Wetland soil characteristics influence the kinetics of dissolved organic carbon sorption: Supplemental File

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Appendix A: Model Parameters

Table A.1. Site and sample descriptions based on experiment ID. Lateral location indicates how many meters upland the sampling site was from the creek edge, vertical location indicates the depth of the sample.

ID	Site	Lateral Location (m)	Vertical Location (cm)	[DOC] (mg L^{-1})	Salinity (psu)
JBHF	Jug Bay	High Marsh (10)	Homogenized (0-40)	High (275)	Fresh (0)
JBHS	Jug Bay	High Marsh (10)	Homogenized (0-40)	High (275)	Saline (35)
JBLF	Jug Bay	High Marsh (10)	Homogenized (0-40)	Low (<5)	Fresh (0)
JBLS	Jug Bay	High Marsh (10)	Homogenized (0-40)	Low (<5)	Saline (35)
TAHF	Taskinas	High Marsh (10)	Homogenized (0-40)	High (275)	Fresh (0)
TAHS	Taskinas	High Marsh (10)	Homogenized (0-40)	High (275)	Saline (35)
TALF	Taskinas	High Marsh (10)	Homogenized (0-40)	Low (<5)	Fresh (0)
TALS	Taskinas	High Marsh (10)	Homogenized (0-40)	Low (<5)	Saline (35)
WCHF	Taskinas	Creek Edge (0)	Shallow (0-5)	High (275)	Fresh (0)
WCHS	Taskinas	Creek Edge (0)	Shallow (0-5)	High (275)	Saline (35)
WCLF	Taskinas	Creek Edge (0)	Shallow (0-5)	Low (<5)	Fresh (0)
WCLS	Taskinas	Creek Edge (0)	Shallow (0-5)	Low (<5)	Saline (35)
WIHF	Taskinas	Intermediate (3)	Shallow (0-5)	High (275)	Fresh (0)
WIHS	Taskinas	Intermediate (3)	Shallow (0-5)	High (275)	Saline (35)
WILF	Taskinas	Intermediate (3)	Shallow (0-5)	Low (<5)	Fresh (0)
WILS	Taskinas	Intermediate (3)	Shallow (0-5)	Low (<5)	Saline (35)
WMHF	Taskinas	High Marsh (10)	Shallow (0-5)	High (275)	Fresh (0)
WMHS	Taskinas	High Marsh (10)	Shallow (0-5)	High (275)	Saline (35)
WMLF	Taskinas	High Marsh (10)	Shallow (0-5)	Low (<5)	Fresh (0)
WMLS	Taskinas	High Marsh (10)	Shallow (0-5)	Low (<5)	Saline (35)

PCHF	Taskinas	Creek Edge (0)	Shallow (0-5)	High (275)	Fresh (0)
PCHS	Taskinas	Creek Edge (0)	Deep (30-40)	High (275)	Saline (35)
PCLF	Taskinas	Creek Edge (0)	Deep (30-40)	Low (<5)	Fresh (0)
PCLS	Taskinas	Creek Edge (0)	Deep (30-40)	Low (<5)	Saline (35)
PIHF	Taskinas	Intermediate (3)	Deep (30-40)	High (275)	Fresh (0)
PIHS	Taskinas	Intermediate (3)	Deep (30-40)	High (275)	Saline (35)
PILF	Taskinas	Intermediate (3)	Deep (30-40)	Low (<5)	Fresh (0)
PILS	Taskinas	Intermediate (3)	Deep (30-40)	Low (<5)	Saline (35)
PMHF	Taskinas	High Marsh (10)	Deep (30-40)	High (275)	Fresh (0)
PMHS	Taskinas	High Marsh (10)	Deep (30-40)	High (275)	Saline (35)
PMLF	Taskinas	High Marsh (10)	Deep (30-40)	Low (<5)	Fresh (0)
PMLS	Taskinas	High Marsh (10)	Deep (30-40)	Low (<5)	Saline (35)

Table A.2. Cs_{t0} & $DOCw_{t0}$ initial values for the analytical solution (C t_0 values) by scenario for all three model formulations, plus Q_{max} for the Langmuir model.

Scenario	**Cs_{t0} (mg)**	**$DOCw_{t0}$ (mg)**	**Q_{max} (mg)**
Description	Concentration of OC on sediment	Concentration of DOC in solution	Maximum sorption capacity
JBHF	4.284	8.867	5.967
JBHS	4.500	8.385	12.500
JBLF	4.242	0.077	5.909
JBLS	4.500	0.105	12.500
TAHF	2.030	8.780	2.254
TAHS	1.930	8.413	10.800
TALF	2.030	0.122	2.254
TALS	1.969	0.124	11.016
WCHF	1.015	3.003	1.127
WCHS	0.939	2.955	5.256
WCLF	0.995	0.042	1.105
WCLS	0.933	0.072	5.220
WIHF	1.048	3.103	1.164
WIHS	0.984	2.955	5.508
WILF	1.022	0.069	1.134
WILS	0.952	0.084	5.328
WMHF	0.968	3.003	1.076
WMHS	0.971	2.955	5.436
WMLF	1.002	0.042	1.112
WMLS	0.991	0.072	5.544
PCHF	0.982	3.038	1.090

PCHS	0.920	3.125	5.148
PCLF	0.995	0.101	1.105
PCLS	0.920	0.086	5.148
PIHF	0.988	3.103	1.098
PIHS	0.933	2.955	5.220
PILF	0.988	0.069	1.098
PILS	0.971	0.084	5.436
PMHF	0.962	3.003	1.068
PMHS	0.926	2.955	5.184
PMLF	0.982	0.042	1.090
PMLS	0.939	0.072	5.256

Table A.3. Optimized Linear, Langmuir, and Time-Dependent model rates. Linear and Langmuir outputs are using the reduced data sets, and Time-Dependent outputs are using the full data sets (with peaks).

	Linear (hr $^{-1}$)		**Langmuir (hr $^{-1}$)**		**Time-Dependent (hr $^{-1}$)**		
Scenario	kdes	kads	kdes	kads ($kads_2$*Q_{max})	kdes _max	kdes _min	kads
JBHF	0.383	0.925	0.527	4.520	51.25	28.62	20.88
JBLF					5.07	4.85	17.58
JBHS	1.107	0.927	2.43	11.703	12.86	8.01	13.21
JBLS					4.73	4.80	17.69
TAHF	-0.001	-0.010	1.841	1.176	6.64	0.44	0.08
TALF					15.49	14.38	8.18
TAHS	0.688	1.957	0.969	0.750	2.43	1.06	0.57
TALS					9.03	5.40	5.75
WCHF	0.269	1.016	0.992	6.501	39.48	1.50	0.71
WCLF					69.80	39.67	65.44
WCHS	0.902	0.841	0.361	0.790	41.26	1.18	1.26
WCLS					868.96	4.93	10.10
WIHF	-0.020	0.298	0.665	0.285	1.14	0.29	0.04
WILF					2.40	0.35	0.20
WIHS	1.364	3.833	2.544	1.076	0.79	1.66	0.90
WILS					6.69	9.44	14.16
WMHF	-0.010	0.227	12.456	4.183	124.61	56.40	7.51
WMLF					402.11	18.82	6.85
WMHS	0.620	2.534	0.851	0.500	9.12	2.21	0.92
WMLS					20.35	8.55	7.65

PCHF	-577.48	3417.05	1.000	1.091	50.00	2.81	0.16
PCLF					7.10	10.59	8.07
PCHS	0.228	1.809	0.502	0.235	1.80	7.46	2.35
PCLS					17.87	25.79	31.72
PIHF	-0.782	12.564	2.200	18.311	2.99	3.18	0.55
PILF					11.54	14.59	14.15
PIHS	0.465	2.149	0.309	0.211	23.54	18.62	8.64
PILS					18.19	22.73	41.30
PMHF	-5.526	39.390	65.475	11.694	130.11	238.13	23.32
PMLF					25.78	55.70	23.55
PMHS	0.673	2.939	0.765	0.385	0.61	0.00	0.01
PMLS					16.14	25.85	24.64

Table A.4a. Generalized equations: versions of manuscript equations 1-7 that account for mass and volume for model application. The units of each parameter are specific to this set of equations and are defined in Table A.4b.

Eq. #	Equation	Model
1	$\frac{dCs}{dt} = -k_{des} \times Cs \ + \ k_{ads} \times DOC \times \frac{V}{M}$	Linear
2	$\frac{dDOC}{dt} = k_{des} \times Cs \times \frac{M}{V} - \ k_{ads} \times DOC$	Linear
3	$Cs(t) = \frac{1}{k_{ads} + k_{des}}\left[Cs(0)\left(k_{ads} + k_{des}e^{-(k_{ads}+k_{des})t}\right) + \ DOC(0) \times \frac{V}{M} \times k_{ads}\left(1 - \ e^{-(k_{ads}+k_{des})t}\right)\right]$	Linear
4	$DOC(t) = \frac{1}{k_{ads} + k_{des}}[Cs(0) \times \frac{M}{V} \times k_{des}\left(1 - \ e^{-(k_{ads}+k_{des})t}\right) + DOC(0)\left(k_{des} + k_{ads}\ e^{-(k_{ads}+k_{des})t}\right)]$	Linear
5	$\frac{dCs}{dt} = -k_{des} \times Cs \ + k_{ads_2} \times DOC \times S$	Langmuir
6	$\frac{dDOC}{dt} = \frac{M}{V} \times \left(k_{des} \times Cs - k_{ads_2} \times DOC \times S\right)$	Langmuir
7	$S \ = \ Qmax \ - \ Cs$	Langmuir

Table A.4b. Model parameters, descriptions, and units for equations listed in Table A.4a.

Parameter	Description	Unit	Model Version
k_{des}	Desorption rate coefficient	hr^{-1}	Linear, Langmuir
k_{ads}	Adsorption rate coefficient	hr^{-1}	Linear
Cs(t)	Concentration of organic carbon adsorbed on soils	$mg\ g^{-1}$	Linear
DOC(t)	Concentration of DOC free in solution	$mg\ L^{-1}$	Linear
S	Saturation coefficient	$mg\ g^{-1}$	Langmuir
Q_{max}	Maximum adsorption capacity	$mg\ g^{-1}$	Langmuir
k_{ads2}	Saturation adsorption rate coefficient	$L\ mg^{-1}\ hr^{-1}$	Langmuir
M/V	Ratio of soil mass to solution volume	$g\ L^{-1}$	Linear, Langmuir
V/M	Ratio of solution volume to soil mass	$L\ g^{-1}$	Linear, Langmuir

Appendix B: Statistics

Table B.1. Ranked RMSE outputs for each model, lowest to highest values. Linear and Langmuir outputs are using the reduced data sets, and Time-Dependent outputs are combined high and low (H & L) [DOC] values using the full data sets (with peaks).

Analytical/Linear		**Langmuir**		**Time-Dependent**	
Scenario	RMSE	Scenario	RMSE	Scenario	RMSE
PIS	0.1296	WMS	0.1034	PIS	0.0508
WIS	0.1316	PMS	0.1136	WIS	0.0520
WCS	0.1363	PCS	0.1209	PIF	0.0560
WCF	0.1862	WIS	0.1230	WIF	0.0693
PCS	0.2374	WMF	0.1255	PMS	0.0709
PMS	0.2627	WIF	0.1292	PMF	0.0907
WMS	0.2641	JBS	0.1552	WMF	0.1092
JBF	0.3192	PIS	0.1571	WMS	0.1177
TAS	0.3706	PMF	0.1648	PCS	0.1200
PIF	0.3967	TAF	0.2056	JBS	0.1837
WIF	0.4716	TAS	0.2139	JBF	0.2521
PCF	0.5578	WCF	0.2183	PCF	0.2636
WMF	0.5765	WCS	0.2957	TAS	0.2715
PMF	0.5785	JBF	0.3398	TAF	0.2860
TAF	0.9532	PIF	0.3478	WCF	0.6853
JBS	1.3656	PCF	0.4119	WCS	0.7212

Appendix C: Linear Model (Analytical) Fits

Figures C.1-7 show the remaining *Linear* model fits for all other experiments (bulk kinetic experiments – results present in this manuscript; spatial experiments – results outlined in Morrissette (2021)). Points are the observed DOC mass over time, and the dashed lines are the corresponding model outputs. The two panels are a) fresh or b) saline initial conditions, and the colors represent either high [DOC] (pink) or low [DOC] (red) initial conditions.

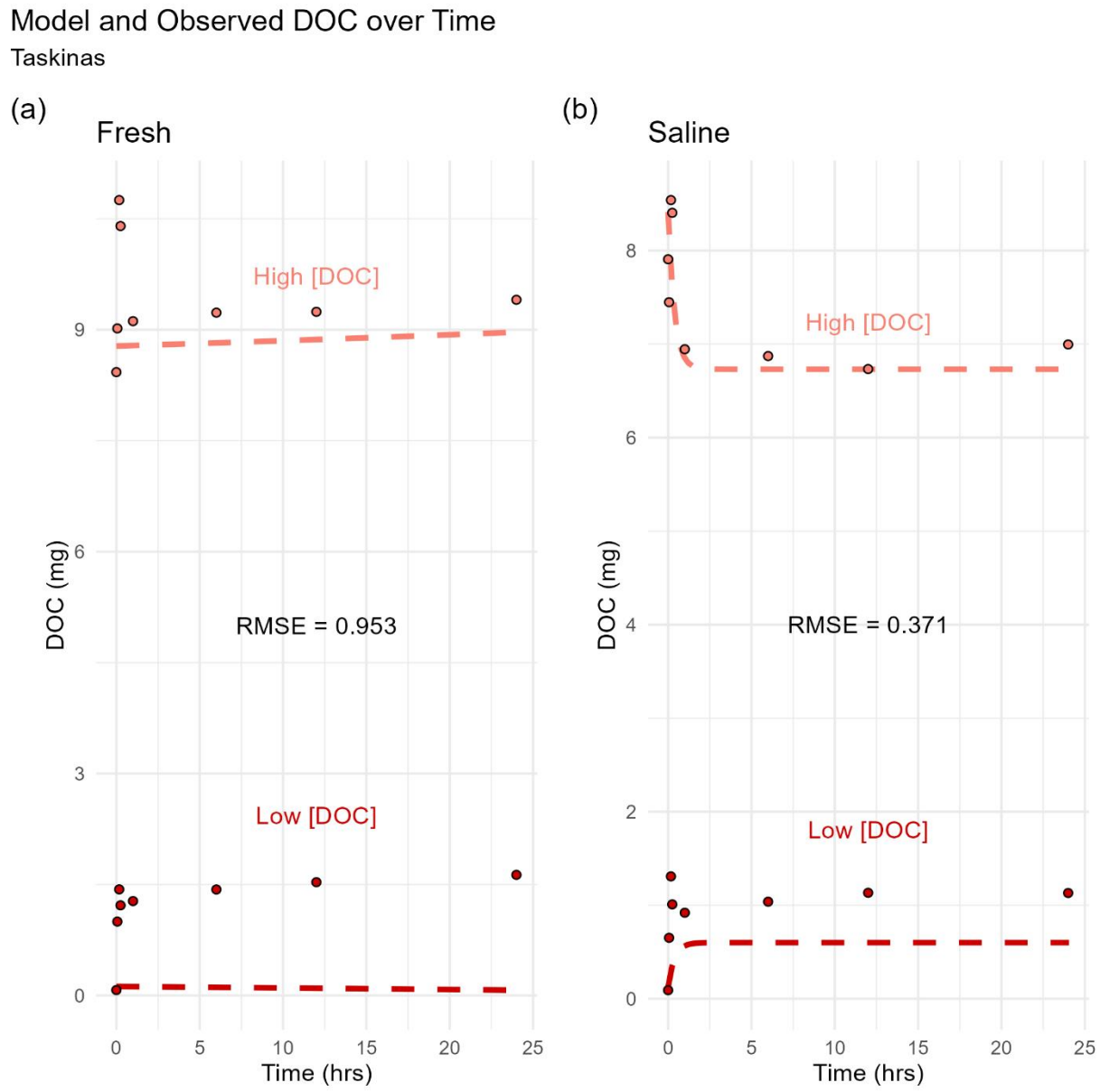

Figure C.1. Taskinas Creek, bulk kinetic experiments.

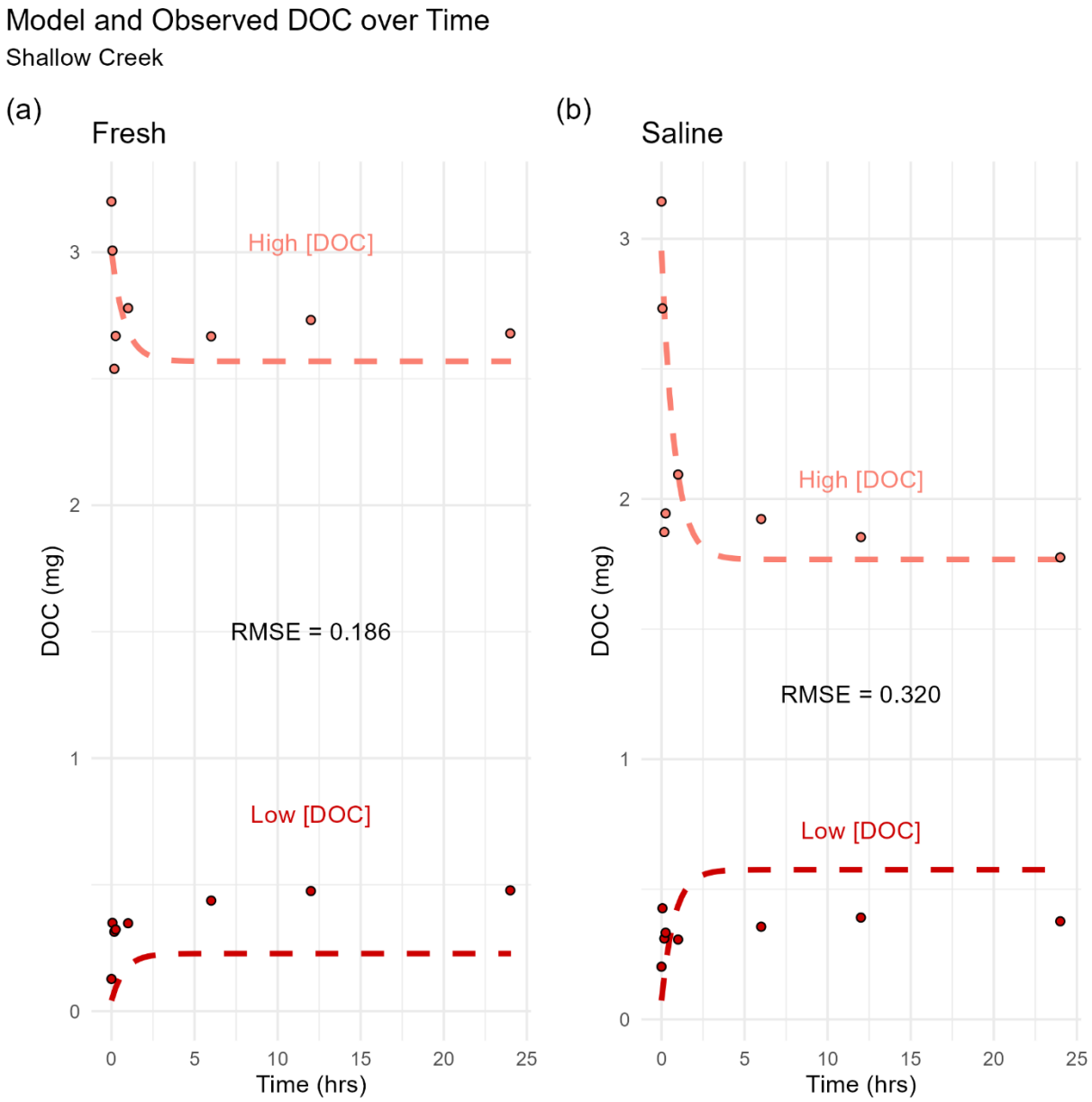

Figure C.2. Shallow Creek Edge, spatial experiments.

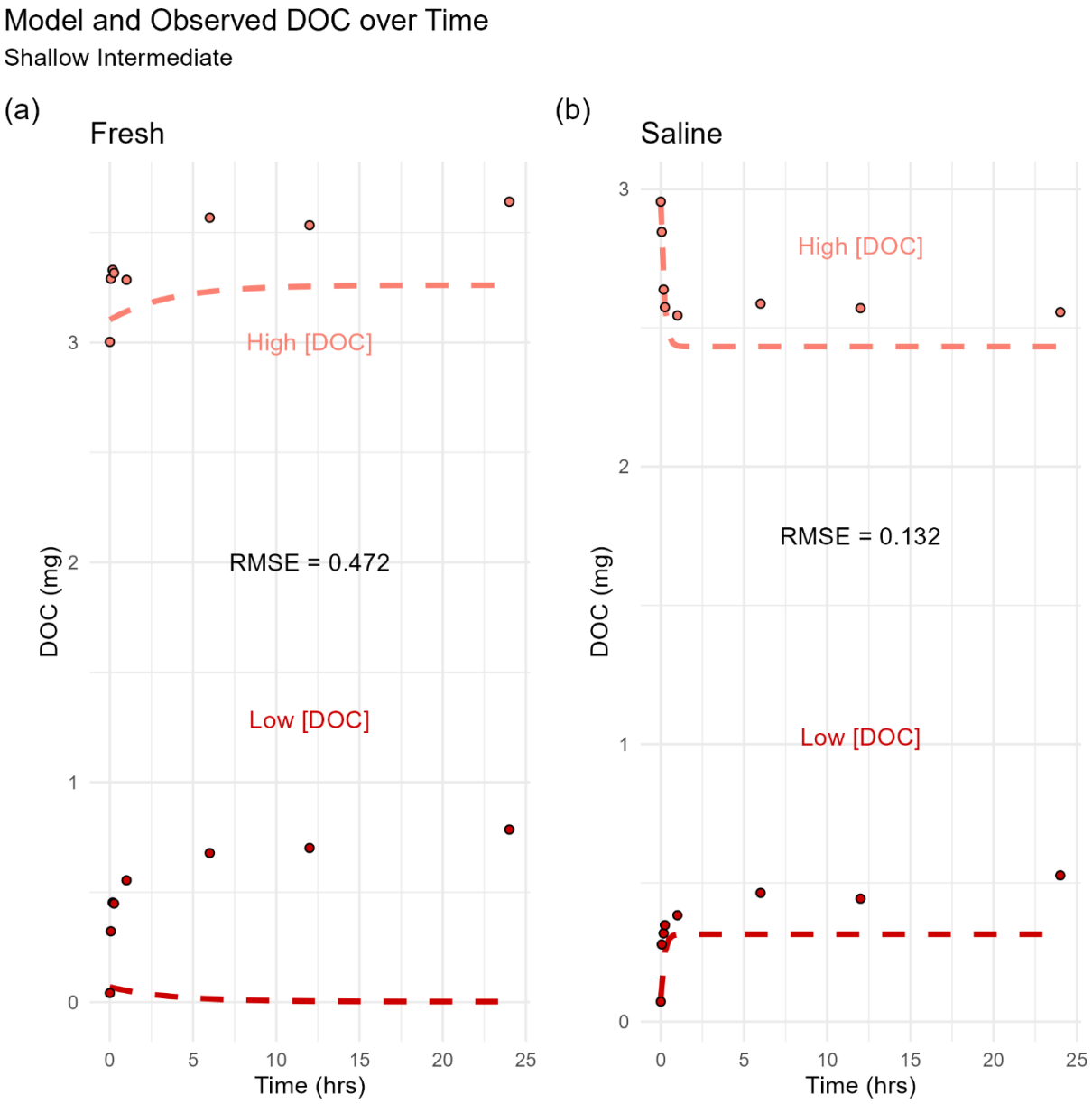

Figure C.3. Shallow Intermediate Plot, spatial experiments.

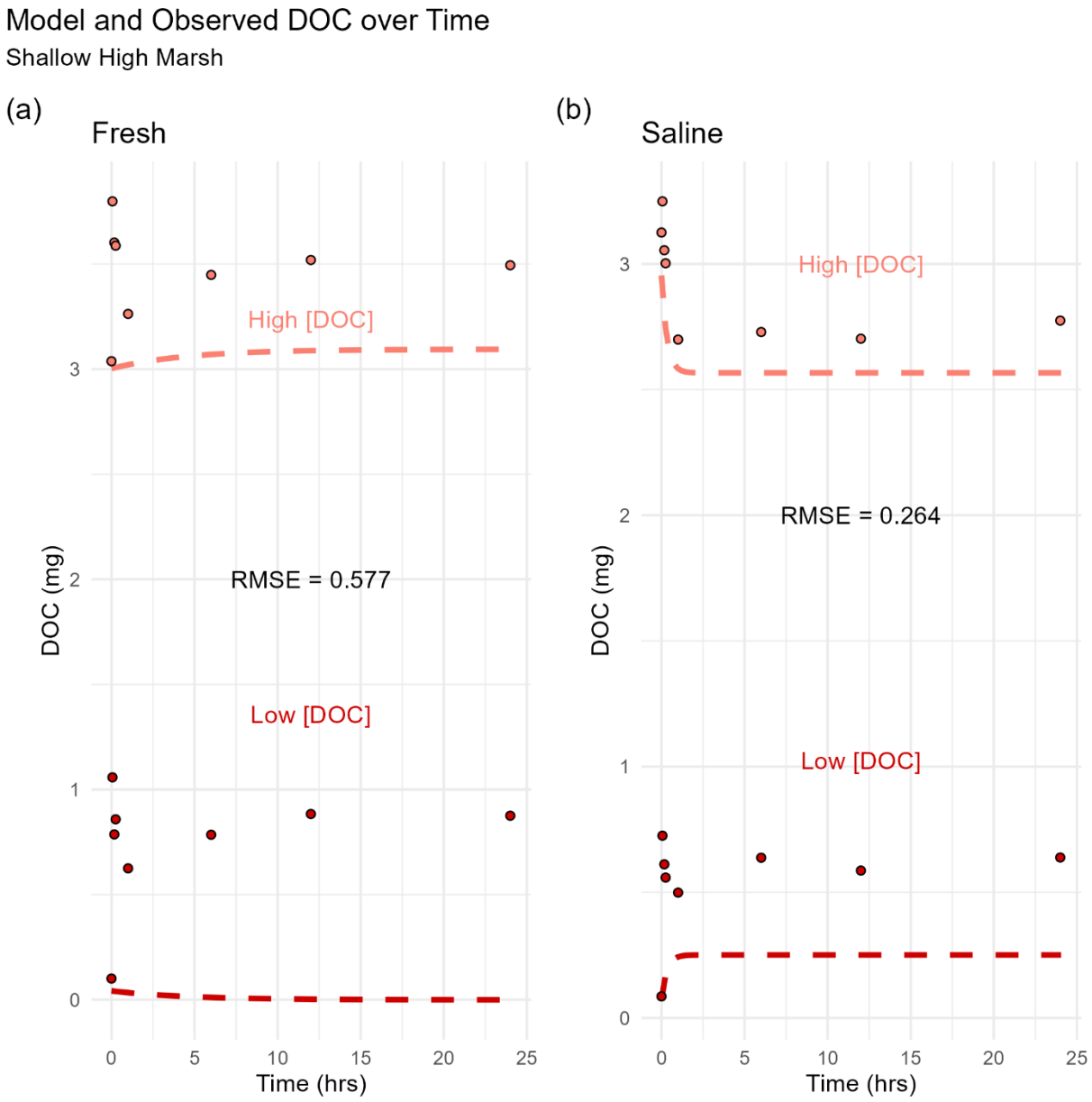

Figure C.4. Shallow High Marsh, spatial experiments.

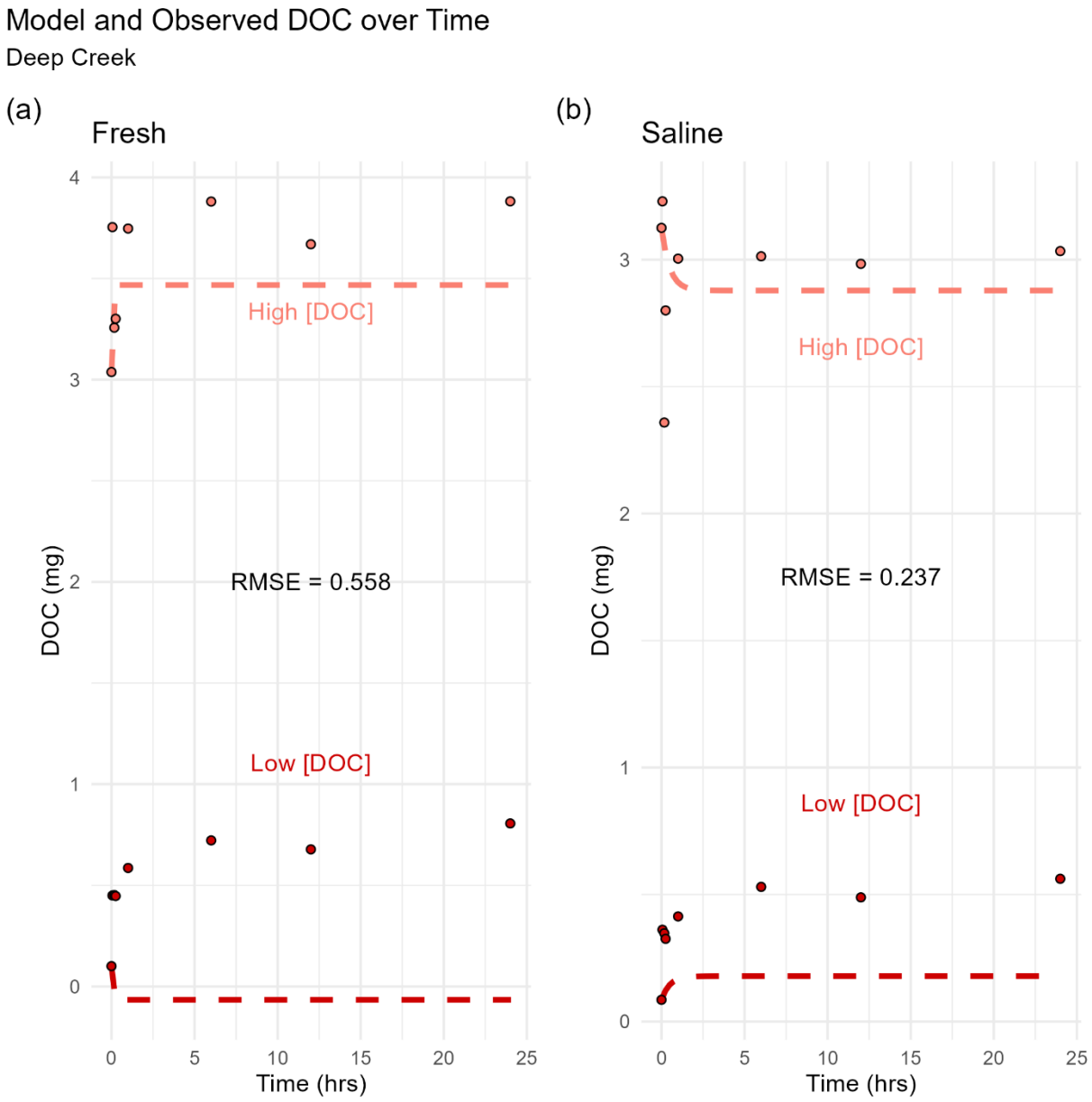

Figure C.5. Deep Creek Edge, spatial experiments.

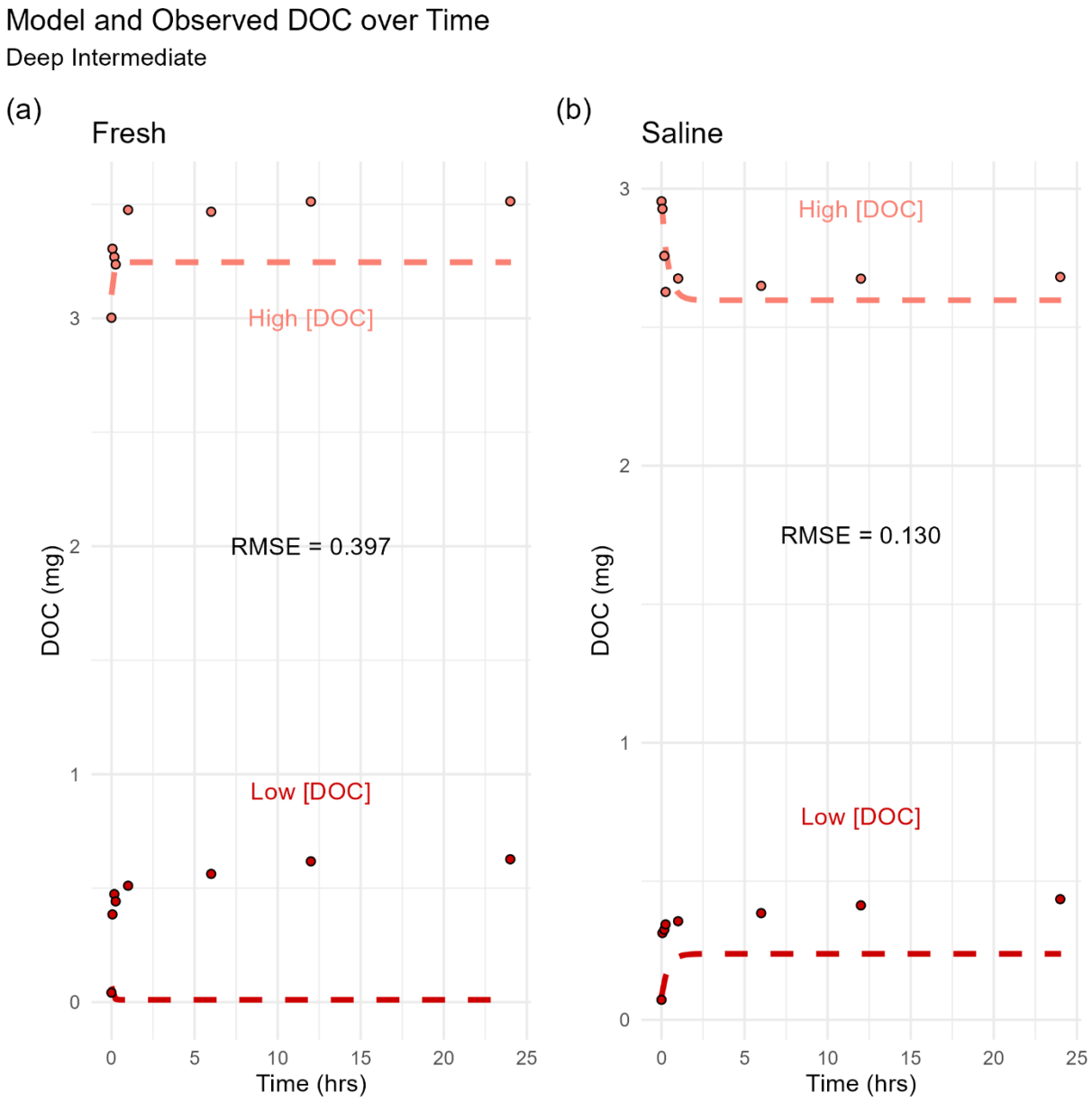

Figure C.6. Deep Intermediate Plot, spatial experiments.

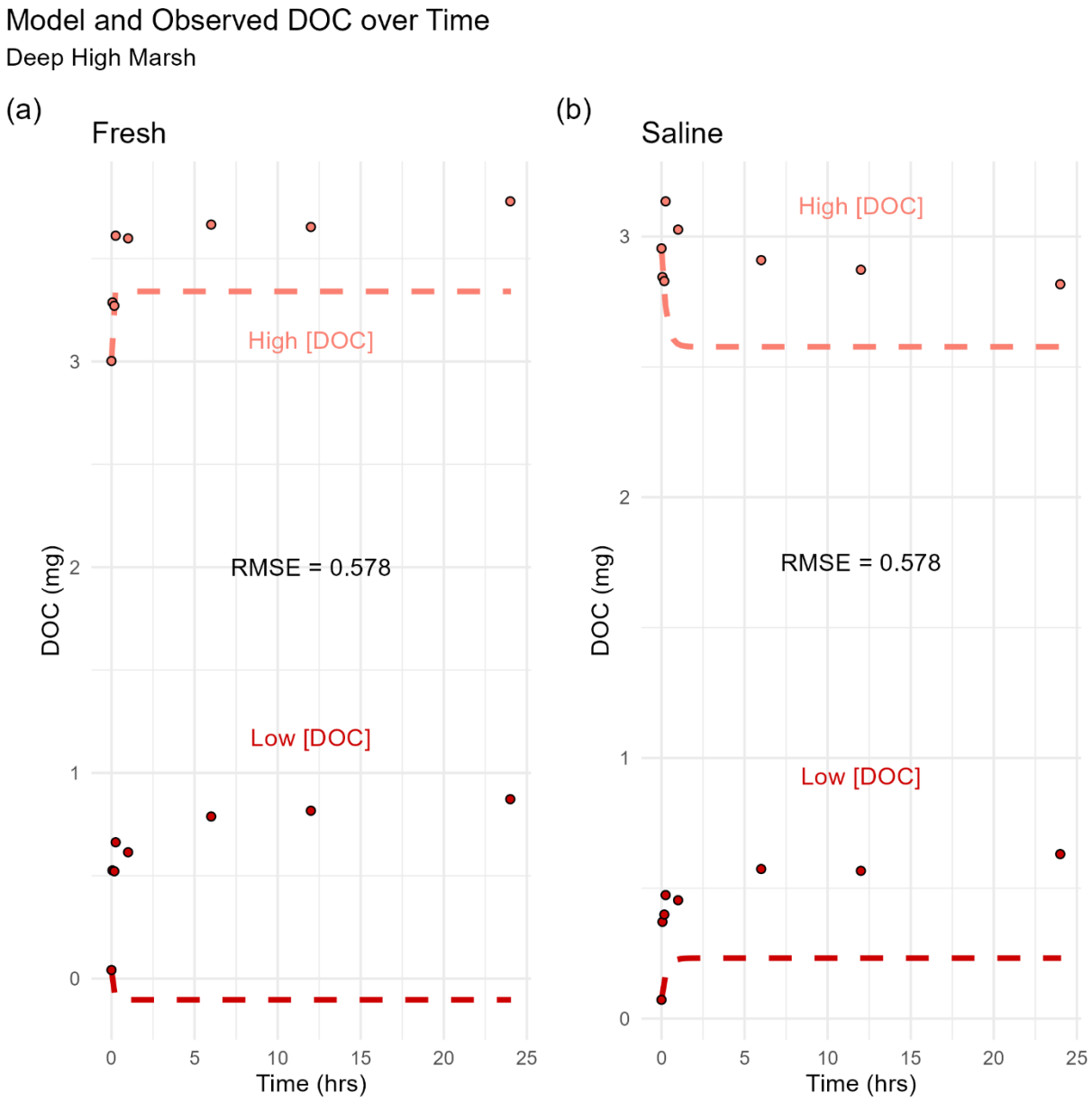

Figure C.7. Deep High Marsh Plot, spatial experiments.

Appendix D: Langmuir Model Fits

Figures D.1-7 show the remaining *Langmuir* model fits for all other experiments (bulk kinetic experiments – results present in this manuscript; spatial experiments – results outlined in Morrissette (2021)). Points are the observed DOC mass over time, and the solid lines are the corresponding model outputs. The two panels are a) fresh or b) saline initial conditions, and the colors represent either high [DOC] (light green) or low [DOC] (dark green) initial conditions.

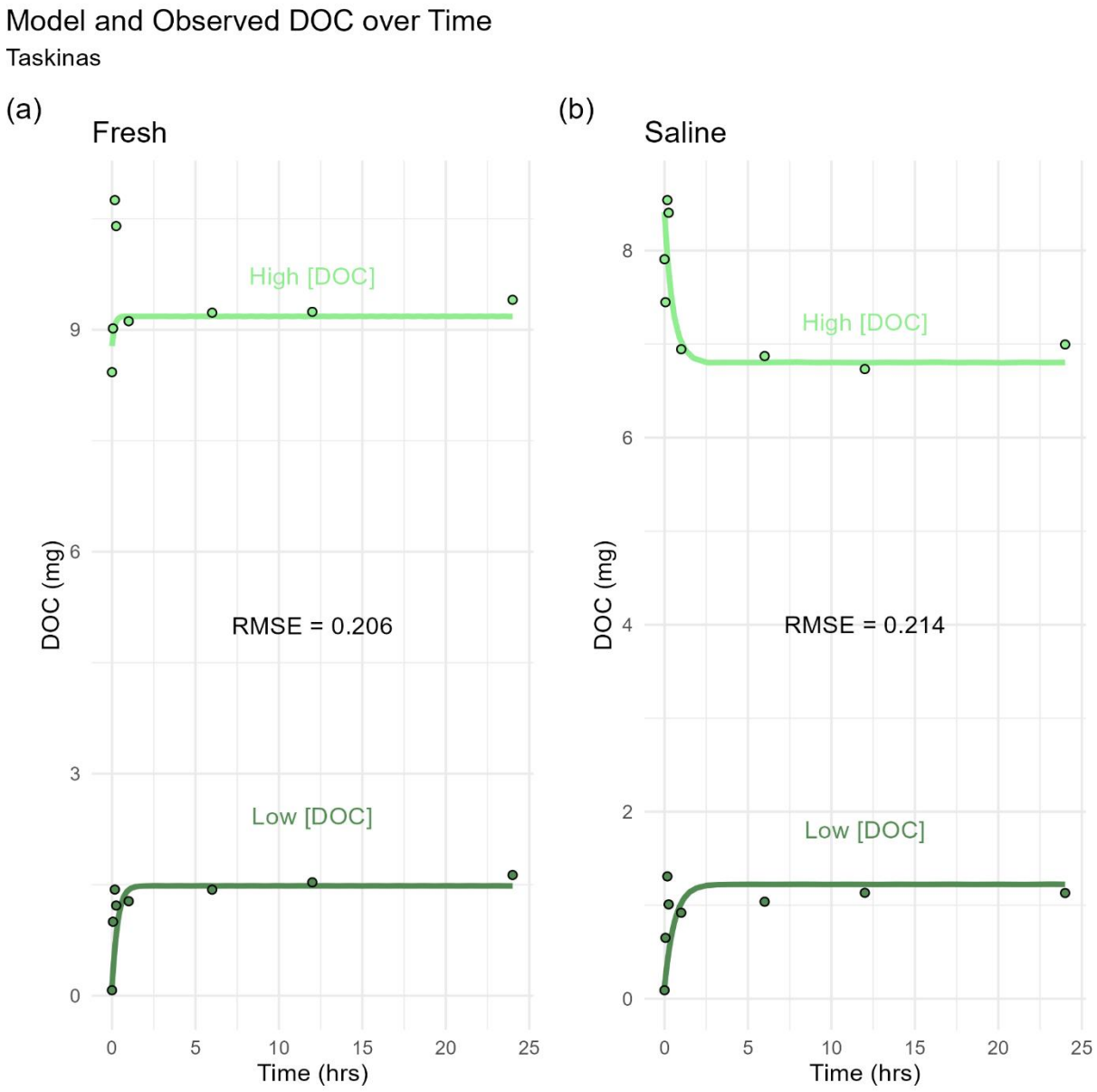

Figure D.1. Taskinas Creek, bulk kinetic experiments.

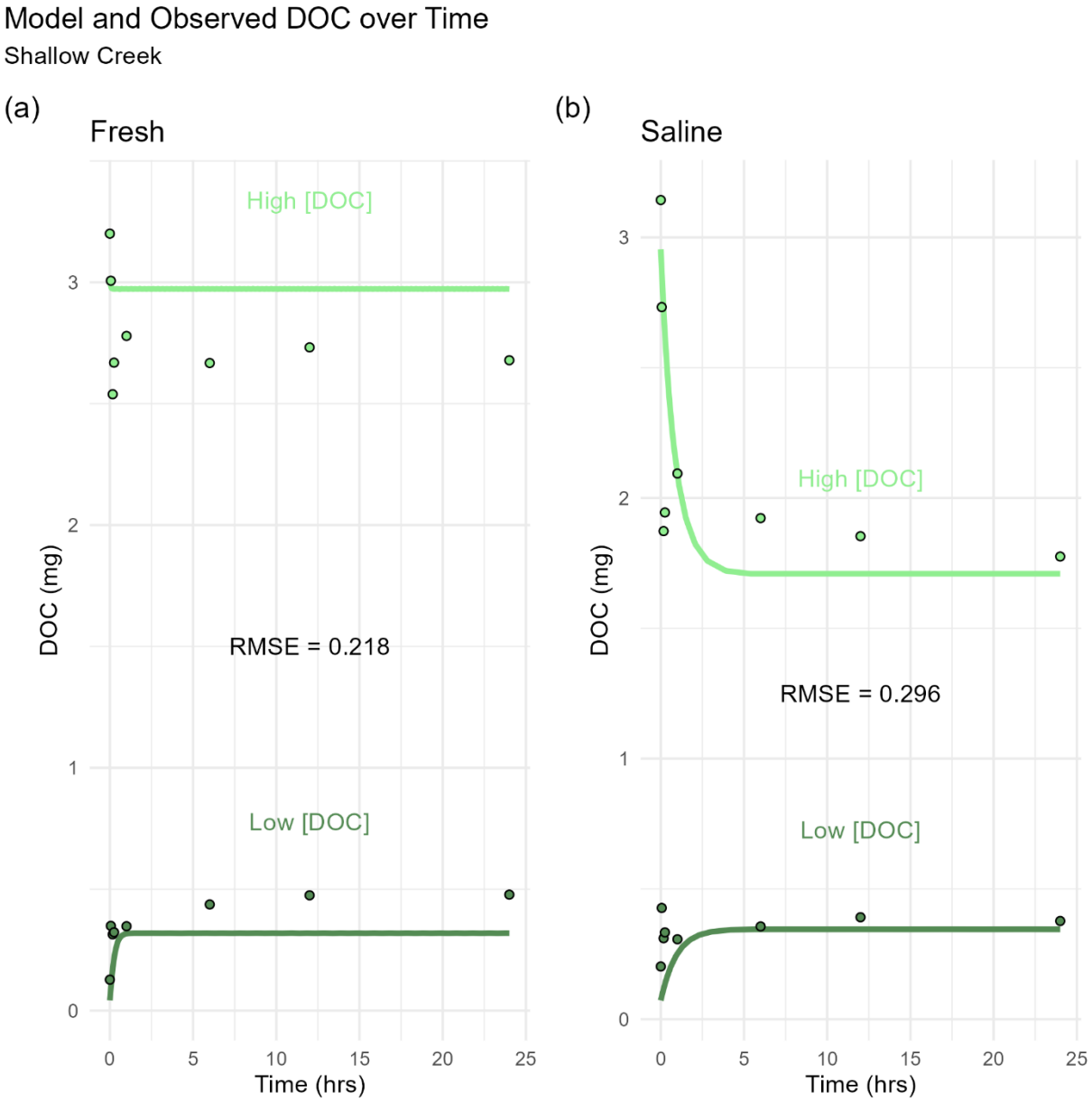

Figure D.2. Shallow Creek Edge, spatial experiments.

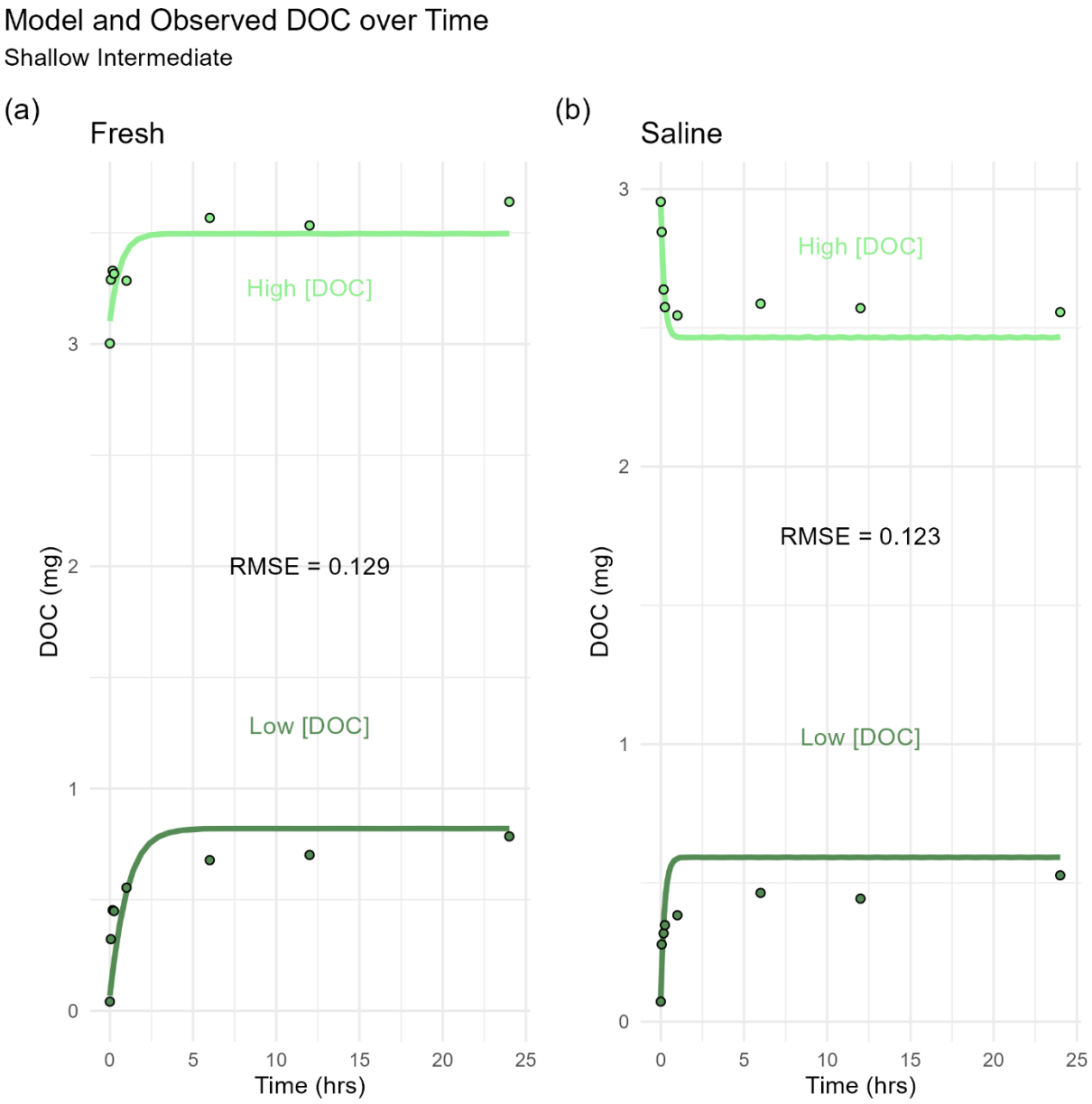

Figure D.3. Shallow Intermediate Plot, spatial experiment.

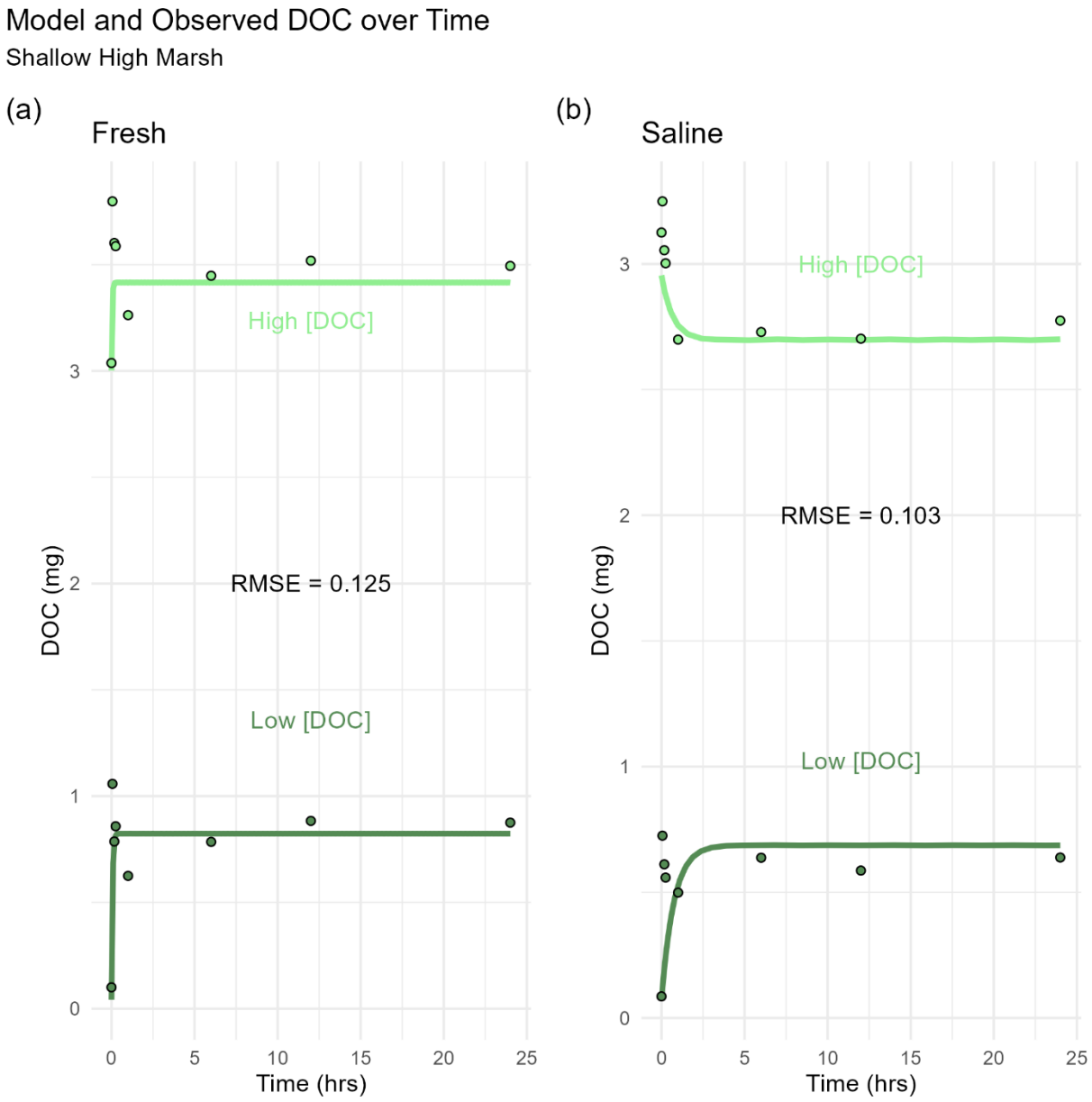

Figure D.4. Shallow High Marsh, spatial experiments.

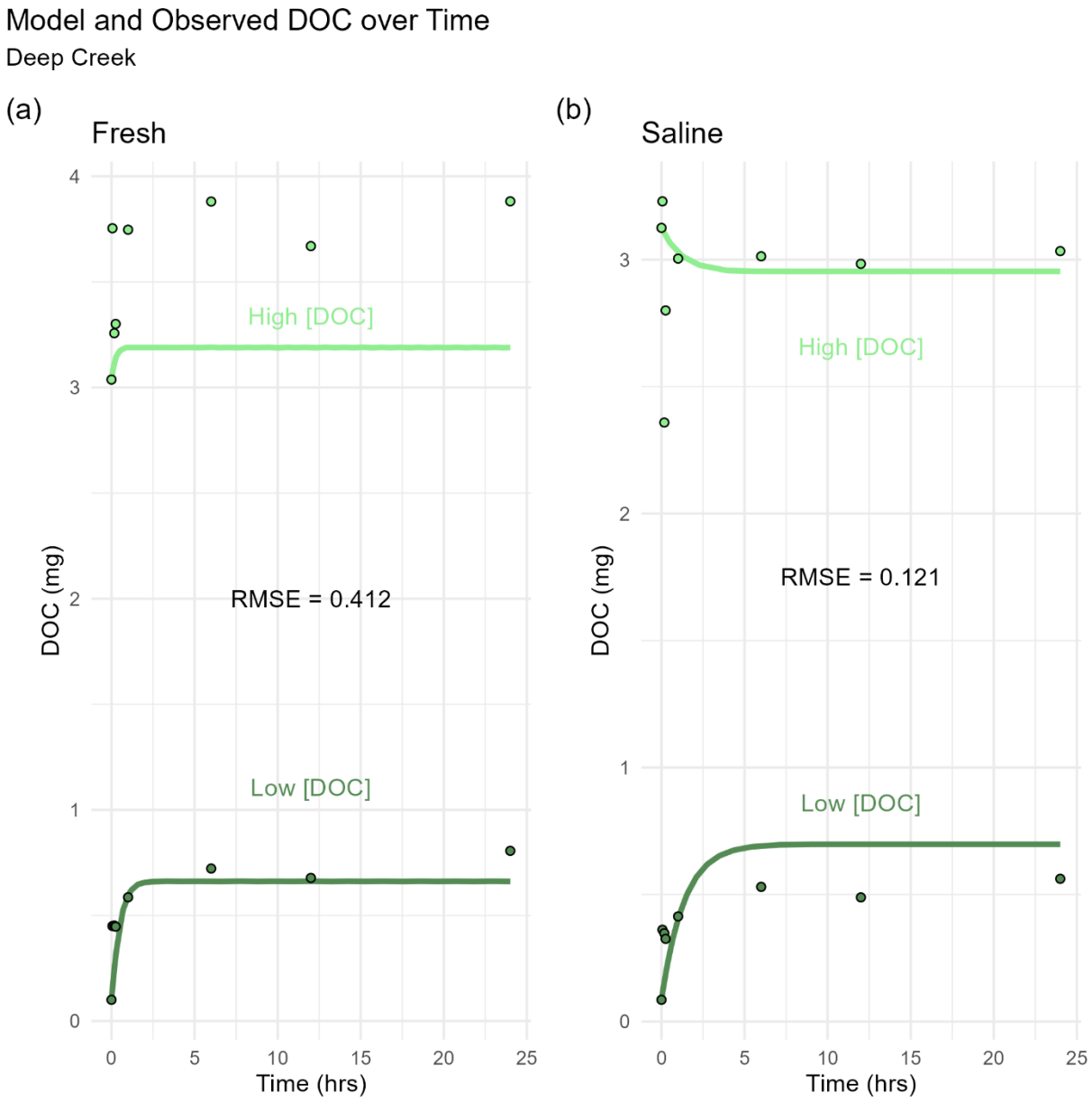

Figure D.5. Deep Creek Edge, spatial experiments.

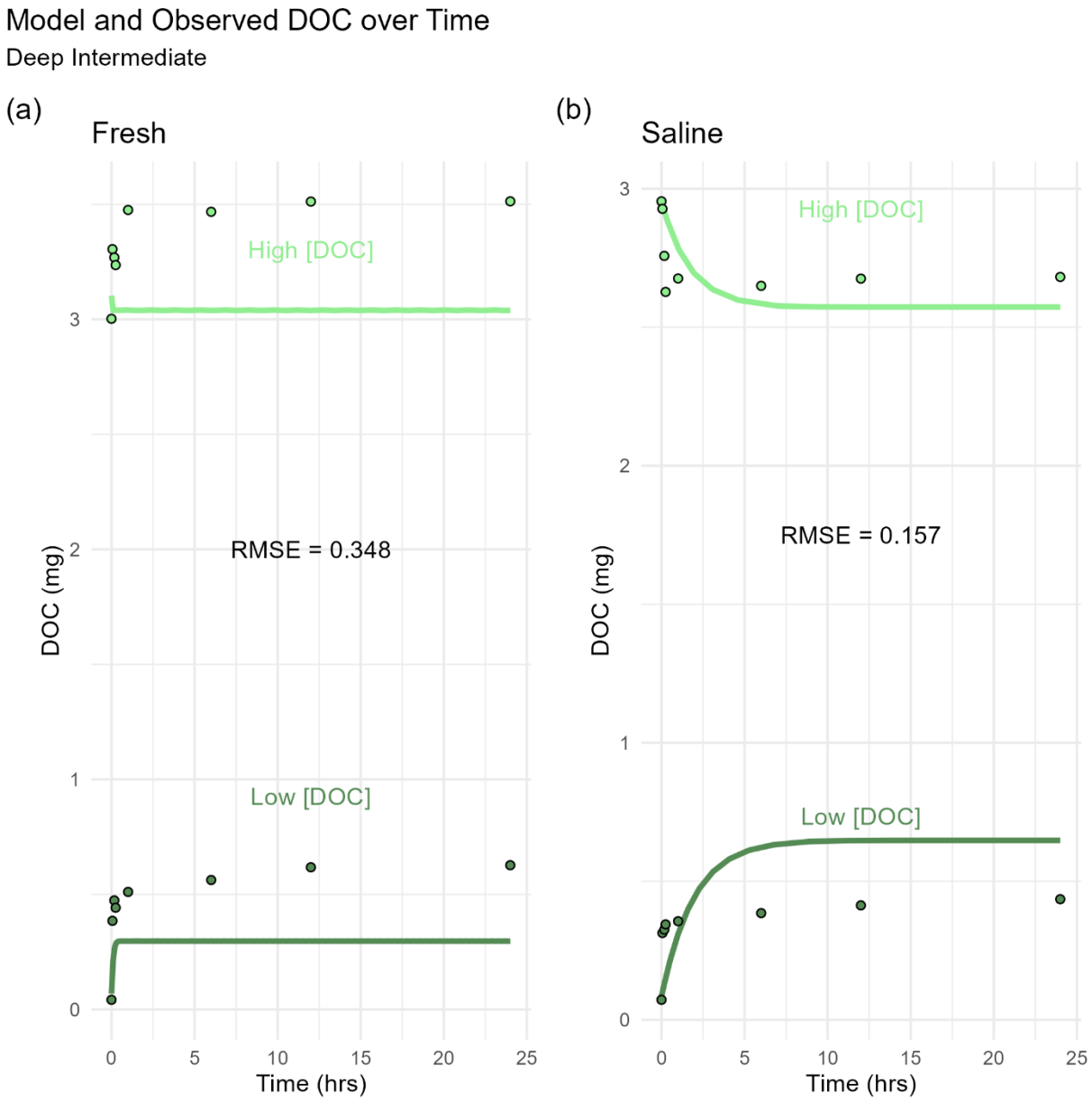

Figure D.6. Deep Intermediate Plot, spatial experiments.

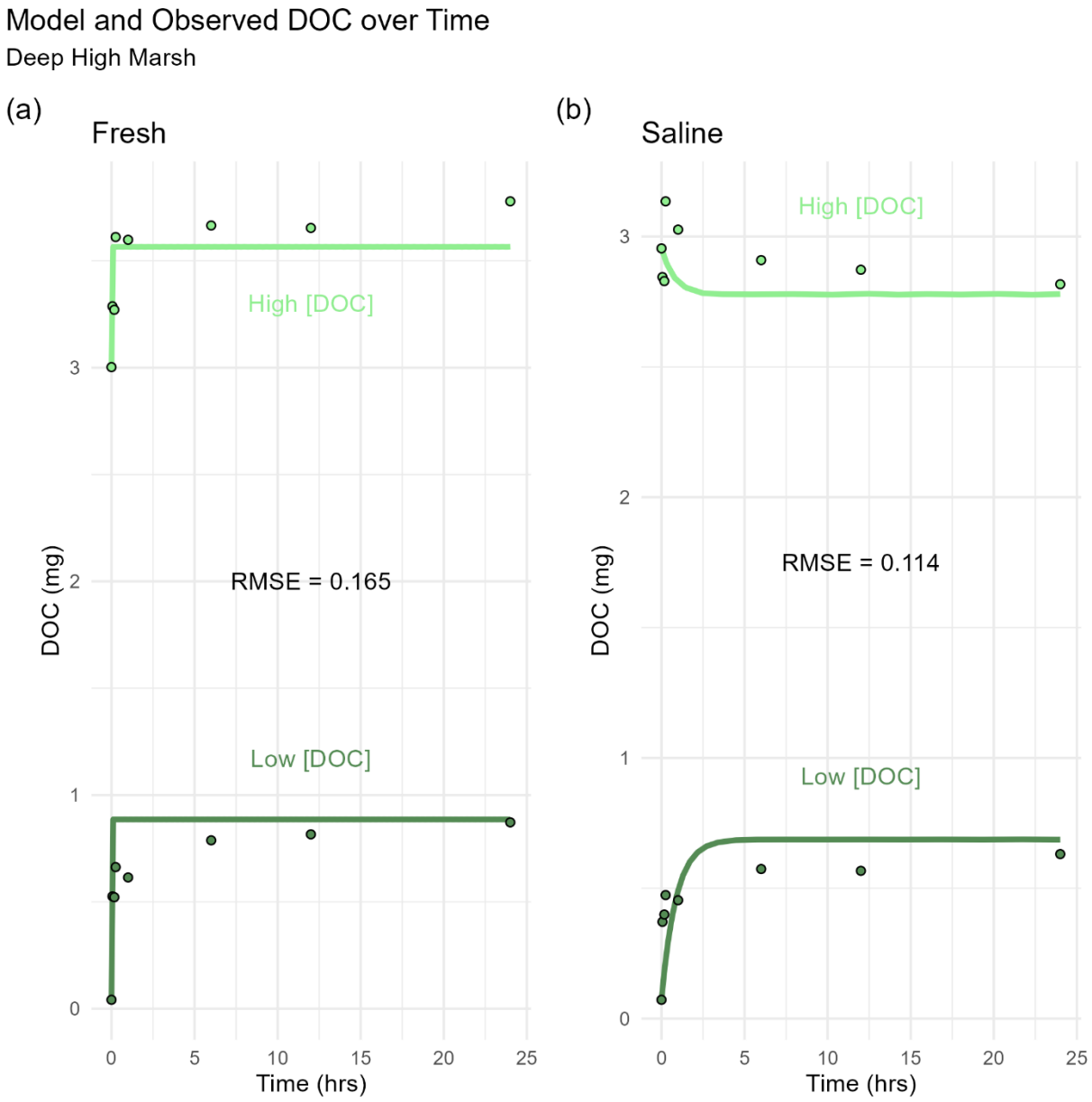

Figure D.7. Deep High Marsh, spatial experiments.

Appendix E: Time-Dependent Model Fits

Figures E.1-8 show the *Time-Dependent* model fits for all other experiments (bulk kinetic experiments – results present in this manuscript; spatial experiments – results outlined in Morrissette (2021)). Points are the observed DOC mass over time, and the dashed lines are the corresponding model outputs. The four panels are the four sets of initial conditions: a) HF; b) HS; c) LF; d) LS.

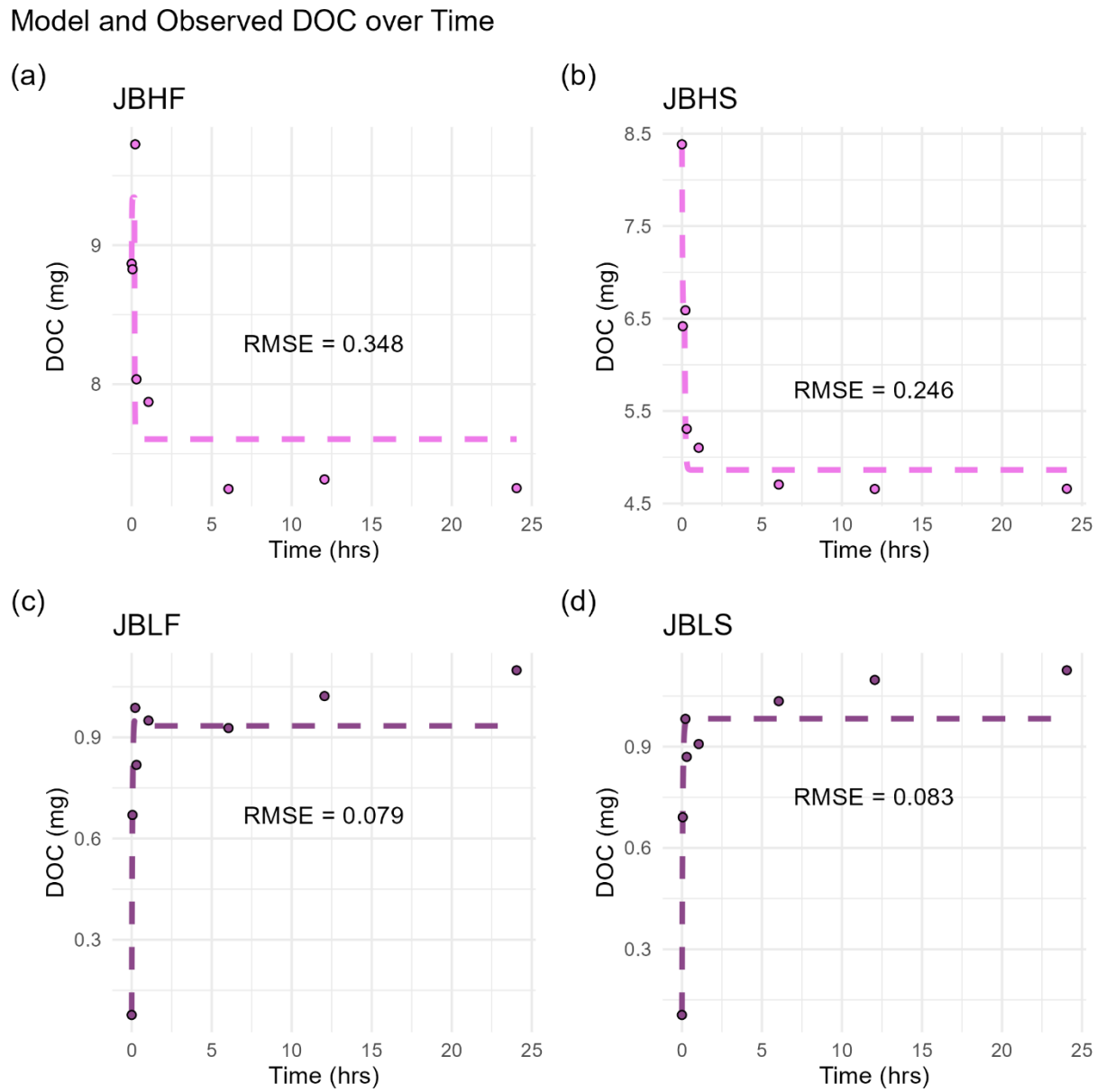

Figure E.1. Jug Bay, bulk kinetic experiments.

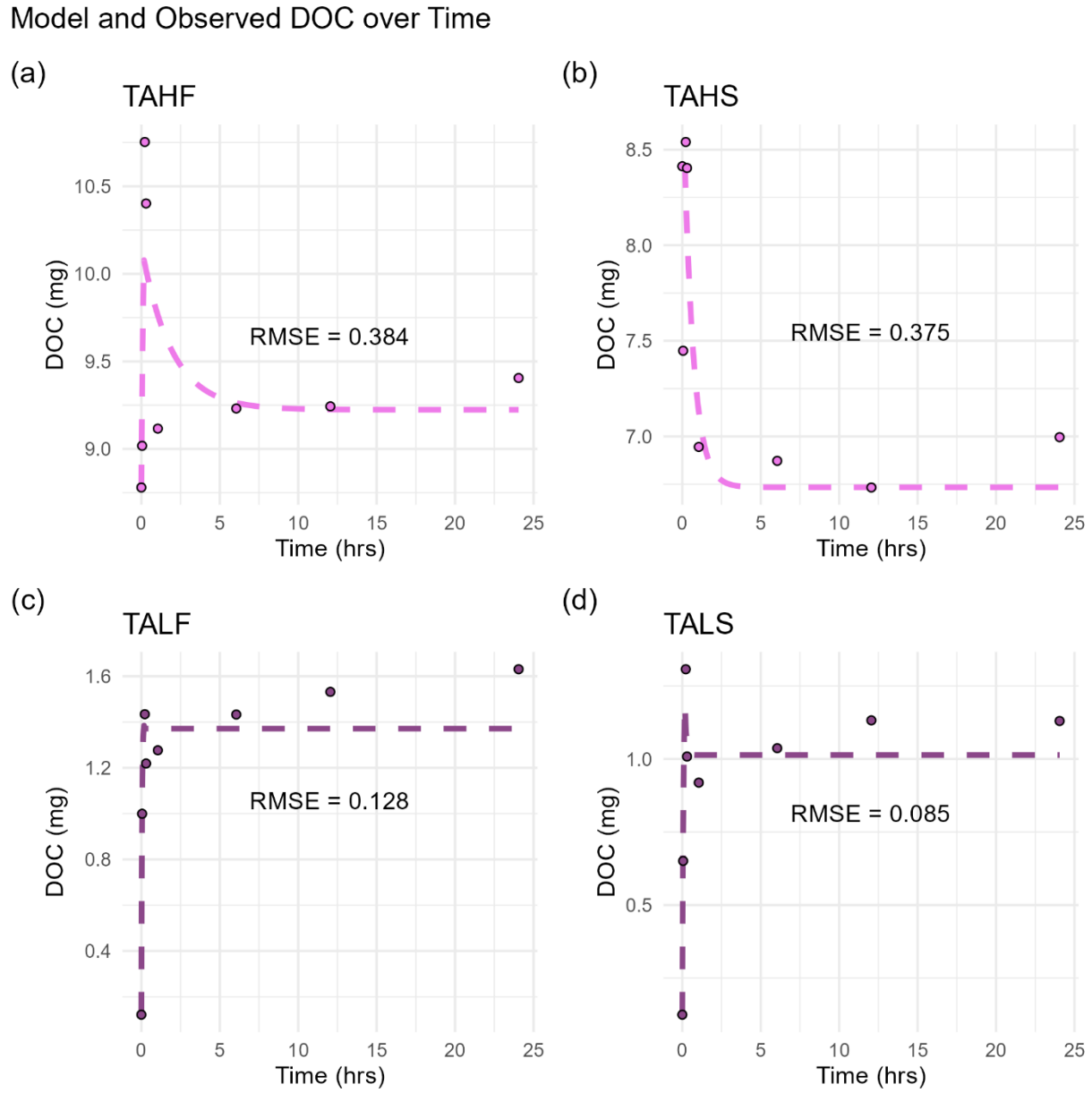

Figure E.2. Taskinas Creek, bulk kinetic experiments.

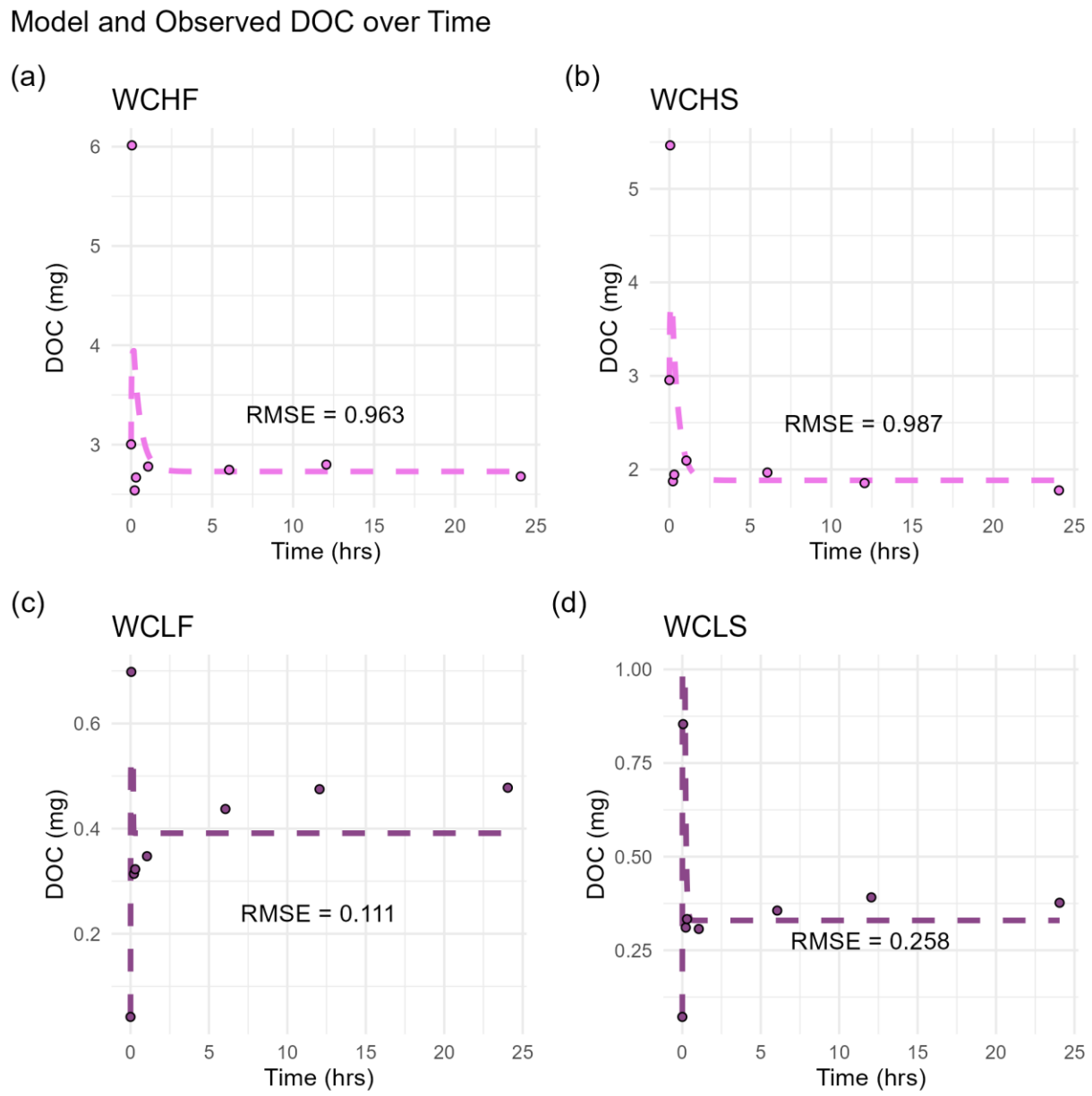

Figure E.3. Shallow Creek Edge, spatial experiments.

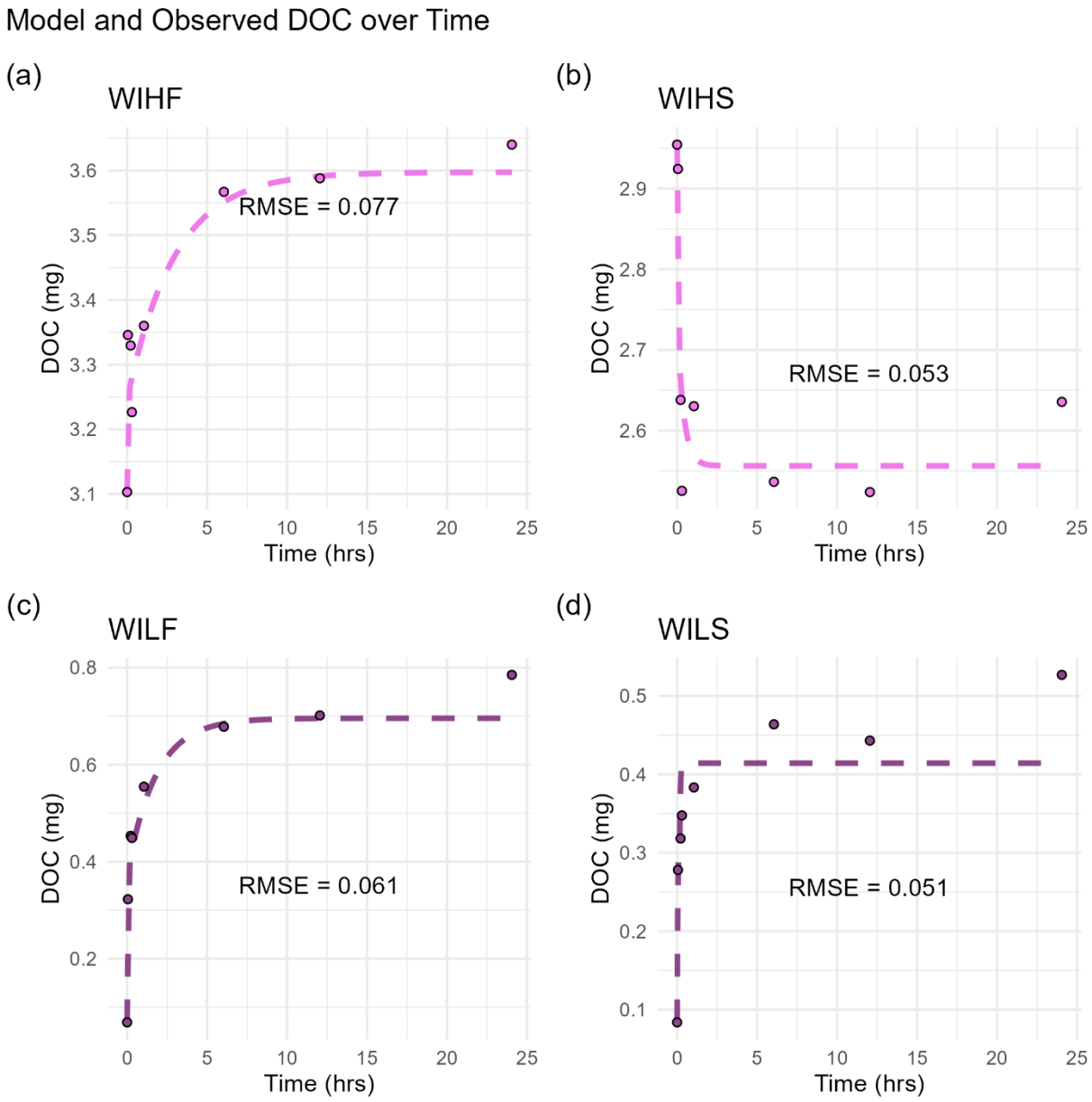

Figure E.4. Shallow Intermediate Plot, spatial experiments.

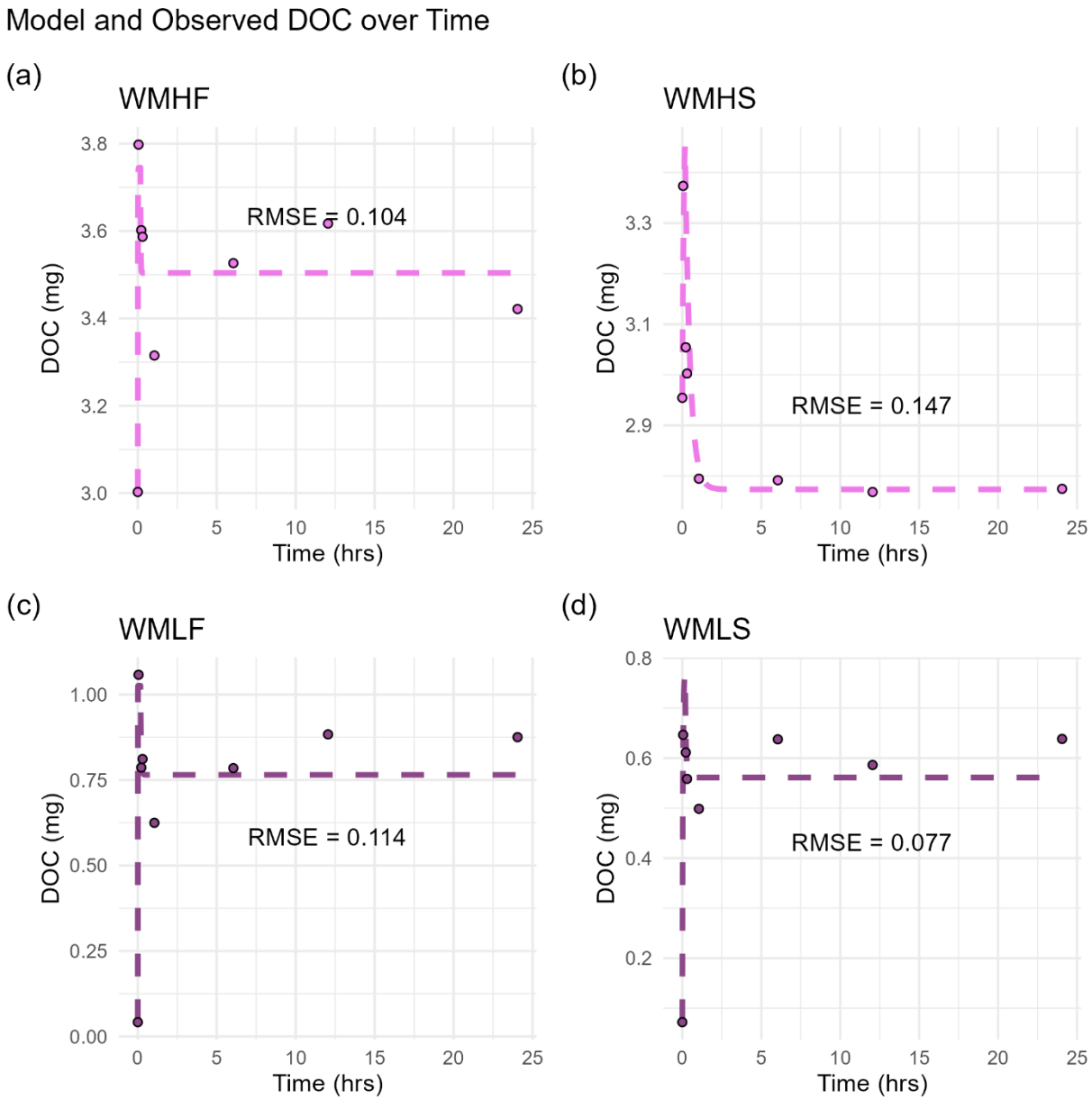

Figure E.5. Shallow High Marsh, spatial experiments.

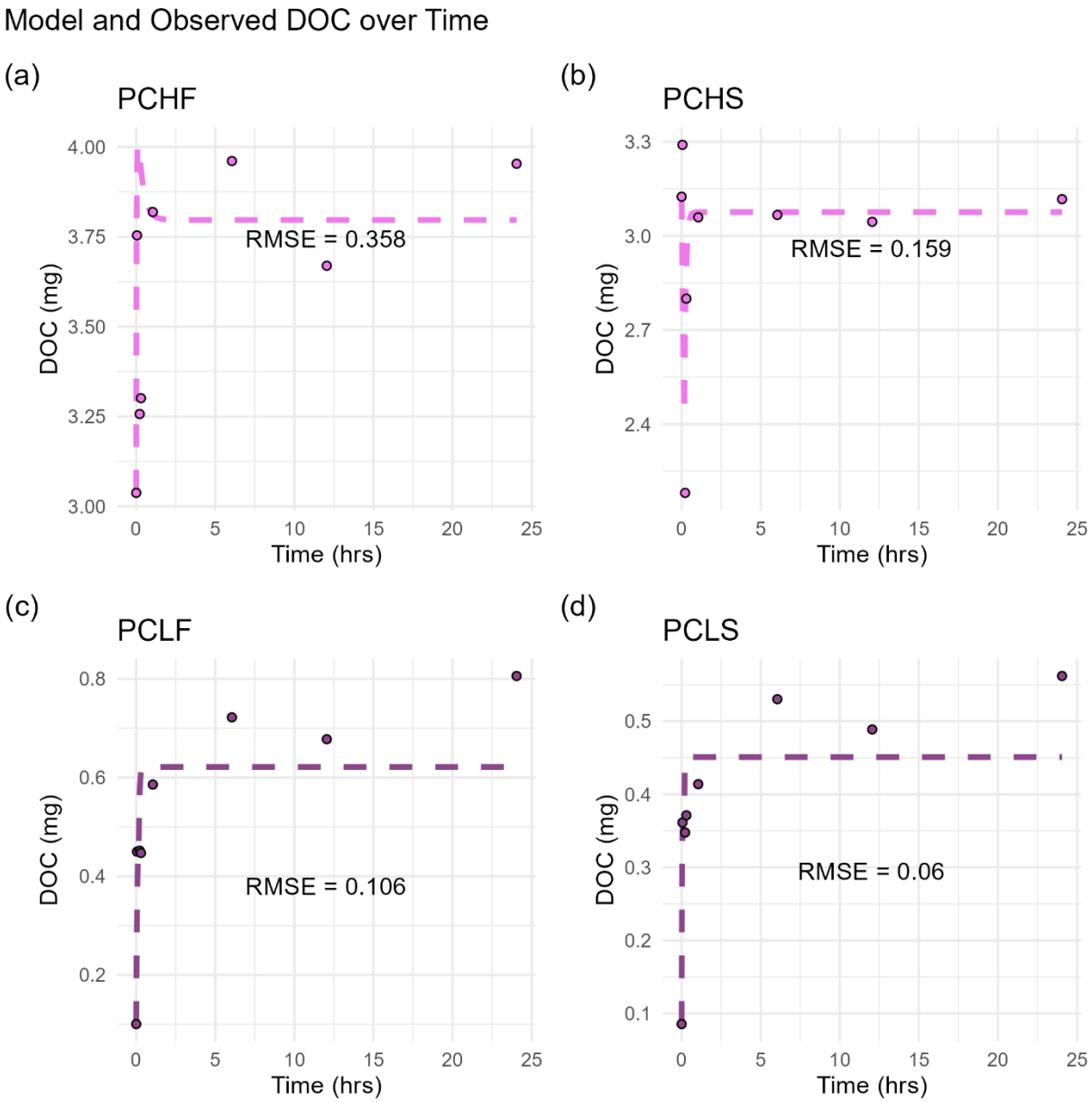

Figure E.6. Deep Creek Edge, spatial experiments.

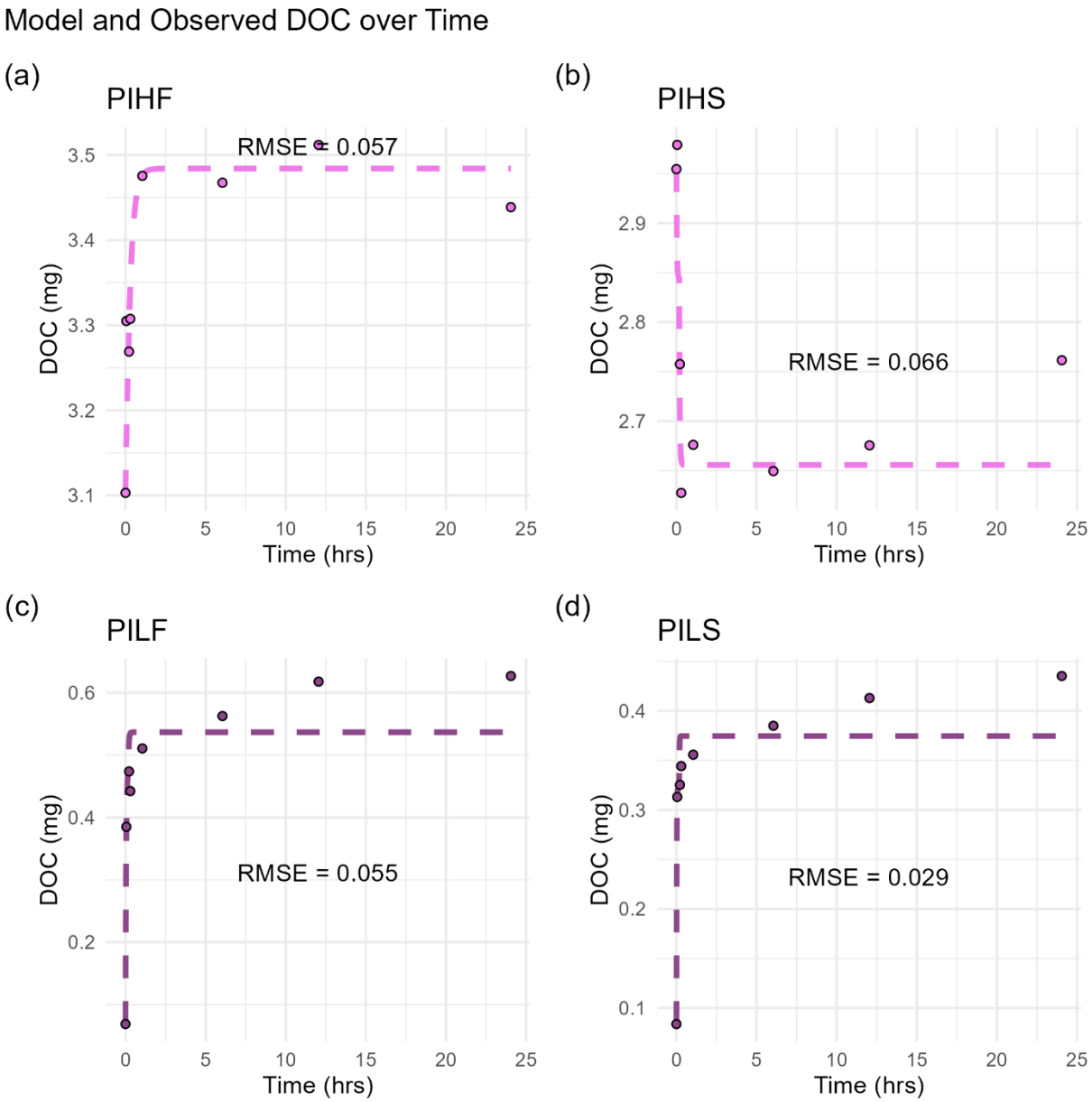

Figure E.7. Deep Intermediate Plot, spatial experiments.

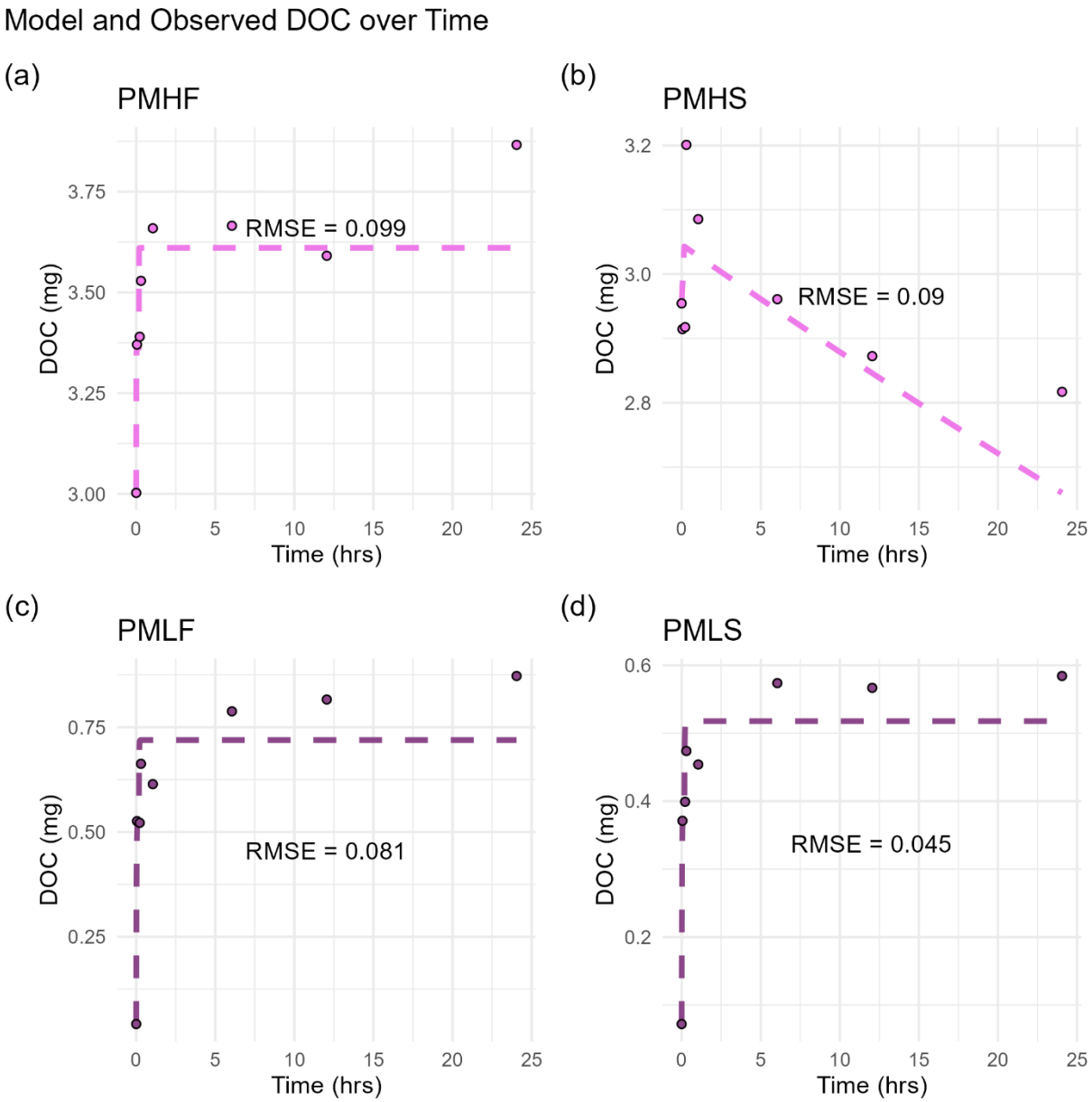

Figure E.8. Deep High Marsh, spatial experiments.

Appendix F: Model Comparisons

Figures F.1-8 show the model comparisons for all other experiments (bulk kinetic experiments – results present in this manuscript; spatial experiments – results outlined in Morrissette (2021)). Black dots are the observed DOC mass over time, while the lines are the corresponding model outputs: *Linear* (orange dot-dashed); *Langmuir* (green solid); *Time-dependent* (purple dashed). The four panels are the four sets of initial conditions: a) HF; b) HS; c) LF; d) LS.

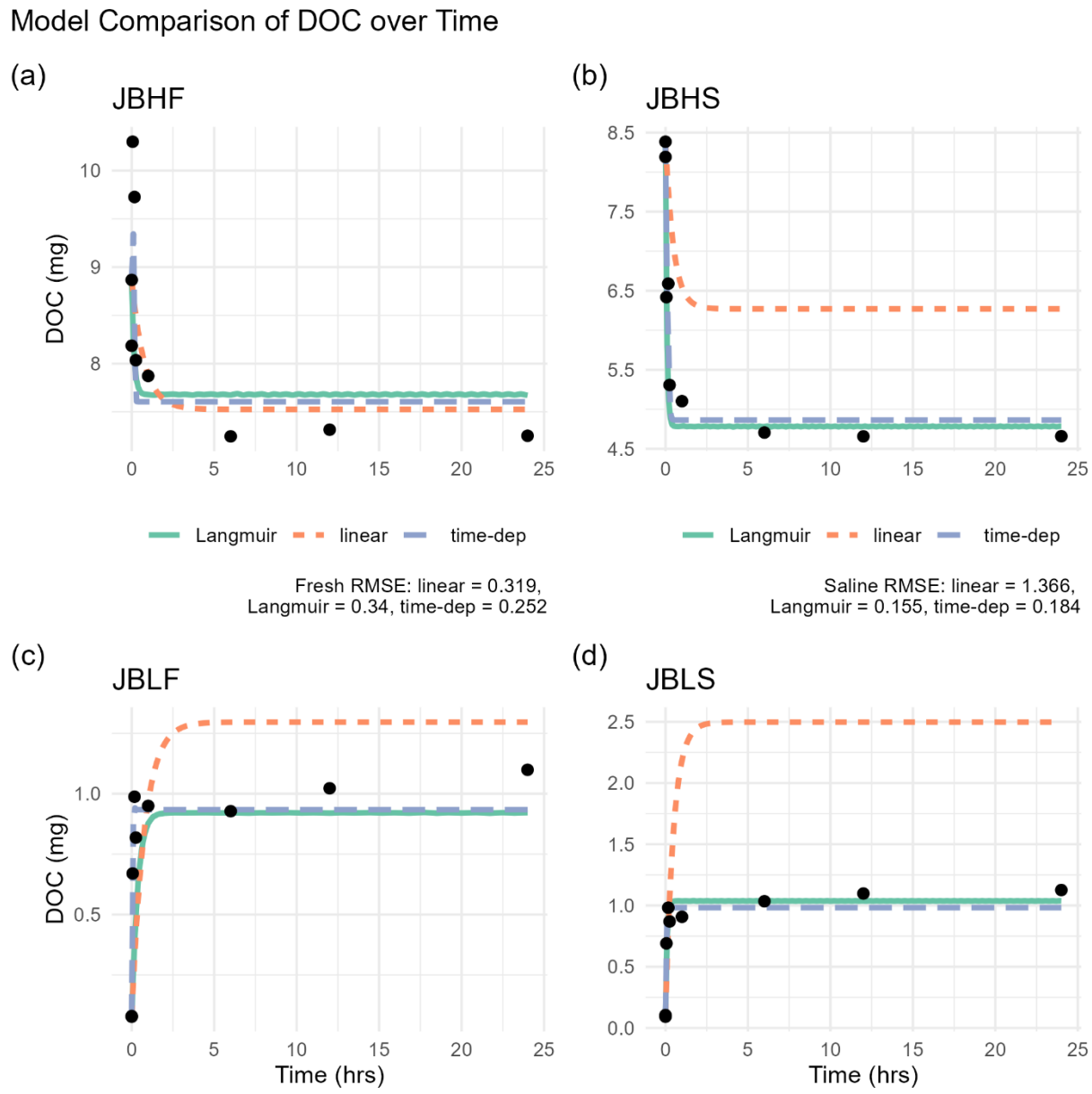

Figure F.1. Jug Bay, bulk kinetic experiments.

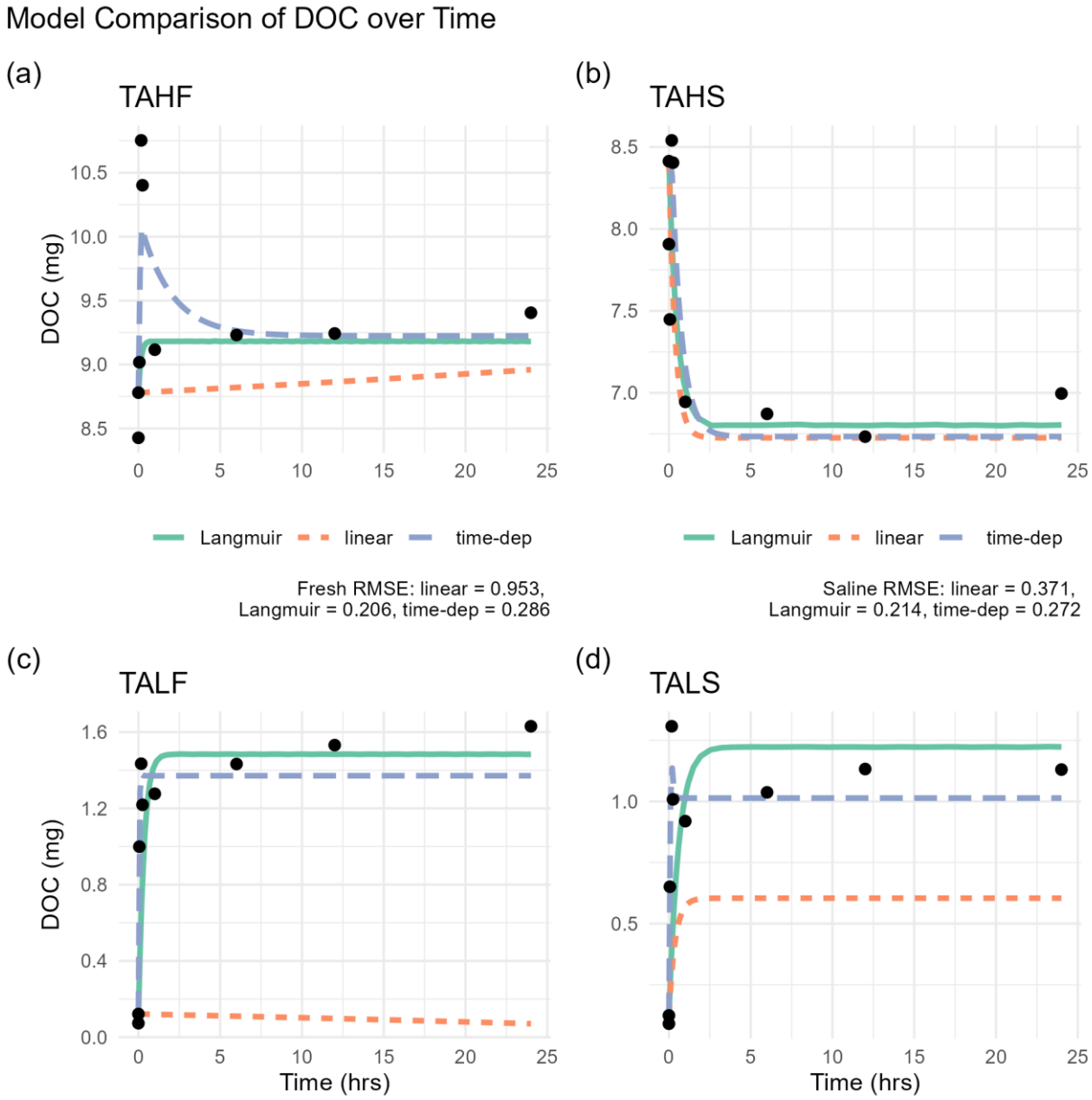

Figure F.2. Taskinas Creek, bulk kinetic experiments.

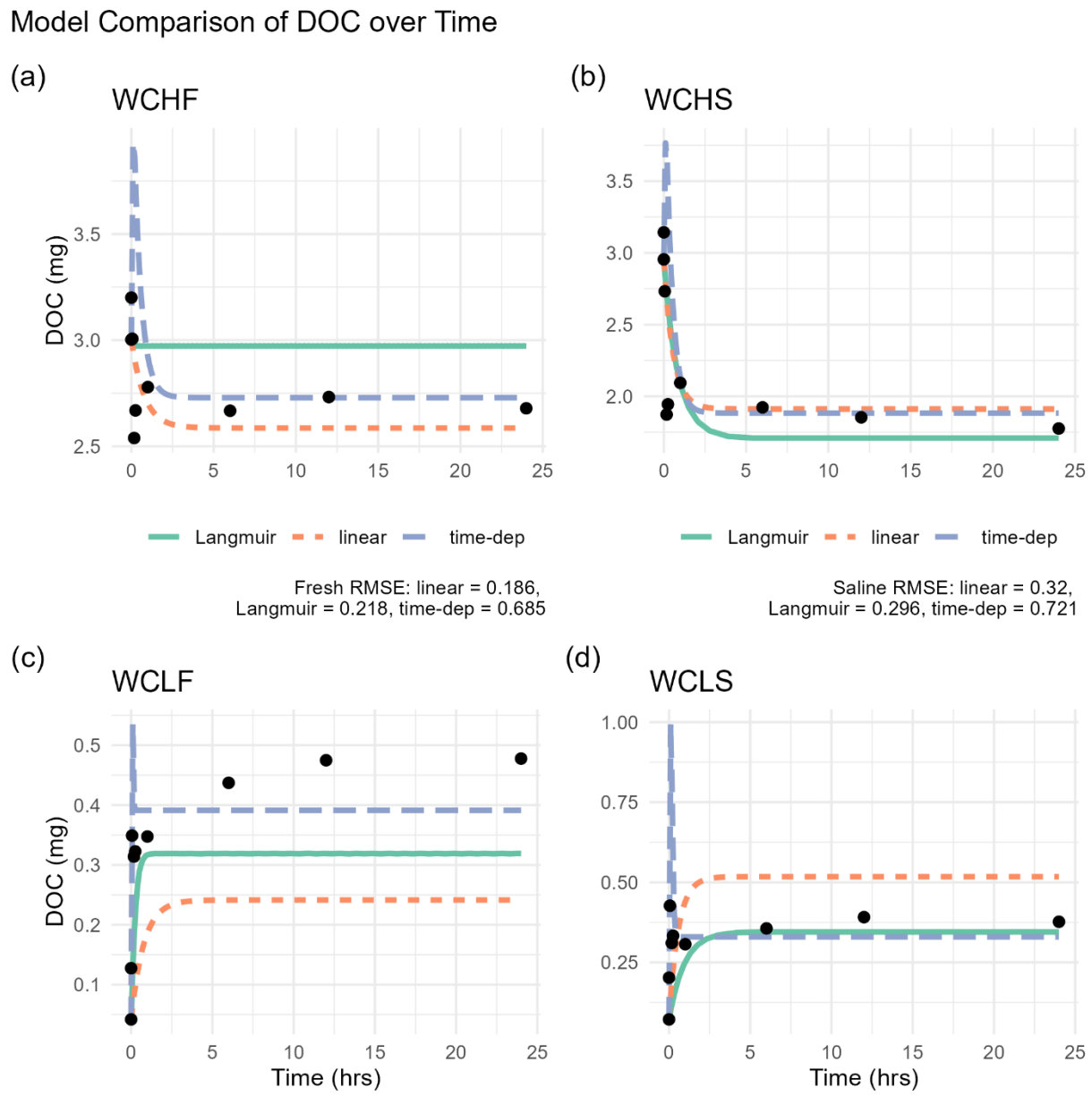

Figure F.3. Shallow Creek Edge, spatial experiments.

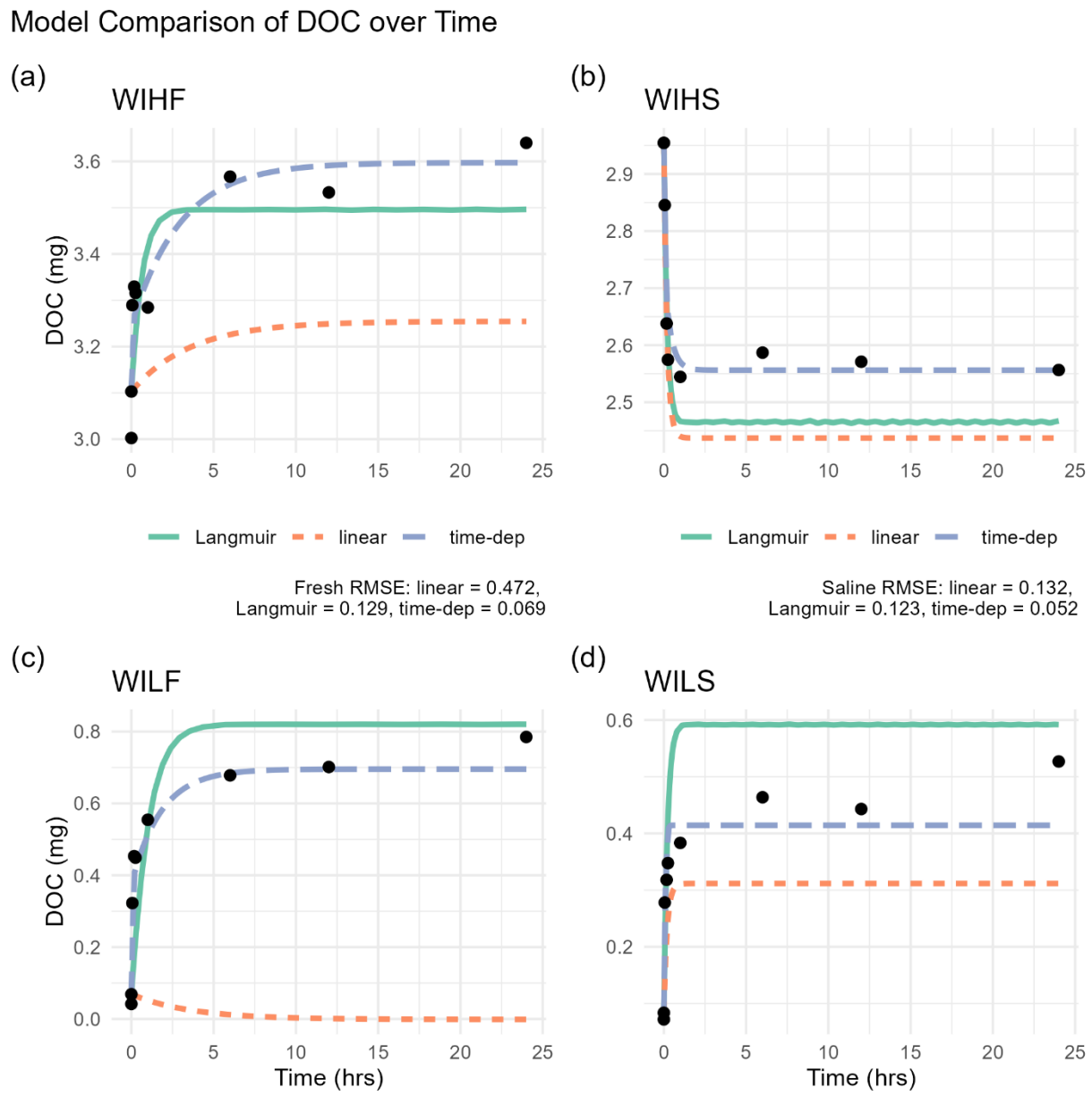

Figure F.4. Shallow Intermediate Plot, spatial experiments.

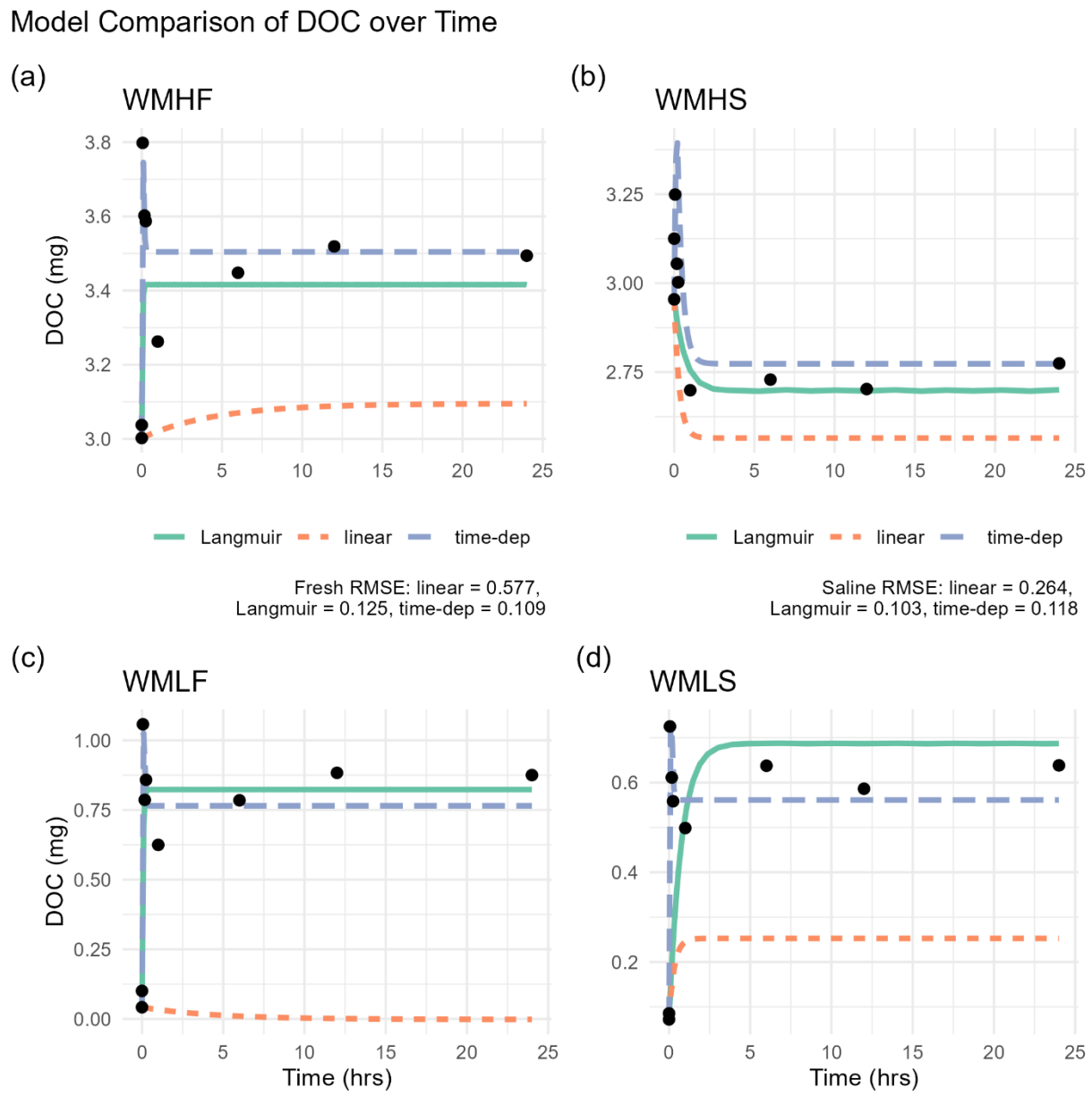

Figure F.5. Shallow High Marsh, spatial experiments.

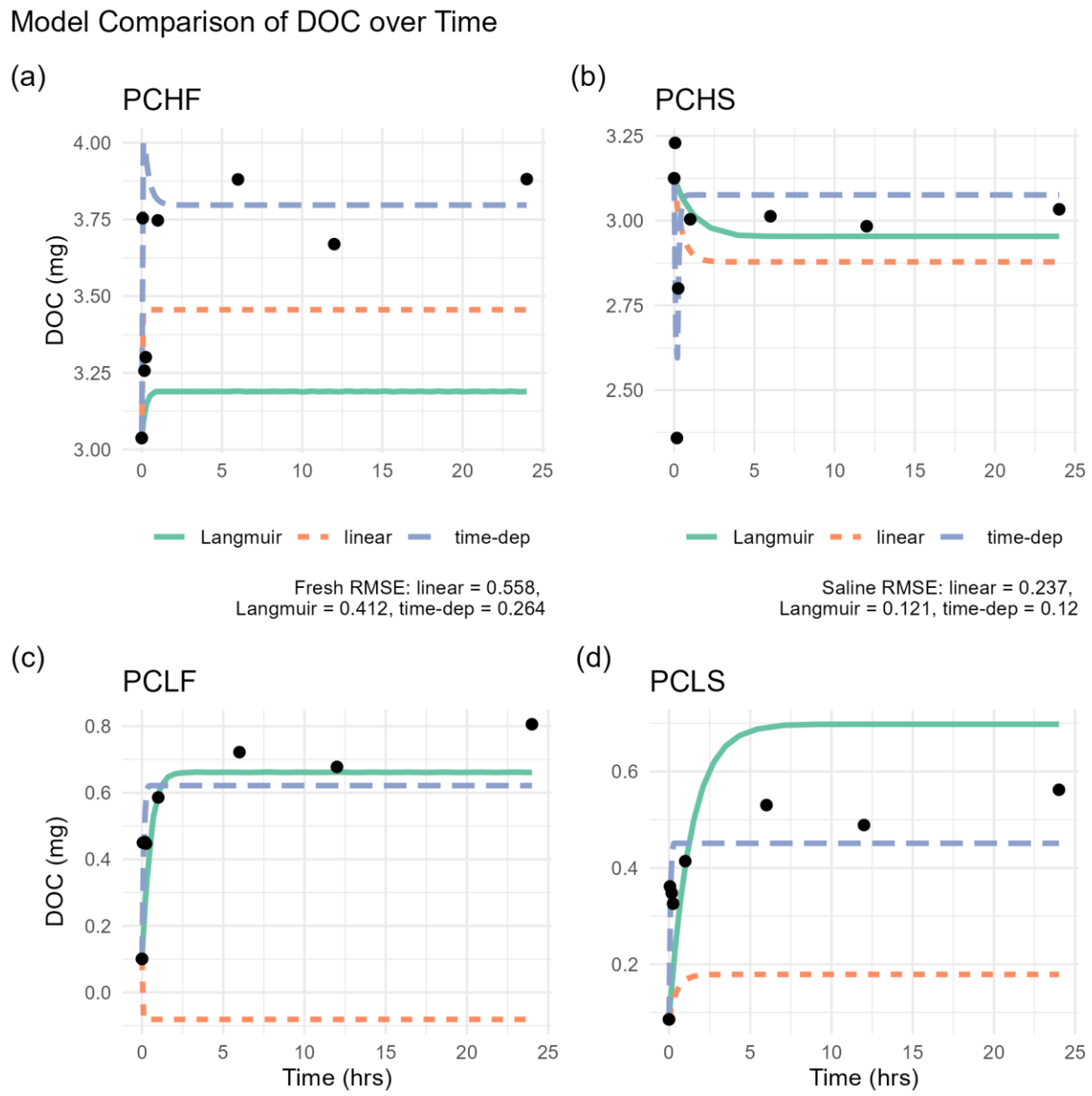

Figure F.6. Deep Creek Edge, spatial experiments.

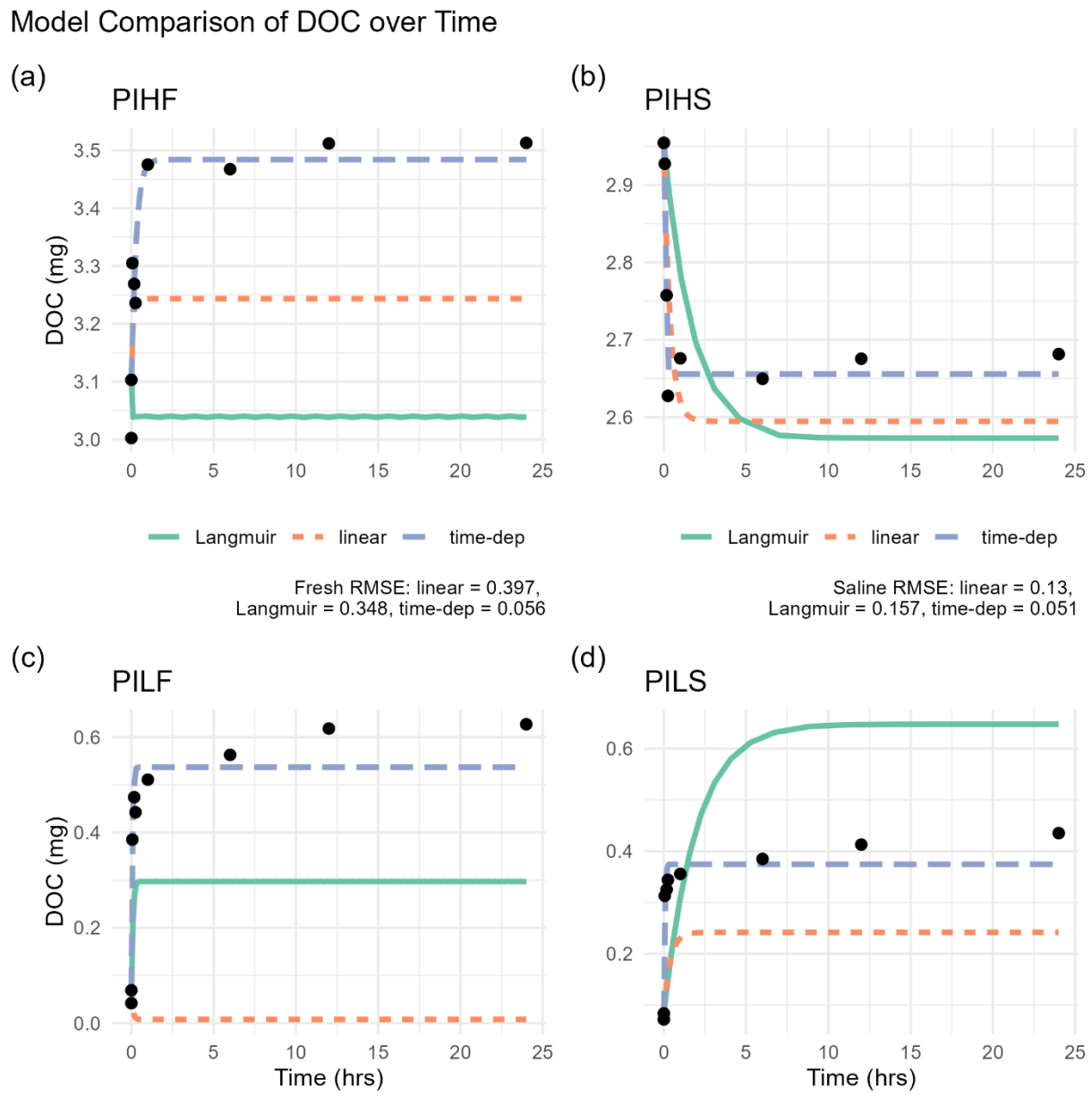

Figure F.7. Deep Intermediate Plot, spatial experiments.

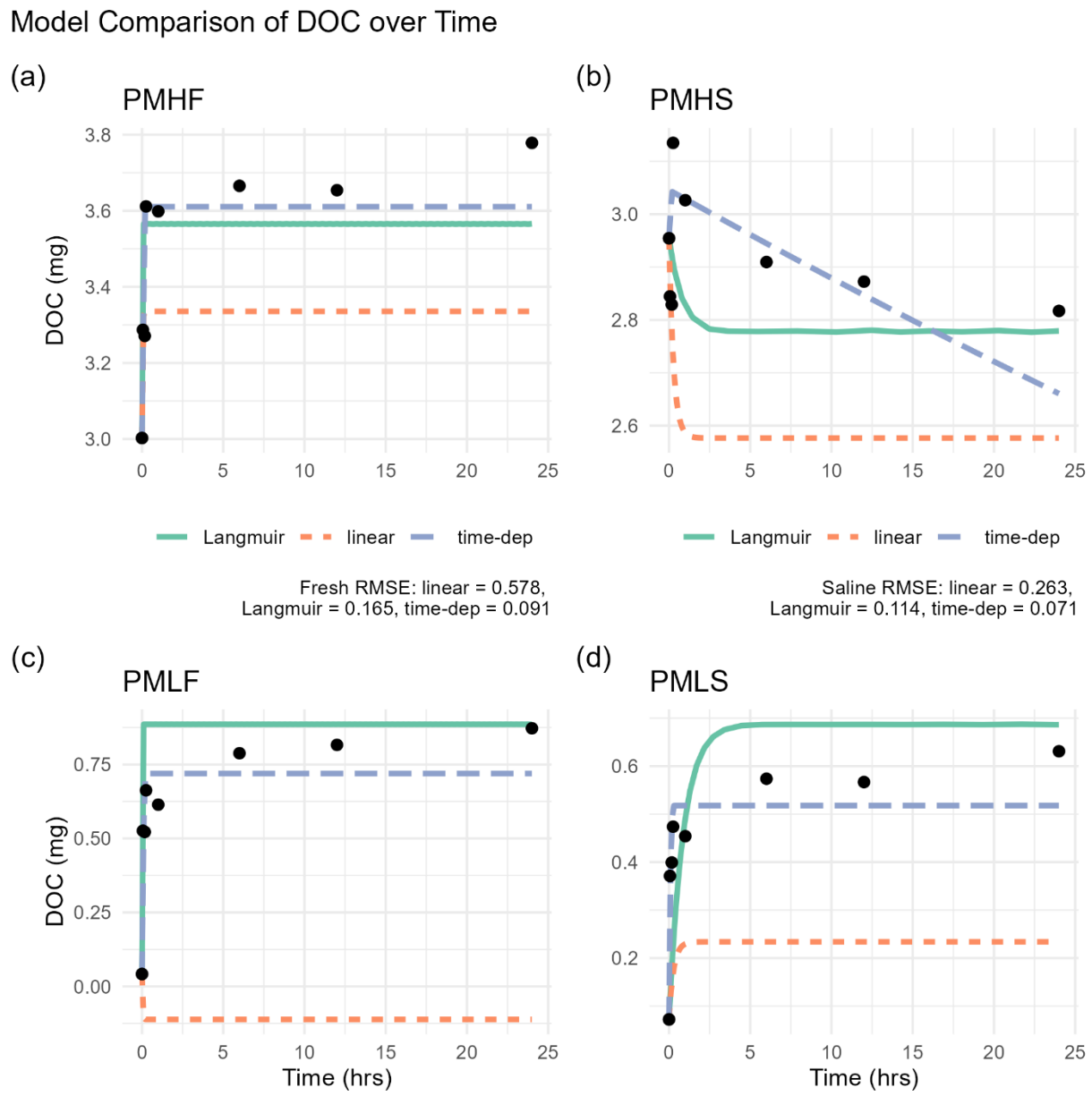

Figure F.8. Deep High Marsh, spatial experiments.