

Supplement Information

Biogeochemical model of CO₂ and CH₄ production in anoxic Arctic soil microcosms

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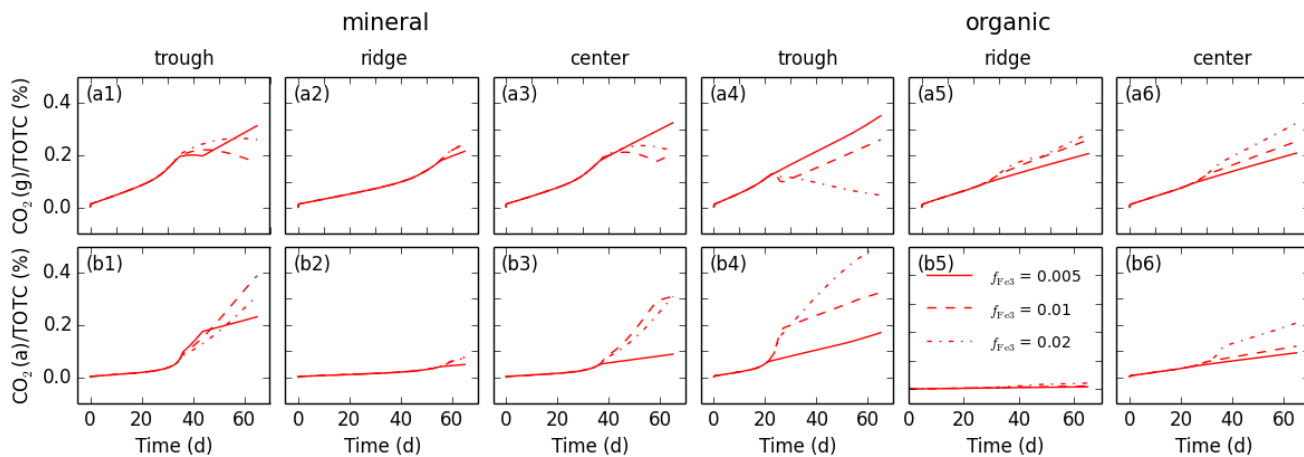
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Table S1. Additional experimental parameter values summarized from (Herndon et al., 2015; Roy Chowdhury et al., 2015).

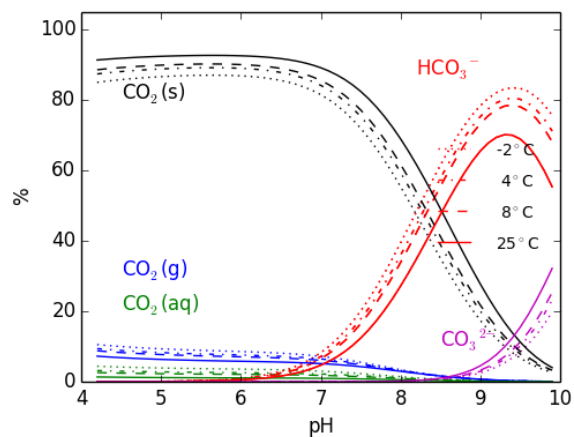
Location	Horizon	Formate (mgC)	Acetate (mgC)	Propionate (mgC)	TOTC/d wt Soil	WEOC /TOTC	Acids/WE OC	f(pH)
Center	Oa	0.3162	1.7185	0.0445	38.35%	1.77%	21.69%	0.486
	Bgh	0.0198	0.3524	0.0213	13.78%	0.31%	10.23%	0.384
Ridge	Oe	0.0012	0.0046	0.0104	38.89%	0.54%	0.24%	0.601
	Bh	0.0270	0.3420	0.0399	14.65%	0.26%	12.46%	0.241
Trough	Oe	0.0016	0.0062	0.0140	20.55%	0.38%	0.66%	0.614
	Bh/ice	0.0204	0.2617	0.0104	7.99%	0.30%	14.53%	0.445

Table S2. Model parameter values for base scenario

Symbol	Value	Description
f_{labile}	0.0005	Initial fraction of LabileC in TOTC
f_{som1}	0.01	Initial fraction of SOM1 in TOTC
f_{som2}	0.02	Initial fraction of SOM2 in TOTC
f_{som3}	0.1	Initial fraction of SOM3 in TOTC
f_{ferb}	2×10^{-6}	Initial fraction of Fe reducers in TOTC
f_{mega}	10^{-6}	Initial fraction of acetoclastic methanogens in TOTC
f_{megh}	10^{-6}	Initial fraction of hydrogenotrophic methanogens in TOTC
f_{mega}	10^{-6}	Initial fraction of SOM4 in TOTC
f_{fe3}	0.0025	Initial Fe(III) as a fraction of soil dry weight
S_{labile}	0.4	Fraction of the original CLM-CN respiration factor goes through labile pool.



5 **Figure S1:** Calculated partition of CO_2 in gas and aqueous phases as a percentage of initial TOTC with different $f_{\text{Fe}3}$ values. The results correspond to Fig. 2 for temperature 8 °C. With increasing $f_{\text{Fe}3}$, the pH increases at the late times, as does the CO_2 solubility.



10 **Figure S2:** Adding 1 mmol $\text{Fe}(\text{OH})_3\text{a}$ into the numerical experiments shown in Fig. 3, the gas-phase fraction is decreased at low pH values.

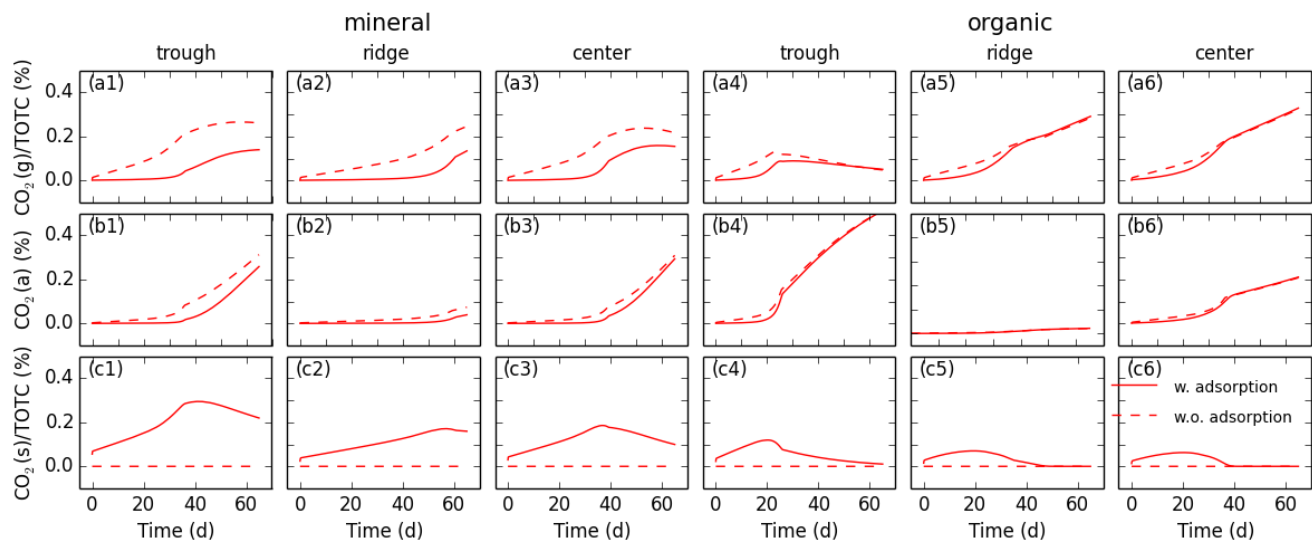


Figure S3: Impact of adsorption of CO_2 to ferric oxide surfaces on the distribution among gas, aqueous and solid phases.

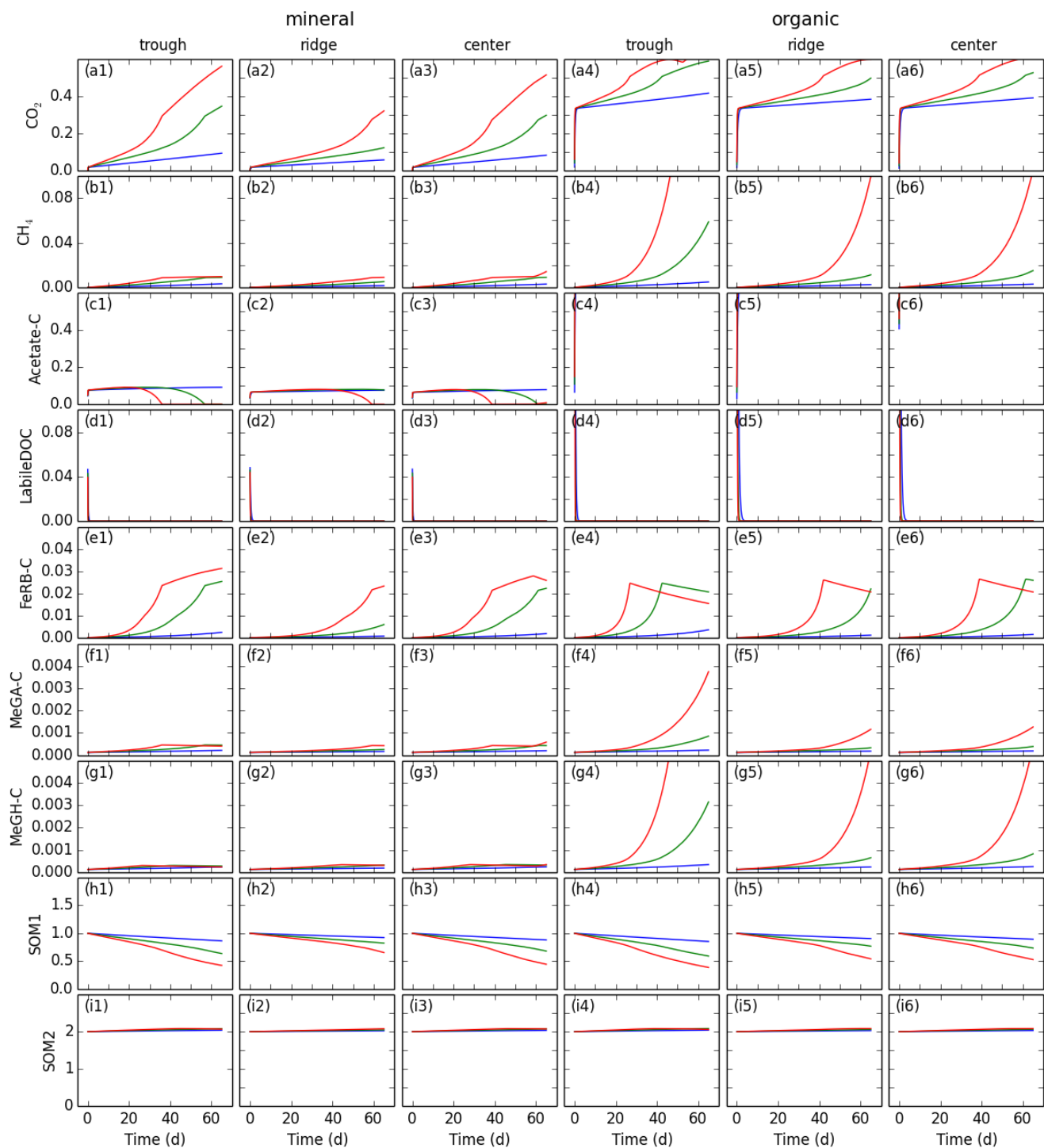


Figure S4: Partition of carbon among various organic pools. a, b, and c are for CO₂ distribution in the gas (head space), aqueous (water), and adsorbed (sorption to Fe(OH)₃a). See Fig.2 caption for more description about the model and experimental parameters.

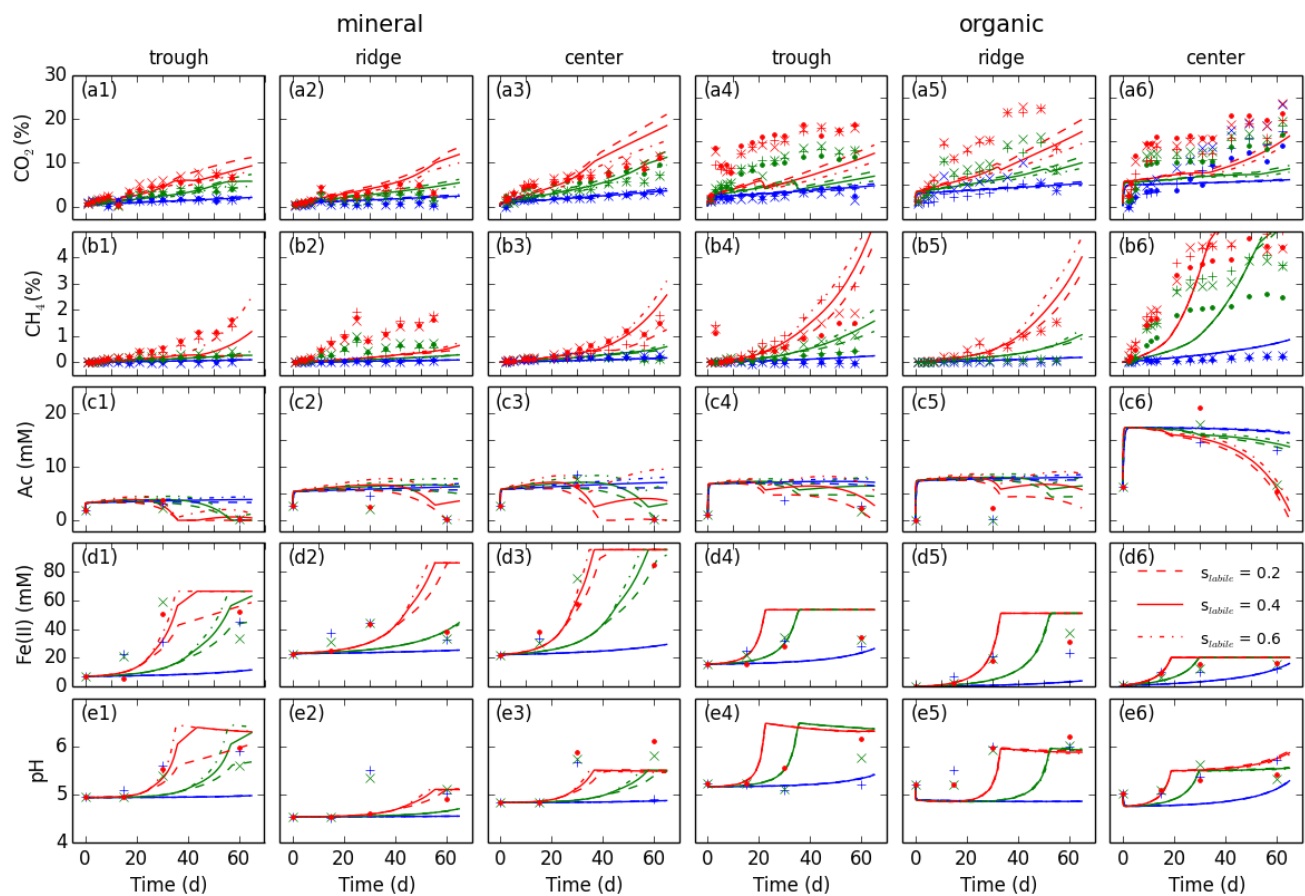


Figure S5: Impact of indirect respiration fraction (s_{stable}) WHAM on predictions. See Fig.2 caption for more description about the model and experimental parameters.

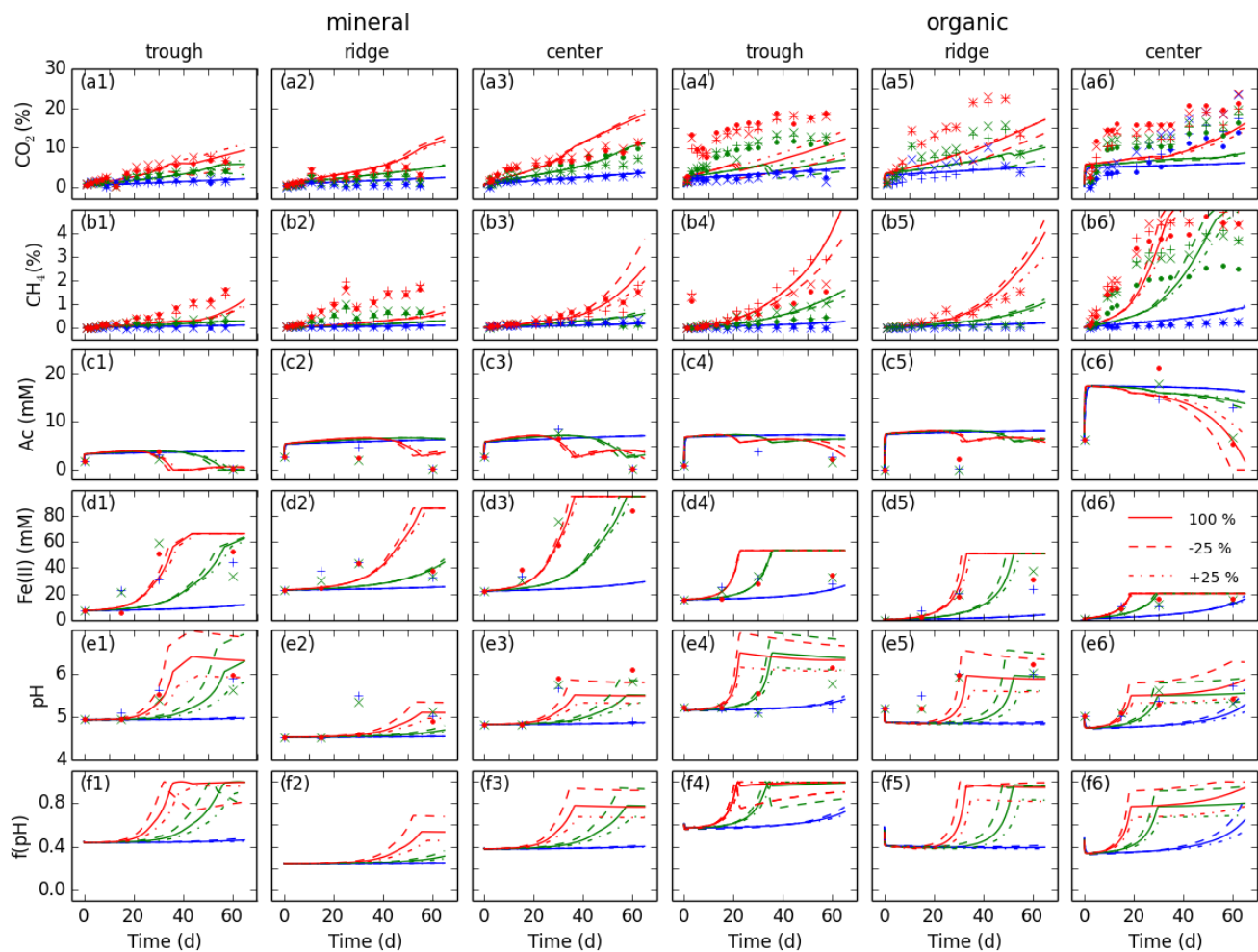


Figure S6: Impact of specified organic matter in WHAM on predictions. See Fig.2 caption for more description about the model and experimental parameters.

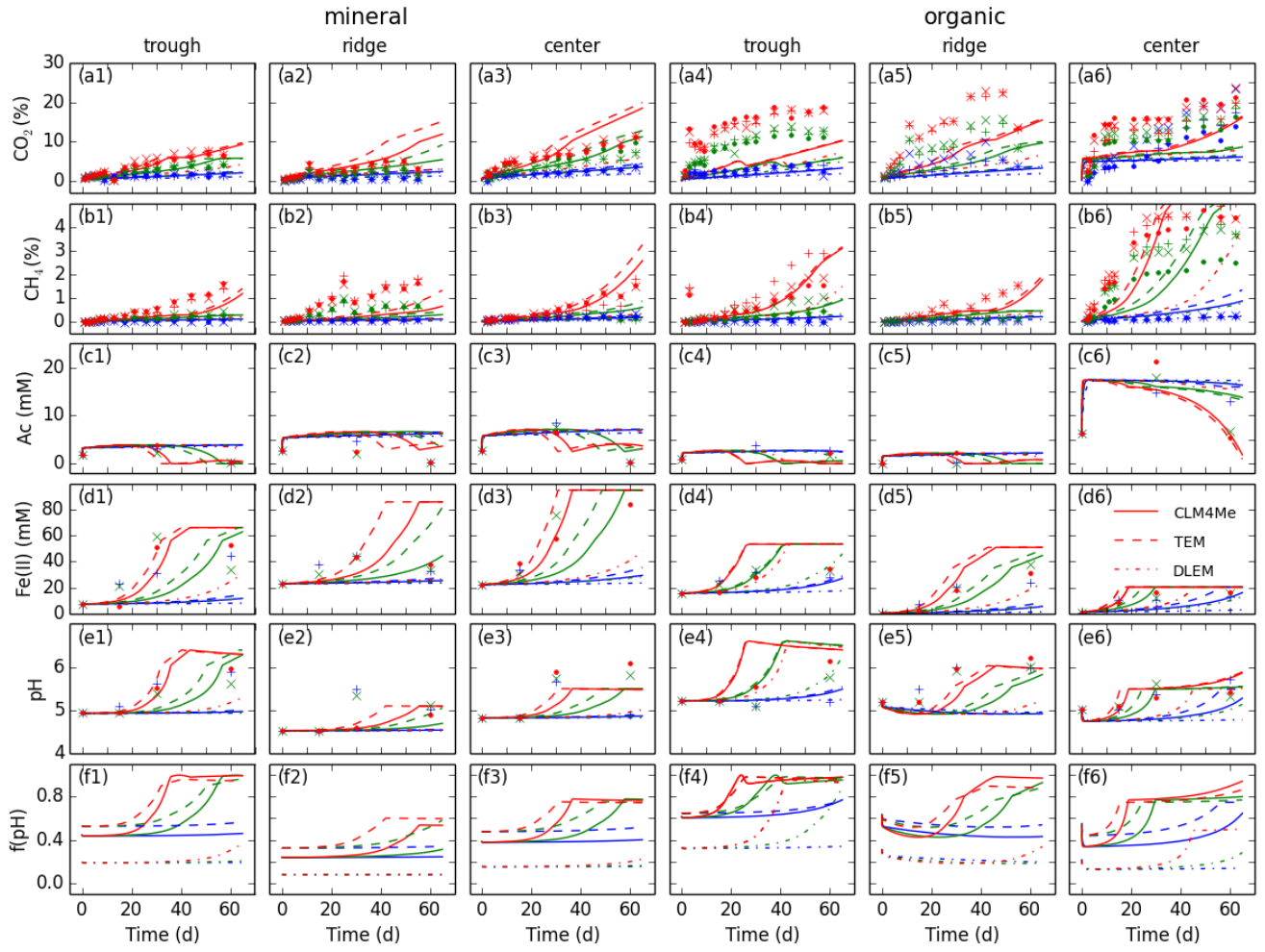


Figure S7: Comparison of the impact of different pH response functions (CLM4Me, TEM, and DLEM) on predictions.

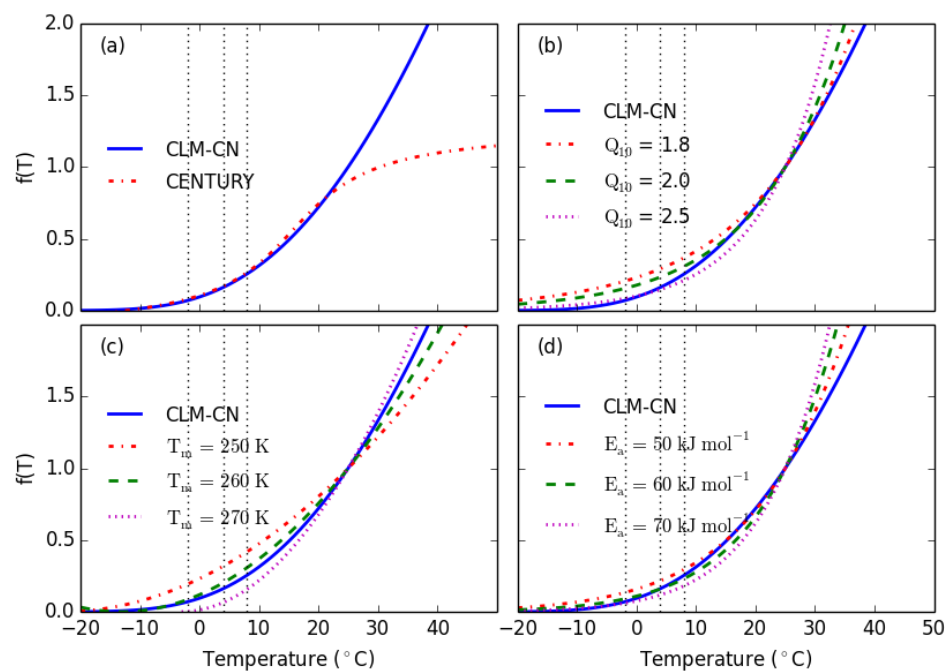


Figure S8: Fig. 7 with arithmetic vertical scale.

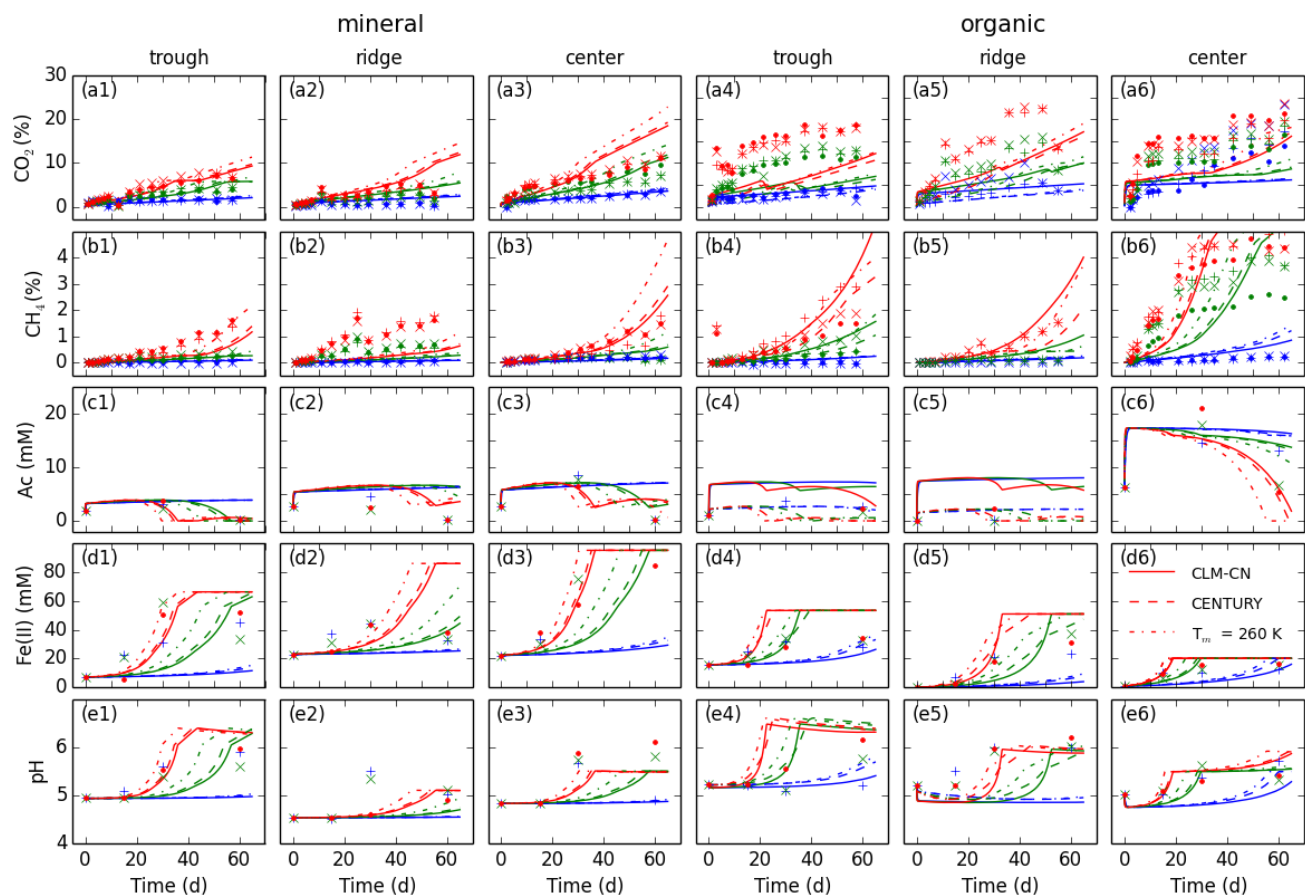


Figure S9: Comparison of impact of different temperature response functions (CLM-CN, CENTURY, Ratkowsky Equation with $T_m = 260$) on predictions.

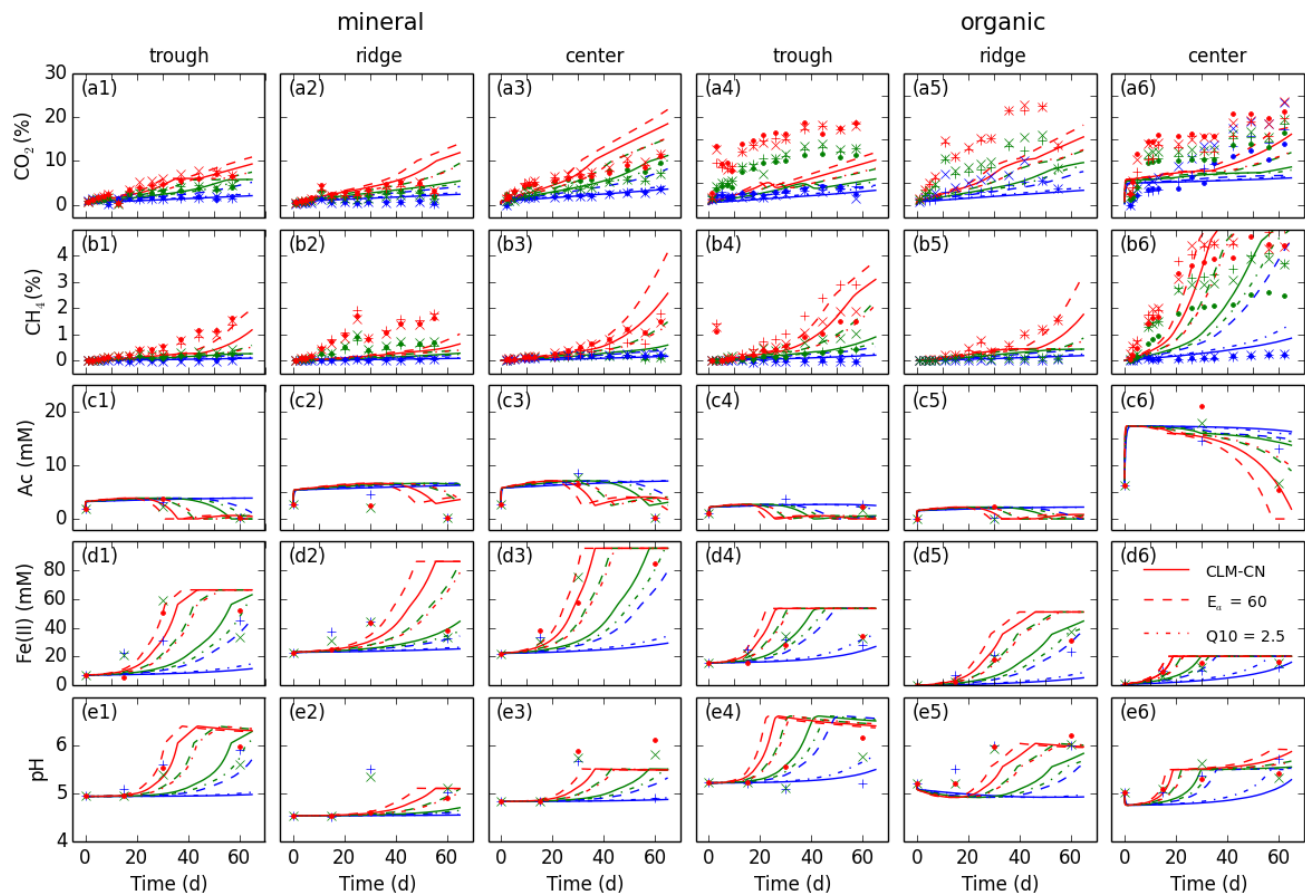


Figure S10: Comparison of impact of different temperature response functions (CLM-CN, Arrhenius equation (E_a), Q_{10} Equation) on predictions

References

- 5 Herndon, E. M., Mann, B. F., Chowdhury, T. R., Yang, Z., Wulfschleger, S. D., Graham, D., Liang, L., and Gu, B.: Pathways of anaerobic organic matter decomposition in tundra soils from Barrow, Alaska, *Journal of Geophysical Research: Biogeosciences*, n/a-n/a, 10.1002/2015JG003147, 2015.
- Roy Chowdhury, T., Herndon, E. M., Phelps, T. J., Elias, D. A., Gu, B., Liang, L., Wulfschleger, S. D., and Graham, D. E.: Stoichiometry and temperature sensitivity of methanogenesis and CO_2 production from saturated polygonal tundra in Barrow, Alaska, *Global Change Biology*, 21, 722-737, 10.1111/gcb.12762, 2015.
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