Supporting Information.

Lambda-PFLOTRAN 1.0: Workflow for Incorporating Organic Matter Chemistry Informed by Ultra High Resolution Mass Spectrometry into Biogeochemical Modeling

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SI.1 Bulk Organic Matter (CH_2O) Reaction Network

The reaction network developed for a generic organic matter molecule of CH_2O is shown in Eq SI.1. This reaction network is used within the Lambda-PFLOTRAN workflow.

$$2.03\ CH_2O + 0.98\ O_2 + 0.2\ NH_4^+ \rightarrow 1.03\ HCO_3^- + 1.23\ H^+ + 0.4\ H_2O + CH_{1.8}O_{0.5}N_{0.2} \quad \text{(SI.1)}$$

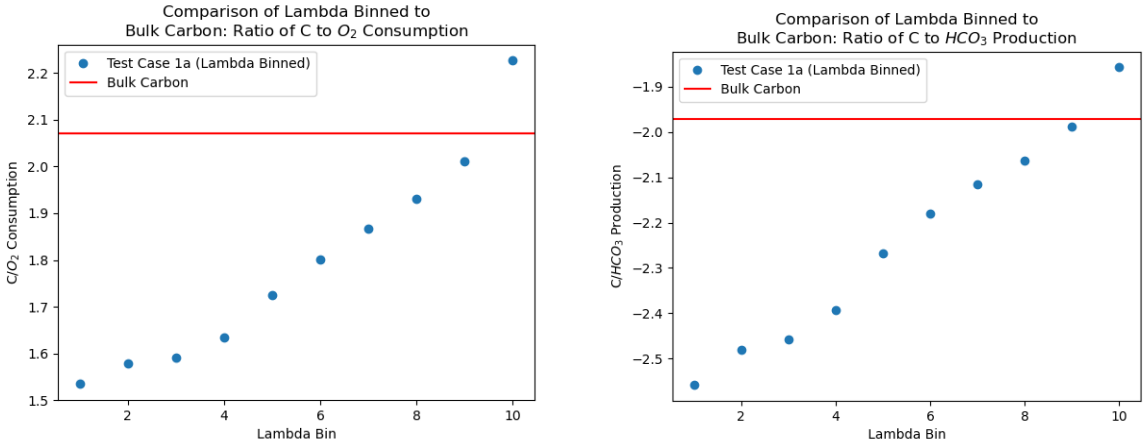

Figure S1. Comparison of Lambda Binned Organic Matter to Bulk Organic Matter (left) Ratio of carbon to oxygen consumption; (right) Ratio of carbon to bicarbonate production.

SI.2 Reaction Networks Developed for Test Case 1b and c

Table S1. Reaction Network Developed from Lambda Theory for Test Case 1b

Bin Number	Representative Organic Matter Species Formula	λ	y_{OC}	y_{HCO3-}	y_{NH4+}	y_{HPO42-}	y_{HS-}	y_{H+}	y_{O2}
1	$C_{32}H_{48}N_{0.24}O_{4.7}P_{0.54}S_{0.42}$	0.019	-0.05	0.62	-0.19	0.03	0.02	0.89	-1.07
2	$C_{27}H_{40}N_{0.16}O_{6.4}P_{0.57}S_{0.14}$	0.025	-0.06	0.66	-0.19	0.04	0.01	0.93	-1.06
3	$C_{23}H_{38}N_{0.15}O_{7.4}P_{0.53}S_{0.1}$	0.029	-0.07	0.67	-0.19	0.04	0.01	0.94	-1.06
4	$C_{21}H_{33}N_{0.17}O_{7.3}P_{0.45}S_{0.1}$	0.033	-0.08	0.70	-0.19	0.04	0.01	0.96	-1.06
5	$C_{20}H_{31}N_{0.36}O_{8.0}P_{0.35}S_{0.12}$	0.038	-0.09	0.75	-0.17	0.03	0.01	1.00	-1.04
6	$C_{19}H_{27}N_{0.35}O_{8}P_{0.24}S_{0.12}$	0.044	-0.10	0.81	-0.17	0.02	0.01	1.03	-1.03
7	$C_{17}H_{25}N_{0.44}O_{8.4}P_{0.2}S_{0.10}$	0.050	-0.11	0.87	-0.15	0.02	0.01	1.07	-1.02
8	$C_{16}H_{22}N_{0.64}O_{7.9}P_{0.14}S_{0.21}$	0.059	-0.12	0.92	-0.12	0.02	0.03	1.10	-1.01
9	$C_{13}H_{19}N_{0.93}O_{7.2}P_{0.12}S_{0.26}$	0.072	-0.15	0.99	-0.06	0.02	0.04	1.12	-1.00
10	$C_{11}H_{15}N_{01.7}O_{6.7}P_{0.08}S_{0.27}$	0.100	-0.21	1.20	0.15	0.02	0.06	1.13	-0.97

Table S2: Reaction Network Developed from Lambda Theory for Test Case 1c

λ Bin	Representative Organic Matter Species Formula	λ	y_{OC}	y_{HCO3-}	y_{NH4+}	y_{HPO42-}	y_{HS-}	y_{H+}	y_{O2}
1	$C_{31}H_{44}N_{0.33}O_{4.8}P_{0.64}S_{0.28}$	0.022	-0.05	0.64	-0.18	0.04	0.02	0.91	-1.07
2	$C_{26}H_{39}N_{0.20}O_{7.0}P_{0.57}S_{0.14}$	0.028	-0.07	0.68	-0.19	0.04	0.01	0.95	-1.06
3	$C_{22}H_{36}N_{0.24}O_{67.5}P_{0.49}S_{0.10}$	0.033	-0.08	0.69	-0.18	0.04	0.01	0.95	-1.06
4	$C_{20}H_{32}N_{0.28}O_{7.3}P_{0.43}S_{0.13}$	0.037	-0.08	0.72	-0.18	0.04	0.01	0.98	-1.05
5	$C_{19}H_{29}N_{0.48}O_{7.9}P_{0.3}S_{0.18}$	0.041	-0.09	0.79	-0.16	0.03	0.02	1.02	-1.04
6	$C_{18}H_{26}N_{0.68}O_{8.1}P_{0.23}S_{0.15}$	0.048	-0.10	0.85	-0.13	0.02	0.02	1.04	-1.03
7	$C_{17}H_{24}N_{0.69}O_{8.1}P_{0.18}S_{0.18}$	0.055	-0.11	0.90	-0.12	0.02	0.02	1.08	-1.02
8	$C_{15}H_{20}N_{0.67}O_{7.6}P_{0.16}S_{0.24}$	0.065	-0.13	0.94	-0.11	0.02	0.03	1.13	-1.00
9	$C_{13}H_{19}N_{1.13}O_{7.4}P_{0.10}S_{0.17}$	0.076	-0.15	1.01	-0.03	0.01	0.03	1.10	-1.00
10	$C_{10}H_{15}N_{1.56}O_{6.5}P_{0.06}S_{0.22}$	0.106	-0.207	1.17	0.12	0.01	0.05	1.11	-0.97

SI.3 Test Case 1b and 1c Results

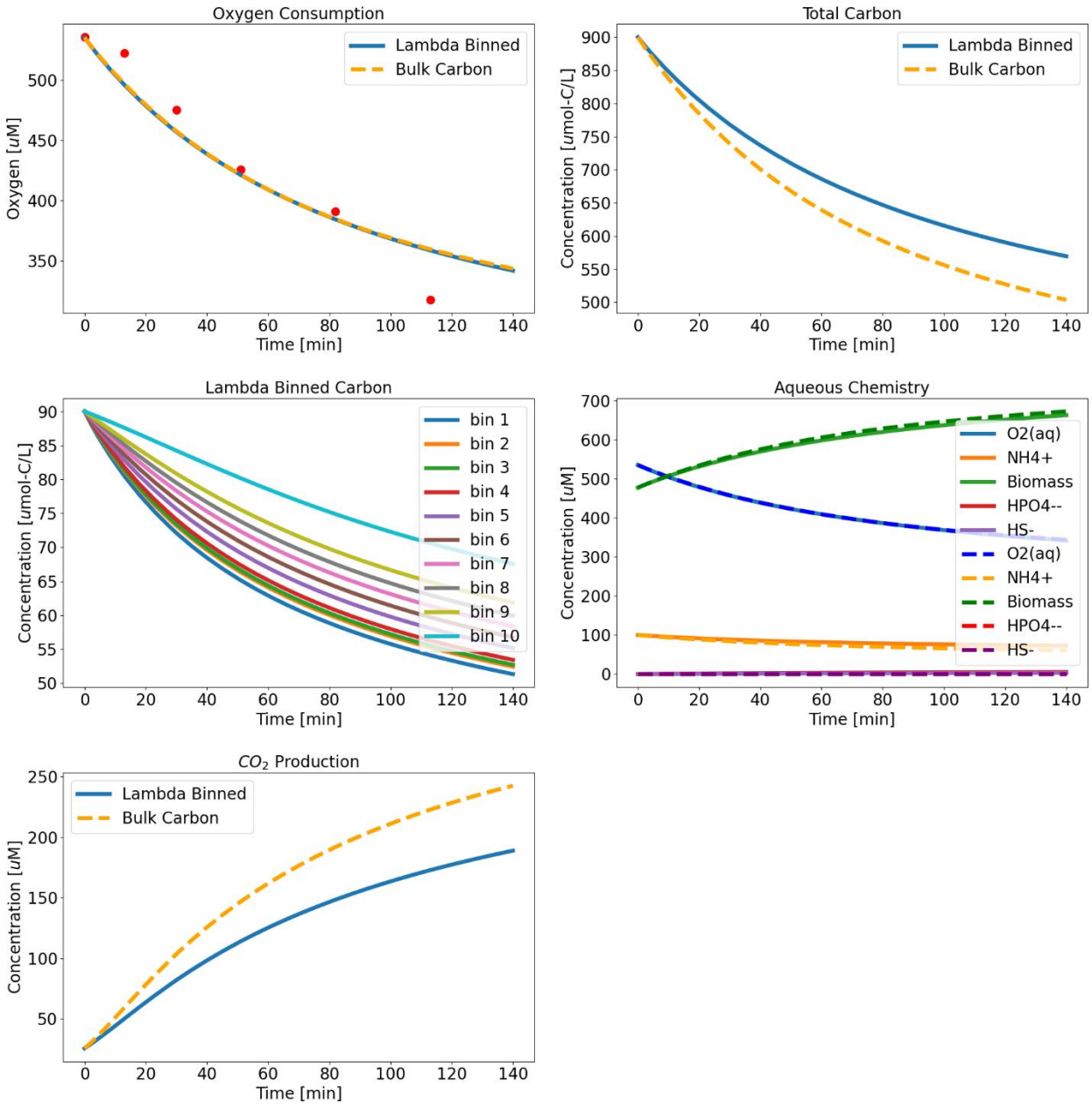

Figure S2: Test Case 1b Results – Oxygen Consumption (top left) where Lambda-PFLOTRAN workflow was used to fit (blue line) to experimental respiration data (red dots) and the corresponding Total Carbon Consumption (top right); Individual OM Consumption by λ bin (middle left); Corresponding biogeochemistry including O_2 (aq) (blue); Biomass (green); NH_4^+ (orange); HS^- (purple); and HPO_4^{--} (red) (middle right) and CO_2 production. The dashed orange lines show simulation results assuming a generic OM species of CH_2O for comparison. Fitted lambda μ_{max}= 0.092 min^{-1}, V_h = 7.5 m^3; CC = 0.65 M (R^2= 0.88). Fitted bulk OM model values were 0.19 min^{-1}, 1.0 m^3, 0.35 M for μ_{max}, V_h, CC, respectively (R^2= 0.88).

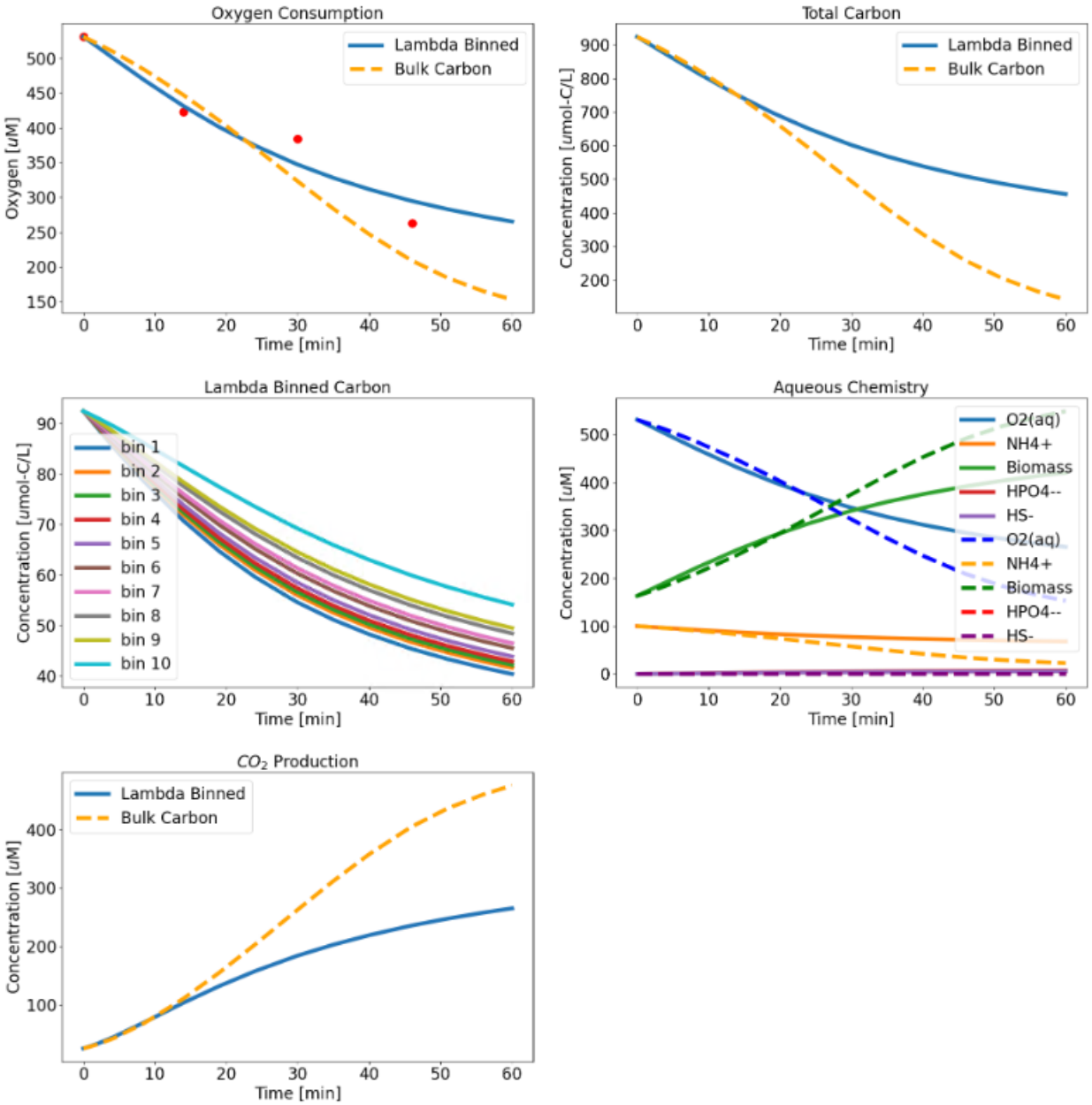

Figure S3: Test Case 1c Results – Oxygen Consumption (top left) where Lambda-PFLOTRAN workflow was used to fit (blue line) to experimental respiration data (red dots) and the corresponding Total Carbon Consumption (top right); Individual OM Consumption by λ bin (middle left); Corresponding biogeochemistry including O_2 (aq) (blue); Biomass (green); NH_4^+ (orange); HS^- (purple); and HPO_4^{--} (red) (middle right); and CO_2 production (bottom left). The dashed orange lines show simulation results assuming a generic OM species of CH_2O for comparison. Fitted lambda μ_{max} = 0.33 min^{-1}, V_h= 10 m^3, CC = 0.27 M (R^2= 0.92). Fitted bulk OM model values were 0.22 min^{-1}, 10 m^3, 0.47 M for μ_{max}, V_h, and CC, respectively (R^2= 0.88).