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Supplement of

A multi-phase biogeochemical model for mitigating earthquake-induced liquefaction via microbially induced desaturation and calcium carbonate precipitation

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COMPARISONS OF PROPOSED AND EXISTING MIDP MODELS

Table S1. Comparison of Existing MIDP Models and the Presented Next Generation MIDP Model

Modeling Component	O'Donnell et al. (2019)	Pham (2017)	Wang et al. (2023)	This Model
Baseline Substrate Recipe Estimation for Desaturation		X	X	X
Baseline Substrate Recipe Estimation for Precipitation			X	X
Complex Acid-base Equilibria		X		X
Denitrifier Growth	X	X	X	X
Denitrifier Decay	X			X
Other Microbe Growth and Decay				X
Microbial Electron Donor Competition				X
Nitrous Acid Inhibition	X	X		X
Alternative MIDP Inhibition				X
Other Microbial Inhibition				X
pH Calculation	X	X		X
$CaCO_3$ Mineral Formation	X	X	X	X
Other Mineral Equilibrium				X
Mineral Precipitation and Dissolution Kinetics				X
N_2 Phase-transfer Kinetics		X		X
Other Gas Production and Phase-transfer Kinetics				X
Ground Improvement Metric Calculations (i.e., desaturation and % precipitation)			X	X
Porosity and Hydraulic Conductivity			X	

CONSTANTS USED IN BIOGEOCHEMICAL MODEL

Table S2. Constants used during modeling; these do not include constants found within the ORCHESTRA database for acid-base speciation (Meeussen, 2003), nor those dependent on electron donor and acceptor (e.g., K_a and K_d).

Parameter	Value	Reference
$\Delta G_c^{0'}$ (kJ e^- eq^{-1}): free energy of the carbon source	Acetate: 27.4 Glucose: 41.0 Molasses: 41.0	(Rittmann & McCarty, 2020)

ΔG_{pc} (kJ e^- eq^{-1}): free energy to convert pyruvate carbon to cellular carbon, depending on the nitrogen source	Nitrate: 14.1 Ammonium: 19.5	(Rittmann & McCarty, 2020)
$\Delta G_a^{0'}$ (kJ e^- eq^{-1}): free energy required to reduce an electron acceptor	Nitrate: -41.65 Nitrite: -92.56 Sulfate: 20.85 Oxygen: -78.72	(Rittmann & McCarty, 2020)
$\Delta G_d^{0'}$ (kJ e^- eq^{-1}): free energy released to oxidize an electron donor	Acetate: 27.4 Glucose: 41.0 Molasses: 41.0	(Rittmann & McCarty, 2020)
$\hat{q}_e$: maximum flow of electrons (e-equivalent g^{-1} biomass d^{-1})	1.0	(Rittmann & McCarty, 2020)
RM_A: (g Chemical Oxygen Demand (donor e^- equivalent)$^{-1}$)	8	(Rittmann & McCarty, 2020)
RM_B: (mol donor g^{-1} Chemical Oxygen Demand)	Acetate: 84 Glucose: 192 Molasses: 192	Calculated from half reactions (Rittmann & McCarty, 2020)
e^-_d (mol electron donor (donor e^- equivalent)$^{-1}$) is the amount of donor per electron equivalent	Acetate: 0.13 Glucose: 0.04 Molasses 0.04	Calculated from RM_A, RM_B, and $\hat{q}_e$
ε: energy transfer efficiency term	0.6	(Rittmann & McCarty, 2020)
n: considers energy efficiency due to thermodynamics, depending on electron donor	Acetate: 1 Glucose: 1 Molasses: 1	(Rittmann & McCarty, 2020)
X_a (mmol biomass L^{-1}): Active biomass concentration	Denitrifiers: 0.5 Sulfate Reducers: 0.25	
k_La (d^{-1}): gas mass transfer constant	0.5	(Yongsiri et al., 2004)
$K_{sp(CaCO_3)}$: speciation constant for calcium carbonate	$10^{-8.3}$	
R (L atm K^{-1} mol^{-1}): universal gas constant	0.082057	
T (K): temperature	298	
K_H (L_{aq} atm mol^{-1}): Henry's Law coefficients	N_2: 1600 CO_2: 29 H_2S: 10	
e (L_{pore} L_{soil}^{-1}): void ratio	0.64	Within a value of acceptable ranges (Christopher et al., 2006)

ka (L d^{-1}): combined coefficient considering a constant mass transfer and the average crystal surface area	100	Within a value of acceptable ranges (Rittmann et al., 2003)
ρ_{soil} (g soil L_{soil}^{-1}): soil density	1950	Within a value of acceptable ranges (Christopher et al., 2006)

DERIVATIONS OF IMPORTANT PARAMETERS

The value of $\hat{q}$ (mol electron donor mol^{-1} biomass d^{-1}) was estimated using Eq. S1 (Rittmann & McCarty, 2020).

$$\hat{q} = \frac{\hat{q}_e e_d^-}{f_e^0} \quad \text{Eq. S1}$$

where $\hat{q}_e$ is the maximum electron flow from the donor to the acceptor for energy production (acceptor e^- eq mol^{-1} biomass d^{-1}), f_e^0 is the fraction of donor electrons used for energy production (acceptor e^- eq (donor e^- eq)$^{-1}$), and e^-_d is the amount of donor per electron equivalent (mol electron donor (donor e^- equivalent)$^{-1}$). The molecular formula for biomass was $CH_{1.8}O_{0.5}N_{0.2}$, and the resulting $\hat{q}_e$ is 24.6 e^- eq mol^{-1} biomass d^{-1}. For acetate, e^-_d is 0.13 electron donor e^- equivalent^{-1}. f_e^0 was determined using Eq. S2 (Rittmann & McCarty, 2020).

$$f_e^0 = 1 - \frac{1}{-\left(\frac{\frac{30.09 - \Delta G_c^{0\prime}}{\varepsilon^n} + \frac{\Delta G_{pc}}{\varepsilon}}{\varepsilon(\Delta G_a^{0\prime} - \Delta G_d^{0\prime})}\right) + 1} \quad \text{Eq. S2}$$

where 30.09 is the amount of energy required to form the representative intermediate during synthesis, acetate (acetyl-CoA) (kJ e^- eq), $\Delta G_c^{0\prime}$ is the energy required to convert the carbon source to forms useful in synthesis (in this case, the carbon source is also the electron donor) (kJ e^- eq^{-1}),

ε is the energy transfer efficiency term (ε = 0.6), n is used to consider energy efficiency when the reaction is thermodynamically positive (n = -1) or negative (n = -1), ΔG_{pc} is the energy required to convert the carbon source (acetate in this case) to carbon used for biomass synthesis, depending on the nitrogen source (kJ e^- eq^{-1}), and ΔG_r is the energy released during each redox reaction (kJ e^- eq^{-1}). ΔG_{pc} was calculated to consider either nitrate or ammonium as the nitrogen source (Rittmann & McCarty, 2020). All free-energy parameters, listed in Table S3, were found in Rittmann and McCarty (2020).

Table S3. Bacterial Energetic Parameters for all Compounds Considered in the Model at pH = 7.

Parameter	Value (kJ e^- eq^{-1})
$\Delta G_c^{0'}$: free energy of the carbon source	Acetate: 27.4 Glucose: 41.0 Molasses: 41.0
ΔG_{pc}: free energy to convert pyruvate carbon to cellular carbon, depending on the nitrogen source	Nitrate: 14.1 Ammonium: 19.5
$\Delta G_a^{0'}$: free energy required to reduce an electron acceptor	Nitrate: -41.65 Nitrite: -92.56 Sulfate: 20.85 Oxygen: -78.72
$\Delta G_d^{0'}$: free energy released to oxidize an electron donor	Acetate: 27.4 Glucose: 41.0 Molasses: 41.0

The model considers biogeochemical reactions that involve alternative electron acceptors and the presence of alternative minerals and metals (i.e., iron, sulfate). Table 2 in the main manuscript details the microbial energetic values used to calculate the expected substrate utilization and maximum specific growth rates (μ_{max}). Within the model, two different nitrogen sources are considered: nitrate and ammonium. Ammonium as a nitrogen source is more thermodynamically favorable, as shown in Table S3. Therefore, more electron equivalents of nitrate are needed to form biomass than ammonium. The thermodynamic favorability of ammonium over nitrate is

reflected in the fraction of electrons going to energy generation (f_e^0) and fraction of electrons going to biomass synthesis (f_s^0) values (Table S4).

Table S4. Microbial Energetics Expected During MIDP, Considering Acetate as the Electron Donor and Natural Electron Acceptors

Electron Acceptor	Nitrogen Source	G_r (kJ e$^-$ eq^{-1})	f_e^0	f_s^0	$\hat{q}$ (mol e$^-$ donor mol^{-1} biomass d^{-1})
Nitrate	Nitrate	-69.05	0.40	0.60	8.12
Nitrite	Nitrate	-119.96	0.28	0.72	11.69
Sulfate	Nitrate	-6.55	0.88	0.12	3.74
Nitrate	Ammonium	-69.05	0.47	0.53	6.95
Nitrite	Ammonium	-119.96	0.34	0.66	9.65
Sulfate	Ammonium	-6.55	0.90	0.10	3.63

Change in Initial Biomass Concentration

To demonstrate the influence of initial biomass concentration on model results, we modeled MIDP assuming that the initial denitrifier biomass concentration of 0.05 mmol L^{-1} and sulfate-reducing biomass concentration of 0.025 mmol L^{-1}. We assumed the same initial treatment recipes detailed in Table 6, environmental characteristics detailed in Table 5, and parameter values detailed in Table 2 through Table 4.

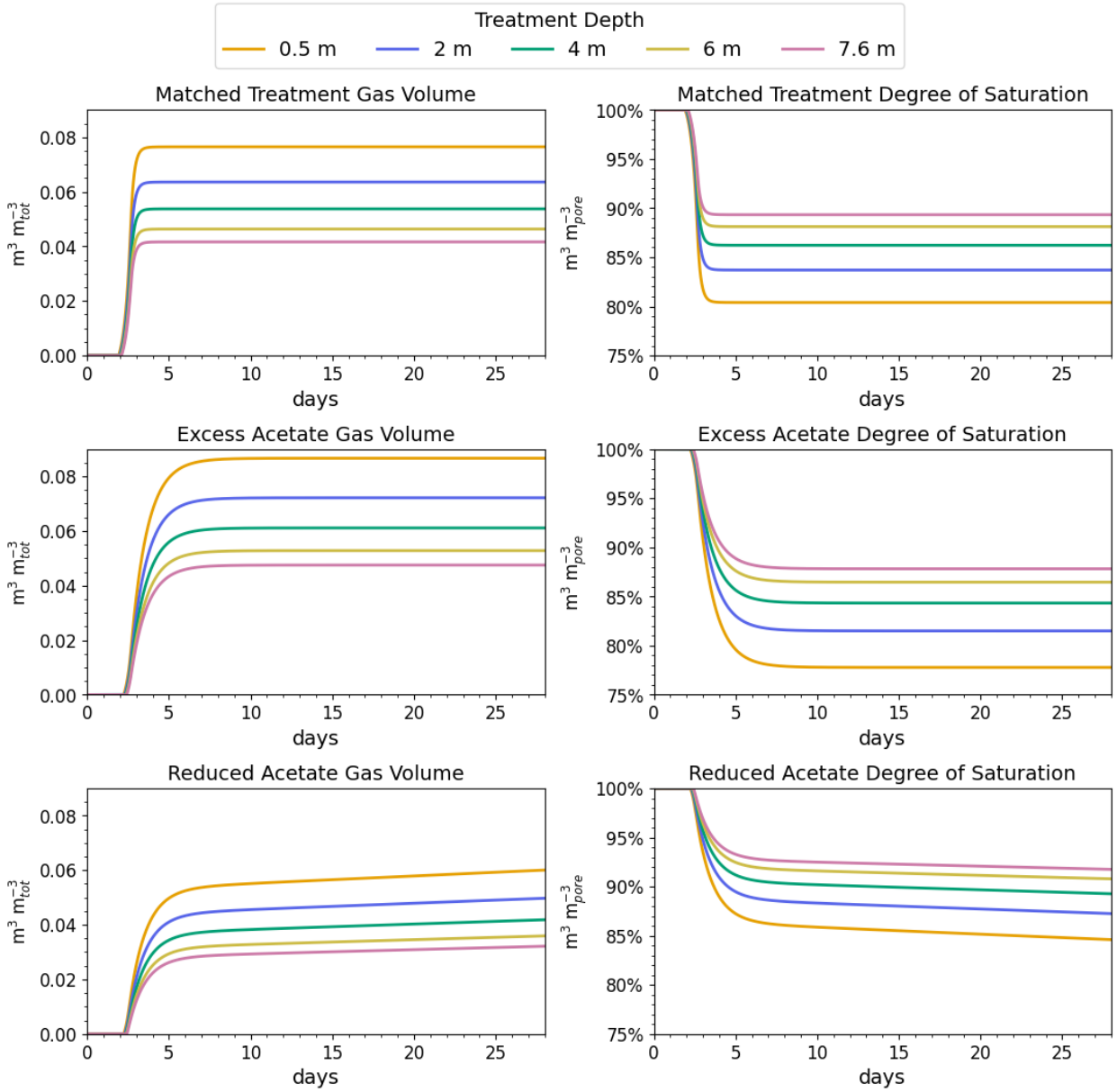

Figure S1. Gas volumes normalized to the total soil volume (left) and degree of saturation by depth for the simulated Coastal seawater conditions with reduced initial biomass concentration. The desaturation target was 10%, or a saturation ratio of 90%.

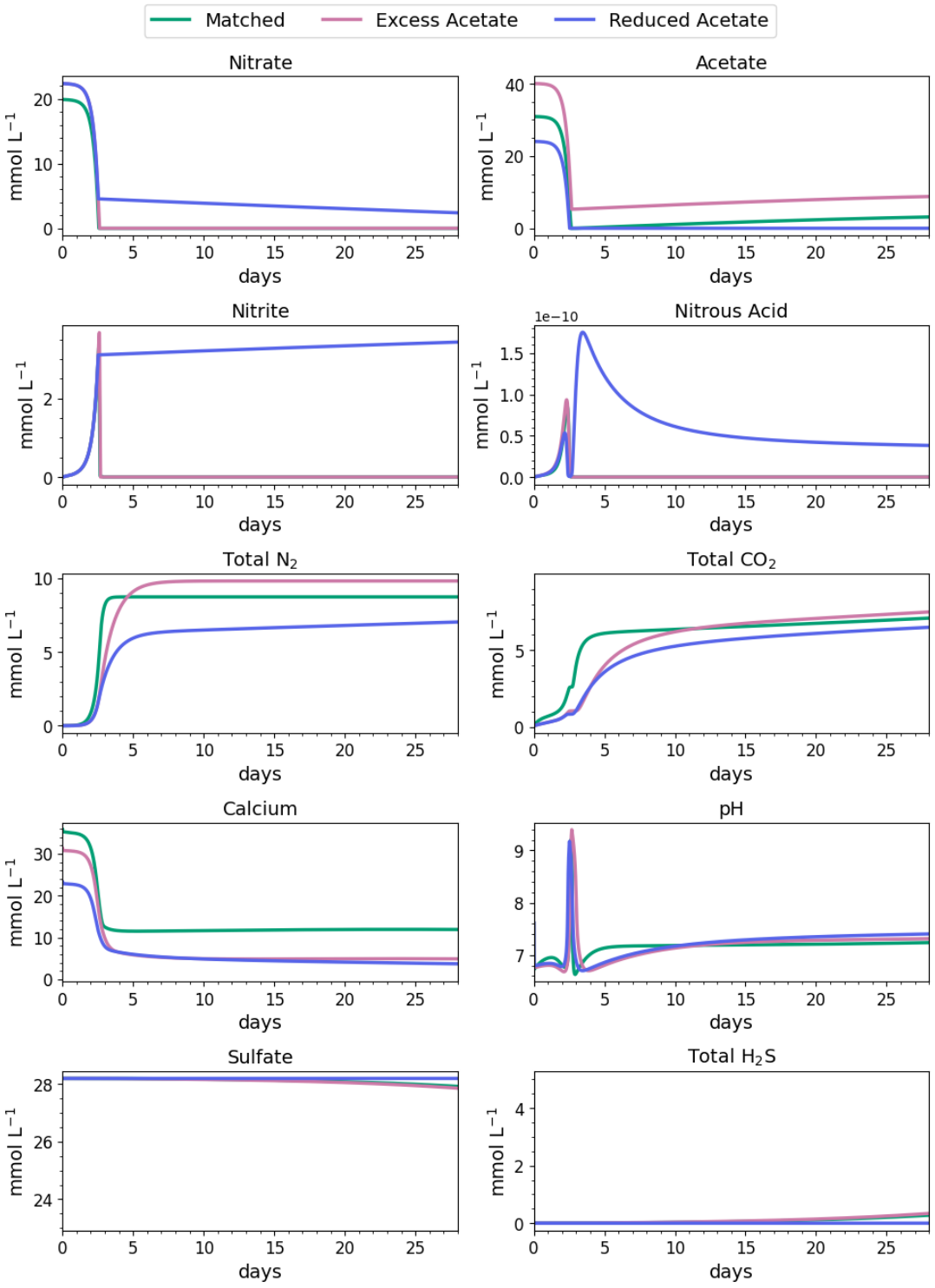

Figure S2. Water-quality results for 28 days of MIDP in coastal seawater conditions targeting a desaturation level of 10% in three different treatment recipes with reduced initial biomass concentration: empirically matched, 25% excess acetate, and 25% reduced acetate.

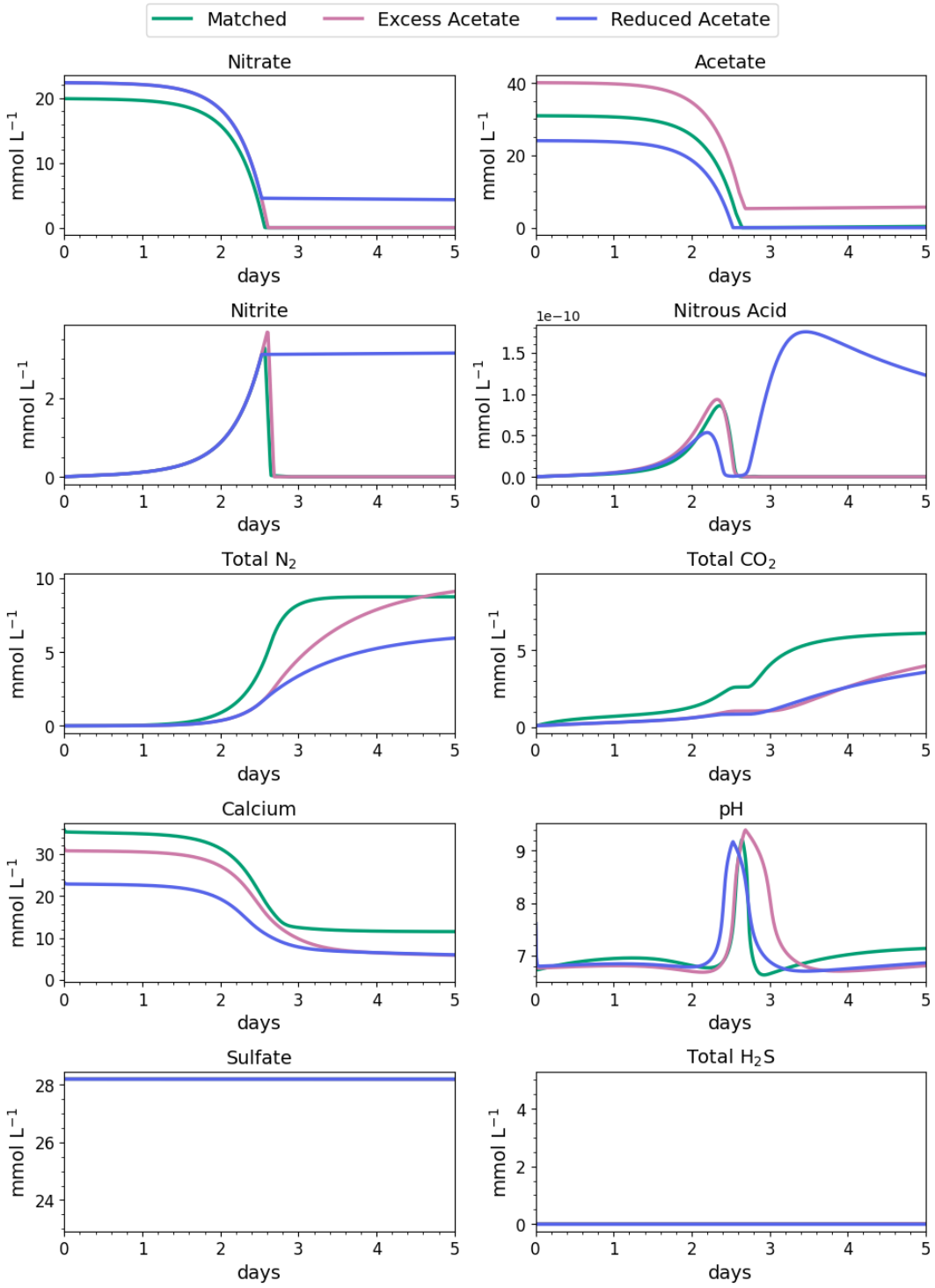

Figure S3. Water-quality results for the first 3 days of MIDP in coastal seawater conditions targeting a desaturation level of 10% in three different treatment recipes with reduced initial biomass concentration: empirically matched, 25% excess acetate, and 25% reduced acetate.

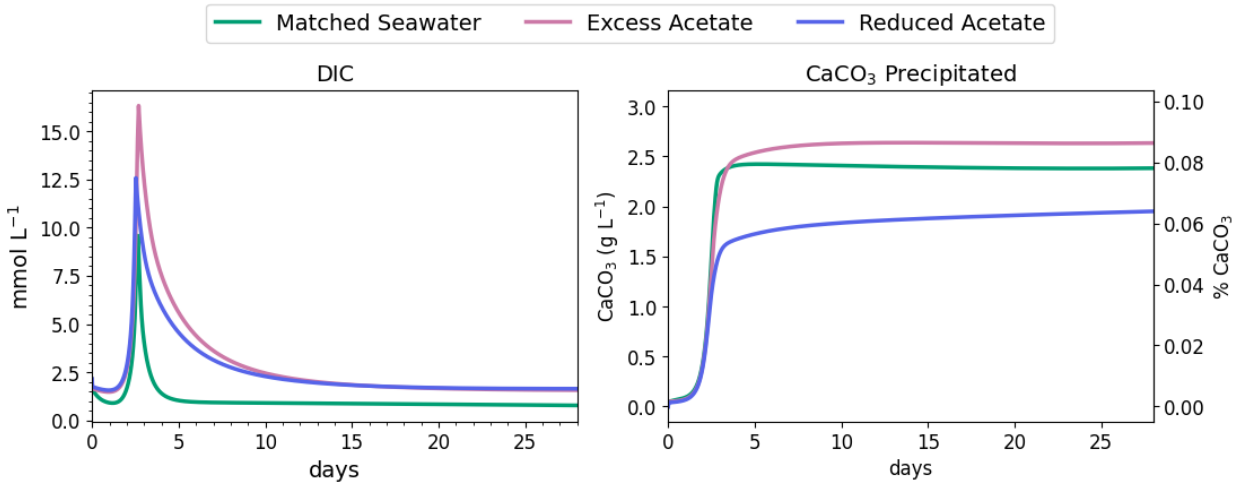

Figure S4. DIC concentration and $CaCO_3$ precipitated during the first 3 days of MIDP in coastal seawater conditions targeting a desaturation level of 10% under reduced initial biomass concentration.