S1 Additional material

S1.1 Additional Plots

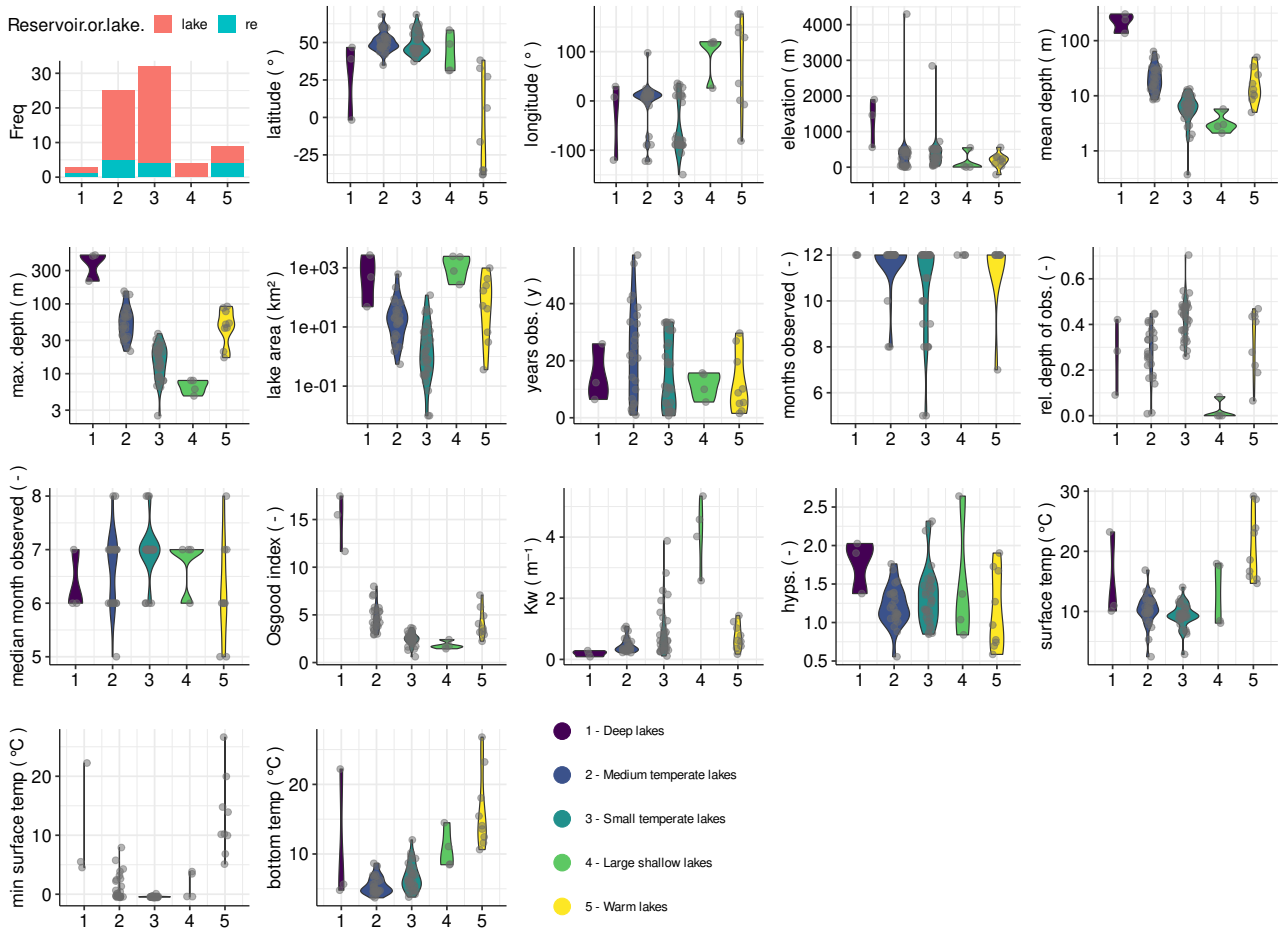

Figure S1: Distribution of lake characteristics for the cluster derived by K-means clustering. The grey points indicate values for individual lakes.

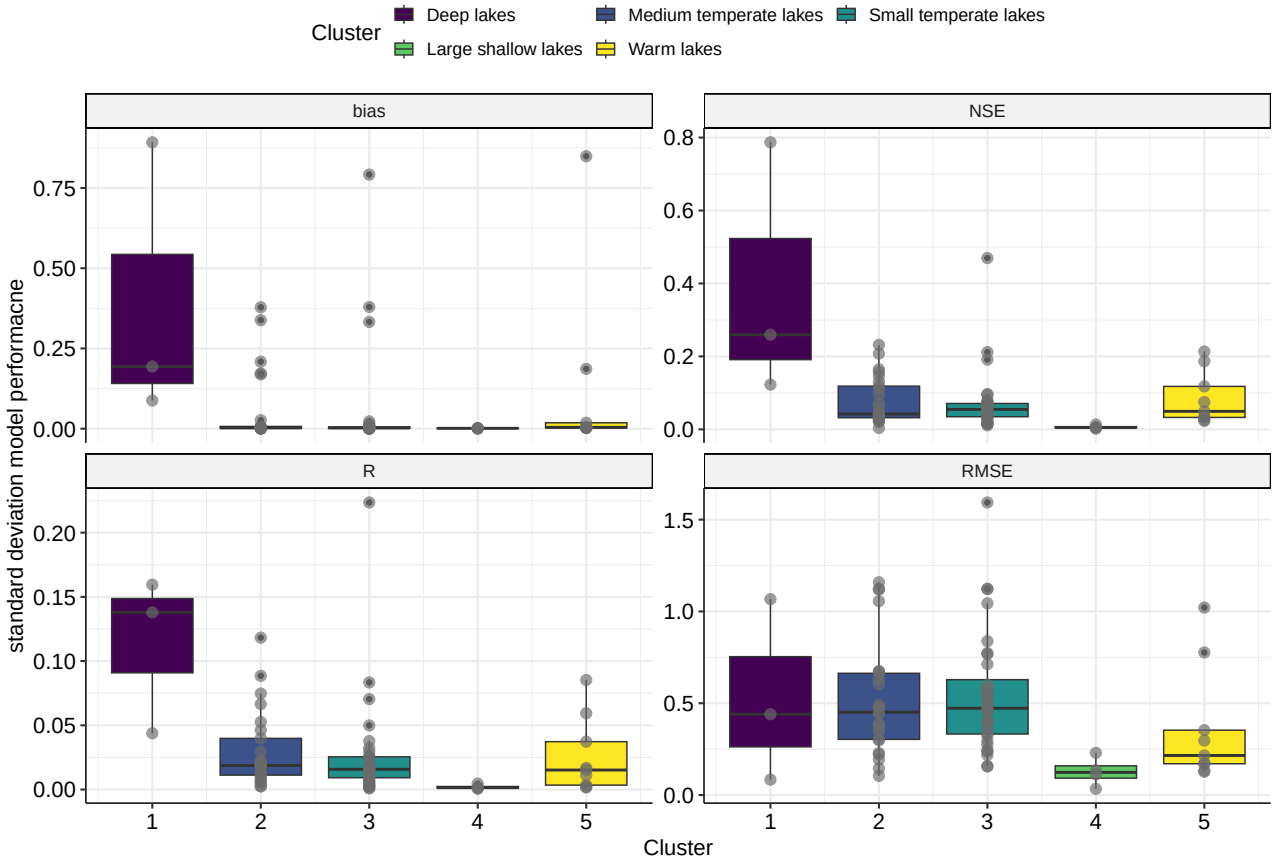

Figure S2: Boxplots of absolute difference between best and worst performing model per lake for the different metrics and lake cluster. The grey points indicate values for individual lakes.

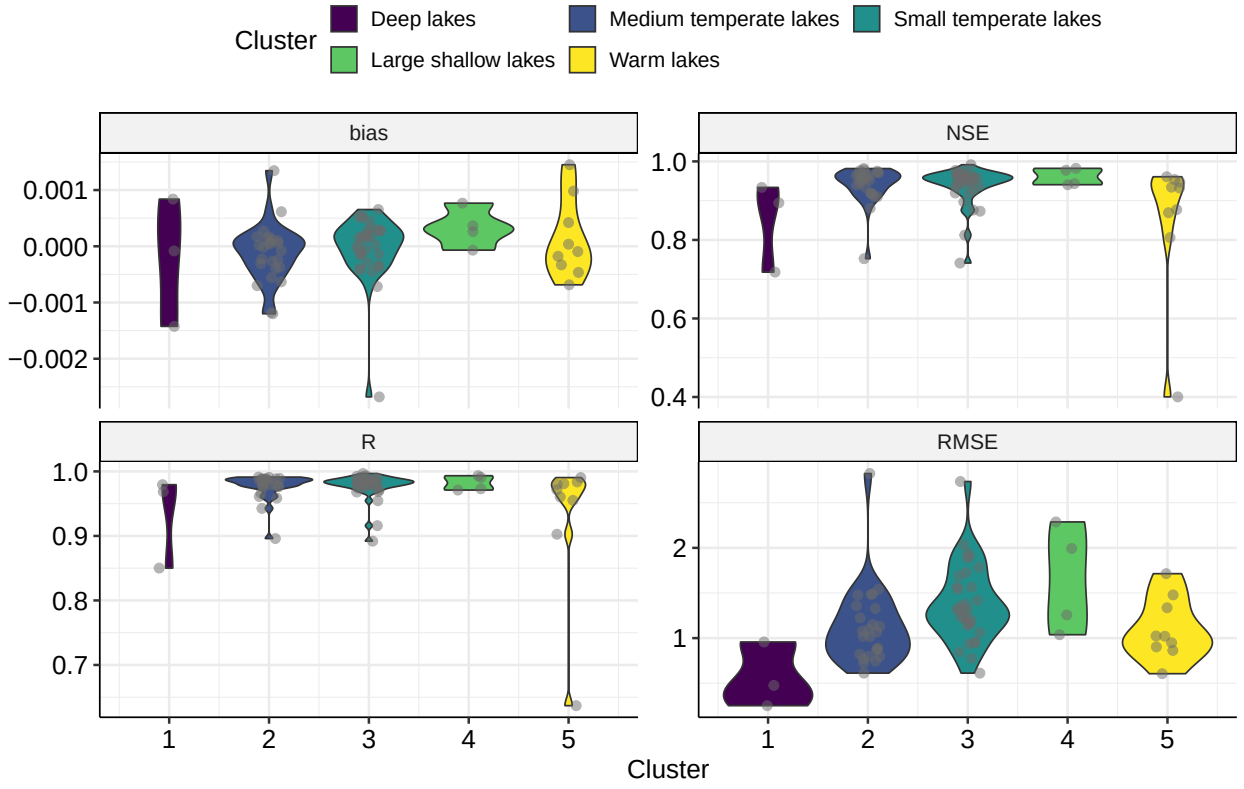

Figure S3: Violin plots of model performance of the best-performing model in each lake, split by lake cluster and performance metric. The grey points indicate values for individual lakes.

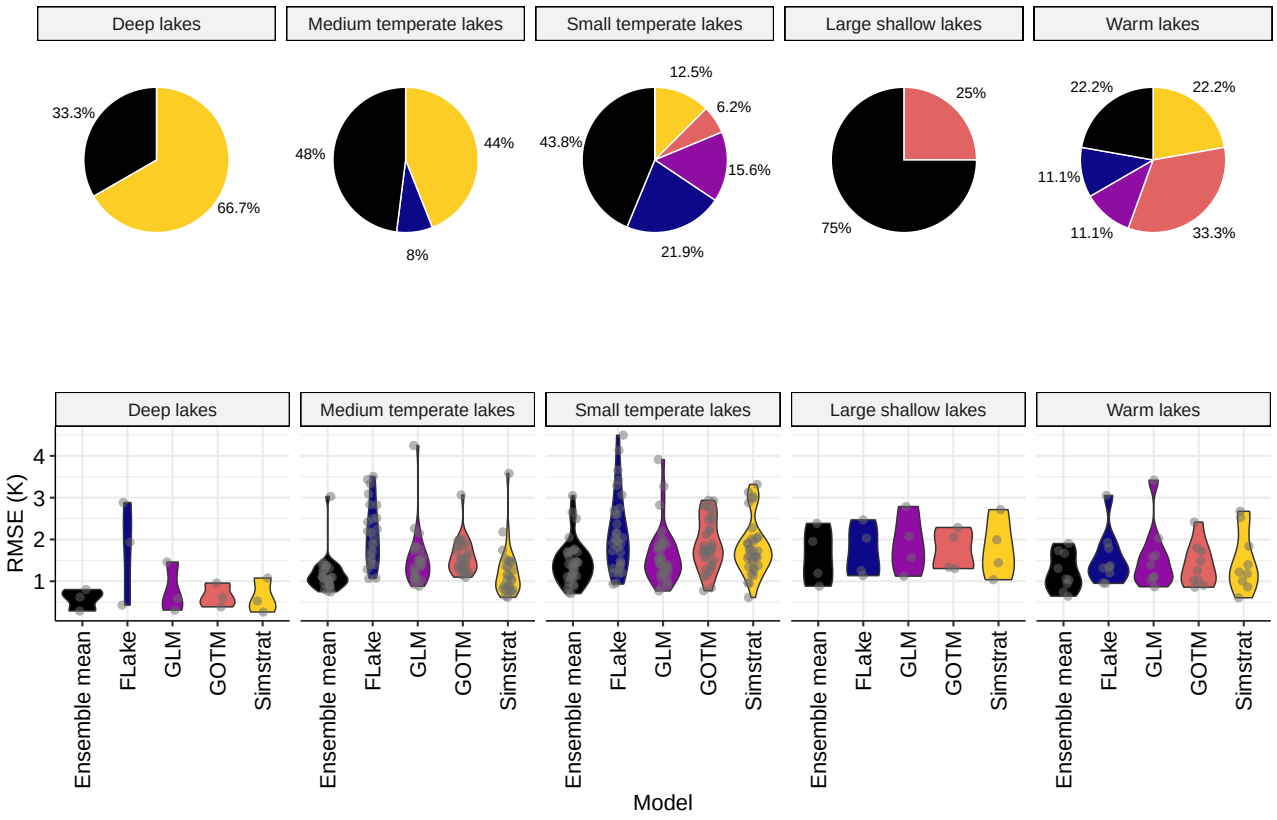

Figure S4: Percentage of lakes where each model performs best in terms of root mean squared error (RMSE), split to the archetype and including the ensemble mean as its own predictor (top, color refers to model or ensemble mean). Distribution of best performing parameter set (RMSE) per archetype (below).

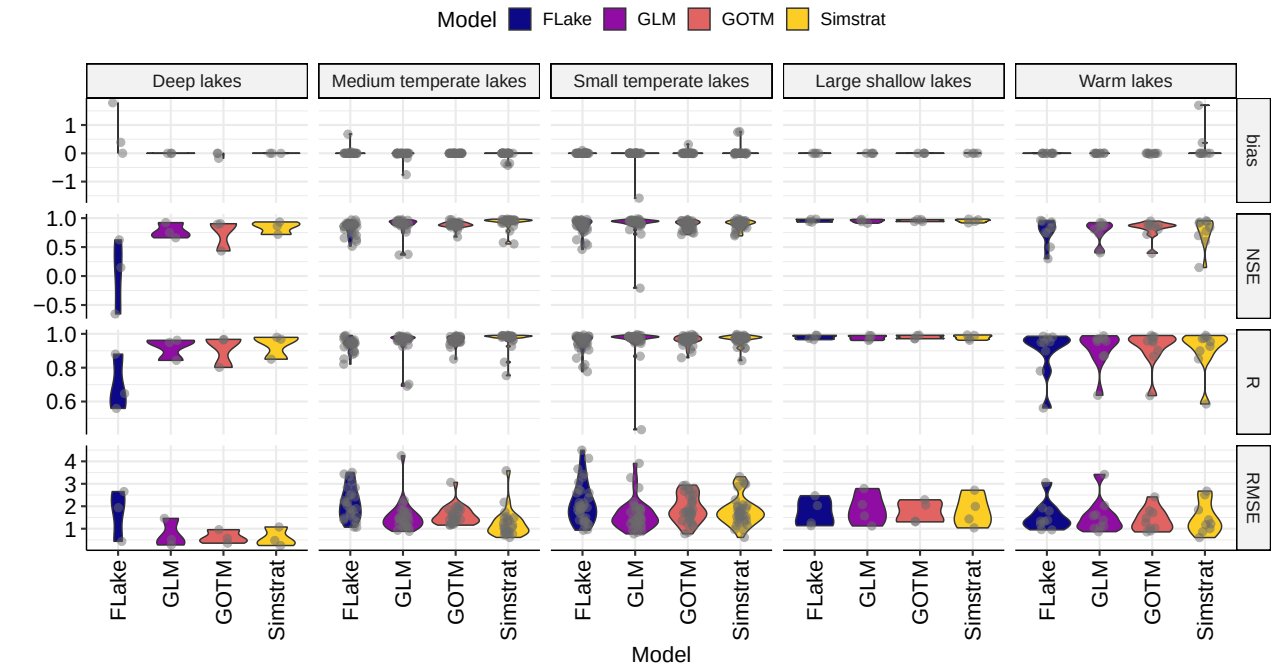

Figure S5: Violin plots of the performance metrics for best performing parameter sets per lake for each model, lake cluster, and performance metirc.

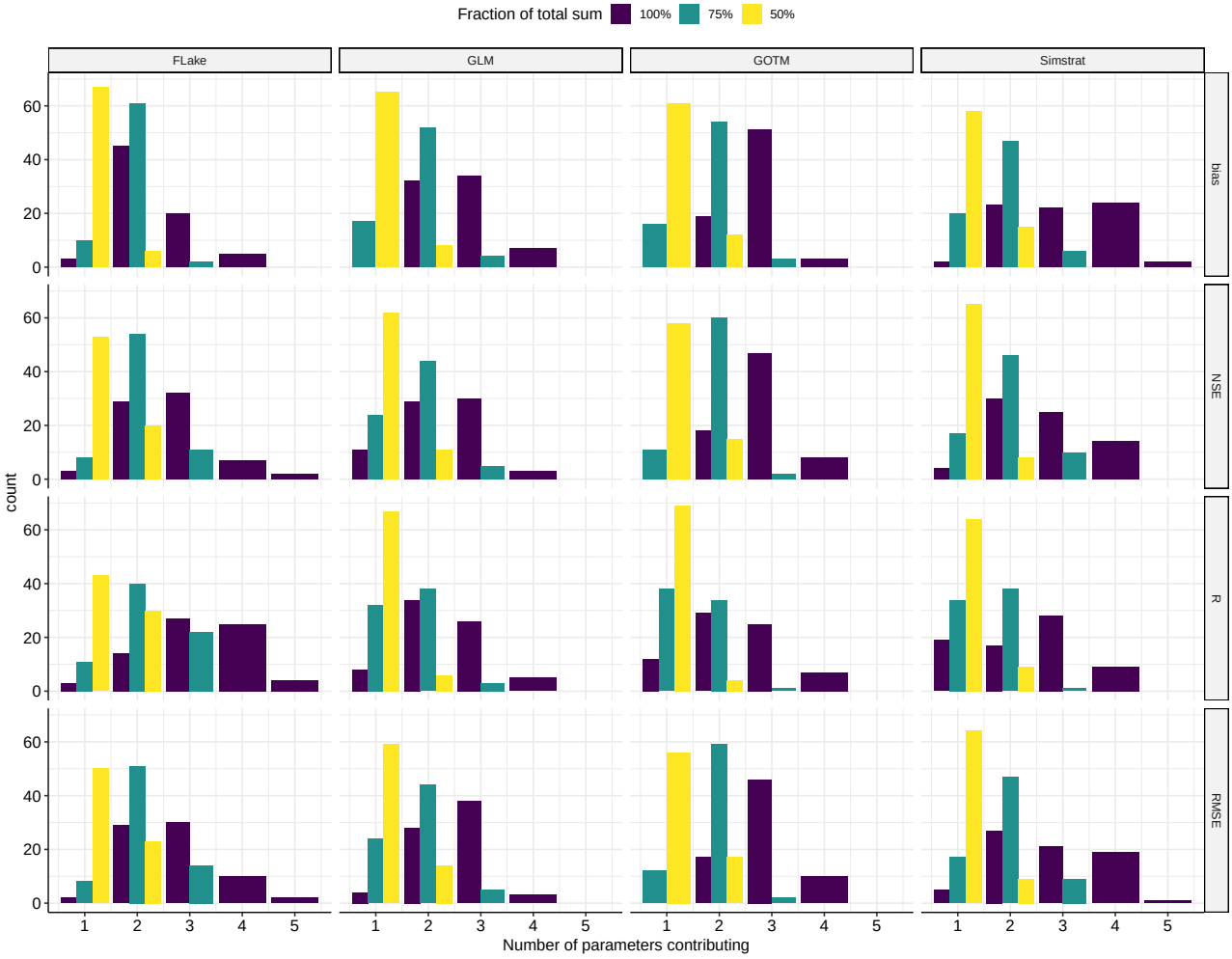

Figure S6: Distribution of the number of parameters that contribute to different fractions of the total sum of sensitivity measure value for each model and performance metric. For example, one contributing parameter for a fraction of 50% means that only one parameter contributes with at least 50% to the sum of all estimated sensitivity measures.

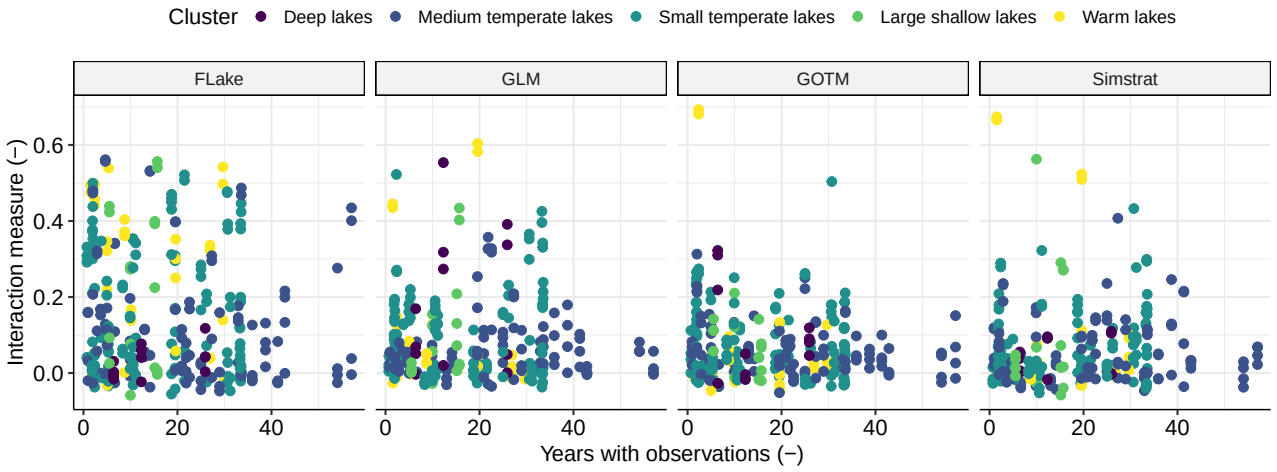

Figure S7: Interaction measure plotted against number of years with observed water temperature for the four models and lake cluster.

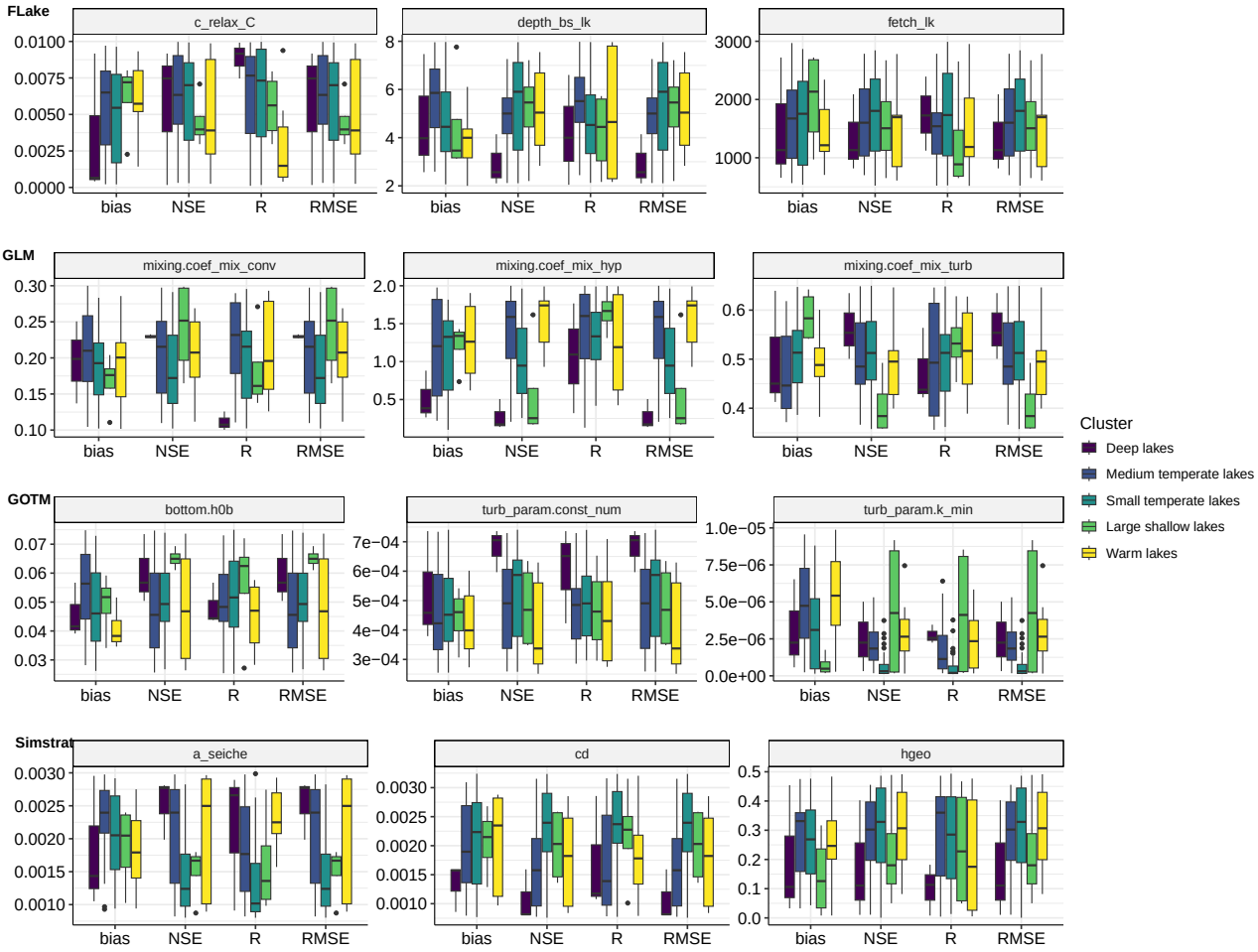

Figure S8: Boxplot of model specific parameters of the best performing parameter set for the different performance measures and lake cluster.

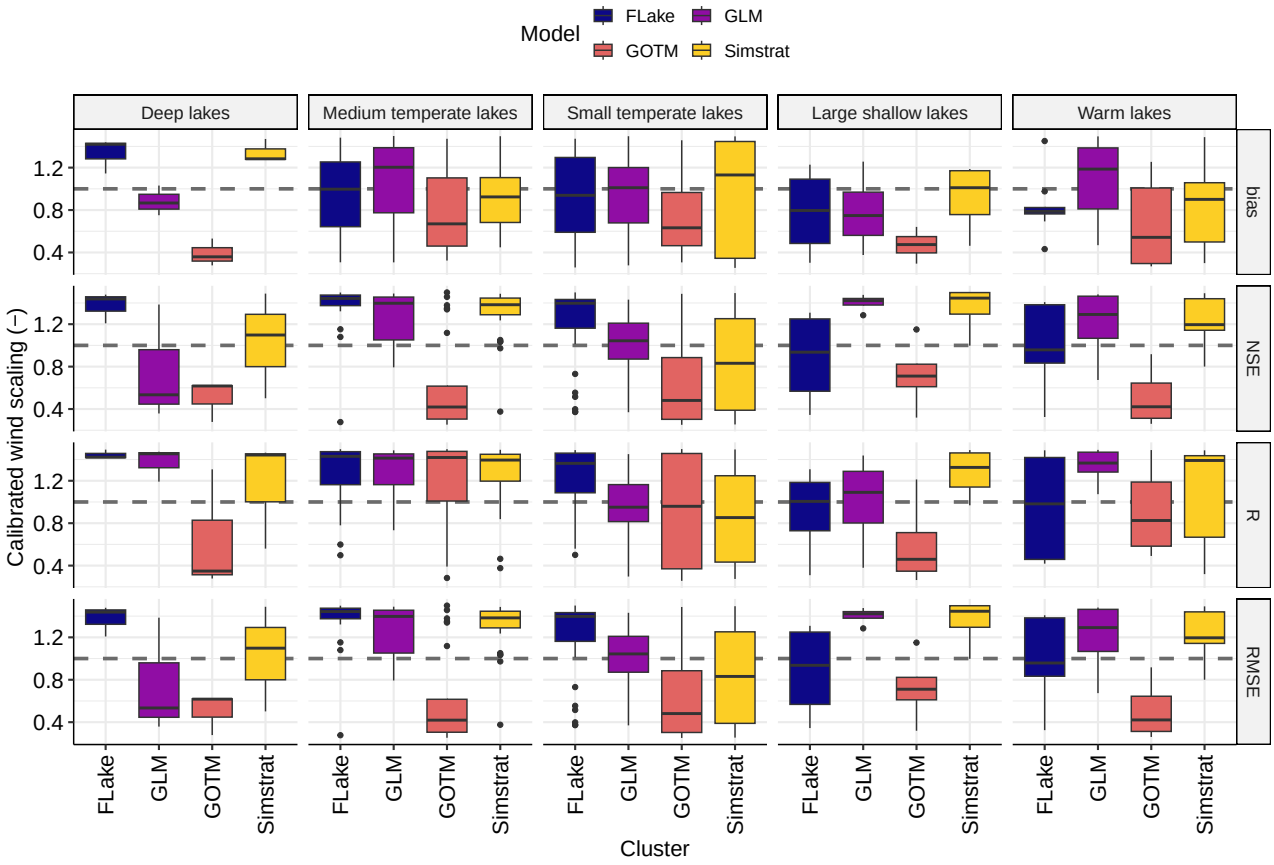

Figure S9: Boxplot of the wind speed scaling factors for the different models, cluster and based on which performance metric was choosen to optimize.

S1.2 Additional Tables

Table S1. Overview of the simulated lakes and their characteristics.

Lake Name	Country	Latitude (°)	Longitude (°)	Elevation (m)	Mean depth (m)	Max depth (m)	Lake area (km^2)	Secchi disk depth (m)	Light extinction (m^{-1})	Lake cluster
Allequash Lake	USA	46.04	-89.62	494	2.9	8	1.64	3.2		Small temperate
Alqueva Reservoir	Portugal	38.2	-7.49	152	16.6	92	250	3.15	0.69	Warm
Lake Annie	USA	27.21	-81.35	33.7	8.57	20.7	0.36			Warm
Lake Arendsee	Germany	52.89	11.47	23	28.8	49	5.11	2.89		Medium temperate
Lake Argyle	Australia	-16.31	128.68	100	10.1	51	980		0.89	Warm
Lake Biel	Switzerland	47.08	7.16	429	30	74	39.3		0.51	Medium temperate
Big Muskellunge Lake	USA	46.02	-89.61	500	7.5	21.3	3.63	6.6		Small temperate
Black Oak Lake	USA	46.16	-89.32	521.51	10.36	25.91	2.28	3.2		Small temperate
Lake Bosumtwi	Ghana	6.3	1.25	210	34	78	52	1.2		Warm
Lake Bryrup	Denmark	56.02	9.52	66	4.6	9	0.37	2.1		Small temperate
Lake Burley Griffin	Australia	-35.3	149.07	556	5	17	6.64	1.4		Warm
Lake Chao	China	31.53	117.53	4.5	3	7.98	780	0.38		Large shallow
Crystal Lake	USA	46	-89.61	501	10.4	20.4	0.38	7.5		Small temperate
Crystal Bog	USA	46.01	-89.61	501.5	1.7	2.5	0.01	1.5		Small temperate
Delavan Lake	USA	42.61	-88.6	282.55	7.61	16.46	6.96	3.53		Small temperate
Dickie Lake	Canada	45.15	-79.09	341	5	12	0.94	3.08		Small temperate
Eagle Lake	Canada	44.68	-76.7	190	10.1	31.1	6.65	4.62		Small temperate
Ekoln basin of Malaren	Sweden	59.75	17.62	0.7	11.5	50	20.18		1.09	Medium temperate
Lake Erken	Sweden	59.84	18.63	10	9	21	24	3.83		Medium temperate
Esthwaite Water	United Kingdom	54.37	-2.99	65	6.9	16	0.96		0.82	Small temperate
Falling Creek Reservoir	USA	37.31	-79.84	507	4	9.3	119		0.87	Small temperate
Lake Feeagh	Ireland	53.9	-9.5	15	14.5	44	3.9	1.74	0.98	Medium temperate
Fish Lake	USA	43.29	-89.65	265	6.6	18.9	0.8	2.4		Small temperate
Great Pond	USA	44.53	-69.89	81	6.3	21	33.83	6.7		Small temperate
Green Lake	USA	43.81	-89	243	33.55	72	29.48	4.8		Medium temperate
Harp Lake	Canada	45.38	-79.13	327	13.32	37.5	0.71	4.08		Small temperate
Hassel Predam	Germany	51.71	10.83	504	5	14	0.26	2.15		Small temperate
Lake Hulun	China	49	117.39	545.6	5.75	8	2339	0.35		Large shallow
Kilpisjarvi	Finland	69.03	20.77	473	20	57	37.3		0.3	Medium temperate
Lake Kinneret	Israel	32.82	35.58	-210	24	45	168	2.95	0.51	Warm
Lake Kivu	Rwanda/DR Congo	-1.73	29.24	1463	240	485	2700	5.21	0.27	Deep
Klicava Reservoir	Czechia	50.07	13.93	294.6	13.1	35	0.55	5.5		Medium temperate
Lake Kuivajarvi	Finland	60.47	23.51	130	6.3	13.2	0.62		0.6	Small temperate
Lake Langtjern	Norway	60.37	9.73	510	2	12	0.23	1.4	2.25	Small temperate
Laramie Lake	USA	40.62	-105.84	2843.8	0.37	6.4	0.14	0.6		Small temperate
Lower Lake Zurich	Switzerland	47.28	8.58	406	49	136	67		0.39	Medium temperate
Lake Mendota	USA	43.1	-89.41	258.5	12.8	25.3	39.61	3		Small temperate
Lake Monona	USA	43.06	-89.36	257	8.2	22.5	13.6	2.4		Small temperate
Mozhaysk reservoir	Russia	55.59	35.82	183	7	23	30.7	1		Small temperate
Mt Bold	Australia	-35.12	138.71	242.9	13	45.4	3.08	1.24	1.16	Warm
Lake Muggelsee	Germany	52.43	13.65	32.3	4.9	7.7	7.4	2	1.48	Small temperate
Lake Murten	Switzerland	46.93	7.08	429	22	45	22.8	3.49		Medium temperate
Lake Neuchatel	Switzerland	46.54	6.52	429	64	152	217		0.25	Medium temperate
Ngoring	China	34.9	97.7	4300	17.6	30.7	611		0.3	Medium temperate
Lake Nohipalo Mustjaerv	Estonia	57.93	27.34	61	3.9	8.9	0.22	0.46		Small temperate

Lake Nohipalo Valgejaerv	Estonia	57.94	27.35	62	6.2	12.5	0.07	4.52		Small temperate
Okauchee Lake	USA	43.13	-88.43	269	7.62	28.65	4.9	6.94		Small temperate
Lake Paaijarvi	Finland	61.07	25.13	102	15	85	13.44	2.2	1.15	Medium temperate
Rappbode Reservoir	Germany	51.74	10.89	415	28.6	89	3.95	4.8	0.25	Medium temperate
Rappbode Predam	Germany	51.71	10.8	533	5.3	16	0.24	2.26		Small temperate
Rimov Reservoir	Czechia	48.85	14.49	471.48	16	44	2.11	2.9		Medium temperate
Lake Rotorua	New Zealand	-38.08	176.28	280	10.8	52.9	425	2.63	0.61	Warm
Lake Sammamish	USA	47.59	-122.1	9	17.7	32	19.8	5		Medium temperate
Sau Reservoir	Spain	41.97	2.4	425	29	65	5.8	2.57	0.84	Medium temperate
Lake Scharmutzelsee	Germany	52.25	14.05	38.3	8.8	29	12.1	2		Medium temperate
Sparkling Lake	USA	46.01	-89.7	495	10.9	20	0.64	6.2		Small temperate
Lake Stechlin	Germany	53.17	13.03	59.8	23.2	69.5	2.23	8.6	0.29	Medium temperate
Lake Sunapee	USA	43.23	-72.5	333	11.4	34	16.55	8.5		Medium temperate
Lake Tahoe	USA	39.09	-120.03	1897	304.8	501	490	19.9		Deep
Lake Taihu	China	31.24	120.17	3.3	2.1	4.8	2445	0.3		Large shallow
Lake Tarawera	New Zealand	-38.21	176.43	300	50	87.5	41.3	8.34	0.18	Warm
Lake Thun	Switzerland	46.7	7.7	558	136	212	48.3	8.05		Deep
Toolik Lake	USA	68.63	-149.6	720	7	25	1.49	4.6		Small temperate
Trout Lake	USA	46.03	-89.67	491.8	14.6	35.7	15.65	4.7		Medium temperate
Trout Bog	USA	46.04	-89.69	495	5.6	7.9	0.01	1.1		Small temperate
Two Sisters Lake	USA	45.77	-89.53	481	9.14	19.2	2.91	17.75		Small temperate
Lake Vendyurskoe	Russia	62.1	33.1	131	5.3	13.4	10.4	3.5	1.5	Small temperate
Lake Vortsjarv	Estonia	58.31	26.01	33	2.8	6	270	0.86	2.76	Large shallow
Lake Washington	USA	47.64	-122.27	5	33	65.2	87.6	5.3		Medium temperate
Windermere	United Kingdom	54.31	-2.95	39	21.3	64	14.76		0.46	Medium temperate
Lake Wingra	USA	43.05	-89.43	254	2.7	6.7	1.36	0.7		Small temperate
Zlutice Reservoir	Czechia	50.09	13.11	507.95	8.5	24	1.5	2.8		Medium temperate
Lake Zurich	Switzerland	47.28	8.6	406	51	136	68.2	5.04		Medium temperate

Table S2: Characteristics of the lakes used for cluster analysis.

Reservoir.or.lake.	either lake or reservoir	-
latitude.dec.deg	coordinates of the lake latitude	°C
longitude.dec.deg	coordinates of the lake longitude	°C
elevation.m	elevation of the lake	m
mean.depth.m	mean depth of the lake	m
max.depth.m	maximum depth of the lake	m
lake.area.sqkm	lake surface area	km^2
Duration	number of years with observations	y
months_meas	number of unique months in which observations were available	-
reldepth_median	median relative depth of the observations (0 means surface, 1 means bottom)	-
months_median	median month of the observations	-
kw	Average calibrated light extinction factor	m^{-1}
vd	Volume development (Håkanson, 1981)	-
osgood	Osgood index (Osgood, 1988)	-
tsurf	average annual surface temperature for the period 1980 – 2000 from simulation	°C
min_tsurf	average annual minimum surface temperature for the period 1980 – 2000 from simulation	°C
tbot	average annual surface bottom for the period 1980 – 2000 from simulation	°C

Table S3: Median RMSE of the calibrated models and the percentage of calibrated fits lower than 2 K

model	Median RMSE (K)	Percentage under 2 K
FLake	1.91	56.2
GLM	1.42	83.6
GOTM	1.58	76.7
Simstrat	1.40	80.8

References

Håkanson, L.: A Manual of Lake Morphometry, Springer Berlin Heidelberg, Berlin, Heidelberg, https://doi.org/10.1007/978-3-642-81563-8, 1981.

Osgood, R. A.: Lake mixis and internal phosphorus dynamics, Archiv für Hydrobiologie, pp. 629–638, https://doi.org/10.1127/archiv-hydrobiol/113/1988/629, publisher: Schweizerbart'sche Verlagsbuchhandlung, 1988.