

Supplementary Material for:

A comprehensive porewater isotope model for simulating benthic nitrogen cycling: Description, application to lake sediments, and uncertainty analysis

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Supplementary Material

15 In this section, additional model outputs are reported. All included figures are referenced in the main text.

S1. Bayesian inference

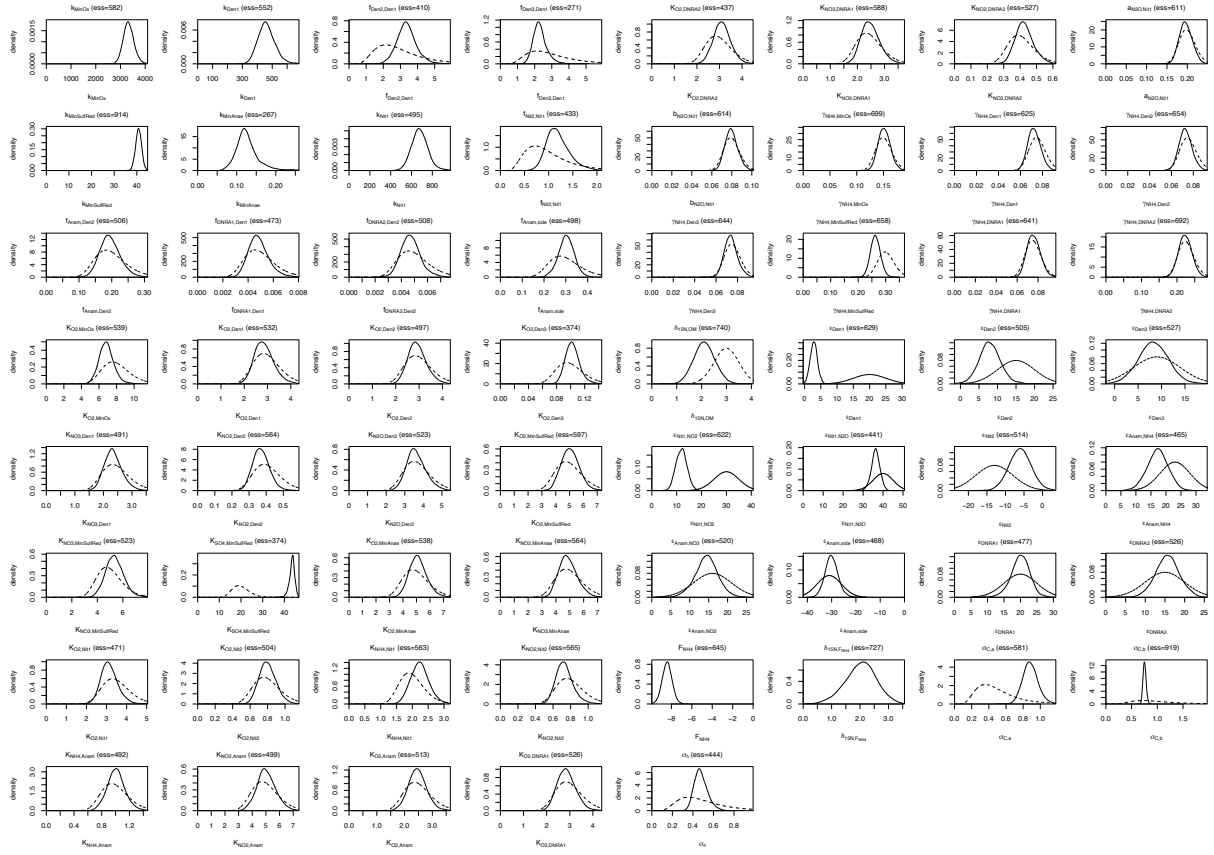


Figure S1. Overview of the marginal prior and posterior distributions for all parameters estimated in the Base scenario.

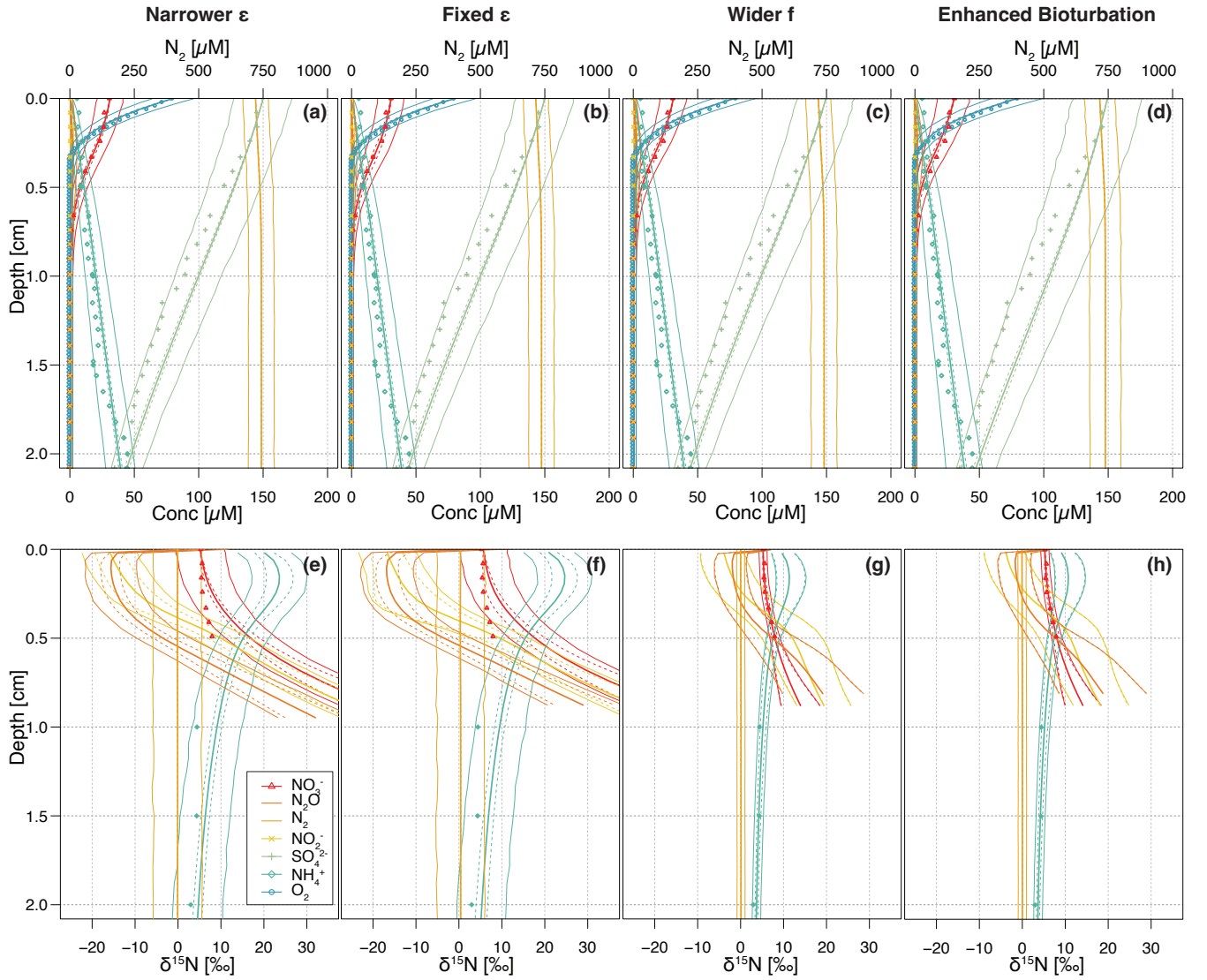


Figure S2. Vertical profiles of concentrations (a-d) and isotopic composition (e-h) of the state variables for the four considered scenarios: Narrower prior for ε values (a,e); fixed ε values based on literature (b,f); wider priors for the fractions of anammox and DNRA (c,g); enhanced bioturbation (d,h). Continuous lines represent the model outputs; symbols represent field-measurement data from Lake Lucerne. For NH_4^+ , open diamonds are based on an interpolation of the high-resolution dataset, using absolute concentrations from the low-resolution data (filled diamonds).

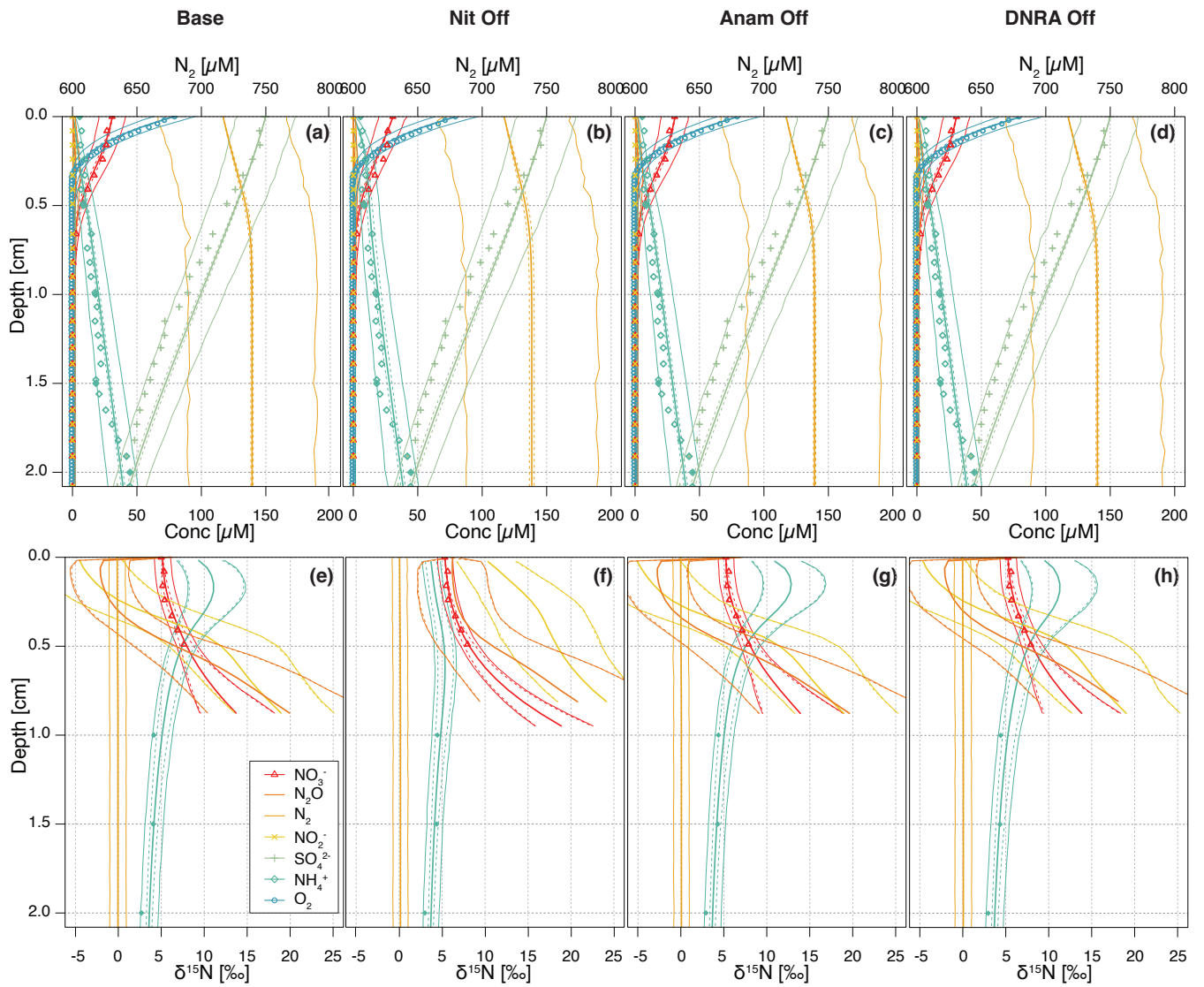
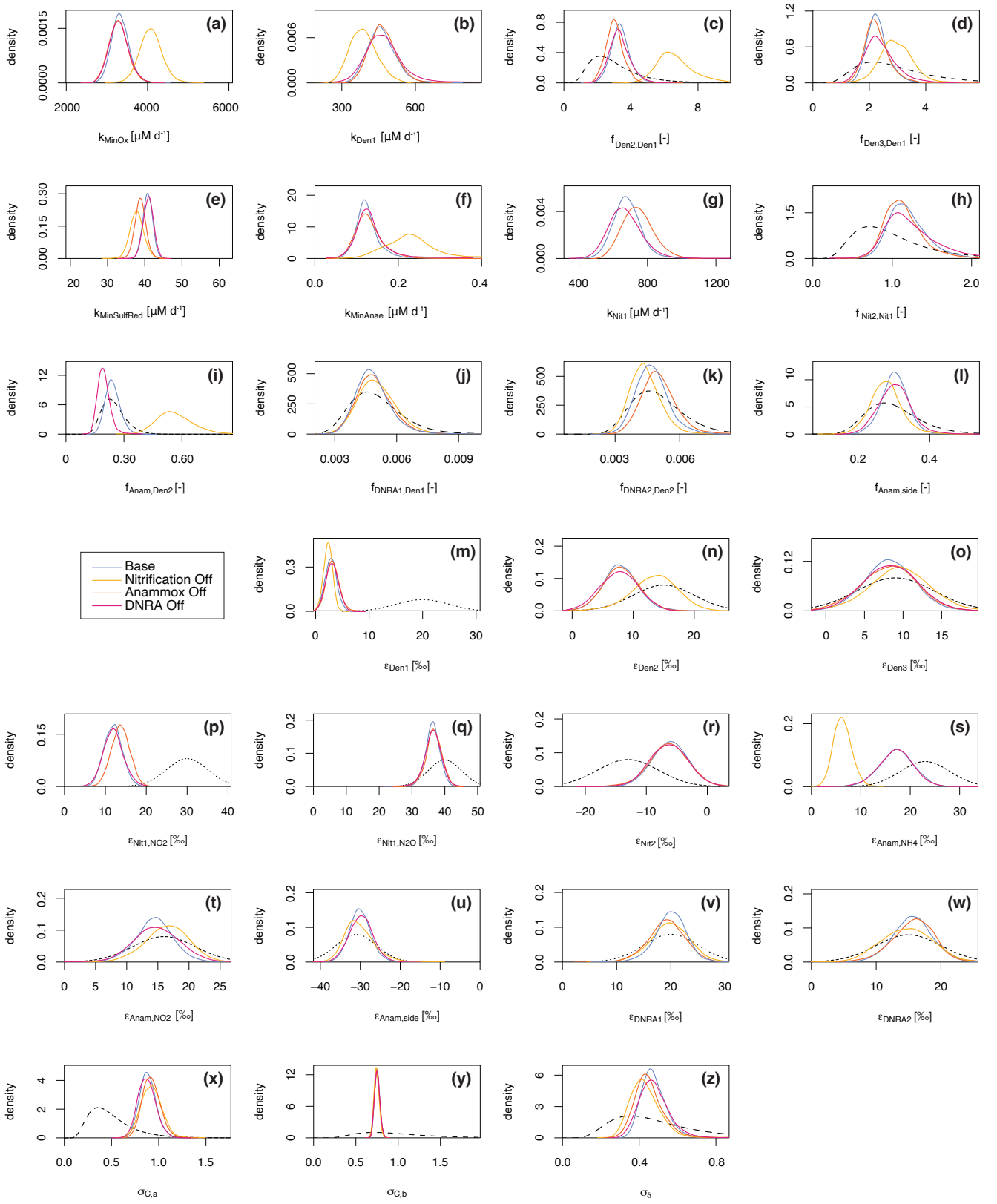
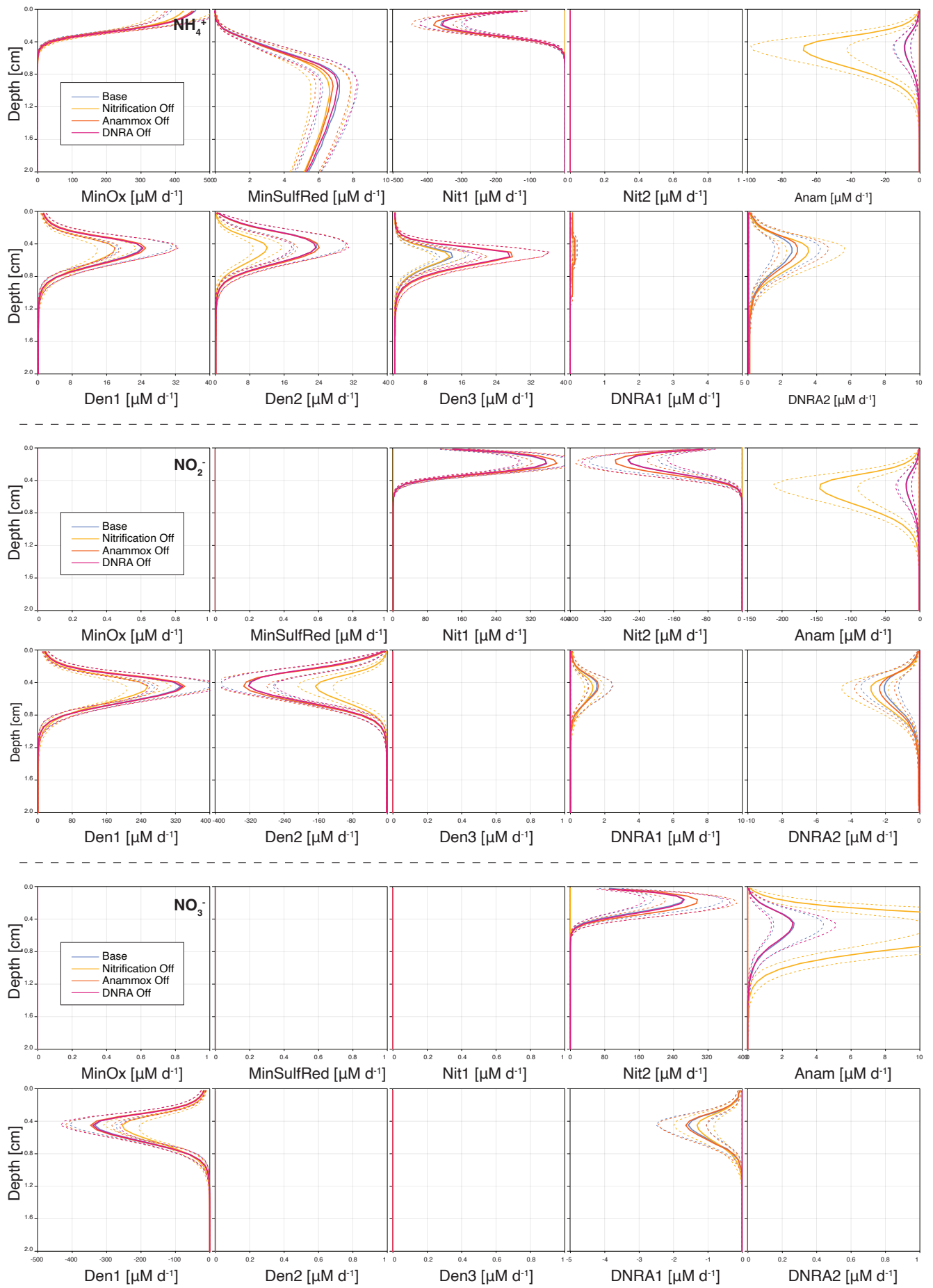


Figure S3. Vertical profiles of concentrations (a-d) and isotopic composition (e-h) profiles of state variables, shown for the full model with all processes included (a,e), and for cases where individual processes were excluded following optimization and inference: nitrification (b,f), anammox (c,g), and DNRA (d,h). Continuous lines represent model outputs; symbols represent experimental data from Lake Lucerne. For NH_4^+ , open diamonds are based on an interpolation of the high-resolution dataset, using absolute concentrations from the low-resolution data (filled diamonds).

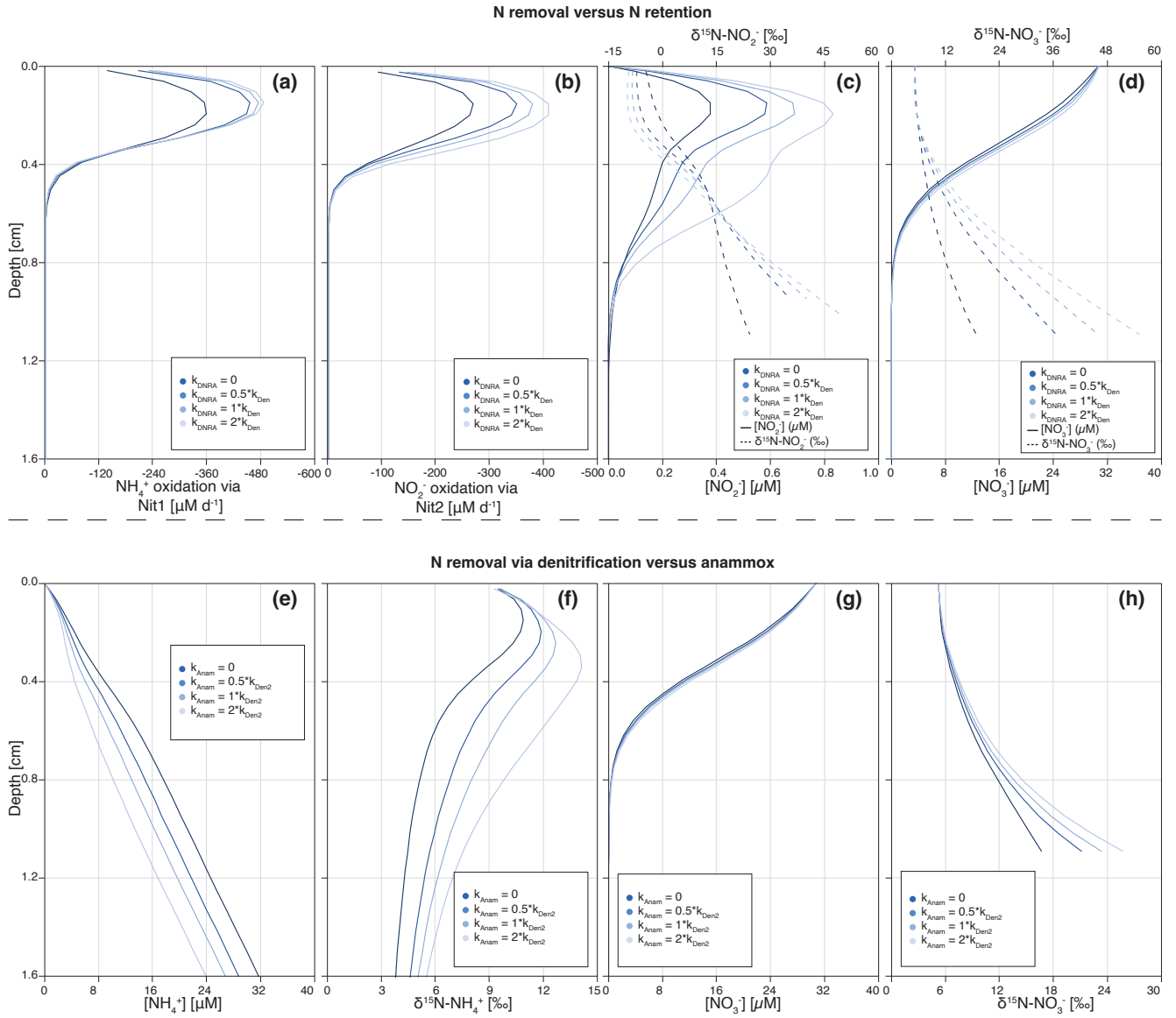


35 **Figure S4. Density distributions of selected estimated parameters, showing prior (dashed line) and posterior (continuous lines) distributions for the full model (all processes included), and for cases where individual processes (nitrification, anammox, and DNRA) were switched off. These results were obtained upon running optimization and inference.**



40 **Figure S5.** Vertical profiles of production and consumption rates (in $\mu\text{M d}^{-1}$) for NH_4^+ , NO_2^- , and NO_3^- under four model configurations: the full model with all processes included and scenarios with nitrification, anammox, or DNRA individually switched off. These results were obtained upon running optimization and inference.

S4. Model applicability in distinct scenarios



45 **Figure S6. Depth profiles of process rates, solute concentrations and $\delta^{15}\text{N}$ values for the two idealized cases investigated: (i) NO_3^- reduction via DNRA and denitrification (a-d), and (ii) N_2 production via anammox and denitrification (e-h). Shadings represent different model scenarios within each case, as defined in the legend. For case (i), colour shading lightens with increasing contribution of DNRA (relative to denitrification) to total NO_2^- reduction. DNRA accounts for 0‰ ($f_{\text{DNRA}} = 0$), 33‰ ($f_{\text{DNRA}} = 0.5$), 50% ($f_{\text{DNRA}} = 1$) and 66% ($f_{\text{DNRA}} = 2$) of total NO_2^- reduction. The resulting effects on nitrification rates (a-b), as well as on the intermediate NO_2^- (c) and substrate NO_3^- (d) pools are shown. For case (ii), colour shading lightens with an increasing proportion of NO_2^- consumed via anammox (relative to denitrification). Anammox contributes 0‰ ($f_{\text{Anam}} = 0$), 33‰ ($f_{\text{Anam}} = 0.5$), 50% ($f_{\text{Anam}} = 1$) and 66% ($f_{\text{Anam}} = 2$) of total NO_2^- consumption/ N_2 production. The resulting effects on NH_4^+ (e-f) and NO_3^- (g-h) concentrations and $\delta^{15}\text{N}$ values are also shown.**

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