

Quantifying aggregation bias in marsh carbon flux estimates caused by rhizosphere oxygen heterogeneity

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Abstract. Rhizosphere oxygen in marsh soils is highly heterogeneous, yet ecosystem models often evaluate respiration at a single mean O₂. This may lead to systematic bias due to the nonlinear response of respiration to O₂. We quantified this potential aggregation error using a Dual Arrhenius Michaelis-Menten scheme calibrated to incubation measurements on marsh-soil samples. With carbon and temperature held constant, we prescribed plausible rhizosphere O₂ distributions (gas and aqueous phase) and compared respiration at the mean O₂ with the mean of respiration across the full O₂ field. For the gas phase, the uniform approach overestimated aerobic CO₂ production by 11.7 %. The bias increases with O₂ variance and with the ratio of mean O₂ to the microbial O₂ half-saturation due to the concavity of the O₂-limitation term. In the aqueous phase, O₂ lies markedly below half-saturation and variance is small, so the bias is ~ 0 %; matching microbial physiology to similar relative saturation, however, leads to a negative bias comparable to the gas phase. Assessing mean O₂, its variance, and the assumed O₂ half-saturation provides a possibility to quantify aggregation error in ecosystem-scale models of marsh soil carbon balance.

1 Introduction

Aerobic heterotrophic respiration in marsh soils is regulated by oxygen (O₂) availability in the rhizosphere. Spatial O₂ heterogeneity arises from trait-mediated root oxygen loss (ROL), sediment structure, and hydrologic state, producing millimetre-scale oxic-anoxic transitions that modulate microbial activity and carbon mineralization (Van Der Nat and Middelburg 1998; Visser et al. 2000; Mueller, Jensen, and Megonigal 2016; Kühl et al. 2021). These processes happen within ecosystems that are major coastal carbon reservoirs, where high primary production and sediment trapping coincide with comparatively slow decomposition (Barbier et al. 2011; Duarte et al. 2013; Kirwan et al. 2016; Granse et al. 2024). The

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Deleted: Estuarine marshes are crucial components of coastal environments around the world and provide numerous ecosystem services, such as carbon sequestration. Plant-microbe interactions are potential key drivers of organic carbon cycling in these ecosystems, but their contribution to the ecosystem-level carbon balance has been rarely quantified so far. This is partly due to the substantial intra- and interspecific variation of plant traits that are affecting microbial functions. Traits such as root oxygen loss and root exudation, for instance, modify soil heterotrophic respiration, but may strongly differ between plant species. Moreover, the non-linearity of the relationships between soil carbon fluxes and effects of plant-microbe interactions may require an explicit representation of trait variation for correctly estimating the carbon balance of estuarine marshes in ecosystem models. However, modelling approaches in this regard so far mostly represent plants as a set of traits that are based on average values of different individuals or species, thus not capturing trait variation. In this study, we implemented a key plant trait, the modification of soil oxygen concentration, into a simple model of heterotrophic respiration in estuarine marsh soils. We then compared two model configurations, one with and one without explicit representation of variation in soil oxygen levels, to estimate the effect on simulated heterotrophic respiration. We found a 10% reduction in the average respiration rate and a deviation from the median of +33%/-47% within the first and third quartile of the distribution in the approach that accounted for trait variation. This illustrates the potentially large impacts that may arise from spatial heterogeneity of plant species or changing community composition of plants on the carbon balance of estuarine marshes. We thus suggest implementing trait variation in marsh ecosystem models.

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resulting carbon balance depends not only on mean environmental conditions but also on the small-scale spatial distribution of O_2 in the root zone, which determines where and when aerobic decomposition can proceed.

Multiple mechanisms make rhizosphere O_2 inherently patchy. ROL varies among species and genotypes, with plant status (growth stage, stress), and through diel and seasonal cycles; aerenchyma development and barriers to ROL alter the effective conductivity of internal gas pathways. Hydrologic dynamics including tidal flooding, drainage fronts, and episodic drying interact with sediment texture to shape air-filled porosity and diffusion pathways. In situ measurements with microelectrodes and optical sensors consistently show steep radial O_2 gradients around roots and strong small-scale variability within and across root neighborhoods (Visser et al. 2000; Kühl et al. 2021). Thus, microbes experience a mosaic of microhabitats in which O_2 ranges from well-oxygenated to effectively anoxic over centimetres or less, a setting in which the nonlinear response of respiration to O_2 becomes pivotal.

Despite this heterogeneity, ecosystem-scale marsh models typically represent drivers of redox reactions in the soil by a single bulk state variable such as mean O_2 level, or a moisture/redox scalar applied uniformly within grid cells or plant functional types (Zhang et al. 2002; Morris et al. 2002; Swanson et al. 2014; Alizad et al. 2016; Kirwan et al. 2016; Rietl et al. 2021). Such simplification is pragmatic but neglects the effects of nonlinearity on predicted fluxes: under a concave O_2 limitation function (saturating, Michaelis-Menten-type), evaluating respiration at the mean O_2 generally differs from averaging respiration across a heterogeneous O_2 field. This is the well-known aggregation (upscaling) bias, a Jensen-type bias that stems directly from the curvature of the response function (Rastetter et al. 1992). For marsh soils, the existence of strong O_2 heterogeneity is well documented, and the physiological basis for concave limitation is well-established; yet the magnitude, direction, and robustness of the resulting aggregation bias remain poorly quantified (Bernal, Megonigal, and Mozdzer 2017; Mueller et al. 2020; Spivak et al. 2019; Bhattacharyya and Furtak 2022).

Here we quantify the potential aggregation bias that arises from spatial heterogeneity in rhizosphere O_2 , focusing on aerobic CO_2 production in the root zone. We do not explicitly simulate plant-internal gas transport or pore-scale advection-diffusion. Instead, we treat ROL and hydrology as drivers that generate local O_2 fields and evaluate their consequences for modeled respiration. To isolate oxygen effects, we use a Dual Arrhenius Michaelis-Menten (DAMM) respiration scheme (Davidson et al. 2012), with an explicit O_2 -limitation term, calibrate its carbon kinetics to marsh-soil incubations, and hold temperature and the substrate-moisture linkage fixed. We prescribe rhizosphere O_2 distributions using (i) a gas-phase proxy (primary driver) and (ii) an aqueous-phase proxy expressed in its native units. For a like-for-like comparison, we also include a diagnostic in which, for the dissolved case, the microbial O_2 half-saturation constant K_{M,O_2} is unit-matched so that the ratio of the spatial mean O_2 to K_{M,O_2} (our “relative saturation”) equals that of the gas case. We then quantify aggregation by contrasting a uniform configuration respiration evaluated at the spatial mean O_2 , with a heterogeneous configuration, the mean of respiration across the full O_2 distribution.

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Deleted: Estuarine marshes are ecosystems at the intersection of land and sea that are distinguished by their salt-tolerant plant species, diverse microorganisms, tidal dynamics, and variation in salinity. These marshes play an essential role for the global coastal environment with regard to ecosystem functions (Kirwan et al., 2016a) and they offer a variety of ecosystem services such as shoreline protection and water purification, i.e. filtering pollutants and excess nutrients before they reach coastal waters (Barbier et al., 2011). Estuarine marshes are crucial for carbon sequestration as they can store large amounts of carbon in their soil, mostly due to trapping of carbon-rich sediments and high primary productivity combined with slow decomposition of organic matter (Granse et al., 2024). The marshes are also important for nutrient cycling and as a habitat for a wide range of species (Duarte et al., 2013).

Plant-microbe interactions are key drivers of carbon cycling in estuarine marshes, as they affect both primary production and soil organic matter decomposition. One crucial process in this regard is root oxygen loss (ROL) by plants, which may create oxygen-rich microenvironments in the soil, thereby affecting microbial activity and pathways and, consequently, decomposition rates (Mueller et al., 2016). Spatial variation in oxygen levels plays a substantial role for the carbon balance of estuarine marsh ecosystem (Spivak et al., 2019), since high oxygen levels promote aerobic decomposition and large emissions of carbon in the form of CO₂, while low oxygen availability results in anaerobic processes that cause small release of carbon as methane (CH₄) (Bhattacharyya and Furtak, 2022). Soil microbes, in turn, affect plants by releasing nutrients during decomposition, thus influencing plant productivity and ecosystem carbon input (Wang et al., 2024). Hence, understanding plant-microbe interactions and their impacts on soil oxygen dynamics is essential for quantifying the carbon balance of estuarine marshes and predicting their response to environmental changes such as sea-level rise and climate change (Crump and Bowen, 2024; Kirwan and Blum, 2011; Spivak et al., 2023; Tang et al., 2021; Weingarten et al., 2023).

In recent years, process-based modelling approaches have been used to examine which biotic and abiotic factors drive the carbon balance of estuarine marshes. These models usually simulate processes such as photosynthesis, respiration, and nutrient cycling to estimate carbon fluxes, and represent plants by several plant functional types (PFTs), while interactions with microbes are often only implicitly considered. The Wetland-DNDC Model, for instance, assumes that soil microbial processes associated with various biogeochemical cycles in wetland ecosystems are driven mostly by plant litter, soil temperature, and hydrology (Zhang et al., 2002). Subsequent models have refined the representation of marsh ecosystem processes (Morris et al., 2002; Swanson et al., 2014), but concentrated mainly on linking marsh elevation changes and vegetation product...

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To assess robustness, we (a) vary kinetic and transport parameters over literature-informed ranges and (b) run a variance experiment at fixed mean O₂ using symmetric two-point mixtures. The first analysis tests sensitivity to plausible parameter uncertainty, while the second isolates the mechanism by linking bias magnitude directly to O₂ variance. Together, these steps provide a transparent, model-structural basis for when replacing heterogeneous rhizosphere O₂ with a single mean is acceptable and when it leads to systematic overestimation of aerobic CO₂ production.

2 Materials and methods

2.1 Model overview: DAMM with explicit O₂ limitation

We use the DAMM framework (Davidson et al. 2012) in which volumetric aerobic CO₂ production R_{ax} (mg C cm⁻³ h⁻¹) depends on temperature, soluble-carbon substrate, and oxygen:

$$R_{sx}(c_{org}, O_2, T) = \alpha_{sx} \times e^{\frac{-Ea_{sx}}{R_{gas}T}} \times \frac{S_x}{K_{m,s} + S_x} \times \frac{[O_2]}{K_{m,o_2} + [O_2]} \quad \text{Equation 1}$$

Here c_{org} is bulk organic C (g C cm⁻³); S_x is the soluble substrate concentration (g C cm⁻³); O_2 is an air-equivalent oxygen proxy expressed as (cm³ O₂ cm⁻³); T is absolute temperature (K); α (mg C cm⁻³ h⁻¹) and Ea (J mol⁻¹) are the pre-exponential factor and activation energy; $K_{m,s}$ (g C cm⁻³) and K_{m,O_2} (cm³ O₂ cm⁻³) are half-saturation constants; and R_{gas} is the universal gas constant. Symbols, units, and baseline values are listed in Table 1.

To isolate O₂ effects in the aggregation experiment, soluble carbon is linked to bulk carbon via a fixed moisture proxy:

$$S_x = c_{org} \times p \times D_{liq} \times \theta_{ref}^3 \quad \text{Equation 2}$$

where p (–) converts bulk to soluble carbon, D_{liq} (–) scales aqueous availability, and θ_{ref} volumetric water content used only inside the substrate term (to isolate oxygen effects). The oxygen-limitation term $O_2 / (K_{m,o_2} + O_2)$ is concave for $O_2 > 0$; this curvature is the source of aggregation bias examined below.

2.2 Incubation medians and calibration

We calibrated α and $K_{M,s}$ against median aerobic respiration rates derived from long-term marsh-soil incubations summarized with a two-pool ICBM framework (ICBM; (André et al. 1997; Knoblauch et al. 2013; Beer et al. 2022)). Incubation rates were converted from $\mu\text{mol CO}_2 \text{ g}^{-1} \text{ d}^{-1}$ to $\text{mg C cm}^{-3} \text{ h}^{-1}$ using soil bulk density and molar-mass factors. Parameters were estimated by bounded direct search (minimizing RMSE between model and medians) at a fixed reference oxygen $O_{2,\text{ref}}$ and fixed θ_{ref} . Uncertainty was quantified by non-parametric bootstrap resampling (500 replicates) to obtain 95 % confidence bands for the calibration curve and confidence intervals for α and $K_{M,s}$. The correlation between $\log_{10} \alpha$ and $\log_{10} K_{m,o_2}$ is reported to indicate identifiability. Fig. 1 shows the fit with bootstrap band and the calibration medians.

2.3 Prescribed rhizosphere O_2 distributions:

We prescribe two rhizosphere O_2 drivers and summarize each by its mean and variance.

■ Gas-phase proxy (primary analysis).

Air-filled porosity α is approximated as

$$\alpha = 1 - \frac{BD}{PD} - \theta \quad \text{Equation 3}$$

where θ is volumetric water content and BD and PD are bulk and particle densities (g cm^{-3}), respectively. Air-equivalent oxygen is then

$$O_2^{gas} = D_{gas} \times 0.209 \times \alpha^{\frac{4}{3}} \quad \text{Equation 4}$$

where D_{gas} (–) represents effective gas-phase diffusivity and 0.209 the atmospheric O_2 mole fraction. This proxy captures aeration in the rhizosphere and is used for all main analyses.

■ Aqueous-phase proxy (Henry's-law dissolved O_2)

An aqueous-phase O_2 proxy is derived from Henry's law equilibrium concentration multiplied by a bulk aqueous mobility factor. We do not rescale dissolved O_2 ; we retain its natural magnitude relative to K_{M,o_2} . In an additional analysis (reported

in the SI), we rescale K_{M,O_2} to the aqueous phase (no O_2 rescaling) so that relative saturation is comparable to the gas phase.

280 As a simple spatial benchmark, we furthermore consider a high- θ case (uniform in θ over a narrow saturated range, mapped to O_2 via the same proxy). All O_2 probability distributions are summarized by their first two moments (mean and variance) for use in the Jensen diagnostic.

2.4 Uniform-versus-heterogeneous experiment (aggregation error)

285 To assess the oxygen effect, the substrate term is held fixed by evaluating S_x at a signal θ_{ref} in all runs. For each C_{org} on a prescribed grid we compute:

- **Uniform configuration:** $R_{uni}(C_{org}) = f(C_{org}, \overline{O_2})$, i.e. evaluate R at the mean oxygen $\overline{O_2} = E[O_2]$.
- **Heterogeneous configuration:** $R_{het}(C_{org}) = E[f(C_{org}, O_2)]$, i.e. average R over the O_2 distribution.

290 Aggregation bias is calculated as:

$$\Delta_s(C_{org}) = \frac{R_{het}(C_{org}) - R_{uni}(C_{org})}{R_{uni}(C_{org})} \times 100\% \text{ Equation 5}$$

295 Unless stated otherwise, all main-text results use the gas-phase proxy; dissolved-phase results are reported as a sensitivity.

2.5 Dependence on O_2 affinity and transport distributions

Since K_{M,O_2} sets the relative O_2 -saturation regime, we performed a structured K_{M,O_2} variation (multipliers $\times 0.25$, $\times 0.5$, $\times 1$, $\times 2$, $\times 4$) for the gas proxy and for the aqueous proxy with unit-matched K_{M,O_2} . We further summarize bias behavior on a response surface as a function of mean(O_2)/ K_{M,O_2} and the coefficient of variation (CV) using a symmetric two-point distribution at fixed mean (reported in the SI).

2.6 Jensen diagnostic (mechanistic check)

300 To link bias magnitude to heterogeneity directly, we fixed the mean oxygen at $\mu = \overline{O_2}$ and constructed symmetric two-point mixtures $\{\mu - d, \mu + d\}$ (equal probability; range constrained to positive values) to vary $\text{Var}[O_2]$ while holding the mean

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305 constant. For each variance level we computed Δ from Sect. 2.5 and compared it to the quadratic approximation implied by the curvature of the O₂-limitation term:

$$\Delta(d) \approx \frac{1}{2} \times \frac{f''(\mu) - \text{Var}[O_2(d)]}{f(\mu)} \times 100 \% \text{ Equation 6}$$

310 Where $f''(\mu)$ is the second derivative of f with respect to O₂ at fixed C_{org} and T.

2.7 Implementation details

All analyses were performed with consistent grid resolution for C_{org} (300 points across 0.001- 0.30 g C cm⁻³). Calibration used bounded least squares; bootstrap size was 500; a fixed random seed was used for reproducibility.

315 **3 Results**

3.1 Model calibration and parameter uncertainty

320 The DAMM calibration reproduces the measured median respiration rates across the observed range of C_{org} (Fig. 1). Best-fit parameters are: $\alpha = 1.48 \times 10^{11}$ mg C cm⁻³ h⁻¹ (95 % CI: $1.04 \times 10^{11} - 9.93 \times 10^{13}$) and $K_{M,s} = 5.98 \times 10^{-6}$ mg C cm⁻³ (95 % CI: $2.64 \times 10^{-6} - 5.90 \times 10^{-3}$) with RMSE = 6.04×10^{-4} (mg C cm⁻³ h⁻¹). Bootstrap resampling (B = 500) yields narrow uncertainty bands at low moderate C_{org} and wider bands at the upper end, reflecting sparser constraints. As expected, log₁₀ α and log₁₀ $K_{M,s}$ are strongly correlated (Spearman's $\rho = 0.96$), indicating partial trade-off between scale and saturation in the carbon term; this does not affect the aggregation analysis because the bias metric Δ defined as the percent difference between the mean of the respiration response over the O₂ distribution and the response evaluated at the mean O₂ is computed with the same substrate term in both evaluations; only the O₂ limitation term differs.

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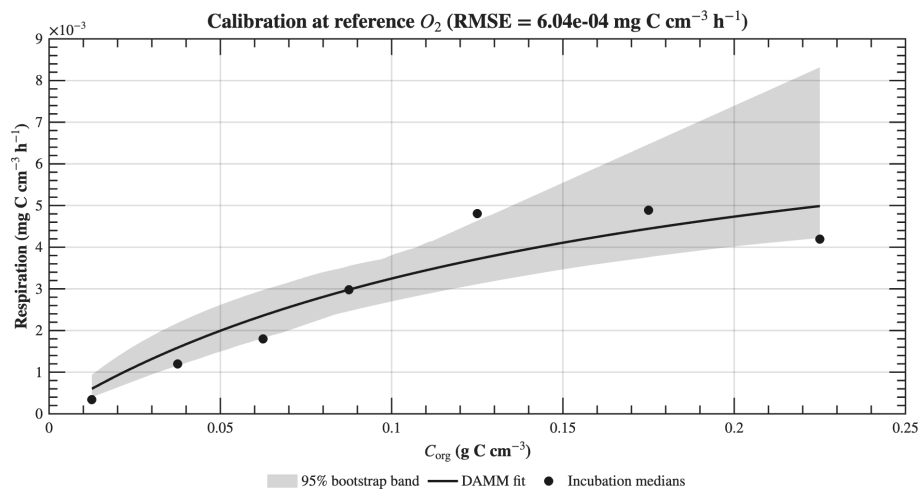


Figure 1: Calibration of the DAMM respiration model to incubation-derived respiration medians under aerobic conditions. Points show median rates for seven bins of bulk organic carbon (C_{org}) obtained from a two-pool ICBM fitted to Elbe estuary incubations (units converted to mg C cm $^{-3}$ h $^{-1}$). The solid line is the best DAMM fit evaluated at the air-equivalent O_2 corresponding to $\theta_{ref} = 0.30$; the shaded envelope is the 95 % bootstrap band ($B = 500$). Best-fit parameters: $\alpha = 1.475 \times 10^{11}$ mg C cm $^{-3}$ h $^{-1}$, $K_{M,S} = 5.98 \times 10^{-6}$ g C cm $^{-3}$; RMSE = 6.04×10^{-4} mg C cm $^{-3}$ h $^{-1}$. Parameter confidence intervals and provenance are summarized in Table 1.

Table 1. Parameters used in the DAMM analyses (fixed and fitted).

All constants are baseline values unless noted; fitted parameters carry 95 % bootstrap CIs.

Symbol	Description	Value / Estimate	Units	Status / Source
T	Temperature	293.15	K	Fixed at 20 °C
E_a	Activation energy	72.26×10^3	J mol $^{-1}$	Fixed; Davidson et al. (2012)

<u>K_{M,O₂}</u>	<u>O₂ half-saturation</u>	<u>0.121</u>	<u>cm³ O₂ cm⁻³ (air-equiv.)</u>	<u>Fixed:</u> <u>Davidson et al. (2012)</u>
<u>p</u>	<u>Soluble C fraction</u>	<u>4.14×10⁻⁴</u>	<u>=</u>	<u>Fixed:</u> <u>Davidson et al. (2012)</u>
<u>D_{liq}</u>	<u>Solute availability scalar</u>	<u>3.17</u>	<u>=</u>	<u>Fixed:</u> <u>Davidson et al. (2012)</u>
<u>D_{gas}</u>	<u>O₂ diffusivity scale</u>	<u>1.67</u>	<u>=</u>	<u>Fixed:</u> <u>Davidson et al. (2012)</u>
<u>BD</u>	<u>Bulk density</u>	<u>0.80</u>	<u>g cm⁻³</u>	<u>Fixed:</u> <u>Davidson et al. (2012)</u>
<u>PD</u>	<u>Particle density</u>	<u>2.52</u>	<u>g cm⁻³</u>	<u>Fixed:</u> <u>Davidson et al. (2012)</u>
<u>θ_{ref}</u>	<u>Reference water content (for S_x)</u>	<u>0.30</u>	<u>cm³ H₂O cm⁻³ soil</u>	<u>Fixed by design</u> <u>(decouple C from O₂)</u>
<u>α</u>	<u>Pre-exponential factor</u>	<u>1.475×10¹¹ [1.043 × 10¹¹, 9.925 × 10¹³]</u>	<u>mg C cm⁻³ h⁻¹</u>	<u>Fitted</u>
<u>K_{M,S}</u>	<u>Carbon half-saturation</u>	<u>5.98×10⁻⁶ [2.64 × 10⁻⁶, 5.90 × 10⁻³]</u>	<u>g C cm⁻³</u>	<u>Fitted</u>

3.2 Rhizosphere O_2 distributions

Both prescribed rhizosphere O_2 distributions are right-tailed on a log scale (Fig. 2). Because the dissolved proxy is $\approx 450\times$ smaller in magnitude than the gas proxy, we show them in separate panels to preserve visibility. For the gas-phase proxy [air-equivalent units], the mean and variance are $\mu = 0.0891$ and $\text{Var} = 3.53 \times 10^{-3}$ ($\text{cm}^3 O_2 \text{ cm}^{-3}$). For the dissolved proxy [native aqueous units], $\mu = 1.97 \times 10^{-4}$ and $\text{Var} = 1.16 \times 10^{-8}$. These moments are utilised in the Jensen diagnostic (Sect. 3.5). We retain each proxy in its native units (without cross-rescaling) so that their positions relative to K_{M,O_2} are preserved.

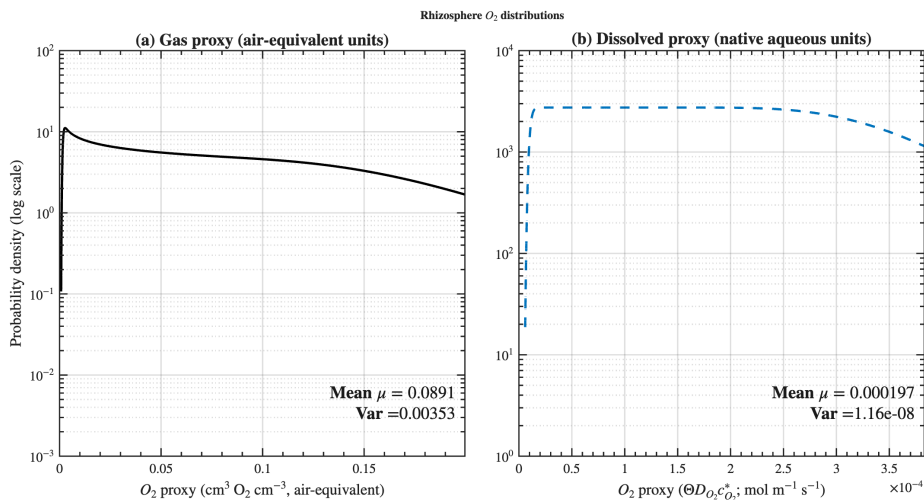
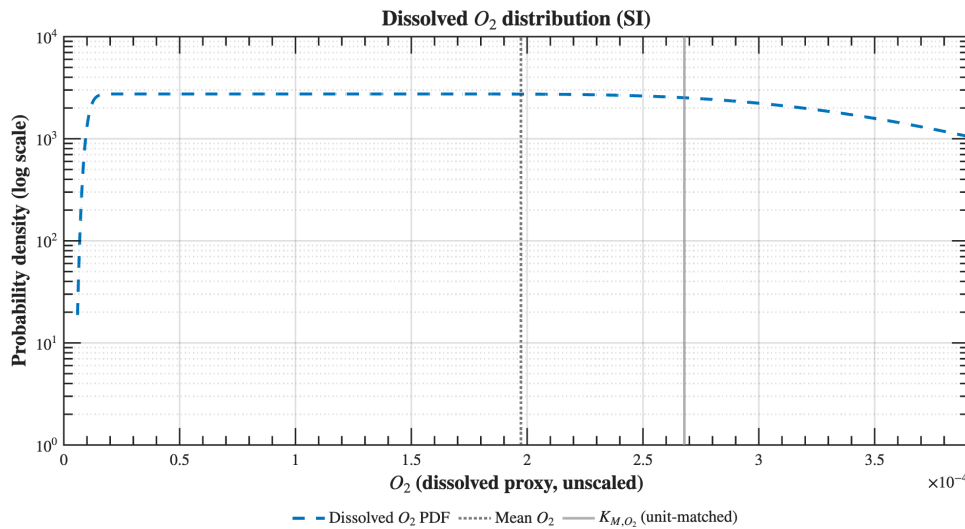


Figure 2a:

Probability density functions (log-scale y-axis) of the prescribed rhizosphere O_2 used to force the DAMM model: (a) gas-phase proxy in air-equivalent units ($\text{cm}^3 O_2 \text{ cm}^{-3}$) and (b) dissolved proxy in native aqueous units. Both distributions are strongly right-tailed. In-panel annotations report the first two moments (gas: $\mu = 0.0891$, $\text{Var} = 3.53 \times 10^{-3}$; dissolved: $\mu = 1.97 \times 10^{-4}$, $\text{Var} = 1.16 \times 10^{-8}$).



355 **Figure 2b:**
 Dissolved-phase O_2 PDF (log scale) with vertical markers for the distribution mean and the unit-matched K_{M,O_2} used in Fig. 4. This places
 dissolved and gas cases on comparable relative saturation without rescaling O_2 itself.

3.3 Aggregation bias: uniform vs heterogeneous O_2

360 Under the gas-phase driver, respiration evaluated at the mean O_2 (uniform configuration) is consistently above the mean of
 the responses to heterogeneous O_2 levels for all values of C_{org} (Fig. 3). The mean aggregation bias is -11.71% , i.e., using a
 single mean O_2 overestimates aerobic respiration by about one-tenth on average. For the dissolved proxy without rescaling,
 the mean O_2 is orders of magnitude below K_{M,O_2} , and the variance is small; the system is therefore near-linear in O_2 , and the
 aggregation bias is negligible (-0.05% ; Fig. S3). As a simple spatial benchmark, tightening the O_2 distribution to a high- θ
 365 range reduces variance and the bias decreases to a small value (-0.51% at $C_{org}=0.15\text{ g C cm}^{-3}$; Fig. S9).

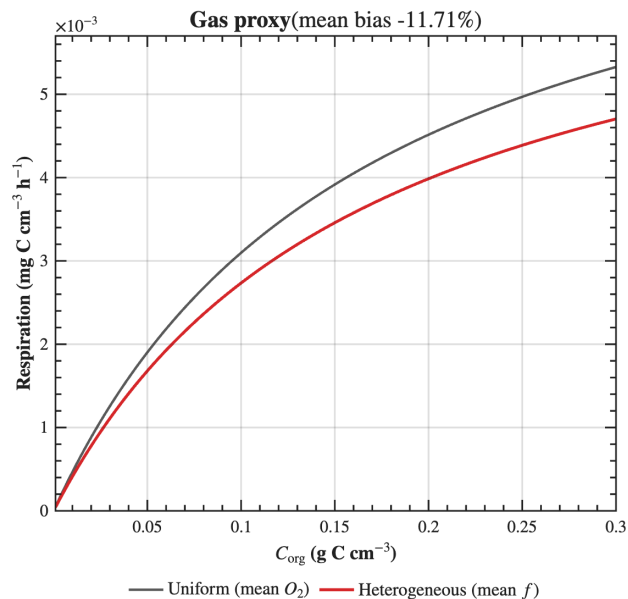


Figure 3:

Aerobic respiration across C_{org} when evaluated at the mean O_2 ("Uniform") versus averaged over the full O_2 distribution ("Heterogeneous"). For the gas-phase proxy, the mean aggregation bias is -11.71% (uniform overestimates respiration).

3.4 Dependence on O_2 affinity and relative saturation

To separate transport from microbial physiology, we varied K_{M,O_2} while holding the O_2 distributions fixed and plot the aggregation bias against the relative saturation ratio $\text{mean}(O_2) / K_{M,O_2}$, which collapses cases onto an interpretable axis (Fig. 4). For the gas proxy, varying K_{M,O_2} by factors of $\times 0.25$, $\times 0.5$, $\times 1$, $\times 2$, $\times 4$ yields a bias range from -13.15 % to -5.80 %. For the dissolved proxy with unit-matched K_{M,O_2} (i.e., chosen so that its mean O_2 concentration correspond to the same relative saturation as the gas case), the range is -8.97% to -3.97%. The baseline points occur at $\text{mean}(O_2) / K_{M,O_2} \approx 0.74$ for both

proxies; biases differ in magnitude because the underlying O_2 PDFs differ in spread. In short, the magnitude of bias increases as the system approaches the nonlinear mid-saturation regime and as O_2 variability increases.

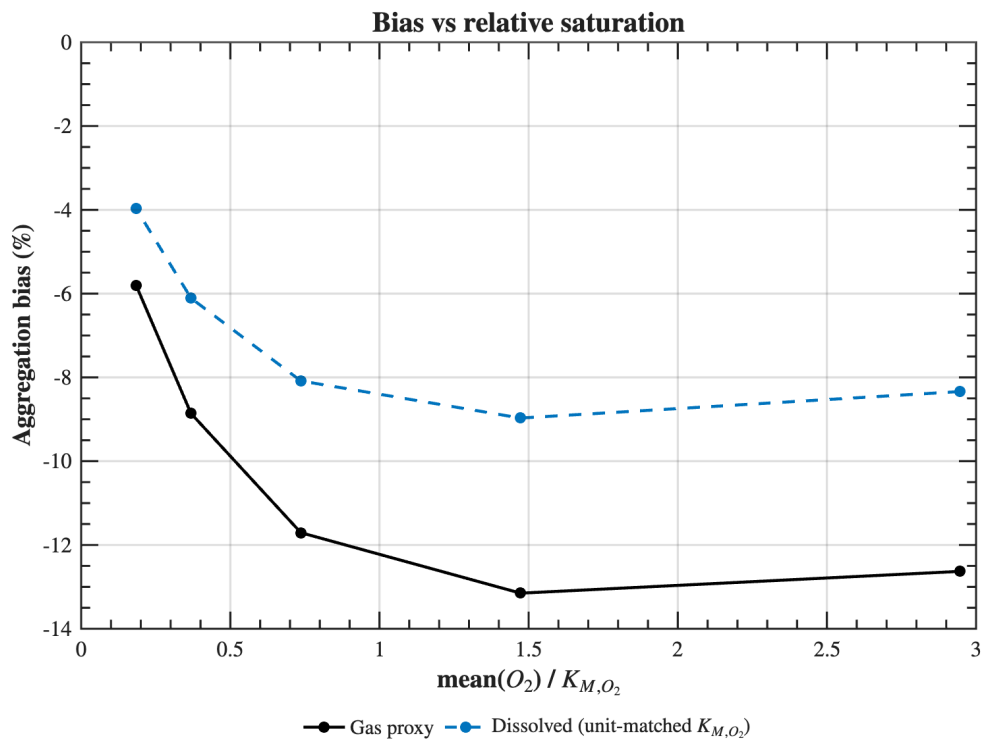


Figure 4: Aggregation bias (%) as a function of $\text{mean}(O_2) / K_{M,O_2}$ for two O_2 drivers: gas proxy (solid black) and dissolved proxy with unit-matched K_{M,O_2} (dashed blue). Bias magnitude increases as mean O_2 approaches K_{M,O_2} and decreases at very low or very high relative saturation.

3.5 Jensen diagnostic

Holding the mean O_2 fixed and increasing $\text{Var}(O_2)$ with symmetric two-point mixtures produces a near-linear growth in bias (Fig. S6). A second-order (quadratic) approximation based on the local curvature of the Michaelis–Menten O_2 term closely tracks the simulations, confirming that the bias is a structural consequence of concavity: averaging a heterogeneous O_2 field

yields $E[f(O_2)] < f(E[O_2])$. A response-surface view in the SI (Fig. S10) shows that bias remains non-positive across the explored domain and peaks when the mean(O_2) is comparable to K_{M, O_2} , and the coefficient of variation is large.

4 Discussion

Spatial heterogeneity in rhizosphere oxygen is a key feature of marsh soils, arising from plant-mediated transport, sediment structure, and hydrology. In this study we aimed to determine the error associated with replacing a heterogeneous rhizosphere O_2 field by a single mean value, as commonly done in large-scale ecosystem models. Based on a Michaelis–Menten-type respiration scheme, we consistently find that evaluating the model at the mean O_2 overestimates the heterogeneous response by about one tenth on average for the gas phase (Fig. 3). This overestimation persists when we vary the microbial O_2 half-saturation across a plausible range (Fig. 4). The comparison is internally controlled: the carbon term and temperature response are identical in both configurations; only the treatment of O_2 variability changes. The bias, therefore, reflects oxygen heterogeneity itself.

Separating diffusive O_2 transport from microbial physiology clarifies the patterns. Transport determines the shape and width of the O_2 distribution, while physiology determines the shape of the response curve relative to that distribution. Narrowing the O_2 distribution alone, for example, by restricting to a high- θ range, reduces variance and reduces the bias toward almost zero (Fig. S9). Varying only physiology via the ratio of mean(O_2) to the half-saturation (Fig. 4), illustrates that, as the system moves away from the near-linear regime and deeper into saturation, the negative bias increases and then decreases again.

This framework also explains why the unscaled aqueous proxy shows almost no bias while the gas proxy does. In native aqueous phase units, dissolved O_2 is orders of magnitude below the half-saturation and has a small variance, so the O_2 response is effectively linear and the bias is negligible (Fig. S3). When we assume that microbial physiology is adapted to average O_2 levels so that dissolved O_2 sits at a similar relative saturation to the gas case, the dissolved bias becomes comparable in sign and magnitude (Fig. 4). The difference between gas and aqueous drivers therefore arises from their position relative to microbial O_2 affinity and from their variance, not from a change in model form. The uniform benchmark must be the model evaluated at the mean O_2 of the imposed distribution. Using O_2 computed from the mean θ can misstate the baseline because the relationship between θ and O_2 is nonlinear, and it can even reverse the apparent sign of the bias. Fig. S8 illustrates this point. Stating the baseline in oxygen space removes this ambiguity.

These findings have direct implications for upscaling. When a model aggregates over heterogeneous rhizosphere conditions and the mean O_2 lies outside the near-linear range of the limitation function, replacing the entire O_2 field with its mean will

Deleted: By comparing the two model configurations (see Fig. 3) we find that the variation of the plant trait root oxygen loss leads to a 10% reduced respiration rate, when averaged over all soil oxygen levels, compared to the model configuration driven only by one average soil oxygen concentration, corresponding to a model with one plant functional type. The percentage reduction is averaged over the range of simulated soil carbon content. The first and third quartiles of the distribution of respiration responses comprise a deviation of +33% and -47% from the median curve, respectively.

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430 systematically overestimate aerobic CO₂ production. The magnitude of this overestimation increases with O₂ variance and with the relative saturation, $\text{mean}(\text{O}_2) / K_{\text{M},\text{O}_2}$. Reporting the O₂ variance and the mean $(\text{O}_2) / K_{\text{M},\text{O}_2}$ ratio (given a plausible K_{M,O_2}) is sufficient to anticipate the aggregation error and to decide when explicit spatial detail is needed.

435 A limitation of our study is that the O₂ drivers are proxies rather than coupled transport reaction simulations; they are designed to bracket realistic heterogeneity and to reveal how bias depends on the first two moments of O₂ and on microbial affinity. Community shifts across O₂ regimes may change the effective half-saturation; we explored this as a sensitivity (Fig. 4) rather than recalibrating by regime without independent evidence. Our calibration uses aerobic incubation medians and a fixed moisture term inside the substrate factor to isolate oxygen effects; therefore our conclusions apply to aerobic respiration and do not address anaerobic pathways or gas-liquid exchange.

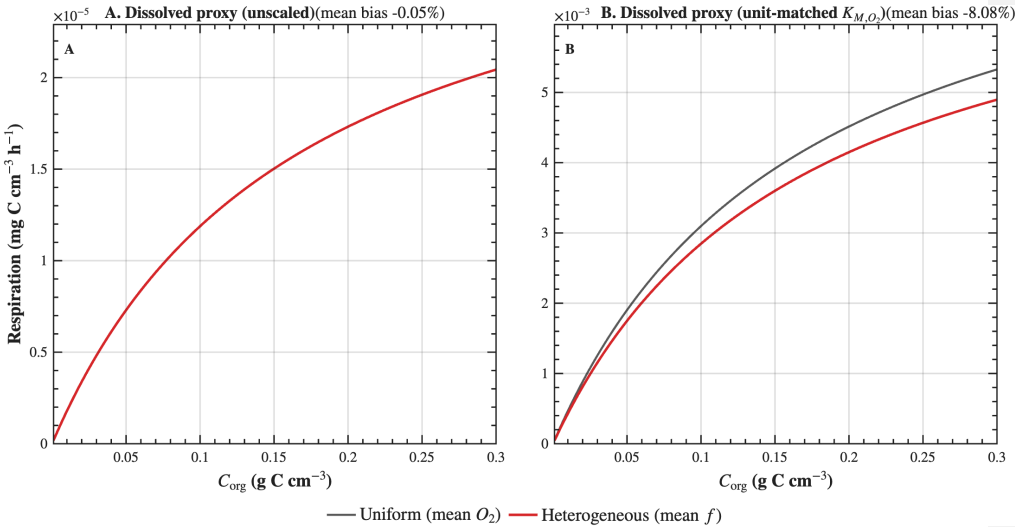
440 Spatial heterogeneity in rhizosphere oxygen produces a predictable, negative aggregation bias in aerobic respiration estimates. The sign is set by concavity, the magnitude scales with relative saturation and variance. Keeping unit integrity, defining the baseline at mean O₂, and reporting mean, variance, and a plausible K_{M,O_2} give ecosystem models a simple, transparent way to quantify and, if needed, correct for aggregation error.

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Appendix:



FigureS3:

A: Aerobic respiration as a function of bulk organic carbon (C_{org}) using the dissolved-phase O_2 proxy in native units (no rescaling). Gray: model evaluated at the mean O_2 (uniform). Red: mean of the model across the full dissolved- O_2 distribution (heterogeneous). The two curves are visually indistinguishable because the $\text{mean}(O_2) \ll K_{M,O_2}$ and the distribution variance is very small, placing the O_2 -limitation term in a near-linear regime. The resulting mean aggregation bias is -0.05% (negligible) across the C_{org} range.

B: Dissolved case with K_{M,O_2} unit-matched to its mean O_2 (no O_2 rescaling). Bias becomes comparable to the gas case (mean -8.08%), demonstrating the role of relative saturation.

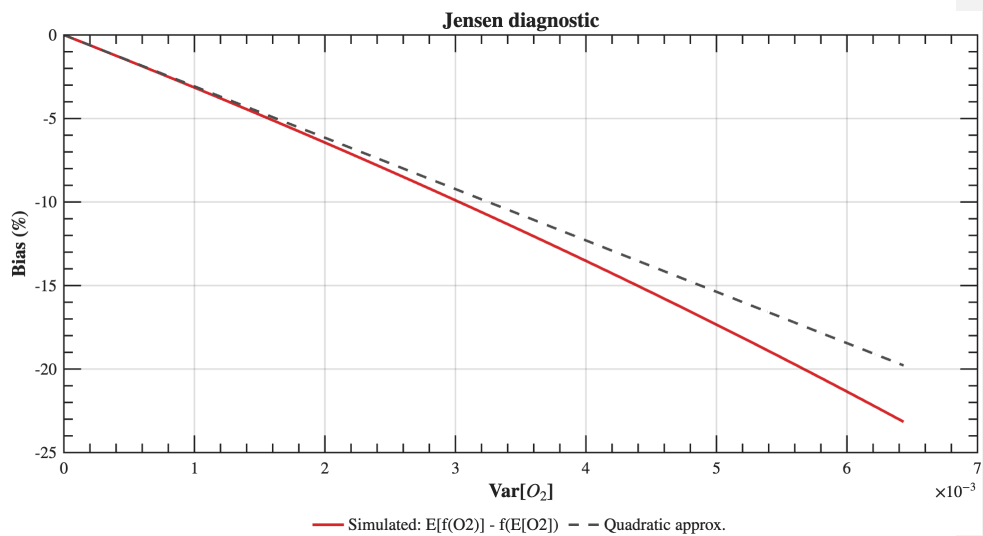


Figure S6:

Mechanistic check at fixed mean O_2 (μ). Red line: simulated $\Delta = E[f(O_2)] - f(E[O_2])$ while increasing $\text{Var}[O_2]$ using symmetric two-point mixtures. Gray dashed line: quadratic approximation from the local curvature of the O_2 -limitation term. Close agreement confirms that bias scales with variance due to concavity.

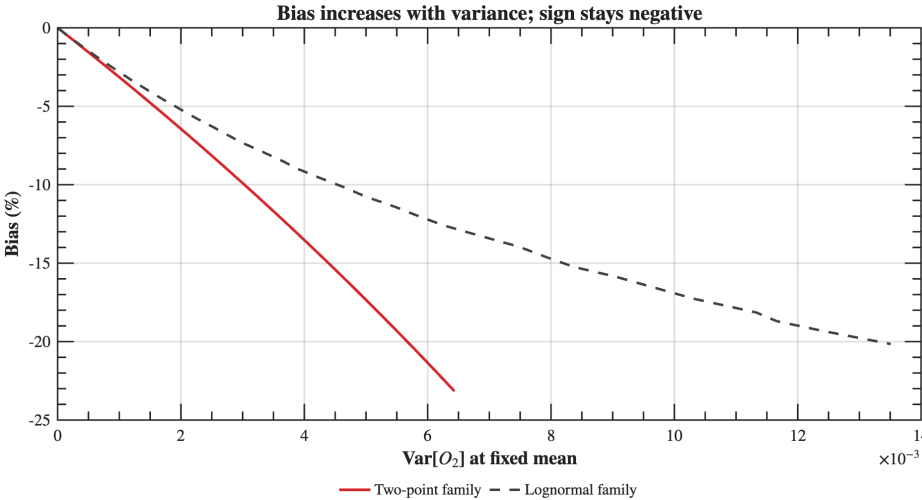


Figure S7:
Bias versus Var[O₂] at fixed mean for two distribution families: two-point mixtures (solid red) and lognormal (dashed gray). Across both families, bias remains negative and increases in magnitude with variance, indicating shape-robust behavior.

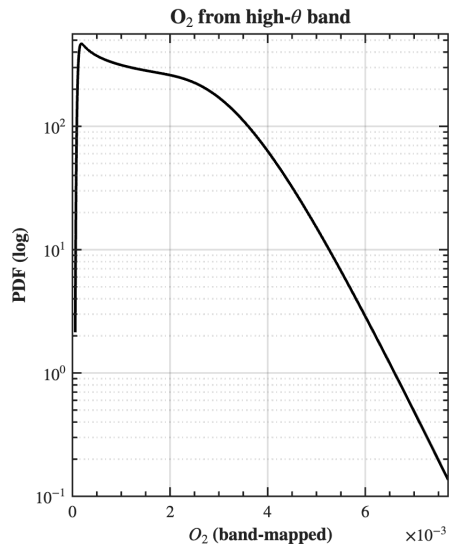


Figure S9:

Probability density of O_2 obtained by mapping a narrow water-content band, $\theta \in [0.65, 0.68]$, to gas-phase O_2 using the same proxy as in the main analysis; the density is shown on a log scale. This “high- θ ” band has much lower variance than the full rhizosphere distribution. Evaluated at $C_{org} = 0.15 \text{ g C cm}^{-3}$, the respiration predicted at the mean O_2 (uniform configuration) is slightly larger than the heterogeneous average $E[f(O_2)]$, giving an aggregation bias of -0.51% (uniform overpredicts). Numerically: $R_{uniform} = 1.2657 \times 10^{-4}$ and $R_{heterogeneous} = 1.2592 \times 10^{-4} \text{ mg C cm}^{-3} \text{ h}^{-1}$ (calibrated DAMM parameters; substrate term evaluated at $\theta_{ref} = 0.30$).

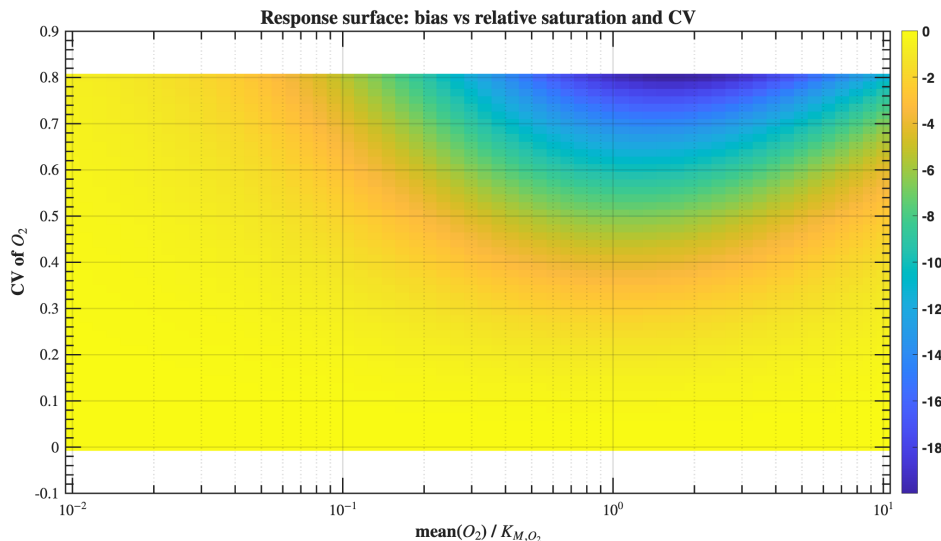


Figure S10

Heat map of aggregation bias (%) computed from a symmetric two-point family while varying $r = \text{mean}(O_2) / K_{M,O_2}$ (x-axis, log) and the coefficient of variation (y-axis). Bias is most negative at intermediate r (nonlinear regime) and large CV, and approaches zero at low r or low CV.

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Figure 3: Comparison of heterotrophic respiration rates assuming an average (black) versus varied (magenta) root oxygen loss.

The solid magenta line represents the average heterotrophic respiration response to soil carbon content across the entire range of oxygen levels, while the red dashed lines denote the first and third quartiles of this range. The black dotted line indicates the simulated respiration response assuming an average soil oxygen concentration.

Our simple model experiment illustrates the potentially substantial impact of variation of plant traits associated with root oxygen loss and microbial respiration for the carbon balance of estuarine marshes. We considered a large range of possible soil oxygen levels in the model. However, also under natural conditions, strong variation in oxygen may occur in the rhizosphere of marsh ecosystems, due to (I) tidal dynamics and associated water table fluctuations (II) increased respiration rates causing short-term oxygen deficiency at small scale or (III) vegetation dynamics that may lead to the occurrence /disappearance of species that have a high rate of root oxygen loss. It should be noted here that we assume a uniform frequency distribution of all possible oxygen levels at a given site in our modelling approach. To develop this further, a representation of all relevant abiotic and biotic factors that cause variation in soil oxygen concentration would be required in marsh ecosystem models. In particular, different plant types /species, each characterized by microbe-related traits, and the (dynamic) abundance of these plants would have to be considered, but also dynamic soil hydrological and thermal conditions. Such a modelling approach would not only be adequate to estimate the role of plant-microbe interactions for the current carbon balance of marsh ecosystems, but it would also allow more realistic predictions of carbon fluxes under climate change pressures, such as warming and sea level rise. Considering only our simple approximation of varied root oxygen loss, and assuming global soil carbon emissions of 31 Tg a^{-1} via heterotrophic respiration from salt marshes (Alongi, 2020), the estimated reduction by 10% would correspond to roughly 8% of global annual anthropogenic carbon emissions (Intergovernmental Panel on Climate Change (IPCC), 2023).

Code availability

The MATLAB codes are available can be downloaded from a repository: <http://doi.org/10.25592/uhhfdm.17912>

Data availability

The data is available upon request from the corresponding author. The ICBM data can be downloaded from a repository; access will be granted upon request. <http://doi.org/10.25592/uhhfdm.14367>.

Author contribution

YS, PP, CB and PM designed the study and YS, PP, and CB carried out the modelling. FN, JNB and AE designed the incubation experiment, FN investigated and provided the incubation data. YS wrote the manuscript with input from all co-authors.

Competing interests

The authors declare that they have no conflict of interest.

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