

The authors present a diagenetic N-isotope model, for use in aquatic sediments. The model is fitted to data and used to estimate the magnitudes of various sedimentary processes. The manuscript is well-written, the model is novel, and the sensitivity analysis and model fitting is state of the art.

We appreciate the insightful feedback from the reviewer and have assessed the implications of each comment. Please refer to the points below for a detailed plan on how we intend to revise the text.

In contrast to other diagenetic models, this model considers only dissolved nitrogen species, imposing the mineralisation rates not by modelling organic matter, but rather by imposing the maximum rates of the separate processes. While the mineralisation processes comprise oxic mineralisation, denitrification and anoxic processes, the sulphate reduction is modelled separately. It is not clear why the authors have distinguished sulphate reduction from the anaerobic mineralisation (but I guess this is because sulphate was measured). However, one could think of a simpler model where sulphate reduction would be part of the anaerobic mineralisation.

We agree that separating sulfate reduction from anaerobic mineralization might not always be a sensible choice. First, in some lacustrine systems the rate of sulfate reduction can exceed rates of anaerobic mineralization by iron or manganese (Lines 241-242) (Steinsberger et al. 2020). Second, sulfate reduction commonly spans a thick layer of sediments in marine systems (Lines 242-243). Third, as mentioned by the reviewer, the availability of sulfate concentration data allowed separate identification sulfate reduction rates (i.e., separately from the other anaerobic mineralization processes). Based on these considerations, we deemed it reasonable to separate sulfate reduction from other anaerobic mineralization pathways in this application. Nonetheless, the model is modular: if future users prefer to have a lumped formulation for anaerobic mineralization, the rate of sulfate reduction, $k_{\text{MinSulfRed}}$, can easily be set to zero in the model, effectively merging it into the broader anaerobic mineralization term.

Ignoring organic matter in the model assumes that the mineralisation is only dependent on the availability of oxidants and not on organic matter. The anaerobic mineralisation is the closure term here and it is not limited by any substrate: it has only inhibition components (p.9). Hence, below the layers where oxygen and nitrate are present, anoxic mineralisation will continue at the same rate for all depths, and integrated anaerobic mineralisation will be infinitely large (theoretically). In the model, this is overcome by imposing an ammonium flux at the lower boundary, which effectively represents a *finite* ammonium production by anaerobic mineralisation. This means that the depth of the model is also an important model parameter, and so one cannot simply extend the model domain, and obtain the

same results, as one could do in other diagenetic models. This should be mentioned in the model assumptions section.

We agree that our assumption of sufficient readily degradable organic matter applies only within a reasonable depth range. At very large, effectively infinite depths, this assumption would no longer hold because mineralization (including anaerobic mineralization) would become substrate-limited. We already note the absence of explicit organic matter as a state variable and limiting factor in section 2.3 (assumptions i and ii). We will add an additional sentence to section 2.3 to clarify that this assumption is intended for layers with sufficient readily degradable organic matter (e.g., top 5 cm of the sediments in Lake Lucerne), and may break down at greater depths.

However, we respectfully disagree that the need for an NH_4^+ flux at the lower boundary arises from not modelling organic matter. The observed NH_4^+ profiles show a clear gradient at 5 cm depth that indicates an upward flux of NH_4^+ in this depth, and for any model of this sediment layer, even one that explicitly accounts for organic matter, a lower boundary condition with an upward flux of NH_4^+ is required. This flux as a lower boundary is not a problematic parameter of the model, as it is well informed by the data (and therefore identifiable even under a uniform prior), because the measured gradient constrains it directly.

We will clarify on line 159 that we estimated the ammonium flux at the lower boundary because the field data display a clear gradient, in contrast to the other state variables. We will also point out that the ammonium flux was estimated alongside $\delta^{15}\text{N}_{\text{FNH}_4}$.

More seriously, is that, when looking at the description of oxygen dynamics, the reoxidation of anoxic substances other than ammonium and nitrite is ignored. This implicitly assumes that the concentrations of Fe^{2+} , Mn^{2+} , H_2S , CH_4 are completely removed in the deep parts of the sediment and therefore do not react with oxygen. While such removal processes may occur in certain sediments, it is rare that they completely remove all of these substances. The authors should also list this important (and perhaps unrealistic) assumption in the model assumptions section (on p 10). A suggestion to make the oxygen dynamics more robust would be to explicitly model a lump-sum of anoxic concentrations in the model that are reoxidised with oxygen, and impose a flux of this lump-sum constituent at the lower boundary.

We agree that it would be a conceptual improvement to include a lumped pool of reduced species and their partial re-oxidation in the upper sediments. However, we do not assume that these substances (Fe^{2+} , Mn^{2+} , H_2S , CH_4) are completely removed at depth (we agree that this would be unrealistic), as

shown by the benthic fluxes presented in Steinsberger et al. (2020) for Lake Lucerne. Nevertheless, their contribution to O₂ consumption by re-oxidation processes in the top sediment layers is expected to be small relative to oxic mineralization and nitrification. We will add this point explicitly to the model assumptions.

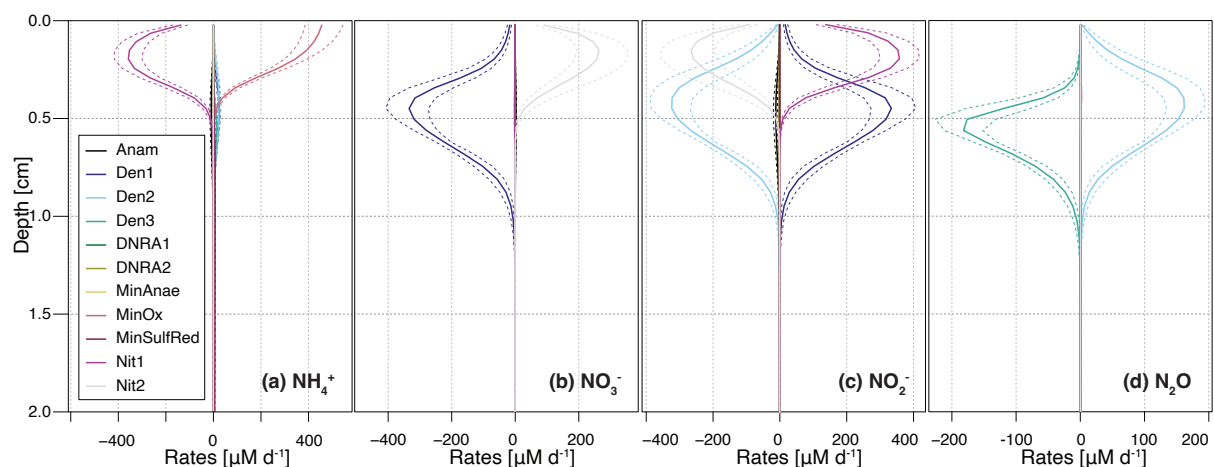
“Re-oxidation of reduced species other than NH₄⁺ and NO₂⁻ (e.g., Fe²⁺, Mn²⁺, H₂S, CH₄) is neglected in the oxygen budget for the modeled interval; this is appropriate where their upward fluxes are minor, but may underestimate O₂ demand in settings with substantial reduced-species fluxes. Future users are encouraged to adapt the model to their research questions and dataset, including adding processes and state variables, provided that they can be constrained.”

We note that adding these processes in the model would introduce additional poorly-identifiable model components without independent constraints, increasing uncertainty or requiring prior knowledge that we do not currently have. We have included a statement in the assumption above about the possibility of modifying the model for specific needs, including considering reoxidation of reduced species.

Some minor comments:

The figures were rather difficult to interpret, due to a color scheme that did not provide enough discriminating power. This made it difficult to follow the discussion.

See comment to Reviewer 1. We provide here an example of revised Figure 3 to show how we plan to change the color scheme to improve readability, while ensuring they remain color-vision-deficiency-friendly:



The ammonium deep boundary flux is imposed. How is this flux divided into 14N-NH₄ and 15N-NH₄?

We parameterized the influx of $^{14}\text{N-NH}_4^+$ and $^{15}\text{N-NH}_4^+$ using the total NH_4^+ flux (F_{NH_4}) and its $\delta^{15}\text{N}_{\text{FNH}_4}$. Both of these parameters are well identifiable from uniform priors, primarily because of the available profile data for NH_4^+ concentrations and $\delta^{15}\text{N}_{\text{NH}_4}$ (see Figure S1 for their marginal posteriors). We will add the prior values for F_{NH_4} and $\delta^{15}\text{N}_{\text{FNH}_4}$ to Table C1 and will mention both of them being estimated on lines 158-159.

The model was dynamically run to steady-state. How was steady-state checked?

We simulated 100 days and plotted profiles every 10 days, which demonstrated that the steady-state was reached to an excellent approximation well before 100 days. Due to the adaptive time-stepping of our numerical integration algorithm, we could be generous with the choice of 100 days as this did not have an essential impact on simulation time because the time step becomes large when changes in the state variables become small.

L 99 sediment reactivity -> organic matter reactivity

We will change the text as suggested by the reviewer.

L176: manganese , iron -> manganese and iron oxides

We will change the text as suggested by the reviewer.

L775: $[\text{NO}_3^-]$ instead of $^{14}\text{NO}_3^- + ^{15}\text{NO}_3^-$?

We cannot find any mentioning of “ $^{14}\text{NO}_3^- + ^{15}\text{NO}_3^-$ ” on Line 775.

L330 Wagenigen -> Wageningen

We will change the text as suggested by the reviewer.

L508. A bioturbation coefficient of $1\text{ cm}^2/\text{day}$ seems to be very high.

Questions about the choice of the bioturbation coefficient were raised also by Reviewer 1 (so please also see our reply to R1). While we have information on the depth affected by bioturbation and an estimate of the bioturbator abundance per unit of volume (Fiskal et al. 2021), substantial uncertainty remains regarding the enhancement of solute diffusion due to their presence/activity. Our analysis is intended to assess model sensitivity to changing bioturbation; therefore, the exact value was not taken from literature but chosen as a representative case. Specifically, a bioturbation coefficient of 1 cm d^{-1} implies an effective solute diffusivity approximately

twice the molecular diffusivity. Nonetheless, we will add this clarification to the description of the "Enhanced bioturbation" scenario (Lines 508-512).

Table 1. The reaction for anammox produces organic matter; however this is not so for the nitrification reactions, which are also autotrophic.

The reviewer raises an important point: organic matter (biomass) production during bacterial growth is a key component of the benthic nitrogen cycling. In our framework, we do not consider/model bacterial growth explicitly (assumption iii); therefore, we formulated all processes (process rate laws) without biomass as state variable or limiting substrate. The only exception is anammox, because the NO_2^- oxidation to NO_3^- requires OM production to close the redox balance (Brunner et al. 2013).

In our model, as mentioned, OM is neither a state variable nor a limiting substrate, and we do not track OM production and consumption. Consequently, this point, while valid, does not affect the present model results. We will clarify this assumption further in the revised manuscript.

Table 1a: (1-ksi) -> (1-ksi/1000)

We respectfully disagree with the reviewer's comment. Our ϵ values (see Table C1) are 5‰ = 0.005, 20‰ = 0.020, etc. For this reason, another division by 1000 is not needed. The unit of "permille" includes the division by 1000 already.

Table C1 shows fractions of NH_4 produced based on aerobic mineralisation, denitrification, DNRA and sulphate reduction. This does not seem to be consistent with the text where it is said that this is determined by the organic matter $^{15}\text{N}/^{14}\text{N}$ composition. Why not use the stoichiometry of the reactions to estimate the NH_4 production from the OM composition?

We appreciate the opportunity to clarify this aspect. Indeed, in our model, the amount of NH_4^+ produced (γ) from OM composition is determined stoichiometrically from the OM composition and the reaction stoichiometries of the respective mineralization pathways. The respective γ values are reported in Table C1. On the other hand, the isotopic composition of the released NH_4^+ is determined by the organic matter $^{15}\text{N}/(^{14}\text{N}+^{15}\text{N})$ composition. Table A1 shows the stoichiometry of all processes and clarifies where R ($^{15}\text{N}/(^{14}\text{N}+^{15}\text{N})$ composition of organic matter) and where the ϵ values for isotope fractionation are used.

fNit2 present in table C2 is not in Table A1.

The f_{Nit_2} term can be found in the equations below Table A1, specifically on Line 783 of the original manuscript.

The default parameter values for most parameters can be found in table C1, but not the rates, and the boundary conditions. All parameter values used for the base run should be presented somewhere in the manuscript.

We agree and will provide information on the boundary conditions (including the F_{NH_4} and $\delta^{15}\text{N}_{\text{FNH}_4}$ mentioned in an earlier comment, which were obtained from field data) with units. As the system-specific rate constants (k values) are estimated using a uniform prior distribution, we will maintain the “-” in Table C1 for these parameters.

At the discretion of the editor, we will add a column to Table C1 with the estimated values (i.e., posterior distributions).