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Supplement of

Lambda-PFLOTRAN 1.0: a workflow for incorporating organic matter chemistry informed by ultra high resolution mass spectrometry into biogeochemical modeling

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SI.1 Test Case 1b and 1c Results

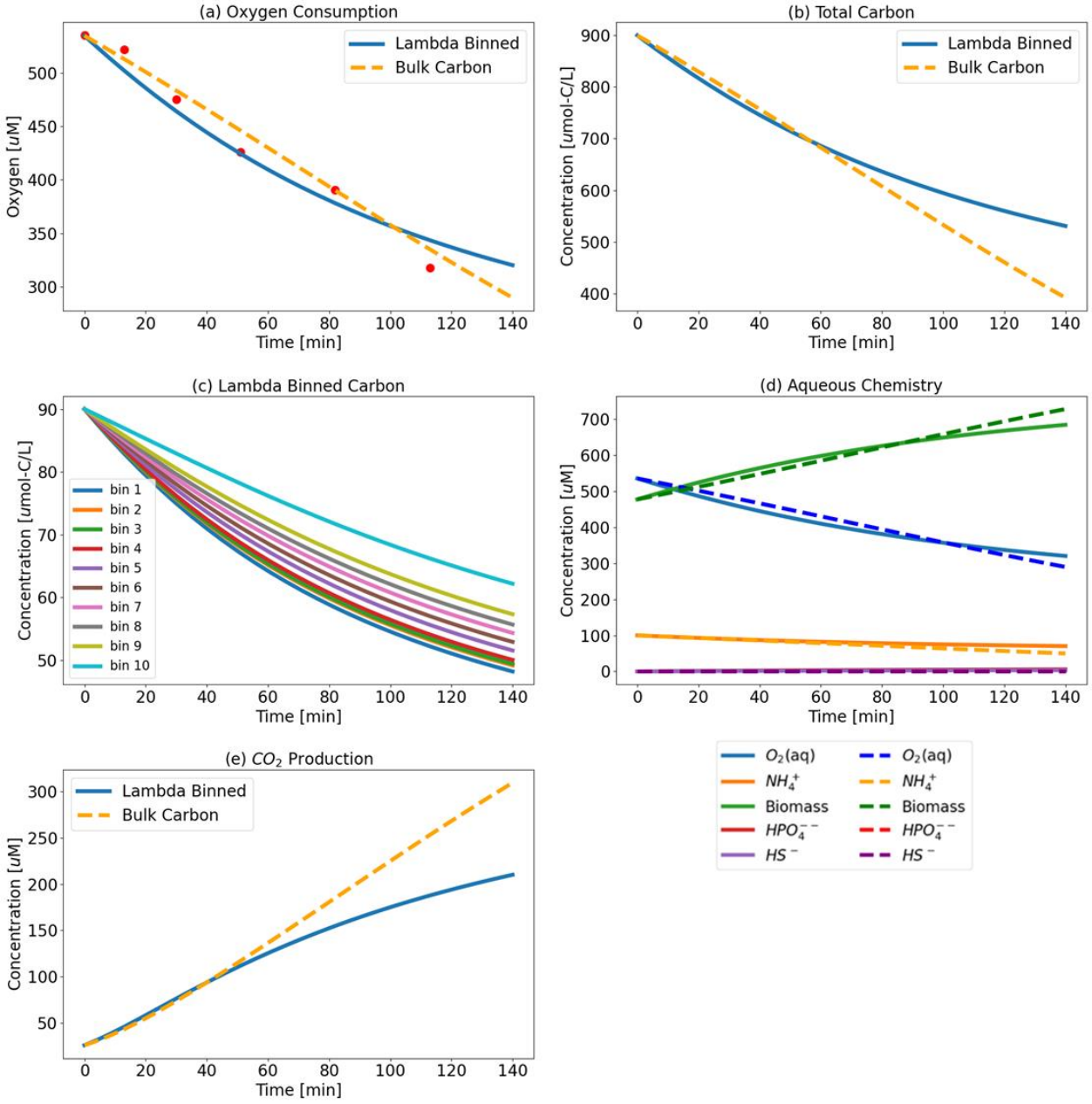

Figure S1: Test Case 1b Results – (a) Oxygen Consumption where Lambda-PFLOTRAN workflow was used to fit (blue line) to experimental respiration data (red dots) and (b) the corresponding Total Carbon Consumption; (c) Individual Organic Matter Consumption by λ bin; and (d) biogeochemistry including O_2 (aq) (blue); Biomass (green); NH_4^+ (orange); HS^- (purple); and HPO_4^{--} (red); and (d) CO_2 production for the upstream incubation. The dashed orange lines in (a, b and e) show simulation results assuming a generic OM species of CH_2O for comparison. Fitted μ_{max} values for the lambda binned model is 0.055 min^{-1} (R^2 = 0.95) and fitted μ_{max} to the bulk OM CH_2O model is 0.0065 min^{-1} (R^2 = 0.97). V_h and CC are fixed at assumed values of 10 m^3 and 1 M, respectively in both simulations.

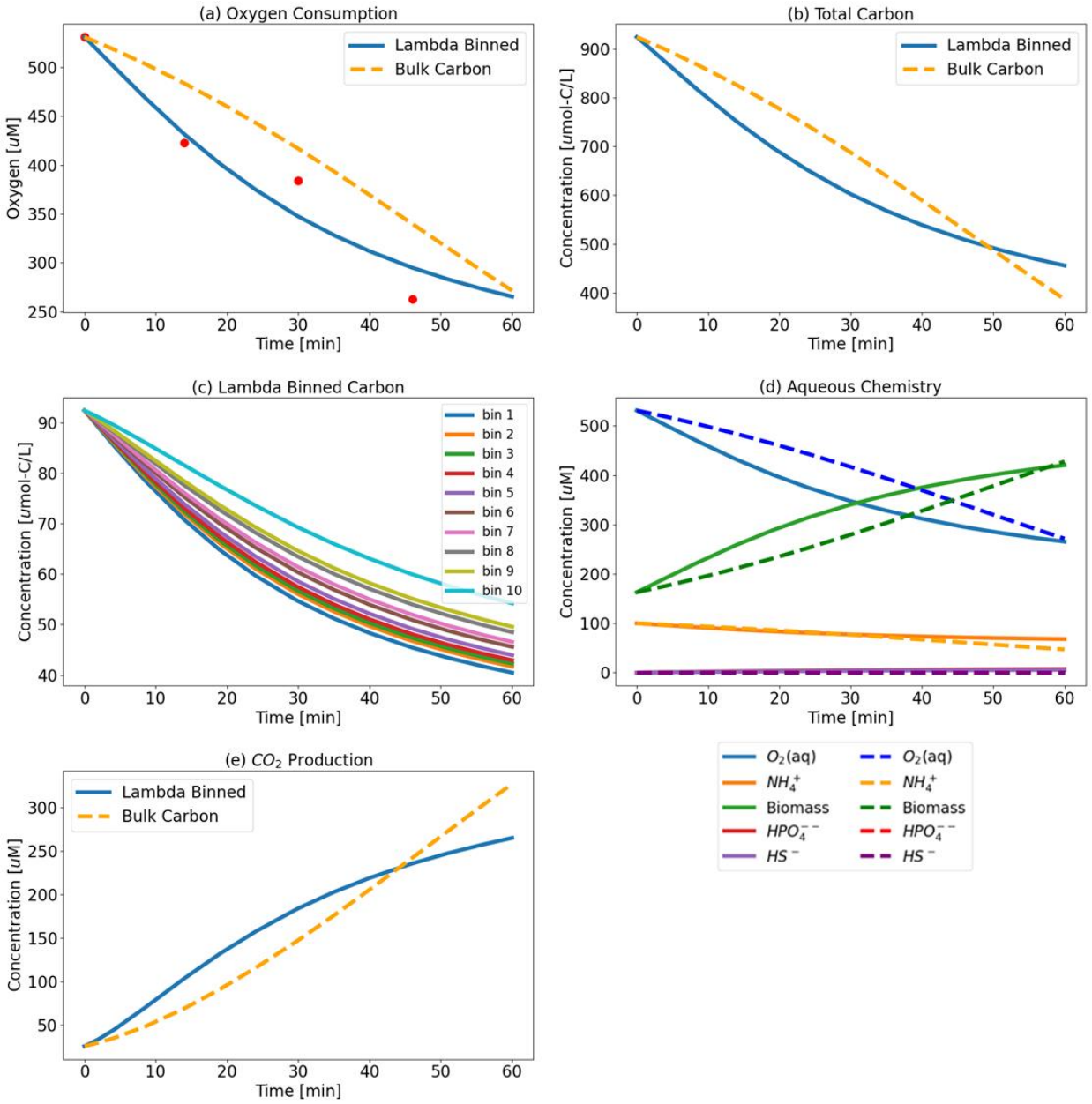

Figure S2: Test Case 1c Results – (a) Oxygen Consumption where Lambda-PFLOTRAN workflow was used to fit (blue line) to experimental respiration data (red dots) and (b) the corresponding Total Carbon Consumption; (c) Individual Organic Matter Consumption by λ bin; and (d) biogeochemistry including O_2 (aq) (blue); Biomass (green); NH_4^+ (orange); HS^- (purple); and HPO_4^{--} (red); and (d) CO_2 production for the upstream incubation. The dashed orange lines in (a, b, and e) show simulation results assuming a generic OM species of CH_2O for comparison. Fitted μ_{max} values for the lambda binned model is 0.35 min^{-1} (R^2 = 0.92) and fitted μ_{max} to the bulk OM CH_2O model is 0.13 min^{-1} (R^2 = 0.48). V_h and CC are fixed at assumed values of 10 m^3 and 1 M, respectively in both simulations.