitive equations. To calculate the distribution of biogeochemical variables, the integration time step was set to 10,800 seconds. The results did not change with increasing temporal resolution, indicating convergence.

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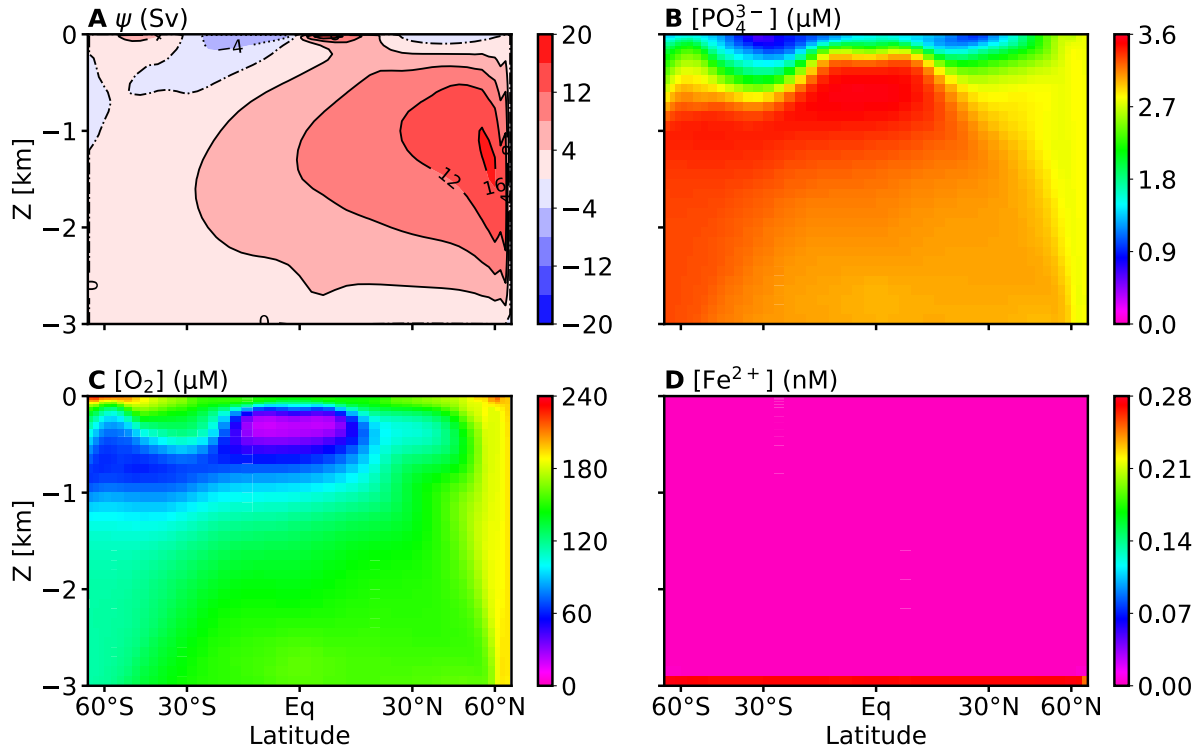


Fig. S1. Results in box configuration simulation. (A) The meridional overturning circulation ($1 \text{ Sv} = 10^6 \text{ m}^3 \text{ s}^{-1}$). The solid contours (streamlines) indicate clockwise circulation, the dotted contours indicate counterclockwise circulation and the dotted-dashed contours mark the zero values. Spatial distribution of (B) $[\text{PO}_4^{3-}]$, (C) O_2 and (D) $[\text{Fe}^{2+}]$. The mean seawater $[\text{PO}_4^{3-}]$ is $3.0 \mu\text{M}$ (100% modern) and stoichiometry of organic matter oxidation is $r_{\text{O}_2:\text{P}} = -150$, which is representative of the modern ocean.

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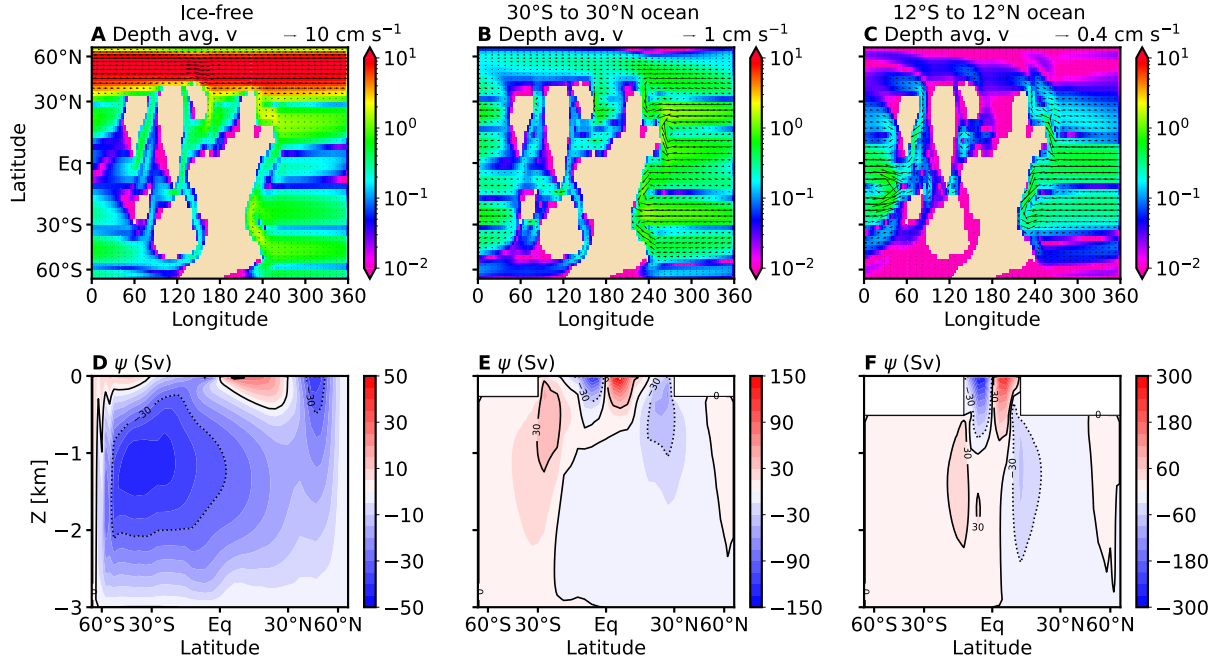


Fig. S2. Ocean circulation in the simulations for different meridional extent of ice-free region. Depth averaged velocity fields (the barotropic flow) and the meridional overturning circulation in the (A),(D) ice-free simulations, and in the snowballs with ice-free ocean between (B),(E) 30°S to 30°N ocean and (C),(F) 12°S to 12°N. The colours in (A)-(C) denote the speed (cm s^{-1}) of the ocean currents. The solid contours (streamlines) in (D)-(F) indicate clockwise circulation, the dotted contours indicate counter clockwise circulation, and the dotted-dashed contours mark the zero values.

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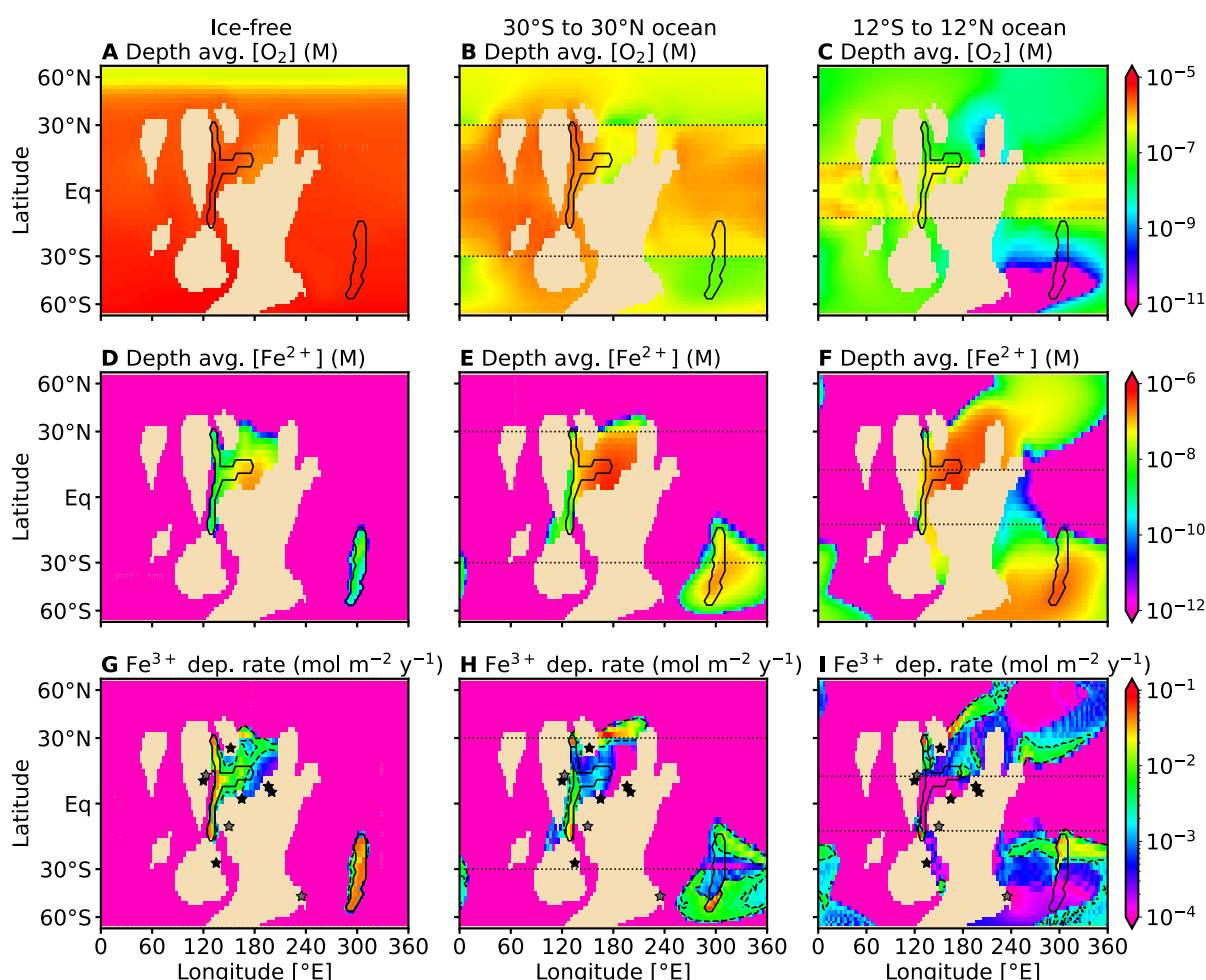


Fig. S3. Results of the 3D ocean model with a mean seawater $[\text{PO}_4^{3-}]$ of $0.03 \mu\text{M}$ (1% modern). (A)-(C) Depth-averaged distribution of $[\text{O}_2]$ and (D)-(F) $[\text{Fe}^{2+}]$ and the (G)-(I) spatial distribution of Fe^{3+} deposition rates in snowballs with different meridional extents of sea glaciers. The solid black contours mark the sites of hydrothermal Fe^{2+} injection, based on estimated locations of mid-oceanic ridges. The dotted black lines denote the extent of the ice-free region. The dashed black lines in (G)-(I) enclose the region where Fe^{3+} deposition rates are within the range estimated from Neoproterozoic BIFs. The stars indicate the approximate location of BIFs associated with the Sturtian pan-glacial. We note that for 1% modern $[\text{PO}_4^{3-}]$ levels, over 10% of the continental margins in the vicinity of Neoproterozoic BIFs are found to be appropriate for precipitation of BIFs, regardless of the extent of marine ice-cover. With ~21% of the margins under consideration viable for precipitation of BIFs, the ice-free ocean with 1% modern $[\text{PO}_4^{3-}]$ is in most agreement with the observed distribution of BIFs, followed by ~18% and ~13% in the 30°S to 30°N and 12°S to 12°N ocean, respectively. While an enhanced adsorption of PO_4^{3-} on iron oxides in an anoxic environment⁸¹ can explain the concurrence between the model results for an ice-free ocean with 1% modern $[\text{PO}_4^{3-}]$ and the distribution of Neoproterozoic BIFs, the precipitation of BIFs in an ice-free ocean is inconsistent with other geochemical evidence that point towards a global glaciation during the Neoproterozoic¹⁰.

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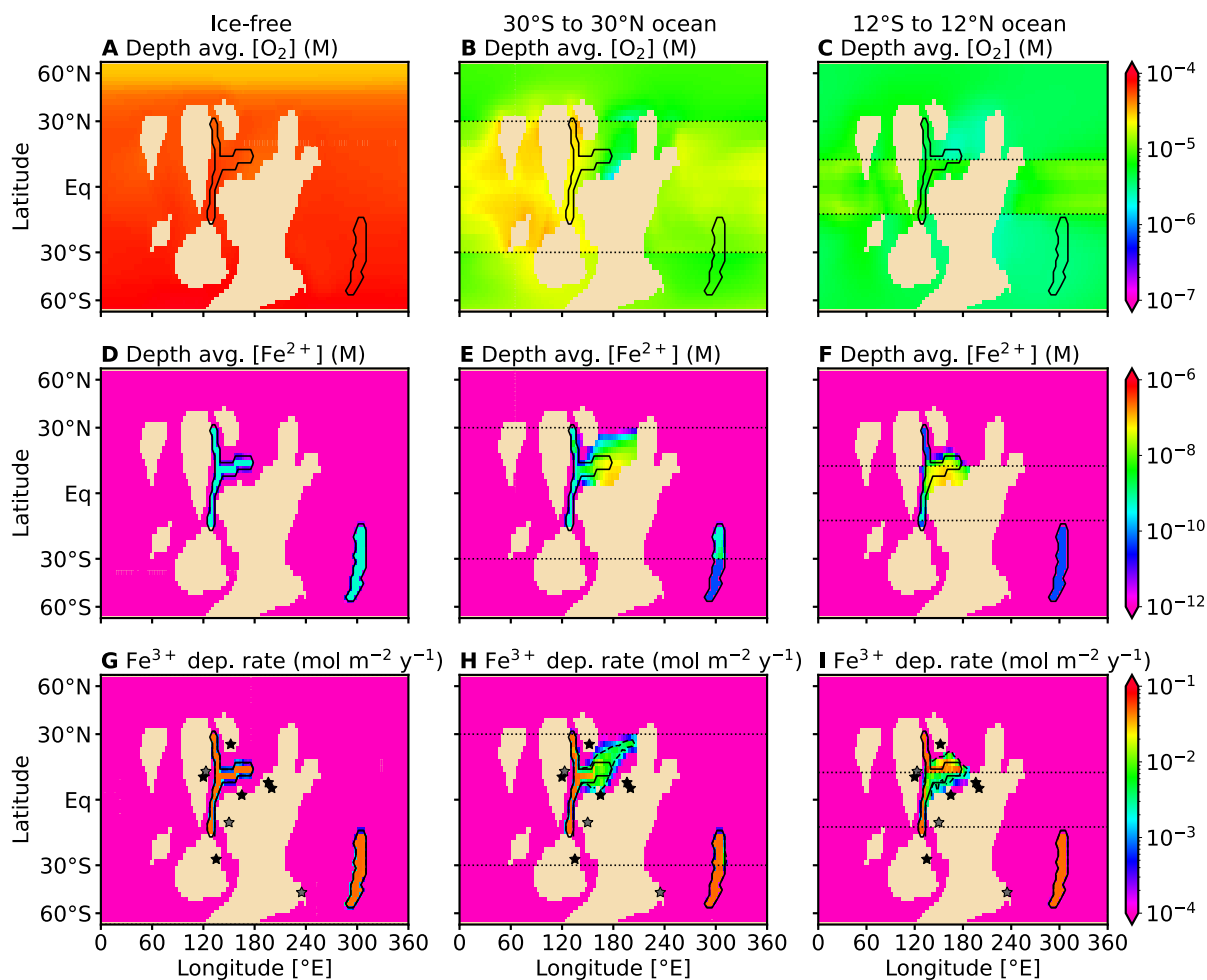


Fig. S4. Results of the 3D ocean model with a mean seawater $[PO_4^{3-}]$ of 0.3 μM (10% modern). See Fig. S3 for the details regarding the different panels.

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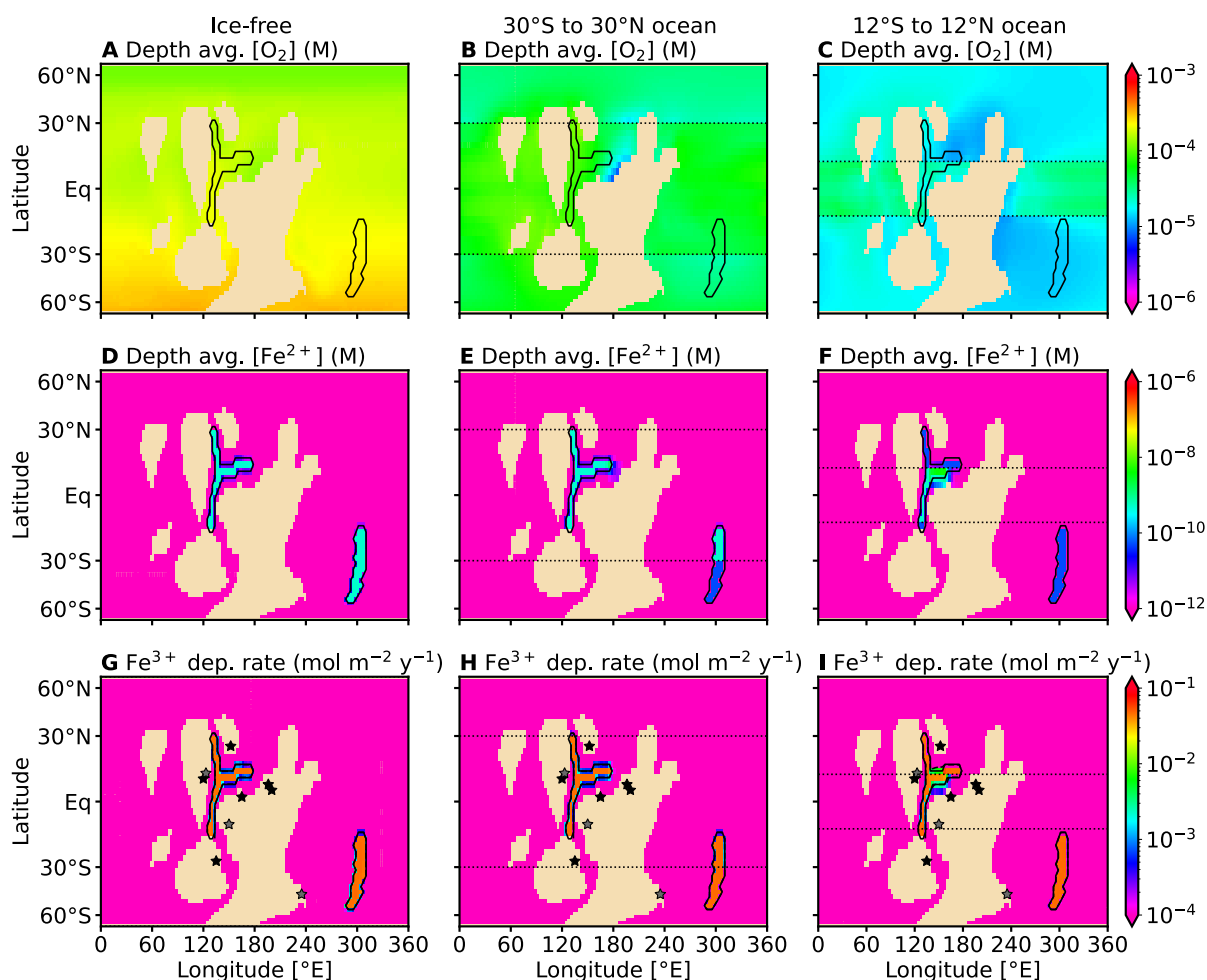


Fig. S5. Results of the 3D ocean model with a mean seawater $[\text{PO}_4^{3-}]$ of $3 \mu\text{M}$ (100% modern).
See Fig. S3 for the details regarding the different panels.

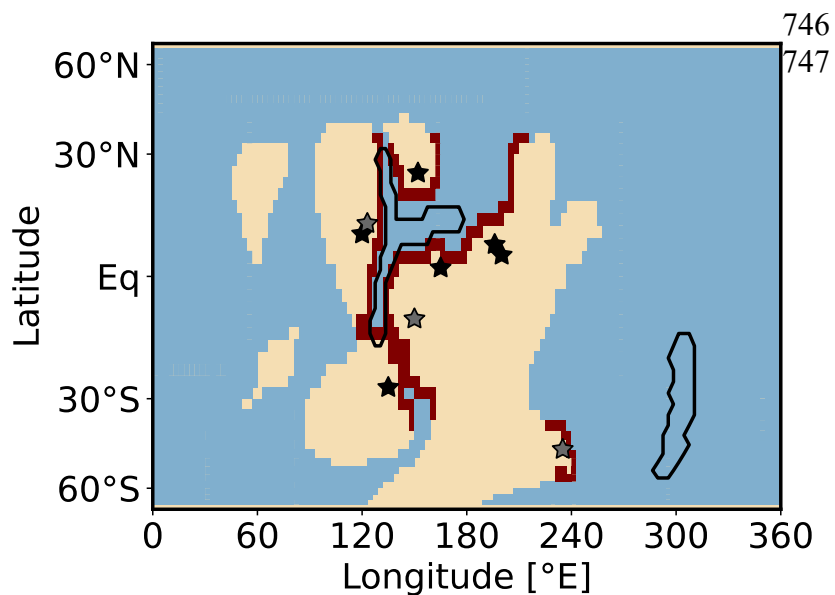


Fig. S6. Continental margins (brown) close to observed BIFs. The fraction of these margins where model Fe deposition occurred at rates between 0.003 and $0.4 \text{ mol m}^{-2} \text{ y}^{-1}$ was calculated to evaluate model-observation agreement. The solid black contours mark the sites of hydrothermal Fe^{2+} injection, based on estimated locations of mid-oceanic ridges. The stars indicate the approximate location of BIFs associated with the Sturtian pan-glacial.

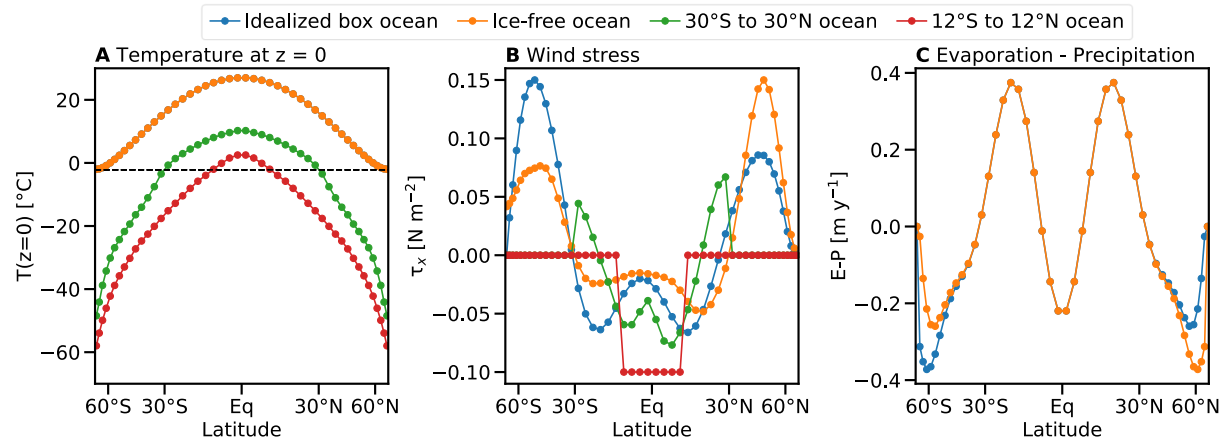


Fig. S7. Forcing (zonal-mean) over the ocean model. (A) Temperature forcing at $z = 0$ for the different meridional extent of sea glaciers. The temperature forcing in the idealized box configuration simulations and in the ice-free Neoproterozoic ocean is the same and the temperature forcing over the two snowballs has been adjusted to account for the fraction of the sea glacier floating above the sea surface. The black dashed line denotes the freezing temperature of seawater at salinity of 40.7 g/kg. (B) Wind stress applied over the ocean surface. The wind over the surface of the sea glaciers in the snowball simulations does not affect the ocean currents and thus is set to zero. (C) Evaporation minus Precipitation (E-P) fields over the ocean's surface in the box configuration simulations and in the ice-free ocean simulations. The slight asymmetry at the high latitudes is added to avoid small oscillations in overturning circulation. To conserve the salinity of the partially ice-covered oceans we do not prescribe an E-P field; instead the freshwater flux due to melting under the ice-shelves is balanced by evaporation in the ice-free region.

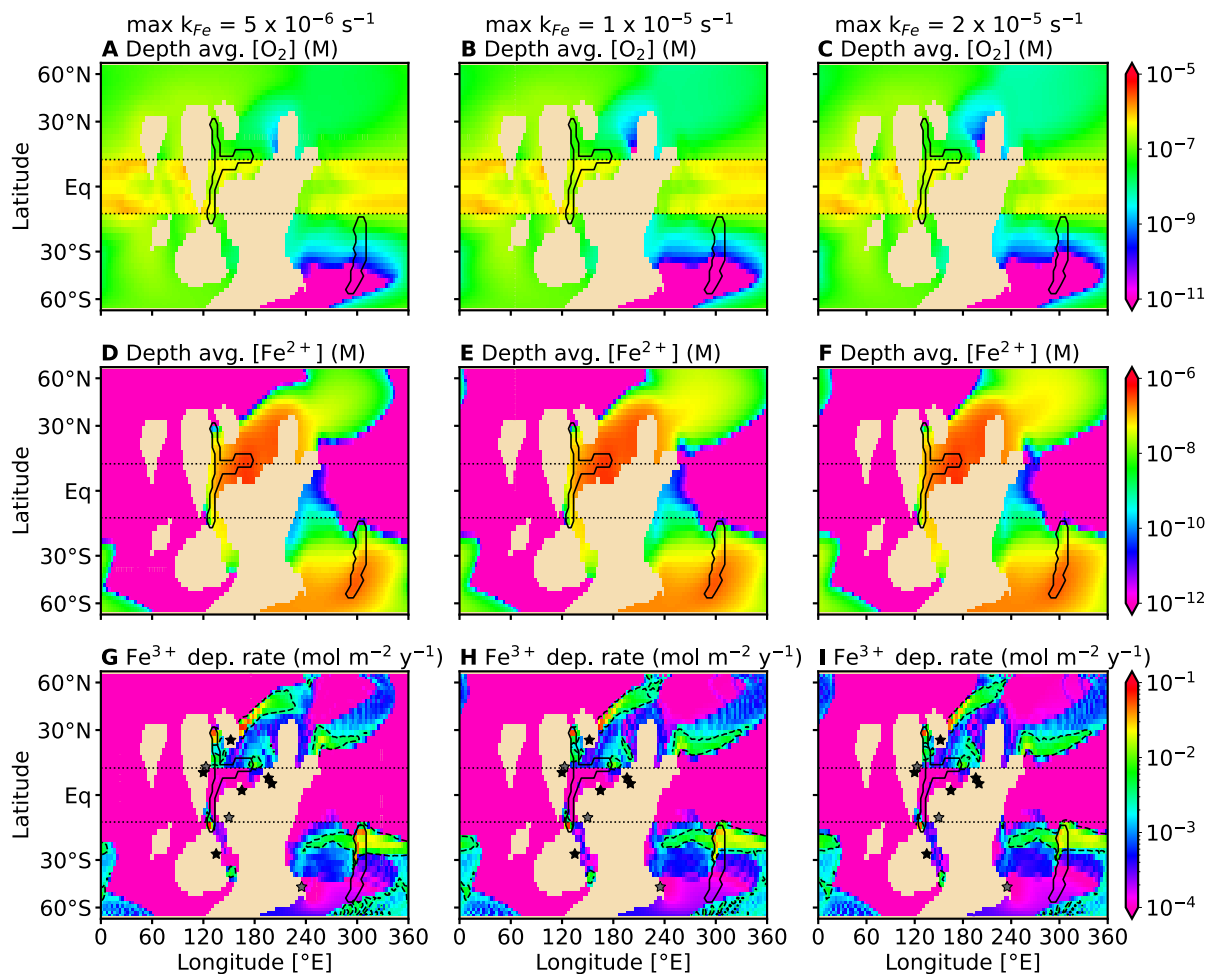


Fig. S8. Summary of profiles for sensitivity to maximum k_{Fe} . (A)-(C) and (D)-(F) show the depth averaged distribution of $[O_2]$ and $[Fe^{2+}]$ for maximum $k_{Fe} = 5 \times 10^{-6} \text{ s}^{-1}$, $1 \times 10^{-5} \text{ s}^{-1}$ and $2 \times 10^{-5} \text{ s}^{-1}$ respectively. (G)-(I) show the deposition rates, calculated by vertical integration of net Fe^{2+} oxidation profiles for the three values of maximum k_{Fe} . In all simulations shown, the ice-free ocean extends from 12°S to 12°N and the mean seawater $[PO_4^{3-}]$ is $0.03 \mu\text{M}$ (1% modern).

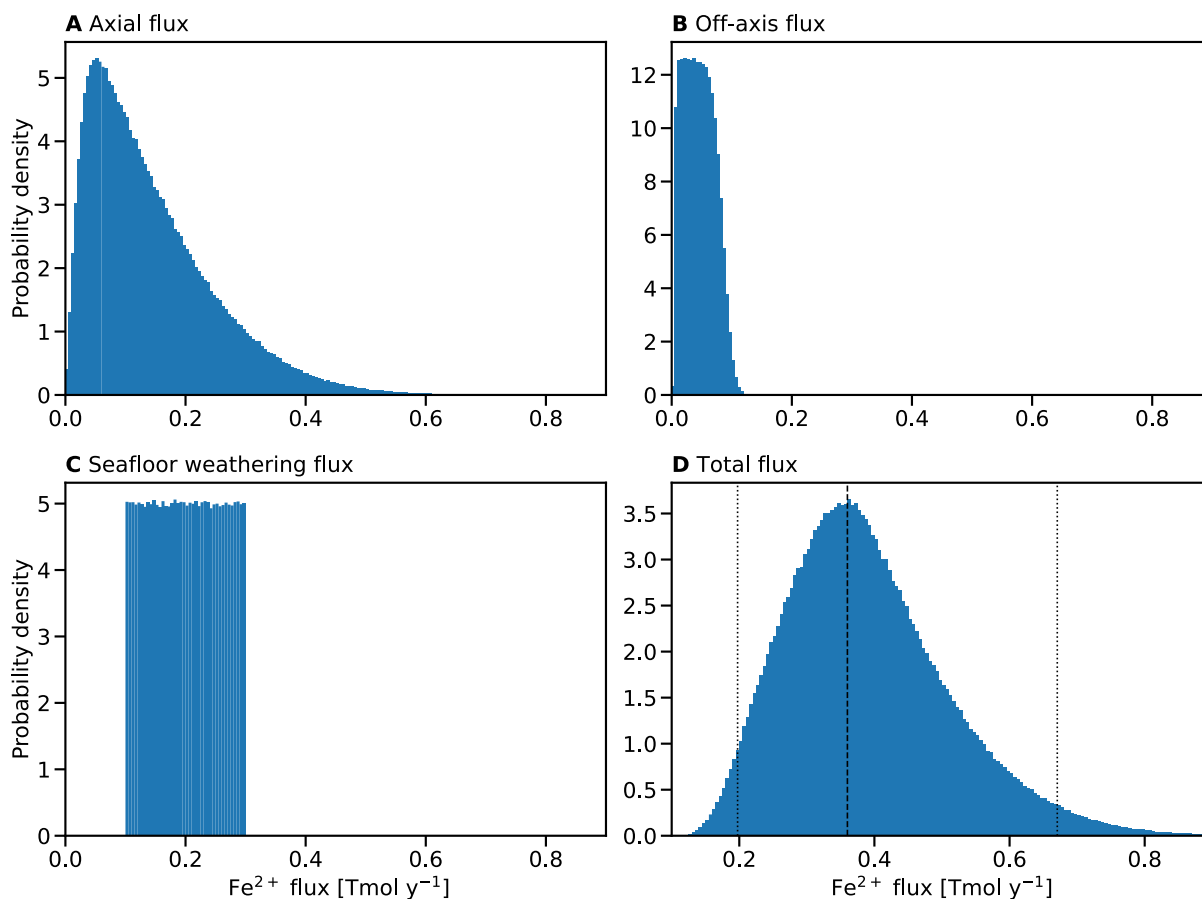


Fig. S9. Probability distribution of estimated Fe^{2+} into the ocean from different sources. (A)-(B) The distribution of axial and off-axis flux of Fe^{2+} from hydrothermal ridges is calculated by assuming that the estimated values of axial and off-axis $[\text{Fe}^{2+}]$ are uniformly distributed and multiplying them with the respective distribution of sea-water flux⁵⁴. (C) The Fe^{2+} influx from seafloor basalt weathering is assumed to be uniformly distributed between its estimated values⁵⁷. (D) The distribution of total Fe^{2+} influx is calculated by convolving the three distributions shown in (A)-(C). The dotted lines denote the 95% confidence interval (0.2 to 0.67 Tmol y^{-1}) and the dashed line marks the mode value (0.36 Tmol y^{-1}).

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Parameter	Symbol	Value	Units	References
Maximum community production	α	3×10^{-3}	$\text{mol P m}^{-3} \text{y}^{-1}$	46
Light half-saturation constant	κ_L	30	W m^{-2}	
Phosphate half-saturation constant	κ_{PO_4}	5×10^{-4}	mol P m^{-3}	
Fraction of SW radiation available for photosynthesis	f_{PAR}	0.4		
Light attenuation constant	k	0.02	m^{-1}	
Semi-labile consumption rate constant for DOP to PO_4^{3-} remineralization	κ_{remin}	0.5	y^{-1}	
Fraction of PO_4^{3-} converted to DOP via production	f_{DOP}	0.7		
Compensation depth	z_c	500	m	
Power law coefficient for POP remineralization	a_{remin}	0.9		This study
Moles of O_2 consumed per mole of P released by remineralization of typical Neoproterozoic marine biomass	$-r_{\text{O}_2, \text{P}}$	216		
Typical Fe^{3+} turnover rate due to anoxic bacterial respiration	μ	100	$\text{mol Fe m}^{-3} \text{y}^{-1}$	73–75
Organic matter half-saturation constant for anoxic bacterial respiration	κ_C	0.5	mol C m^{-3}	74
Iron half-saturation constant for anoxic bacterial respiration	κ_{Fe}	5	mol Fe m^{-3}	75
Vertical gradient of particle sinking velocity	a	12.6	y^{-1}	76
Fraction of Fe^{3+} preserved during anoxic bacterial respiration	$f_{\text{preserved}}$	0.1		This study
Mole equivalent rate of O_2 consumption to balance the flux of reduced gases into the atmosphere.	Φ_{red}	1.0	T mol y^{-1}	This study

758 **Table S1. Parameters of the biogeochemical model.**

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Gas	Annual flux (T mol y ⁻¹)	O ₂ flux required for oxidation (T mol y ⁻¹)
SO ₂	0.30	0.30
H ₂ S	0.18	0.27
CO	0.06	0.03
CH ₄	0.05	0.1
H ₂	0.03	0.015

Table S2. Volcanic flux of reducing gases. Studies indicate that the CO:CO₂ ratio for volcanic emissions is between 10⁻³ and 10⁻¹ ⁷⁷⁻⁷⁹, and the flux of CO stated in Table S1 is calculated from the flux of CO₂ estimated in Ref. ⁸⁰ multiplied by the higher end of this range of ratios.

Iron formation	Age	T _{deposition} (million years)	h (m)	Fe ₂ O ₃ (% wt.)	ρ _{BIF} (kg m ⁻³)	R _{Fe³⁺} (mol m ⁻² y ⁻¹)
Core Y5, Snake River deposit, Rapitan BIF	717 ± 0.5 Ma to 711.34 ± 0.25 Ma ^{10,66}	4.9 – 6.4	81.9 ¹⁶	48.5 ¹⁶	3894.4	0.3 – 0.4
Core N7, Snake River deposit, Rapitan BIF	717 ± 0.5 Ma to 711.34 ± 0.25 Ma ^{10,66}	4.9 – 6.4	25.9 ¹⁶	41.7 ¹⁶	3648.7	0.08 – 0.1
T709, Hard Luck Creek, Tatonduk BIF	717 ± 0.5 Ma to 711.34 ± 0.25 Ma ^{10,66}	4.9 – 6.4	2.7 ¹⁷	17.2 ²⁵	3155.2	0.003 – 0.004
Section C-C', Kingston Range, Kingston Peak BIF	705.4 ± 0.3 Ma to 645 Ma ^{8,10}	58	27.6 ¹⁸	49.6 ¹⁸	3969.5	0.01
Zhongjiajiang section, Fulu BIF	715.9 ± 2.8 Ma to 691.9 ± 8.0 Ma ¹⁹	13.2 – 34.8	21.9 ¹⁹	19.6 ¹⁹	3195.8	0.005 – 0.01
Lanyang section, Fulu BIF	715.9 ± 2.8 Ma to 691.9 ± 8.0 Ma ¹⁹	13.2 – 34.8	50.4 ¹⁹	24.2 ¹⁹	3312.8	0.01 – 0.04
BR52, BR53, Braemar Ironstone	717 ± 0.5 Ma to 680 ± 23 Ma ^{10,69}	13.5 – 58	24.2 – 76.1 ²⁰	58 ²⁰	4199.7	0.01 – 0.2
Mitten Fold, Chuos BIF	760 ± 1 Ma to 635 ± 1 Ma ^{70,71}	58	25.1 ²¹	88.7 ²¹	4920.8	0.02

Table S3. Summary of Fe³⁺ deposition rates estimated from Sturtian BIFs. The approximate deposition duration corresponding to the formation, based on the difference in ages of the deposits above and below the formation, is given by T_{deposition}. If the difference is greater than the duration of the Sturtian glaciation, we assume that the deposition duration is equal to the glaciation duration. The thickness of BIFs, given by h, is calculated from the thickness of layered ironstone in the stratigraphic sections. The fraction of Fe₂O₃ in the BIF samples is used to estimate the density ρ_{BIF}. The Fe³⁺ deposition rate is determined using the formula discussed in the text.