

Iron cycle interactions with hydrological dynamics reduce methane production in a simulated Arctic soil

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Introduction

This supporting information includes four supplemental figures. Figure S1 shows the pH response function used for methanogenesis along with the data points used to parameterize it. Figures S2 and S3 show the results of simulations using a range of fermentation rate constant and acetate half saturation constants. Figure S4 shows time series of various quantities from a simulation of repeated oxic-anoxic cycling in an organic horizon. Figures S5 and S6 show time series comparisons between measured and modeled quantities for simulations with and without direct inhibition of methanogenesis by Fe(III), respectively.

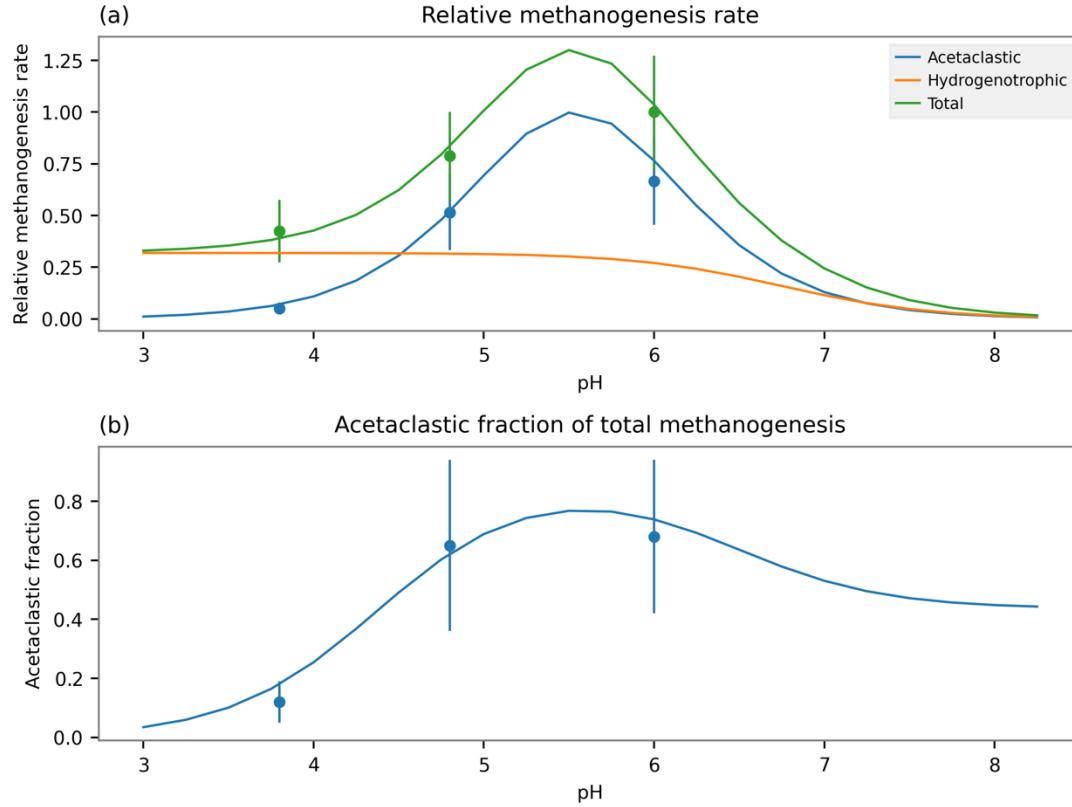


Figure S1: pH dependence of acetoclastic and hydrogenotrophic methanogenesis. Measurements show reported mean and uncertainty values from Kotsyurbenko et al. (2007). Lines show a least squares optimization of Eq. (1). (a): Optimization (lines) and measurements (circles) of acetoclastic and hydrogenotrophic methanogenesis rates as a function of pH, normalized to the maximum acetoclastic rate. (b) Acetoclastic methanogenesis rate as a fraction of total methanogenesis rate.

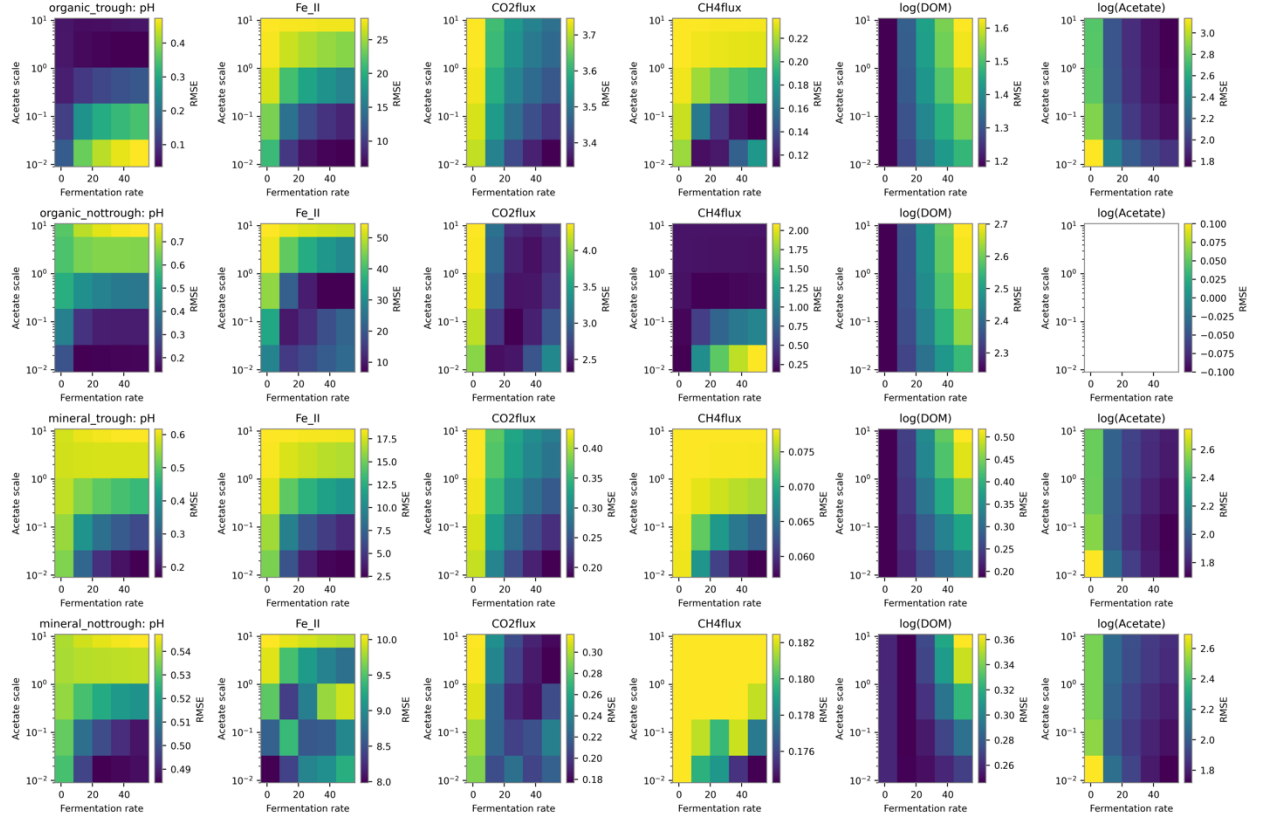


Fig. S2: RMSE between measured and modeled quantities for different values of fermentation reaction rate constant (“Fermentation rate”) and K_s parameter associated with acetate (“Acetate scale”). Each column shows a different quantity (from left to right: pH, Fe(II), CO₂ flux, CH₄ flux, log DOM concentration, and log acetate concentration). Each row shows a different incubated soil core (from top to bottom: Trough organic horizon, rim organic horizon, trough mineral horizon, rim mineral horizon). Lower RMSE (bluer colors) indicate better fit between model and measurements.

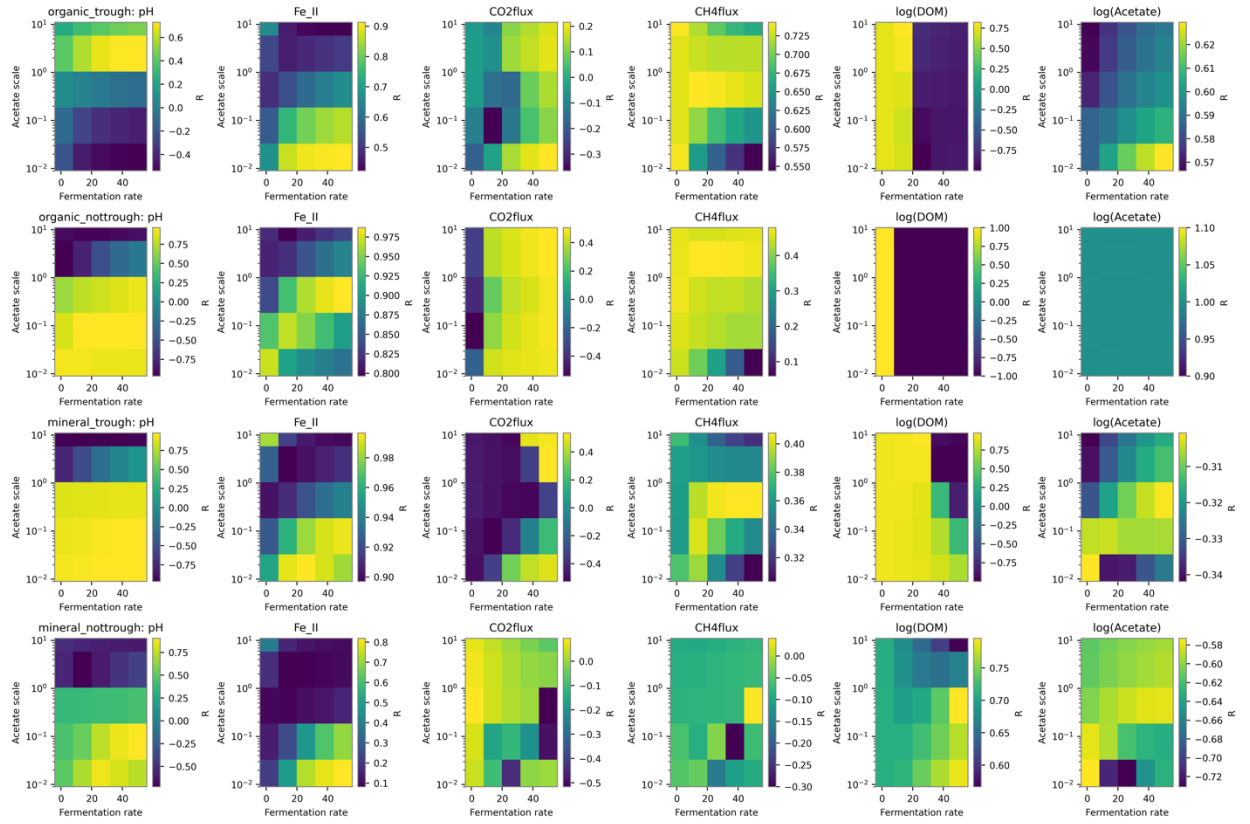


Fig. S3: Correlation coefficient (R) between measured and modeled quantities for different values of fermentation reaction rate constant (“Fermentation rate”) and K_s parameter associated with acetate (“Acetate scale”). Each column shows a different quantity (from left to right: pH, Fe(II), CO₂ flux, CH₄ flux, log DOM concentration, and log acetate concentration). Each row shows a different incubated soil core (from top to bottom: Trough organic horizon, rim organic horizon, trough mineral horizon, rim mineral horizon). R closer to 1 (yellow colors) indicate better fit between model and measurements.

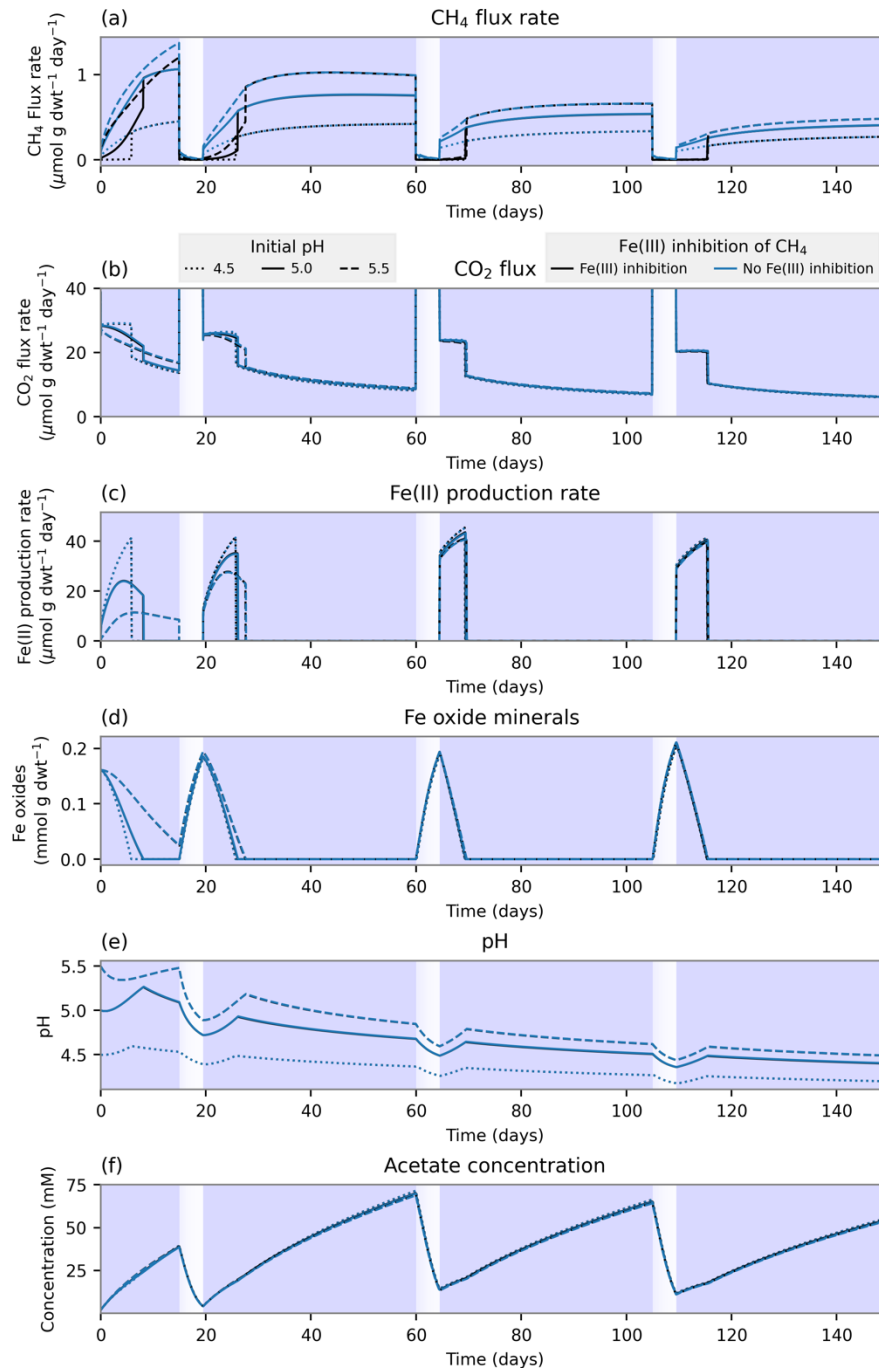


Figure S4: Simulated oxic-anoxic cycles for an organic horizon. Blue backgrounds indicate anoxic conditions and white backgrounds indicate oxic conditions. Black lines show simulations with direct inhibition of methanogenesis by Fe(III) and blue lines show simulations without direct inhibition (a): CH₄ flux rate. (b): CO₂ flux rate. (c): Fe(II) production rate via Fe(III) reduction. (d): Fe oxide mineral concentration. (e): pH. (f): Acetate concentration.

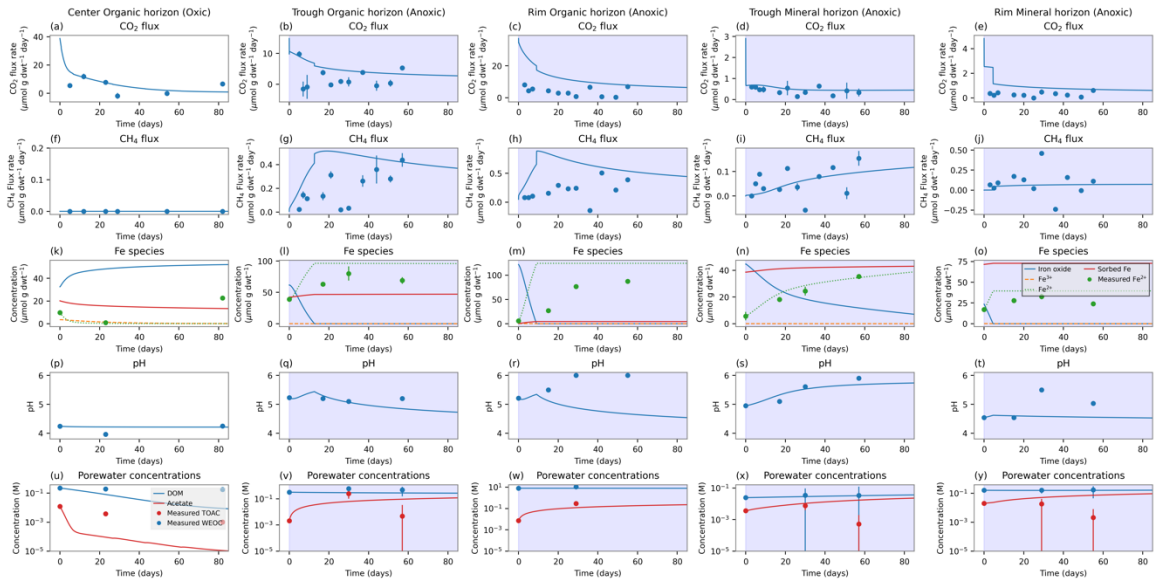


Figure S5: Time series comparison between incubation measurements and model simulations for the model version including direct inhibition of methanogenesis by Fe(III). Each column shows results from an individual incubation. Each row shows a different measured quantity. Lines show model simulation results and circles show measurements. Oxic conditions are shown with a white background and anoxic conditions are shown with a blue background.

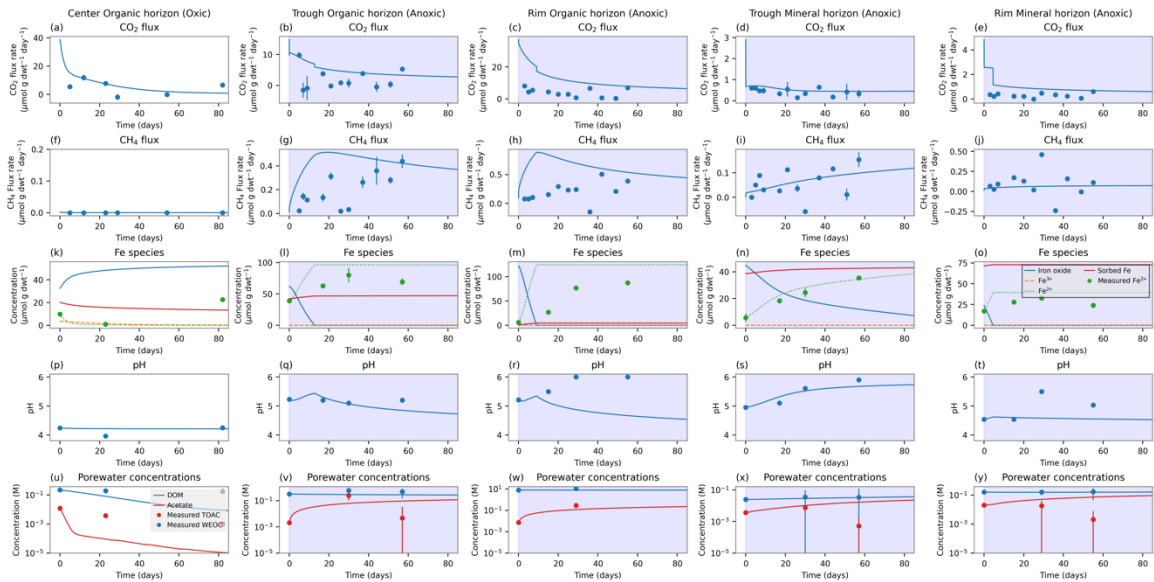


Figure S6: Time series comparison between incubation measurements and model simulations for the model version without direct inhibition of methanogenesis by Fe(III). Each column shows results from an individual incubation. Each row shows a different measured quantity. Lines show model simulation results and circles show measurements. Oxic conditions are shown with a white background and anoxic conditions are shown with a blue background.