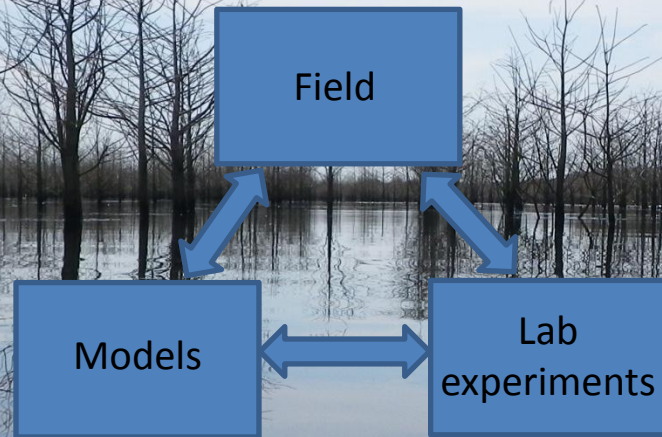


Simulating the Influence of Saltwater Intrusion on Coupled Element Cycles in Coastal Plain Wetlands



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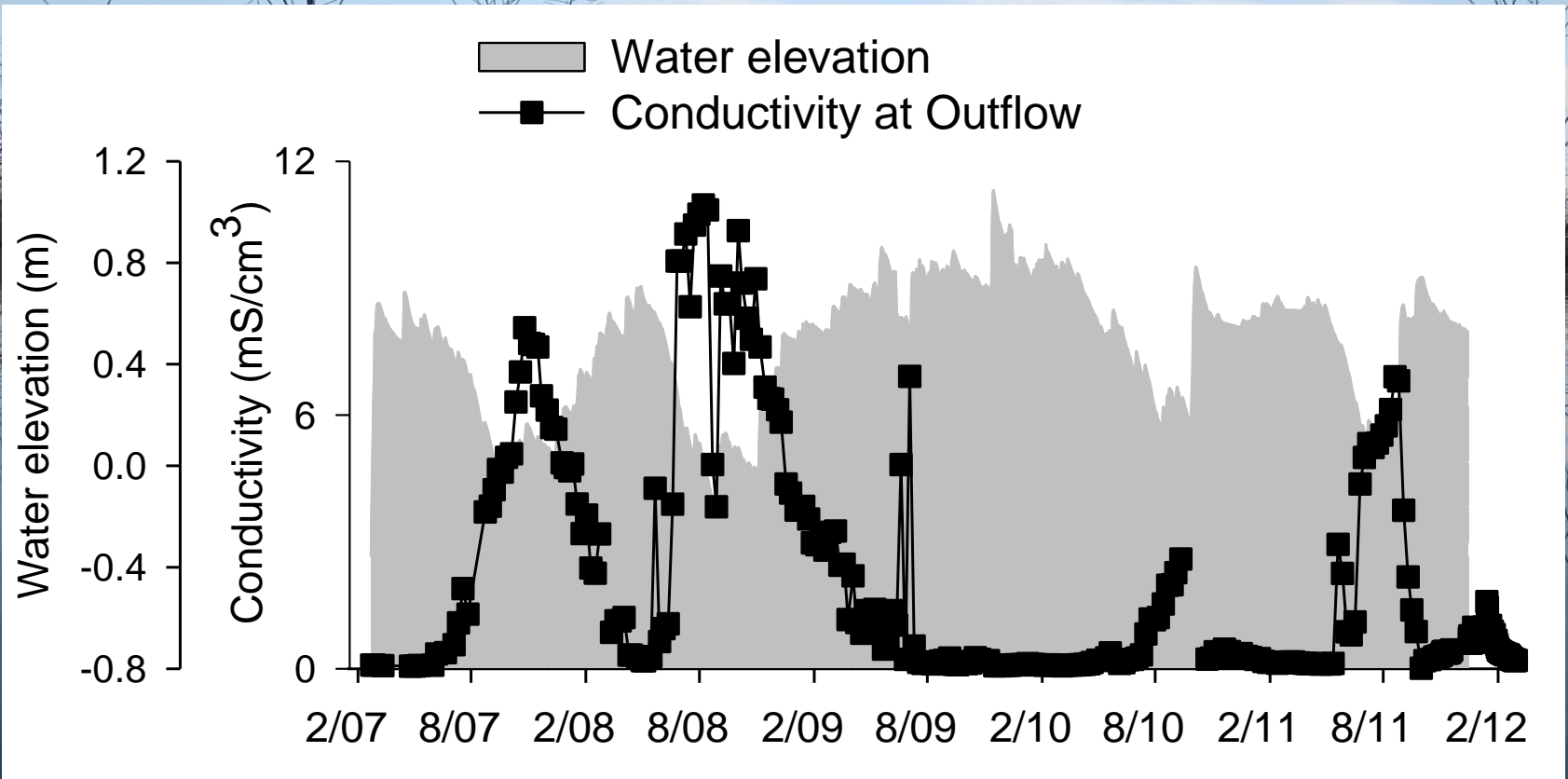
²Department of Land Resources and Environmental Sciences, Montana State University, Bozeman, MT, USA

³Computer Science Department, Montana State University, Bozeman, MT, USA

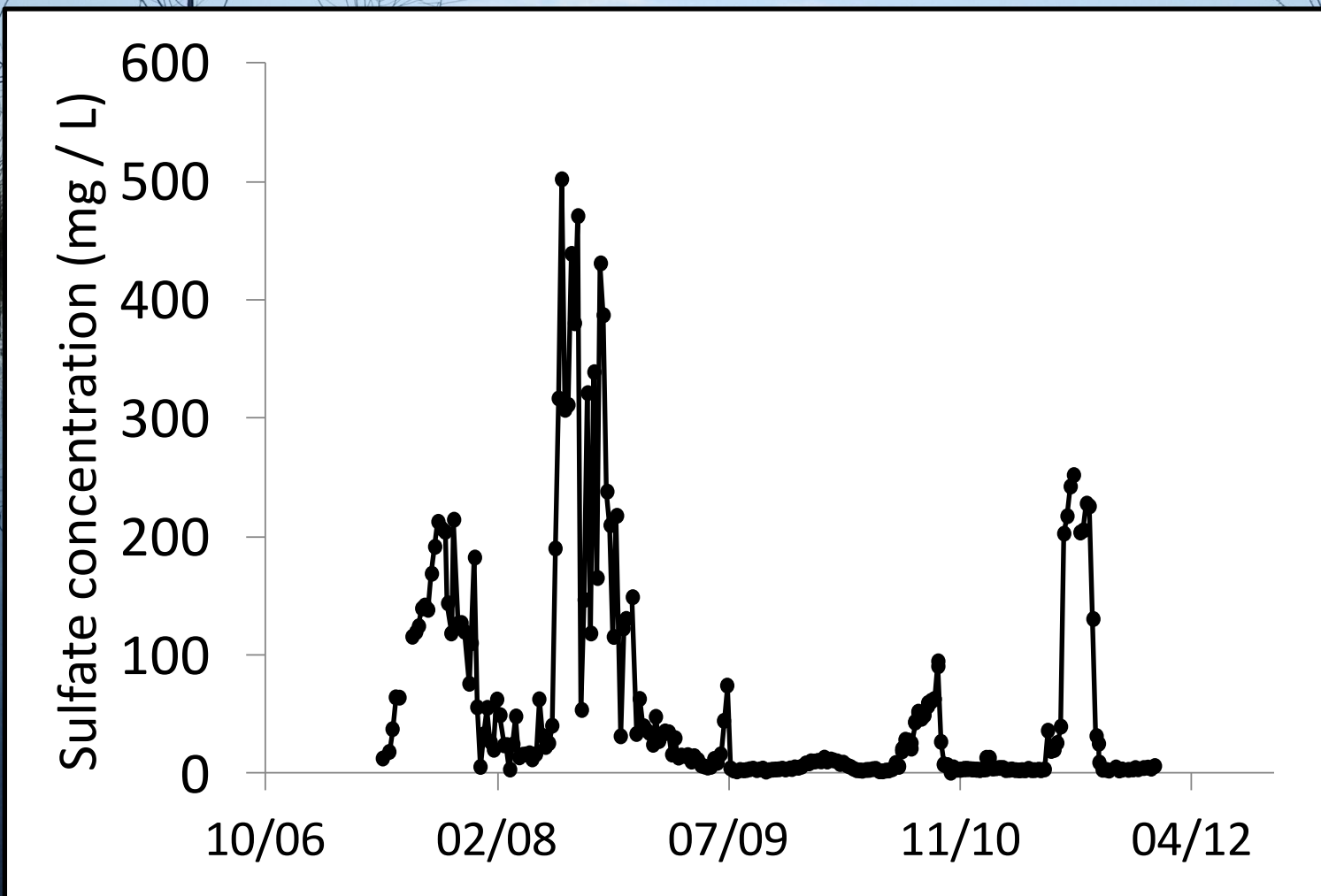
⁴School of Natural Resources, University of Nebraska-Lincoln, Lincoln, NE, USA

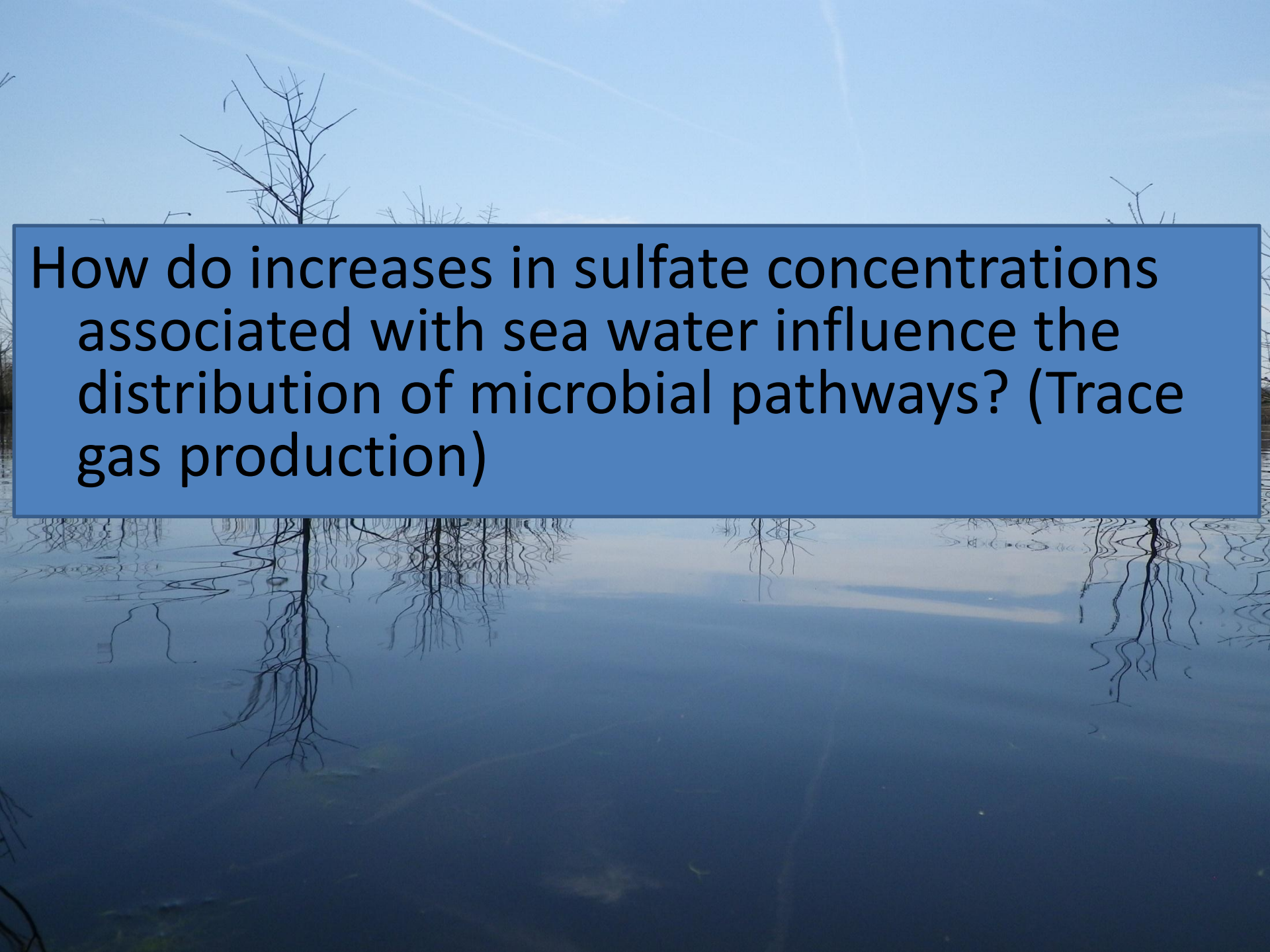
Funded by the National Science Foundation.

Biogeochemistry of salt water intrusion



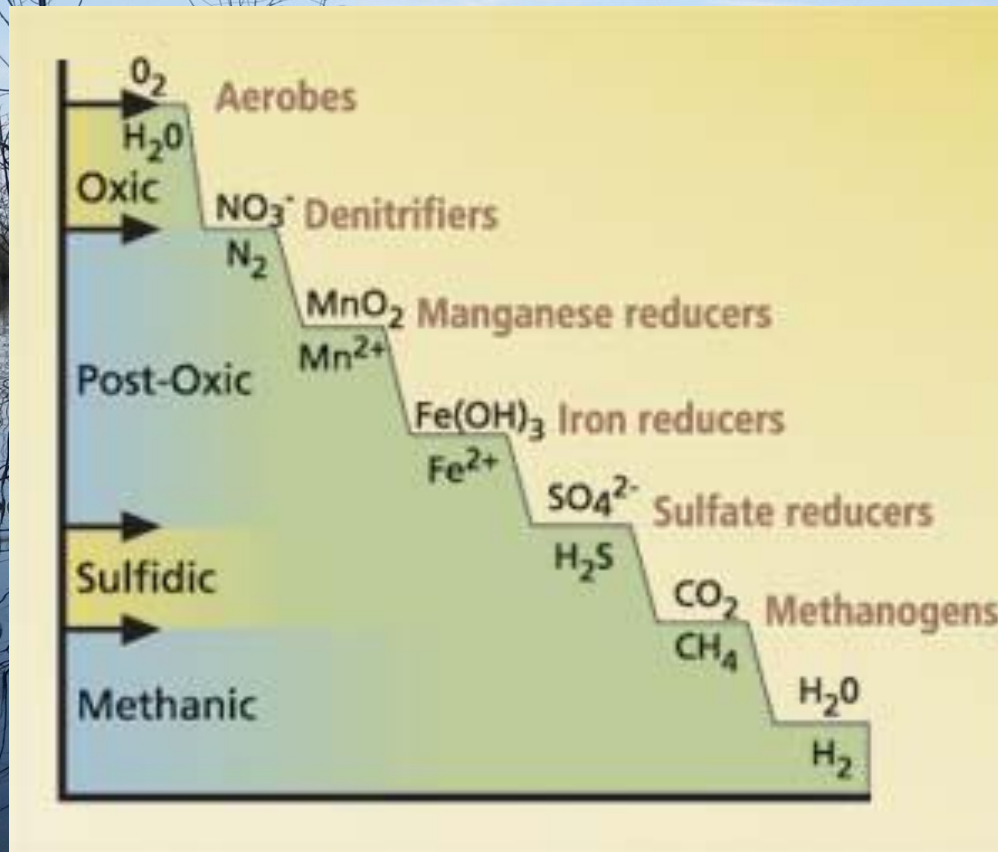
Biogeochemistry of salt water intrusion



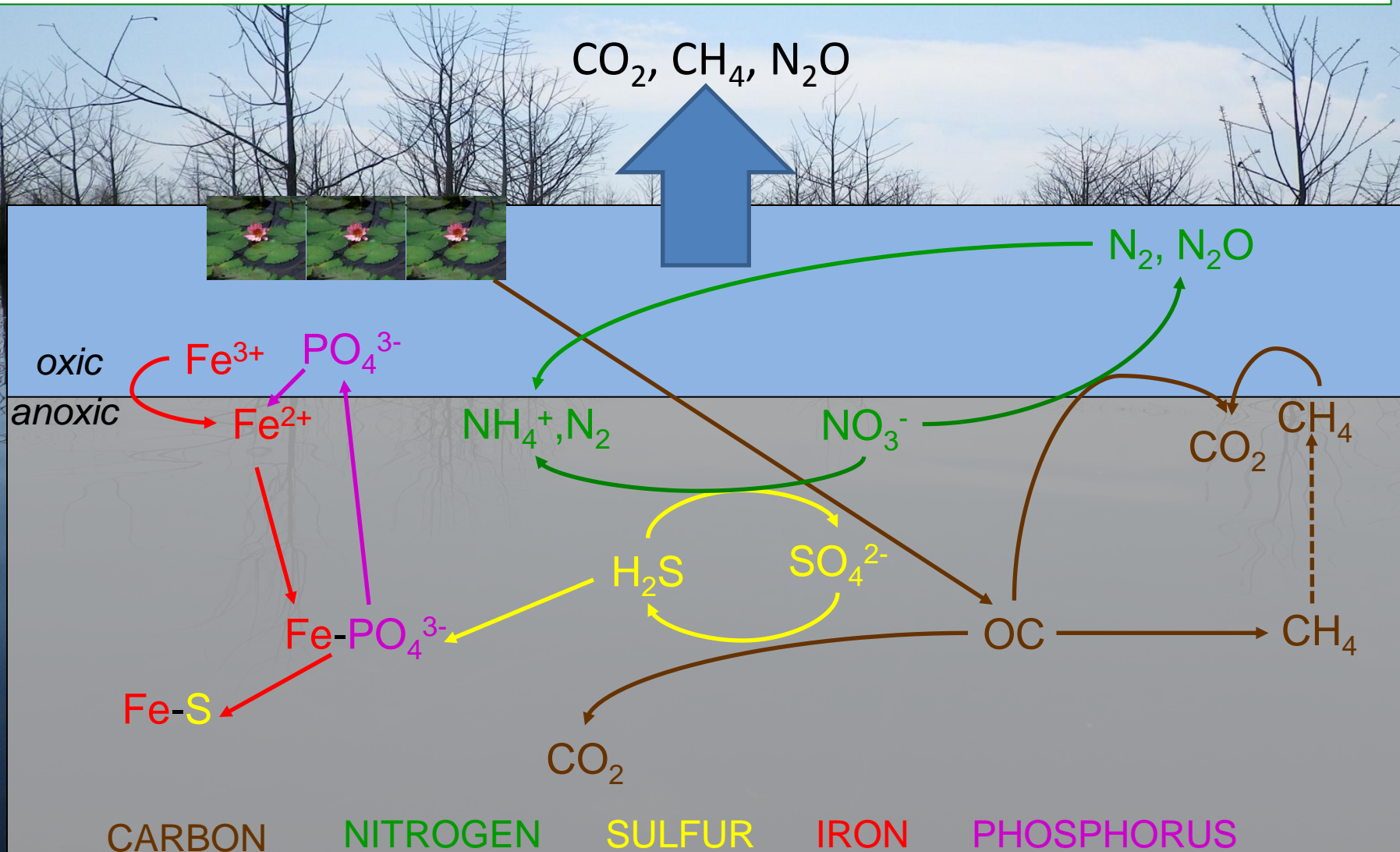


How do increases in sulfate concentrations associated with sea water influence the distribution of microbial pathways? (Trace gas production)

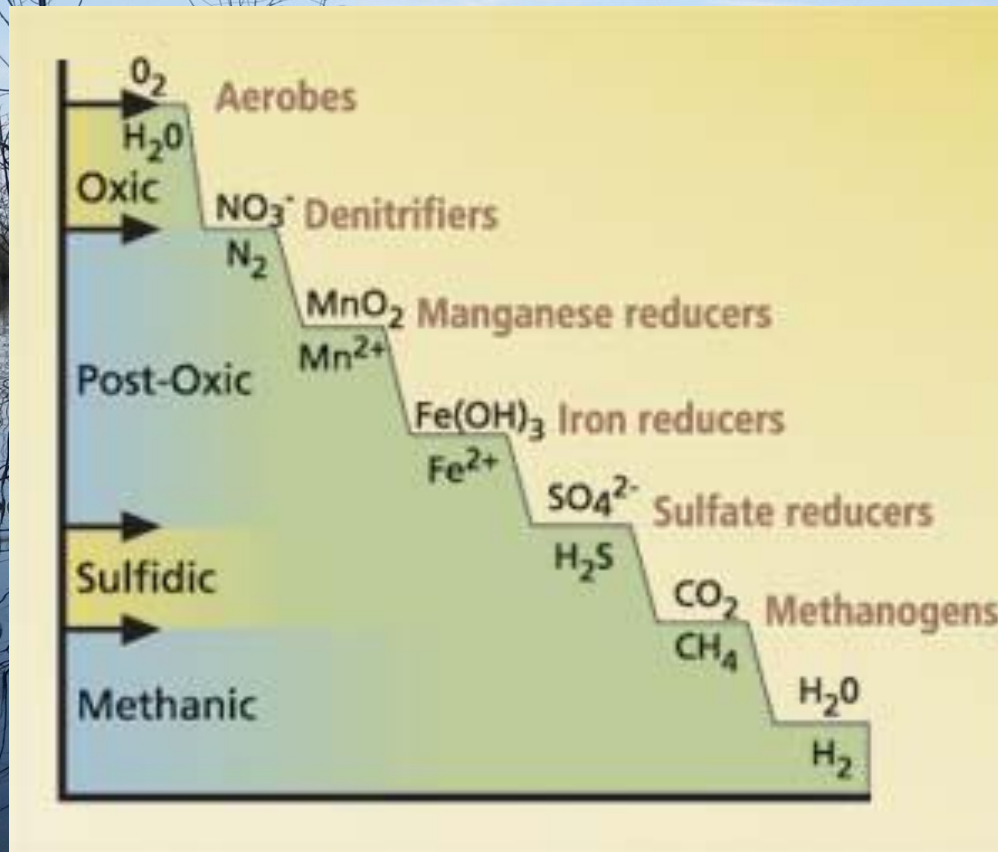
Redox Ladder as Organizing Concept



Connections in elemental cycles often lead to **multi-dimensional, non-linear feedbacks** both on the cycle of interest and other cycles

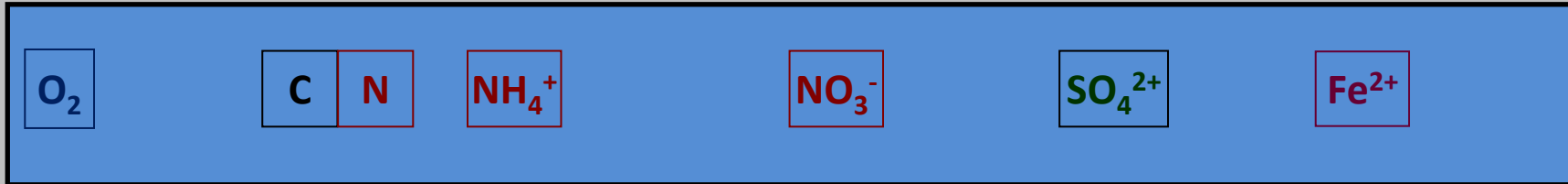


Redox Ladder as Organizing Concept



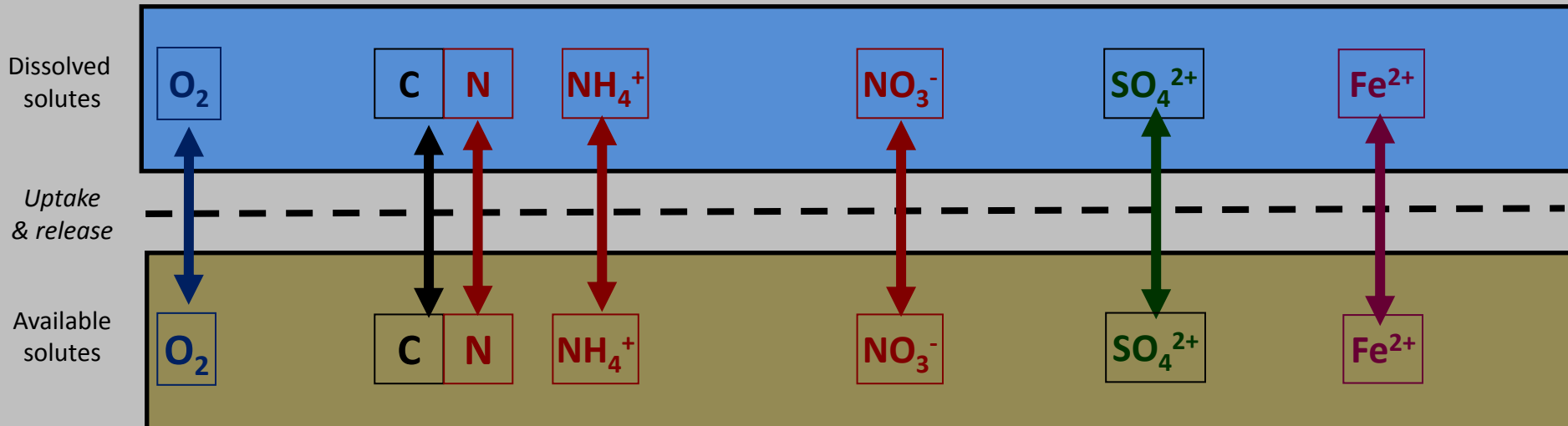
Model Structure

Dissolved
solute



Measured distribution from 5 years of surface and piezometer samples from coastal North Carolina wetland.

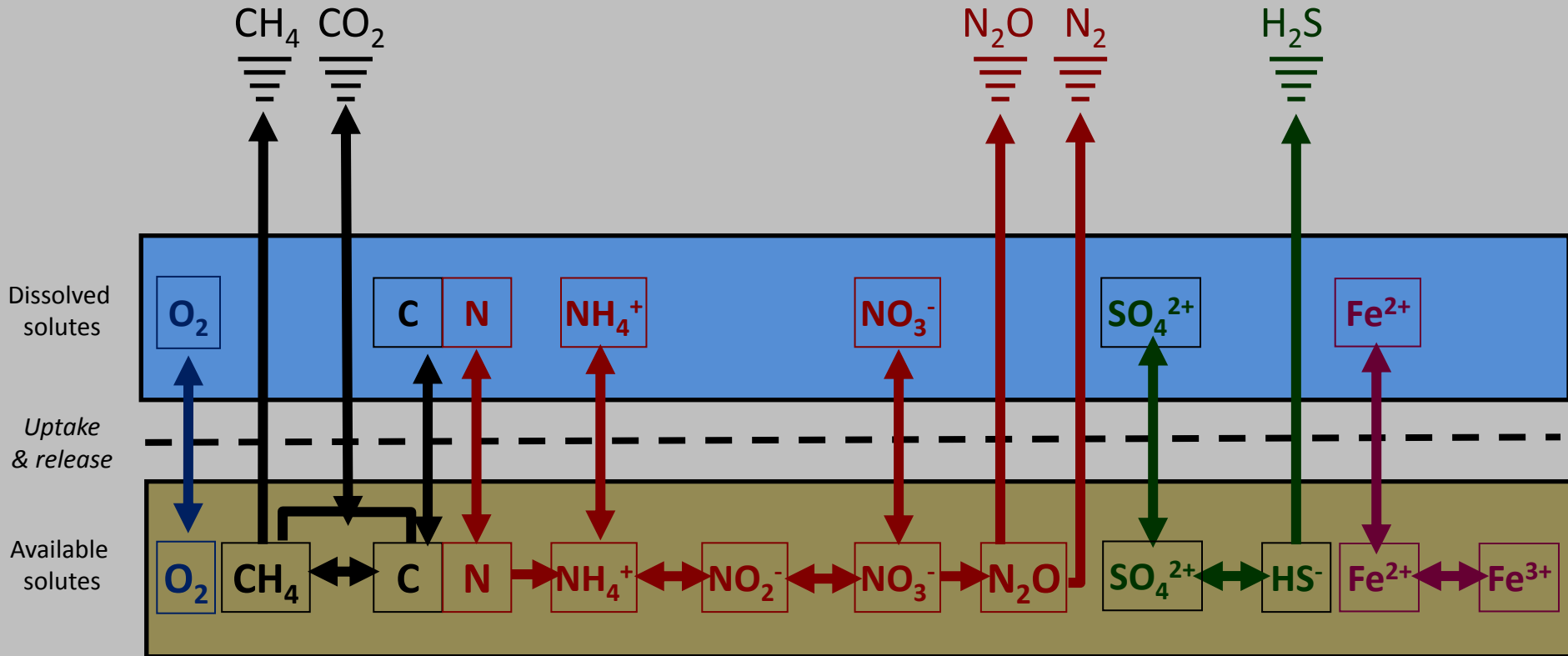
Model Structure



Michaelis-Menten Uptake: $U_c = [C] \times \mu_{max} / ([C] + K_s)$

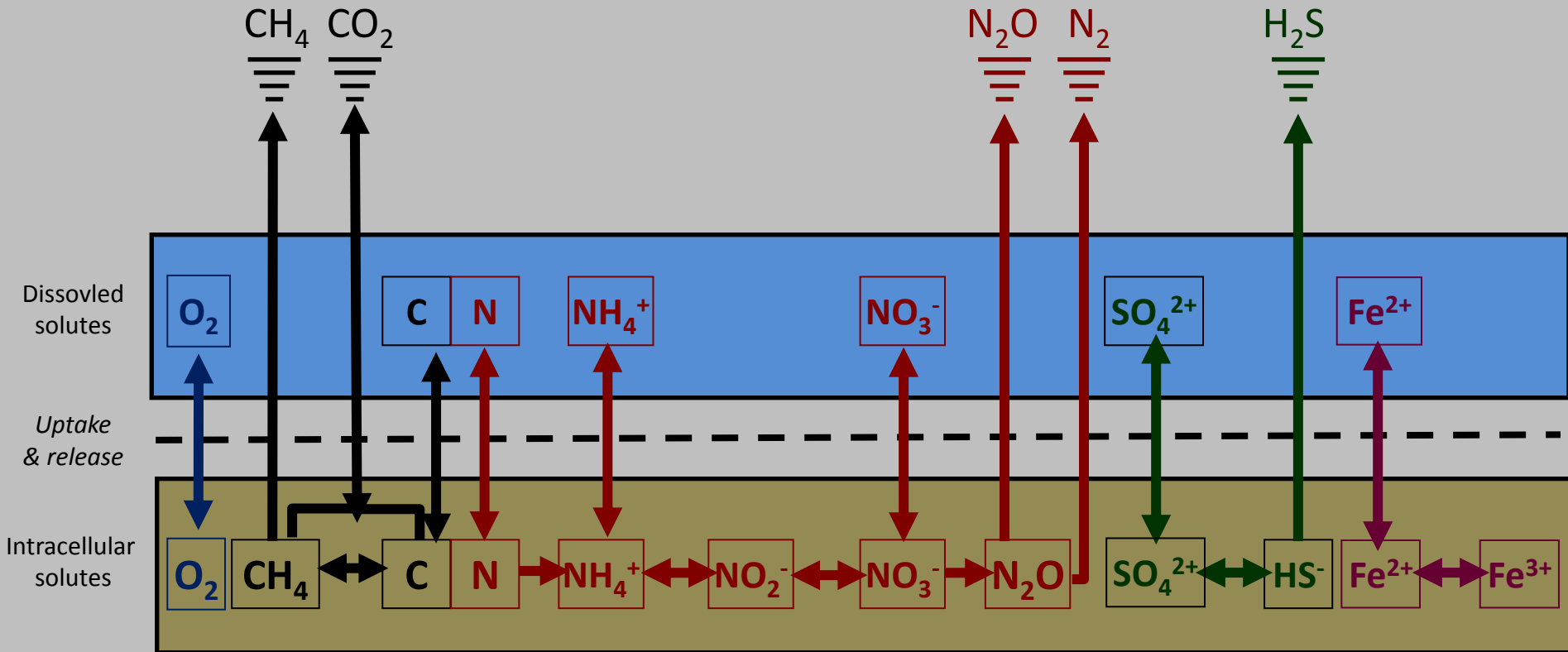
Average μ_{max} and K_s from Piel and Gaudy,
1971, Appl. Microbiol., 21 pp. 253–256

Model Structure



Microbial Process	Reaction	$\Delta G_0'$ (kJ)
Aerobic organic carbon oxidation	$\text{CH}_2\text{O} + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O}$	-502
Denitrification:		
Nitrate reduction	$\text{CH}_2\text{O} + 2\text{NO}_3^- \rightarrow \text{CO}_2 + 2\text{NO}_2^- + \text{H}_2\text{O}$	-354
Nitrite reduction	$\text{CH}_2\text{O} + 2\text{NO}_2^- + 2\text{H}^+ \rightarrow \text{CO}_2 + \text{N}_2\text{O} + 2\text{H}_2\text{O}$	-481
Nitrous oxide reduction	$\text{CH}_2\text{O} + 2\text{N}_2\text{O} \rightarrow \text{CO}_2 + 2\text{N}_2 + \text{H}_2\text{O}$	-710
Nitrification:		
Ammonium oxidation	$\text{O}_2 + 2/3\text{NH}_4^+ \rightarrow 2/3\text{NO}_2^- + 4/3\text{H}^+ + 2/3\text{H}_2\text{O}$	-183
Nitrite oxidation	$\text{O}_2 + 2\text{NO}_2^- \rightarrow 2\text{NO}_3^-$	-148
Methanogenesis	$\text{CH}_2\text{O} \rightarrow 1/2\text{CO}_2 + 1/2\text{CH}_4$	-93
Methane oxidation	$\text{O}_2 + 1/2\text{CH}_4 \rightarrow 1/2\text{CO}_2 + \text{H}_2\text{O}$	-409
Dissimilatory nitrite reduction to ammonium	$\text{CH}_2\text{O} + 2/3\text{NO}_2^- + 4/3\text{H}^+ \rightarrow \text{CO}_2 + 2/3\text{NH}_4^+ + 1/3\text{H}_2\text{O}$	-319
Anaerobic ammonium oxidation	$\text{NH}_4^+ + \text{NO}_2^- \rightarrow 2\text{H}_2\text{O} + \text{N}_2$	-358
Sulfate reduction	$\text{CH}_2\text{O} + 1/2\text{SO}_4^{-2} + 1/2\text{H}^+ \rightarrow 1/2\text{HS}^- + \text{CO}_2 + \text{H}_2\text{O}$	-104
Sulfide oxidation	$\text{O}_2 + 1/2\text{HS}^- \rightarrow 1/2\text{SO}_4^{-2} + 1/2\text{H}^+$	-398
Iron reduction	$\text{CH}_2\text{O} + 4\text{Fe}(\text{OH})_3 + 8\text{H}^+ \rightarrow 4\text{Fe}^{+2} + \text{CO}_2 + 11\text{H}_2\text{O}$	-232
Iron oxidation	$\text{O}_2 + 4\text{Fe}^{+2} + 6\text{H}_2\text{O} \rightarrow 4\text{FeOOH} + 8\text{H}^+$	-429

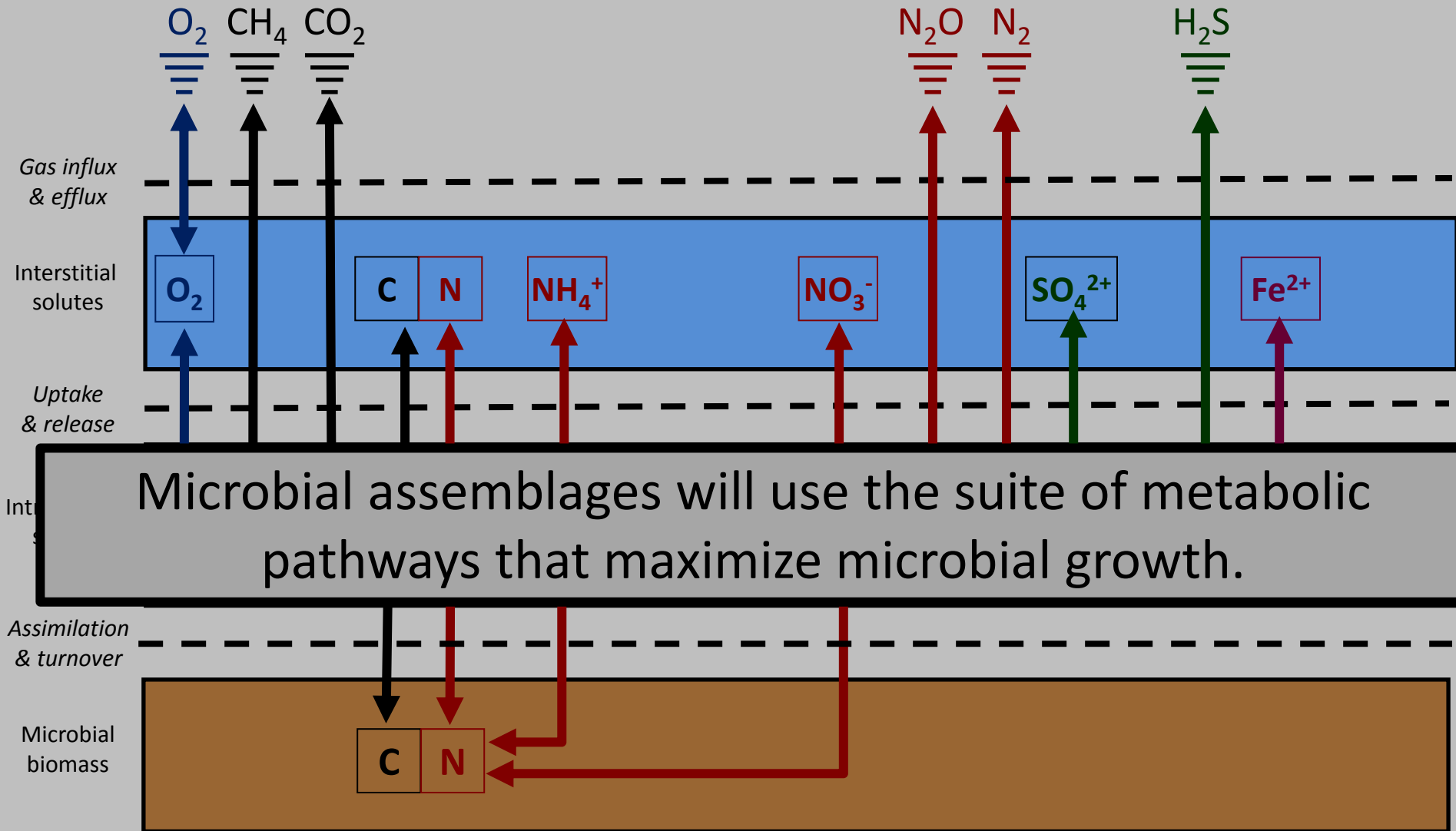
Model Structure



Important Assumptions:

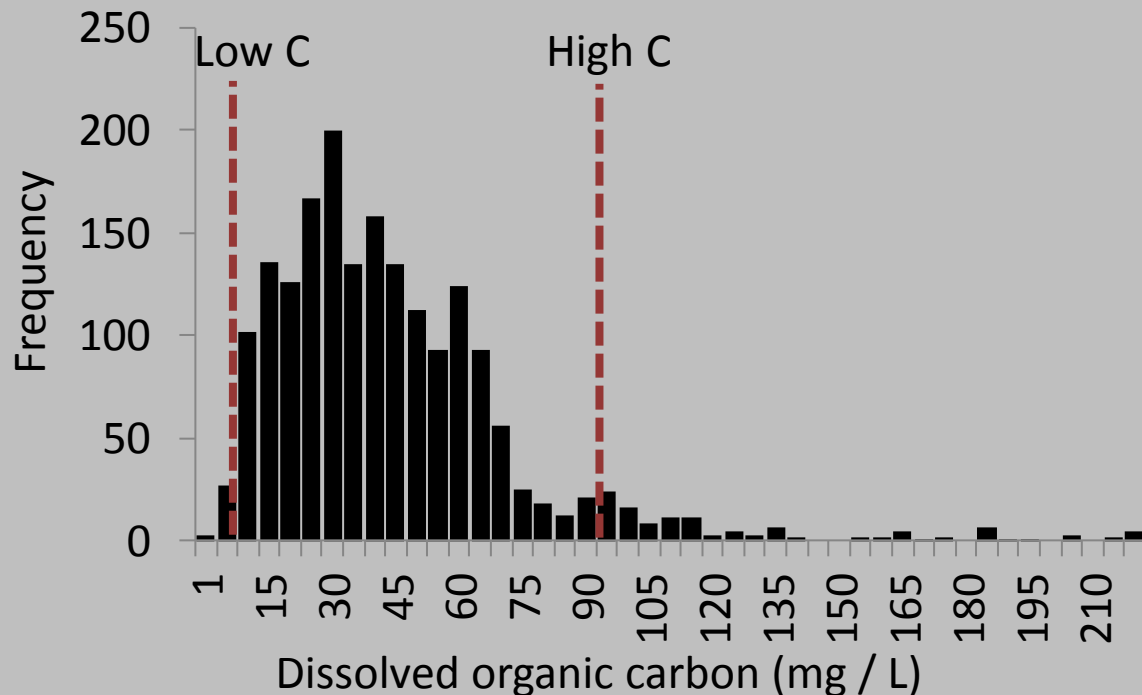
- Energy yields static. Standard free energy at pH = 7.
- Energy requirement (biomass maintenance; heterotrophic growth; chemoautotrophic CO_2 fixation; methanotrophic growth). Tijhuis et al. 1993. Biotechnology and bioengineering 42:509-19.
- Chemoautotrophic growth rates (CO_2 fixed per mol ED; CH_4 growth per mol ED for methanotrophs). Heijnen and Van Dijken. 1992. Biotechnology and bioengineering 39:833-58.

Model Structure



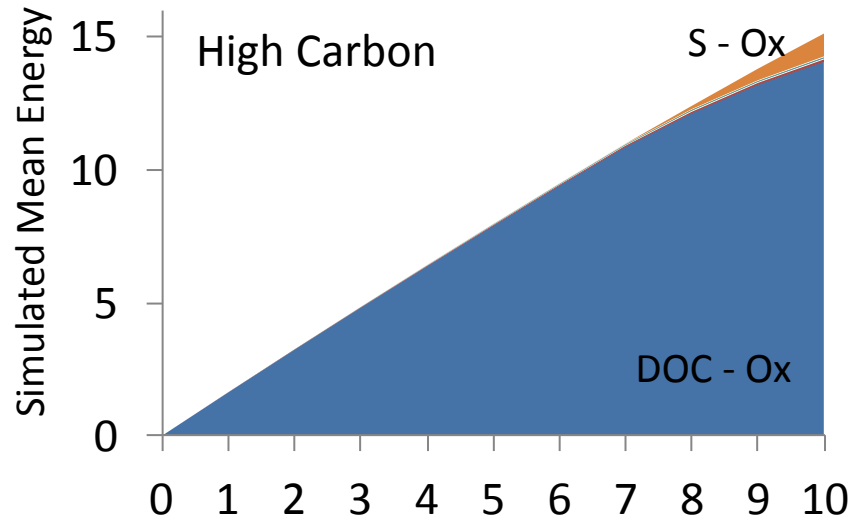
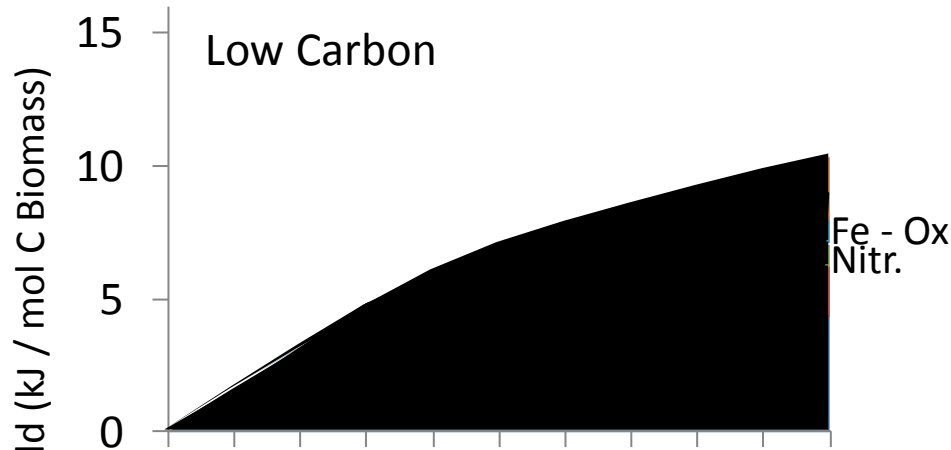
Model Simulations

- Model implemented in linear programming (LPSolve) with Monte Carlo wrapper (Java)
- 10,000 values for each solute based on distributions from coastal NC wetland across range of DO concentration (0 – 10 mg / L)
- >300,000 single time step model runs



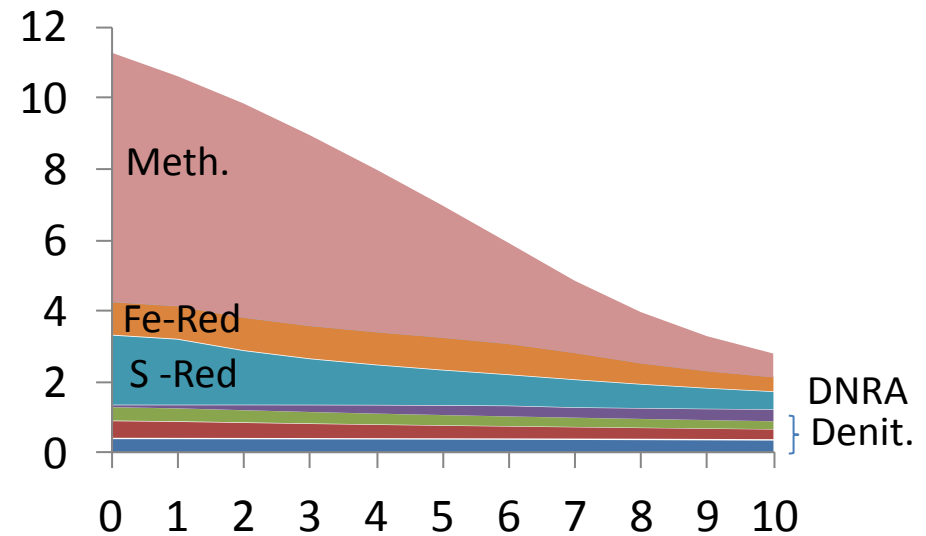
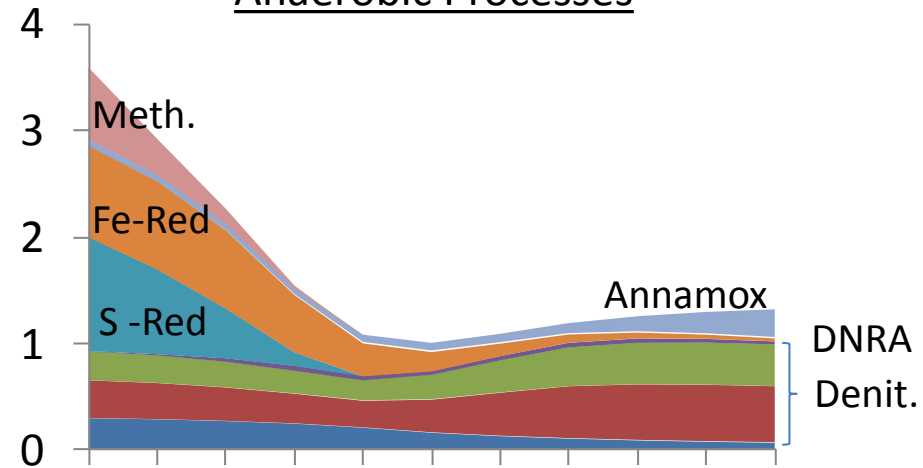
Example of model simulation results

Aerobic Processes

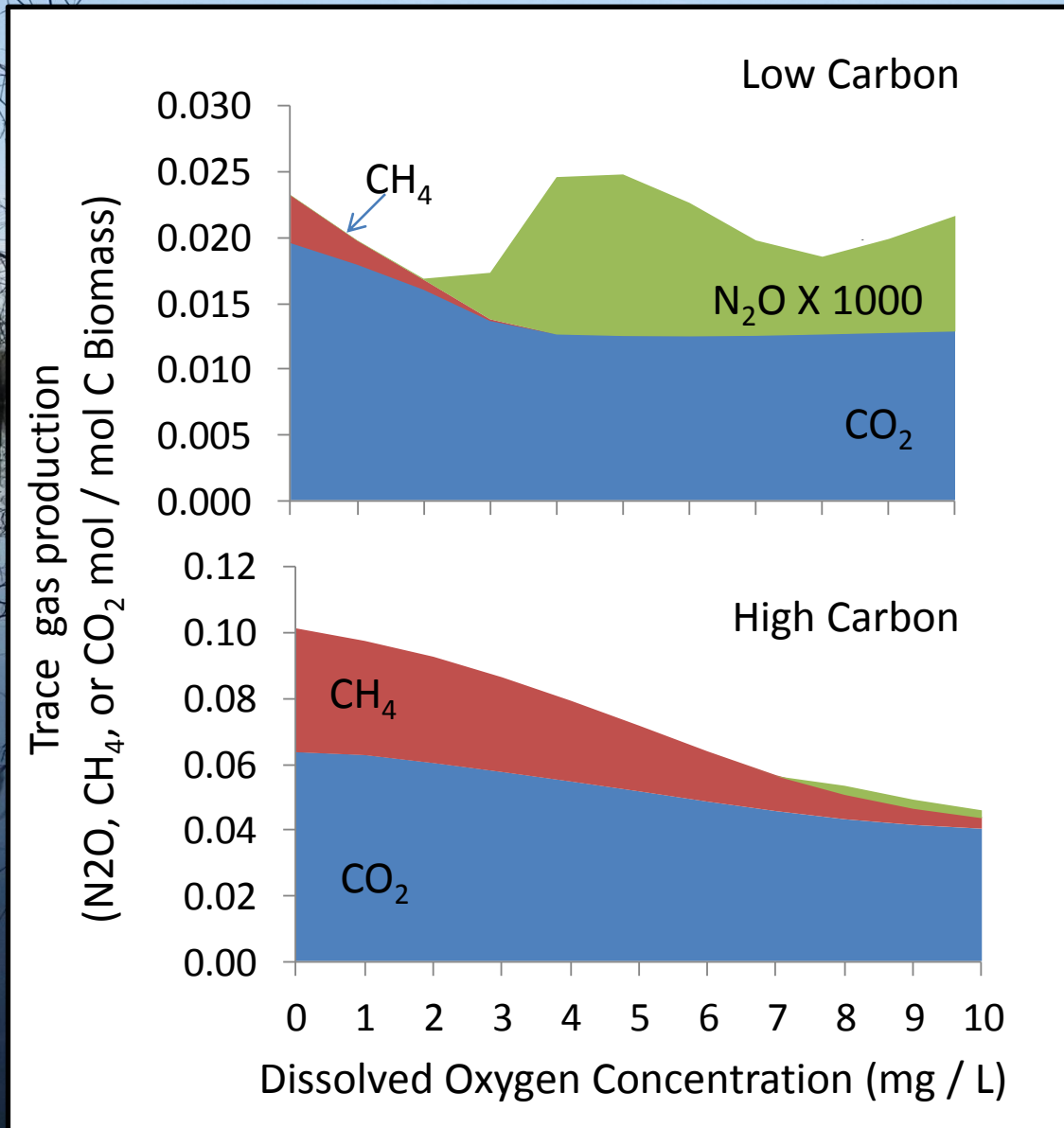


Dissolved Oxygen Concentration (mg / L)

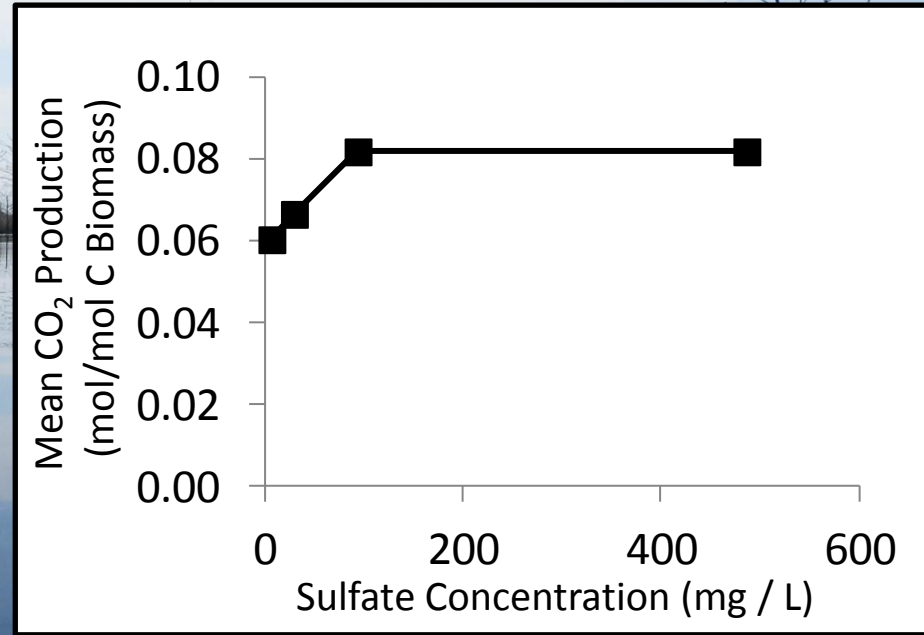
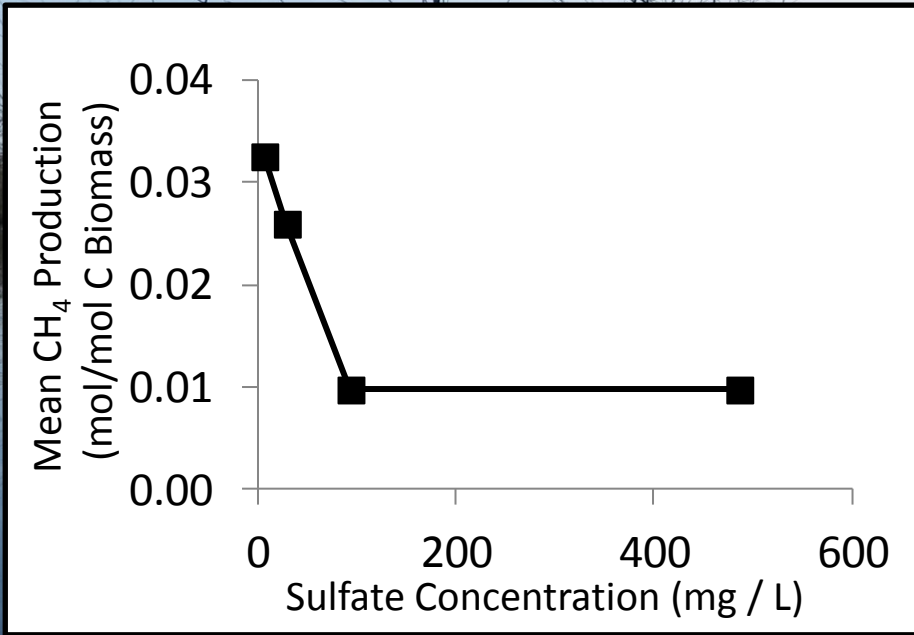
Anaerobic Processes



Model-derived trace gas production

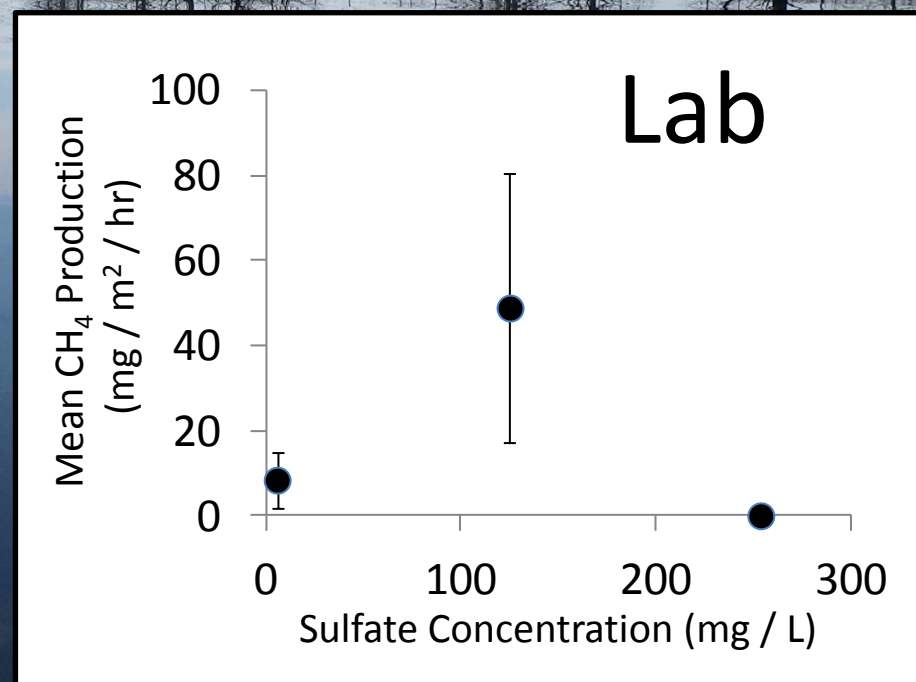
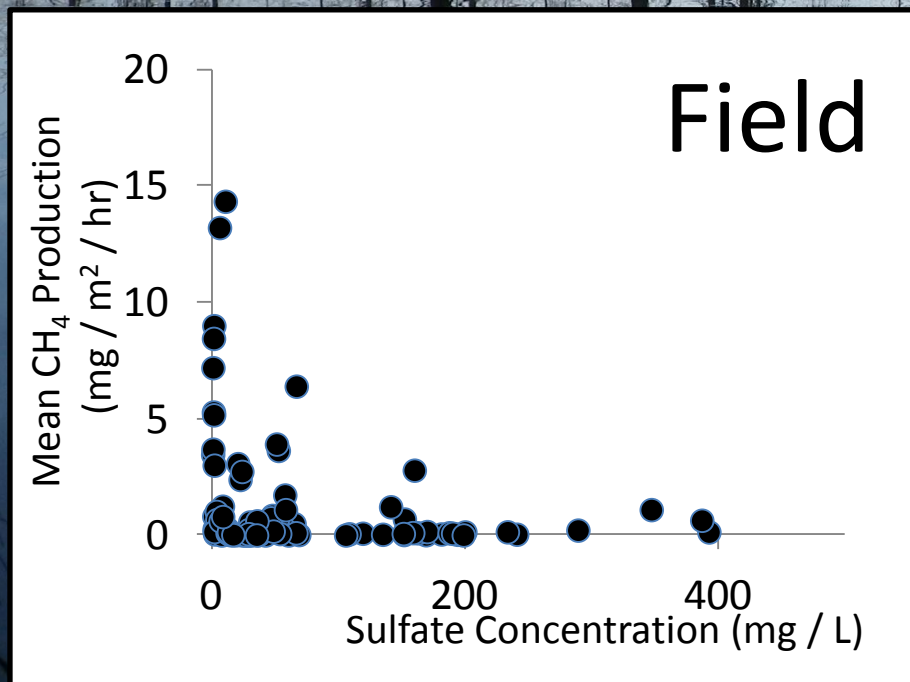
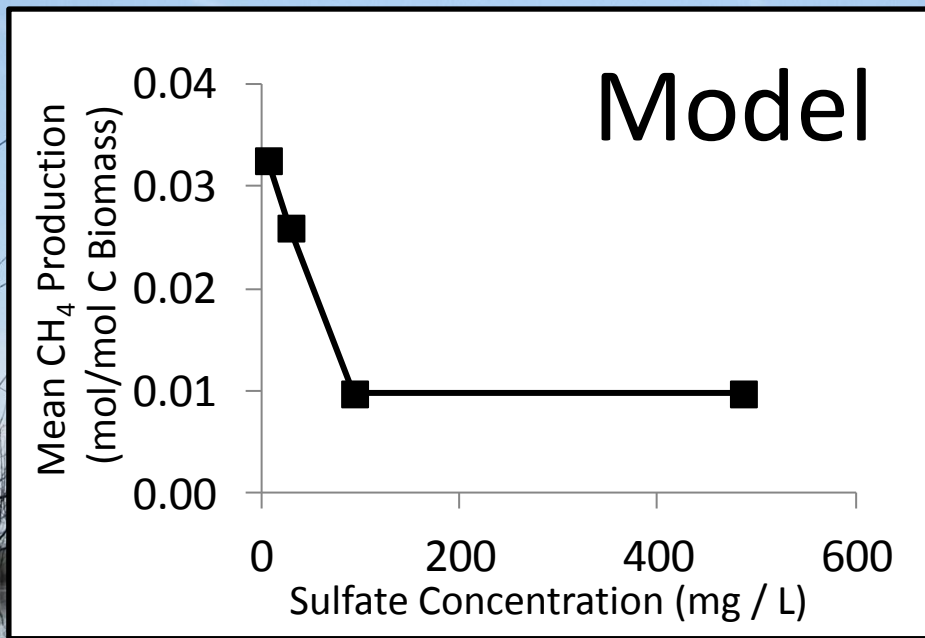


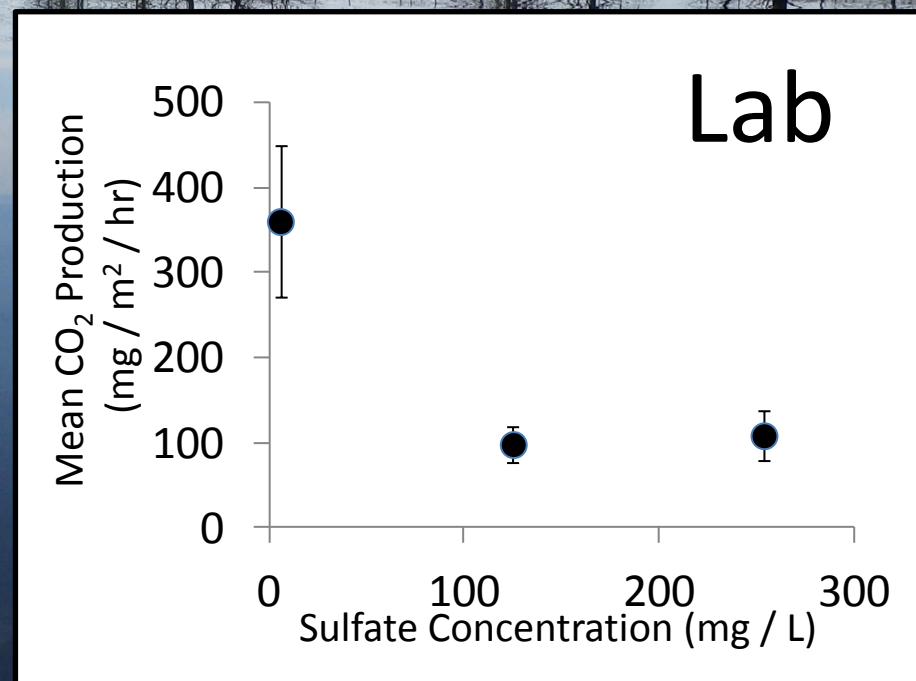
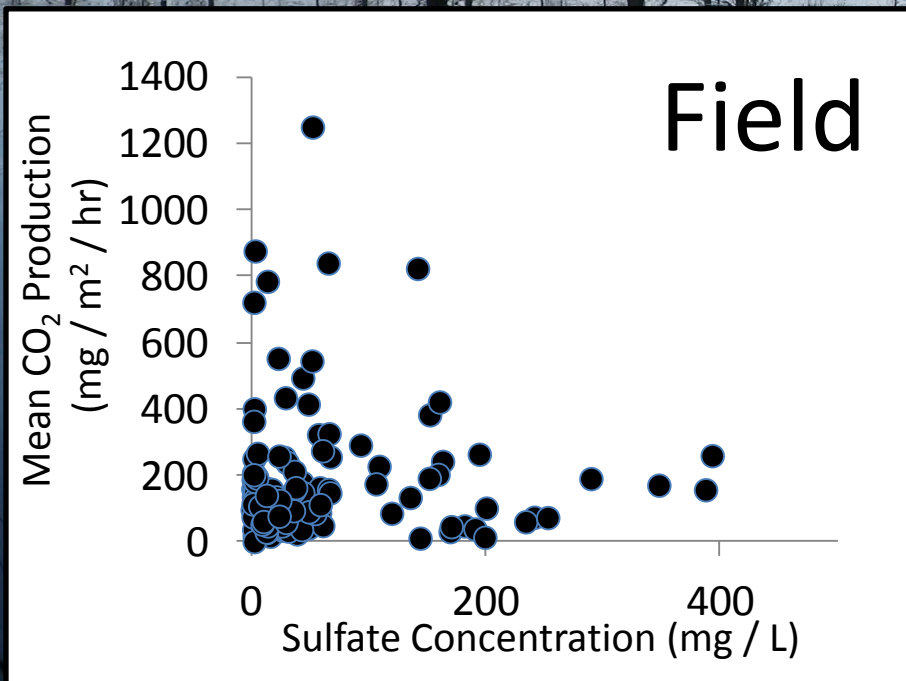
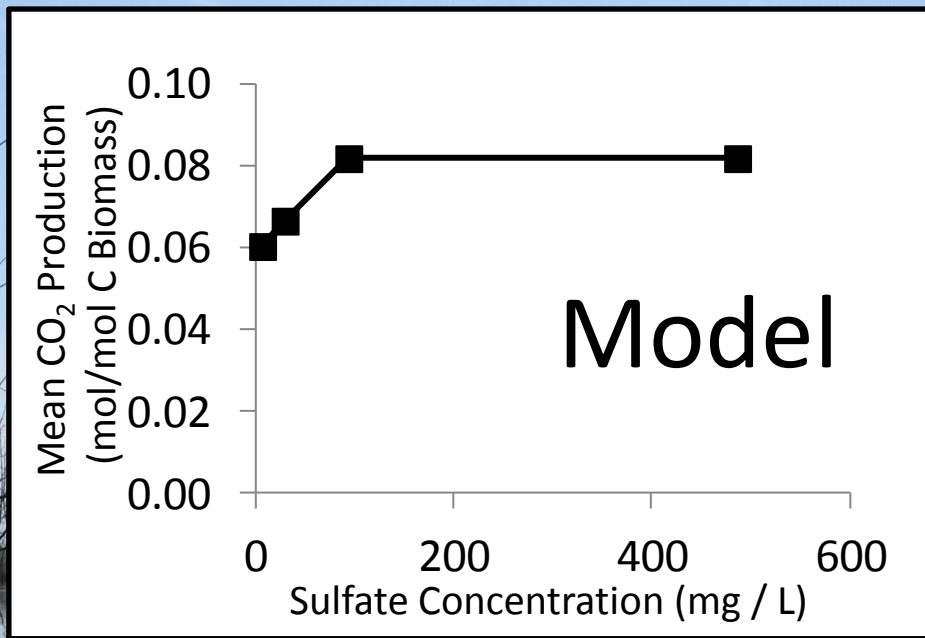
Trace gas production and sulfate loading: Model generated hypotheses



Redox Ladder Hypotheses:

1. CH₄ decreases because sulfate reducers outcompete methanogens.
2. CO₂ increases because sulfate provides new source of electron acceptors to sulfate reducers.





Summary

With increasing SO_4 concentrations:

1. CH_4 : In the model, field, and lab CH_4 emissions decrease EXCEPT high salt concentrations in the lab increase CH_4 emissions.
2. CO_2 : In the model, CO_2 emissions increase. Field results are inconclusive. Laboratory CO_2 emissions decrease.

Additional drivers and next steps

Geochemical

- NH_4^+ released from sediments
- DOC flocculation

Hydrologic: Wet v. Dry

Biological

- Actual free energy yield.
- Novel pathways (AOM, AOS).
- Carbon breakdown (fermentation).
- Competition for H_2 (hydrogenotrophic methanogenesis).
- Stress.

**Field
Measurements**

**Model
Simulations**

**Lab
Experiments**

Model simulations

