

RC2:

The authors constructed a high spatial resolution reaction transport model for oxygen dynamics driven by micro benthic plants (MPBs) in intertidal muddy sediments, and constrained and validated it using microsensor experimental data (including light photosynthesis curve PI, temperature gradient TR, and flooding/exposure IE experiments) from sediments in Oosterschelde tidal bay in the Netherlands. They found that the MPB community adapts to low light environments and responds to changes in light through vertical redistribution; Under low light conditions, the re oxidation of reduced inorganic substances dominates the consumption of sedimentary oxygen. As light intensity increases, the proportion of aerobic mineralization increases to about 50%. Under high light conditions, photorespiration, as an additional oxygen sink, can account for up to 20% of the total generated oxygen; Temperature exhibits different Cardinal responses to production and consumption processes, with photosynthesis reaching its peak at around 35 ° C and collapsing at 40-45 ° C, while the re oxidation process has higher heat resistance (peak at around 45 ° C); Sedimentation exposure leads to a decrease of approximately 60% in photosynthesis. The model is released in the open source R package O2DIA/O2DIAshiny, providing a transferable framework for the interpretation and prediction of intertidal sedimentary oxygen dynamics. This study is the first to couple processes such as MPB vertical migration, photorespiration, re oxidation, and aerobic mineralization into a predictable mechanistic model at the sub millimeter scale, filling the gap of previous inversion methods that could only diagnose but not predict; The fusion of high-resolution microsensor data and mechanistic models provides a paradigm for sedimentary biogeochemical research, and it is recommended to publish it after substantial modifications. Main issues and suggested modifications:

1. Insufficient discussion on parameter identifiability and calibration uncertainty (lines 280-298, section 3.2): The manuscript acknowledges that due to the fact that light field measurement and O<sub>2</sub> measurement are not located at the same position, parameters such as  $k_{ext}$ ,  $\mu$ ,  $\sigma$ ,  $kl$ ,  $w$  cannot be independently constrained, but are jointly estimated through O<sub>2</sub> production rate profiles. This is a substantive model recognizability issue, but the manuscript does not provide: results of parameter sensitivity analysis; Correlation and covariance estimation between parameters; Is the objective function used for calibration the weighted least squares of the O<sub>2</sub> concentration profile and GPP profile? How to determine the weight?); The propagation of parameter uncertainty to the quantitative evaluation of simulation results.

**Response:**

*We thank the reviewer for emphasizing parameter identifiability and calibration uncertainty as points that have not been sufficiently developed in the original manuscript. In the revised manuscript, we have clarified the calibration procedure, added post-calibration local sensitivity and practical-identifiability diagnostics, and explicitly distinguished these diagnostics from formal statistical covariance estimation.*

*The calibration was conducted sequentially by manual, profile-by-profile visual matching of the measured  $O_2$  and gross-production profiles. Consequently, no weighted least-squares objective function, profile-specific weighting scheme, likelihood function, or formal parameter covariance matrix was defined. We now state this explicitly in the Methods.*

*We added a local normalized sensitivity analysis using the measured  $O_2$  profiles and the gross-production profiles. For each analysis, the fitted value of one parameter was increased by 0.1% simultaneously in all PI conditions, while retaining the original fitted core- and condition-specific parameter values. This assesses whether the PI observations distinguish the effects of parameter classes; it does not assume that parameters such as  $\mu$  and  $\sigma$  have one common value across all cores and irradiances. The  $O_2$  profiles were most sensitive to light attenuation and deep ODU concentration, whereas the gross-production profiles were most sensitive to light attenuation, MPB-distribution parameters, the photosynthetic rate coefficient, and the P-I response parameters.*

*We further added an FME collinearity analysis of the same profile sensitivities. All possible two-, three-, and four-parameter combinations among the 14 PI-fitted parameters were evaluated, and we additionally evaluated the five-parameter group highlighted by the reviewer ( $k_{ext}$ ,  $\mu$ ,  $\sigma$ ,  $kl$ , and  $w$ ). The  $kl$ - $w$  pair had a collinearity index of 36.0, the reviewer-highlighted five-parameter group had an index of 40.7, and the photorespiration-ebullition group ( $c_{photoresp}$ ,  $m_{photoresp}$ ,  $f_{O_2,ebul}$ , and  $r_{O_2,ebul}$ ) had an index of 30.0. These results show that these parameter groups cannot be independently resolved from the PI profile data alone. The diagnostics quantify local practical identifiability: a high collinearity index indicates that simultaneous changes in a parameter group generate nearly indistinguishable changes in the measured profiles. They are not formal parameter correlations or covariances, because the original calibration did not define a statistical objective function or residual-error model.*

*Finally, uncertainty propagation to the standardized-system predictions was already evaluated through the Monte Carlo simulations shown in Figs. 3 and 4. In these forward simulations, selected parameters were independently varied by  $\pm 10\%$ , and the resulting ranges in vertical profiles and depth-integrated  $O_2$  budgets are shown as shaded envelopes. We have clarified that these ranges represent robustness to assumed plausible*

*parameter ranges, rather than formal confidence intervals inferred from calibration residuals.*

2. The steady-state assumption does not match the time scale of the dynamic experiment (lines 143-148, lines 555-562): The authors have self-questioned in lines 555-562 that the "5-fold difference in light/dark re oxidation rate coefficients" observed in the PI experiment may be due to the fact that the ODU profile did not reach true steady state (ODU comes from a much thicker sedimentary layer than the oxide layer, and its response is much slower than O<sub>2</sub>). But the model calibration still assumes steady state: this assumption directly affects the estimation of  $r_{\text{reox}}$ , which in turn affects the quantitative reliability of the core conclusion that "re oxidation dominates low light oxygen consumption"; The manuscript does not provide any evidence to demonstrate whether the processing time of each experiment is sufficient to achieve steady state of O<sub>2</sub>, nor does it evaluate the impact of ODU quasi steady state error on parameter estimation.

**Response:**

*We thank the reviewer for the opportunity to clarify this point. The potential mismatch between the rapid adjustment of the O<sub>2</sub> profile and the slower adjustment of the reduced-compound pool was already recognized and discussed in the manuscript. Each PI condition lasted approximately 2–3 h, including O<sub>2</sub> profiles before and after the depth-resolved GPP measurements. Although this duration is sufficient for repeated O<sub>2</sub>-profile measurements, the attainment of a true whole-system steady state additionally requires equilibration of the ODU profile.*

*As stated in the manuscript, ODU concentrations were not measured independently, and the present model represents all reduced compounds as one lumped dissolved ODU pool. It therefore does not explicitly describe the production, storage, transport, and oxidation of individual dissolved and solid-phase reduced compounds. For this reason, a dynamic simulation with the present model cannot provide an independent test of whether the real sedimentary ODU pool reached steady state during the PI treatments: it would only describe the equilibration behavior implied by the assumed simplified ODU formulation. We therefore do not add additional dynamic-model analyses to the revised Supplementary Information.*

*The steady-state representation of ODU is thus an explicit and necessary modelling assumption, required to infer O<sub>2</sub>-consumption pathways from the available O<sub>2</sub> and GPP measurements. We have strengthened the Discussion to state this more clearly and to emphasize that resolving the apparent light/dark contrast in  $r_{\text{reox}}$  requires time-resolved*

*measurements of relevant dissolved and solid-phase reduced compounds, together with a mechanistic multi-component ODU model. The present results therefore identify a clear direction for future measurements and model development.*

3. The parameterization of MPB vertical migration is too empirical (lines 365-372, formula 15): formula 15 linearly relates  $\sigma$  to incident light  $I_2$ :  $\sigma(I_2) \approx 2 \times 10^{-3} + 2.25 \times 10^{-7} \cdot I_2$ . This relationship is only based on fitting three core samples from PI experiments, and the variation of  $\mu$  with light is "statistically insignificant ( $p=0.357$ )" and lacks mechanistic basis (such as biophysical mechanisms of phototaxis/avoidance response). Its applicability has not been verified under different temperatures or exposure conditions - the model only "fine tuned"  $\mu$  and  $\sigma$  in TR and IE experiments, but... Whether to still follow formula 15 without explanation.

**Response:**

*We would first like to clarify how this empirical relationship was derived and used. The MPB distribution parameters  $u_{\text{bio}}$  and  $sd_{\text{bio}}$  were fitted independently for each measured profile based on the corresponding  $O_2$  production profile. The relationship between  $sd_{\text{bio}}$  and incident irradiance was derived only afterwards from these independently fitted values. Thus, Eq. 15 was not used to prescribe the MPB distribution during model calibration, and the fitted distributions of the individual profiles were not constrained to follow this relationship. We have clarified this point in the revised Methods.*

*The representation of MPB redistribution is intentionally empirical. Our aim was to describe the observed vertical redistribution of active MPB biomass with the simplest possible formulation, using only two parameters that define its vertical position and spread, rather than to construct a mechanistic model of MPB migration. Explicit representation of phototaxis, photoprotection and other behavioral or physiological controls on migration would require additional state variables, processes and parameters that cannot be constrained by the measurements available here. This is consistent with the deliberately parsimonious design of O2DIA, which is intended to reproduce the dominant  $O_2$  dynamics under the investigated conditions rather than resolve all underlying physiological mechanisms.*

*We have therefore retained the empirical formulation but revised the manuscript to clarify its derivation, its role in the model, and its limited applicability. In particular, Eq. 15 should be interpreted as an empirical relationship observed across the PI profiles rather than a generally applicable mechanistic law of MPB migration.*

4. The heuristic function for the tidal exposure effect lacks a mechanistic explanation (lines 225-228, formula 8, lines 605-618): the function  $g(h) = g_0 + (1 - g_0) \cdot h^2 / (h^2 + k_h^2)$  is purely a mathematical fit, with  $g_0$  ranging from 0.4 to 0.5. Section 4.5 discusses possible mechanisms (CO<sub>2</sub> availability, nutrient supply, sediment physical compaction), but: no additional experimental or literature quantitative data has been used to constrain  $g_0$  and  $k_h$ ; The response differences among the three IE cores are significant (core 8 decreases to <5%, core 7 remains almost unchanged), but the model only characterizes it with a single  $g_0 \approx 0.4-0.5$ , masking this heterogeneity; The treatment of compressing the diffusion layer (DBL) to zero under exposed conditions is too idealized.

**Response:**

*Indeed, the emersion function  $g(h)$  was introduced as a phenomenological representation of the observed reduction in photosynthetic activity during emersion, rather than as a mechanistic description of the physiological processes responsible for this response. Although reduced MPB productivity during emersion has been reported previously, including by Lara et al. (2018), we are not aware of quantitative relationships that could be used to independently parameterize the dependence of photosynthesis on water height. The parameters  $g_0$  and  $k_h$  were therefore roughly estimated based on the present experimental observations.*

*The strong differences among the three IE cores represent an important limitation of this formulation. Interestingly, these differences could be reproduced while keeping the parameters of the emersion response function approximately constant and adjusting the MPB biomass distribution among the individual cores. We therefore chose not to introduce additional core-specific parameters into  $g(h)$ . This represents a deliberate trade-off between reproducing the observations and avoiding additional parameters that cannot be independently constrained. Determining whether the contrasting responses among cores arise from differences in CO<sub>2</sub> availability, nutrient supply, sediment physical properties, MPB physiology, or other mechanisms requires dedicated experiments beyond those available in the present study.*

*We are aware that setting the DBL thickness to zero during emersion is an idealization. In reality, residual surface water films and microscale variations in surface wetness may persist and affect diffusive transport. These features were not measured and therefore cannot be quantitatively represented with the present data. We have retained this simplifying assumption but now state it explicitly as a limitation. More generally, we have revised the manuscript to clarify that  $g(h)$  and the treatment of the DBL are effective representations developed for the experimental conditions investigated here, rather than mechanistic descriptions expected to apply universally.*

5. The boundary description of the model is not prominent enough (lines 650-658): The model currently only considers molecular diffusion and ignores: wave driven pore water exchange in permeable sediments; Biological disturbance and biological irrigation; Horizontal processes and tidal gradients. These are mentioned as "future development" in lines 655-658, but the statement "predicting O<sub>2</sub> dynamics in intertidal dimensions" in the abstract and introduction may lead readers to mistakenly believe that the model is universally applicable to intertidal zones. In fact, the model is strictly applicable to intertidal sediments dominated by mud, low permeability, and MPB.

**Response:**

*Although we are fully aware that the model is only applicable under diffusion-governed transport, we acknowledge that we did not communicate this with a sufficient emphasis. To correct this, the title has been changed to specify diffusion-dominated intertidal sediments, and the Abstract, Discussion and Conclusions now also explicitly restrict the present model to cohesive, diffusion-dominated intertidal sediments. We also clarify that application to permeable sediments, where advective porewater transport becomes important, would require further model development to explicitly represent advective transport. Broader statements implying general applicability to intertidal sediments have been revised accordingly.*

6. Add references in lines 18-19 of the introduction  
( <https://doi.org/10.1016/j.scitotenv.2023.168299> )

**Response:**

*Thank you for the suggested reference. We have added it to the revised manuscript.*