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Using empirical orthogonal functions derived from remote-sensing reflectance for the prediction of phytoplankton pigment concentrations

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1 Supplement: Additional tables

Table 1. List of cruises from which HPLC surface pigment data sets were used for the field (upper panel) and the satellite-based (lower panel) data set, including database (DB) or citation (ref.), cruise name, number of pigment data matched by 5x5 collocation criterium (N), investigator, date and region.

Pigment data matched with field reflectances data

DB/ref.	Cruise	Dates	Investigator	Region	N
Own data	ANTXXIV/4	25 Apr-6 May 08	Bettina Taylor	35°N-10°S, 42°-23°W	11
Own data	ANTXXV/1	10-24 Nov 08	Bettina Taylor	35°N-9°S, 21°-14°W	22
Own data	ANTXXVI/4	24 Apr-9 May 10	Bettina Taylor	35°N-9°S, 27°-13°W	20

Pigment data match with satellite reflectances data

DB/ref.	Cruise	Dates	Investigator	Region	N
BODC	AMT 12	27-31 May 03	Tim Jickells	12°N-10°S, 35°-14°W	3
BODC	AMT 14	12-23 May 04	Patrick Holligans	32°N-7°S, 36°-25°W	5
BODC	AMT 15	4-12 Oct 04	Andy Rees	34°N-8°S, 25°-17°W	5
BODC	AMT 16	7-12 Jun 05	Patrick Holligans	14°N-2°S, 32°-25°W	5
Own data	ANTXXIII/1	26 Oct-8 Nov 05	Rüdiger Röttgers	39°N-10°S, 21°-4°W	6
SEABASS	EGEE3	29 May-4 Jul 05	A.Subramamanian	6°-10°S, 10°-3°E	13
SEABASS	Amma-rb-06	25 Jun-3 Jul 06	Norman Nelson	14°N-5°S, 23°W	3
SEABASS	EGEE5	10-11 Jun 07	A Subramamanian	8°-5°N, 6°-2°W	2
Own data	ANTXXIV/1	1-15 Nov 07	Bettina Taylor	35°N-6°S, 22°-2°W	15
BODC	D325	17 Nov-15 Dec 07	Ruth Airs	26°-16°N, 25°-22°W	9
LOV	BonusGoodH	14-28 Feb 08	Josephine Ras	18°-8°N, 42°-33°W	2
BODC	AMT 18	12-26 Oct 08	Victor Martinez	33°N-10°S, 41°-24°W	8
Own data	ANTXXIV/4	25 Apr-6 May 08	Bettina Taylor	35°N-10°S, 42°-23°W	13
Own data	ANTXXV/1	10-24 Nov 08	Bettina Taylor	35°N-9°S, 21°-14°W	4
BODC	AMT 19	22 Oct-10 Nov 09	Victor Martinez	33°N-9°S, 41°-24°W	28
Own data	ANTXXVI/4	24 Apr-9 May 10	Bettina Taylor	35°N-9°S, 27°-13°W	6
Own data	MSM18-3	30 Jun-18 Jul 11	Bettina Taylor	3°N-6°S,21°W-0°	34

Table 2. Specific pigments measured in samples collocated to the satellite-based 5x5 pixels (s) and field (f) reflectance data sets: Maximum (max), minimum (min), mean and standard deviation (stdv) in mg m^{-3} (for PE relative units are given), number and percentage of samples where specific pigments had a concentration of 0 mg m^{-3} (nd and nd %, respectively) or were not measured in most samples (nm). Prasino, Allo, Lut, β-caroten, TPhaeo and chlorophyllide-*a* were only detected in less than 60% of the samples at both data sets and are not listed here. Full pigment names and abbreviations are given in chapter 2.3.1.

Pigment	MVChla	DVChla	TChla	TChlb	Chl-*c*1/2	Chl-*c*3	Fuco	But	Hex
max-s	2.9920	0.1439	3.5529	0.1203	0.2607	0.1123	1.7931	0.1950	0.4752
min-s	0.0048	0.0052	0.0048	0.0014	0.0003	0.0001	0.0010	0.0013	0.0030
mean-s	0.4075	0.0501	0.4681	0.0318	0.0645	0.0177	0.0887	0.0455	0.1229
stdv-s	0.4677	0.0374	0.5214	0.0352	0.0630	0.0313	0.2596	0.0478	0.1253
nd-s	0	15	0	41	14	51	15	14	8
nd-s [%]	0%	9%	0%	24%	8%	30%	9%	8%	5%
max-f	3.9759	0.2356	4.1505	1.1164	1.1568	0.6877	1.7890	0.3455	1.5512
min-f	0.0228	0.0097	0.0326	0.0034	0.0022	0.0015	0.0017	0.0019	0.0074
mean-f	0.0408	0.0627	0.4745	0.0560	0.0689	0.0413	0.0913	0.0303	0.1137
stdv-f	0.8091	0.0509	0.8126	0.1641	0.1809	0.1025	0.2840	0.0529	0.2437
nd-f	0	4	0	18	0	1	1	0	0
nd-f [%]	0%	8%	0%	34%	0%	2%	2%	0%	0%

Pigment	Peri	PSC	Diadino	Diato	Viola	Zea	Caro	PPC	PE	Neo
max-s	0.0585	1.8917	0.3825	0.0482	0.0235	0.4660	0.1909	0.5332	nm	nm
min-s	0.0005	0.0028	0.0001	0.0006	0.0001	0.0086	0.0014	0.0178	nm	nm
mean-s	0.0146	0.2787	0.0532	0.0078	0.0016	0.1214	0.0316	0.1567	nm	nm
stdv-s	0.0160	0.3267	0.0677	0.0116	0.0039	0.0868	0.0296	0.1069	nm	nm
nd-s	58	0	9	66	87	1	23	0	nm	nm
nd-s [%]	35%	0%	5%	39%	52%	1%	14%	0%	nm	nm
max-f	0.0477	3.6995	0.6315	0.0797	0.2532	0.3526	0.2626	1.0107	0.7296	0.1417
min-f	0.0017	0.0092	0.0045	0.0008	0.0006	0.0225	0.0029	0.0302	0.0008	0.0013
mean-f	0.0051	0.2404	0.0517	0.0081	0.0104	0.0933	0.0311	0.2004	0.0983	0.0066
stdv-f	0.0084	0.5666	0.1046	0.0143	0.0371	0.534	0.0426	0.2233	0.1496	0.0222
nd-f	17	0	1	8	14	0	0	0	0	29
nd-f[%]	32%	0%	2%	15%	26%	0%	0%	0%	0%	55%

Table 3. Statistics of linear models using EOF modes based on full fit (*MDPD*, *MPD*, *PB*, *a*, *RMSE*, and R^2) and the mean values of validation over all permutations (*MDPDcv*, *MPDcv*, *RMSEcv*, and R^2cv) for all models established for all pigment and pigment groups and based on the six reflectance data sets: field data set with hyperspectral resolution (hyper_R_{RS}) a) from 350 to 700nm and b) from 380 to 700nm, c) field data set with multispectral (band_R_{RS}) resolution and satellite data set with multispectral resolution (MERIS ρ_{wN} data) using d) 1x1, e) 3x3, and f) 5x5 matchups.

a) Field data set hyperspectral resolution 350-700 nm

Pigment	N	*MDPD*	*MPD*	*PB*	*a*	*RMSE*	R^2	$MDPD_{cv}$	MPD_{cv}	$RMSE_{cv}$	R^2_{cv}
TChla	53	23	33	9	-0.25	0.43	0.82	33	48	0.60	0.67
TChlb	53	85	251	195	-1.62	1.61	0.70	93	514	2.00	0.60
PSC	53	35	45	15	-0.47	0.53	0.80	39	58	0.65	0.71
PPC	53	18	35	11	-0.61	0.42	0.68	27	49	0.56	0.52
MVChla	53	27	34	9	-0.23	0.41	0.87	35	47	0.57	0.76
DVChla	53	32	99	65	-0.57	0.74	0.83	40	1.E+04	1.45	0.56
MVChlb	53	79	220	164	-1.49	1.48	0.74	90	321	1.79	0.65
DVChlb	53	97	255	199	-5.71	1.85	0.28	100	382	2.32	NA
$Chlc_{1/2}$	53	31	38	11	-0.48	0.45	0.87	39	53	0.63	0.75
$Chlc_3$	53	37	94	59	-1.12	0.74	0.74	50	134	0.98	0.61
But	53	35	62	26	-1.50	0.67	0.64	43	81	0.82	0.55
Hex	53	36	44	13	-0.7	0.54	0.77	42	57	0.67	0.66
Fuco	53	36	89	53	-0.96	0.77	0.76	44	149	1.01	0.64
Peridin	53	80	305	238	-3.79	1.50	0.41	83	424	1.74	0.32
Allo	53	28	110	79	-1.81	1.05	0.78	47	266	1.53	NA
Diadino	53	31	619	581	-2.22	0.97	0.42	38	1208	1.20	0.39
Diato	53	48	284	226	-3.63	1.27	0.37	59	658	1.76	0.21
Zea	53	19	31	7	-1.11	0.36	0.56	28	42	0.48	0.35
Caro	53	29	38	11	-1.08	0.44	0.72	34	57	0.67	0.52
Lutein	53	80	117	71	-6.27	1.19	0.26	87	245	1.56	NA
Viola	53	71	191	131	-2.55	1.22	0.61	78	314	1.55	0.44
Neo	53	47	71	33	-1.13	0.82	0.85	64	94	1.02	0.77
PE	53	65	106	60	-0.99	1.01	0.73	72	585	1.34	0.62

b) Field data set hyperspectral resolution 380-700 nm

Pigment	N	*MDPD*	*MPD*	*PB*	*a*	*RMSE*	R^2	$MDPD_{cv}$	MPD_{cv}	$RMSE_{cv}$	R^2_{cv}
TChla	53	30	38	10	-0.22	0.40	0.84	32	43	0.49	0.77
TChlb	53	86	245	190	-1.58	1.58	0.71	92	316	1.82	0.65
PSC	53	32	46	16	-0.43	0.51	0.82	34	53	0.62	0.75
PPC	53	22	33	10	0.70	0.40	0.70	27	49	0.58	0.46
MVChla	53	29	39	10	-0.28	0.45	0.84	34	44	0.50	0.79
DVChla	53	30	82	47	-0.50	0.69	0.85	41	7289	1.35	0.59
MVChlb	53	78	218	163	-1.43	1.45	0.75	88	285	1.66	0.69
DVChlb	53	100	243	188	-6.22	1.93	0.22	108	370	2.41	NA
$Chlc_{1/2}$	53	32	43	13	-0.58	0.49	0.85	36	49	0.56	0.80
$Chlc_3$	53	34	94	59	-1.16	0.76	0.73	42	130	0.92	0.66
But	53	44	58	22	0.68	0.63	0.68	50	102	0.91	0.49
Hex	53	31	45	15	-0.59	0.49	0.80	36	53	0.60	0.70
Fuco	53	31	106	71	-1.06	0.81	0.74	43	171	1.08	0.59
Peridin	53	82	298	232	0.40	1.51	0.40	85	534	1.78	0.33
Allo	53	33	86	54	-1.63	1.00	0.80	40	197	1.33	NA
Diadino	53	36	418	381	-2.11	0.95	0.45	40	1061	1.19	0.39
Diato	53	56	295	231	0.34	1.30	0.34	60	663	1.77	0.18
Zea	53	20	32	8	0.52	0.37	0.52	29	45	0.52	0.26
Caro	53	31	42	13	-1.24	0.47	0.68	33	50	0.54	0.62
Lutein	53	72	115	65	0.35	1.12	0.35	84	310	1.54	NA
Viola	53	70	175	116	0.62	1.20	0.62	74	248	1.42	0.51
Neo	53	46	71	33	-1.12	0.82	0.85	65	100	1.05	0.76
PE	53	61	121	71	-1.12	1.07	0.70	65	139	1.16	0.69

c) Field data set MERIS band resolution

Pigment	N	*MDPD*	*MPD*	*PB*	*a*	*RMSE*	R^2	$MDPD_{cv}$	MPD_{cv}	$RMSE_{cv}$	R^2_{cv}
TChla	53	21	33	8	-0.23	0.41	0.83	28	42	0.54	0.72
TChlb	53	77	219	168	-1.52	1.55	0.72	87	265	1.74	0.67
PSC	53	27	45	15	-0.47	0.53	0.80	32	51	0.62	0.75
PPC	53	26	36	11	-0.66	0.43	0.66	28	51	0.57	0.52
MVChla	53	26	36	10	-0.28	0.45	0.84	31	45	0.54	0.77
DVChla	53	31	90	57	-0.70	0.82	0.79	40	76569	1.50	0.54
MVChlb	53	86	205	148	-1.49	1.48	0.74	90	251	1.63	0.71
DVChlb	53	110	226	167	-5.78	1.86	0.27	100	1522	2.32	NA
$Chlc_{1/2}$	53	32	41	12	-0.56	0.49	0.85	34	48	0.57	0.79
$Chlc_3$	53	30	90	53	-1.18	0.76	0.72	39	115	0.89	0.69
But	53	37	65	29	-1.60	0.69	0.62	44	95	0.90	0.50
Hex	53	28	44	14	-0.68	0.53	0.77	37	57	0.69	0.64
Fuco	53	38	106	68	-1.10	0.82	0.73	43	191	1.04	0.63
Peridin	53	66	287	222	-3.79	1.50	0.41	85	438	1.83	0.32
Allo	53	36	118	83	-2.06	1.12	0.75	46	1068190	1.52	NA
Diadino	53	33	522	484	-2.40	1.01	0.37	40	959	1.16	0.37
Diato	53	51	357	294	-4.43	1.40	0.23	59	499	1.68	0.18
Zea	53	27	33	7	-1.23	0.38	0.51	31	45	0.52	0.28
Caro	53	29	39	11	-1.13	0.45	0.71	34	55	0.62	0.55
Lutein	53	72	123	75	-5.81	1.15	0.31	84	270	1.38	NA
Viola	53	71	203	142	-2.65	1.24	0.59	75	276	1.45	0.49
Neo	53	54	78	38	-1.21	0.86	0.84	64	123	1.00	0.78
PE	53	56	117	69	-1.09	1.05	0.70	67	156	1.28	0.65

d) MERIS 1x1 matchup data set

Pigment	N	*MDPD*	*MPD*	*PB*	*a*	*RMSE*	R^2	$MDPD_{cv}$	MPD_{cv}	$RMSE_{cv}$	R^2_{cv}
TChla	139	29	37	10	-0.49	0.54	0.72	32	47	0.64	0.67
TChlb	139	77	1417	1325	-3.97	2.14	0.26	80	4760	2.27	0.23
PSC	139	42	65	29	-0.74	0.71	0.74	42	59	0.79	0.70
PPC	139	24	36	10	-1.23	0.44	0.50	27	40	0.49	0.50
MVChla	139	38	51	19	-0.57	0.61	0.74	40	55	0.67	0.72
DVChla	139	58	902	838	-2.82	1.73	0.26	61	1141	1.90	0.19
MVChlb	139	91	965	873	-4.44	2.22	0.28	91	3.E+06	2.44	0.24
DVChlb	139	129	204	151	-7.30	1.80	0.09	123	262	2.06	0.05
$Chlc_{1/2}$	139	54	1039	977	-2.73	1.47	0.41	56	1296	1.67	0.34
$Chlc_3$	139	86	716	629	-5.90	2.29	0.03	89	964	2.44	NA
But	139	46	311	257	-2.10	1.21	0.56	52	374	1.31	0.53
Hex	139	44	584	534	-1.82	1.22	0.50	51	602	1.25	0.50
Fuco	139	41	954	901	-2.49	1.41	0.47	47	1535	1.60	0.41
Peridin	139	79	643	561	-4.44	1.79	0.32	81	953	1.92	0.26
Allo	139	77	126	88	-6.66	1.42	0.21	78	168	1.56	0.14
Diadino	139	54	266	217	-2.30	1.14	0.50	55	300	1.26	0.46
Diato	139	89	317	242	-6.41	1.75	0.11	92	2.E+05	2.09	NA
Zea	139	27	350	320	-2.00	0.72	0.27	31	1210	0.86	0.21
Caro	139	53	585	522	-3.37	1.49	0.29	55	860	1.63	0.21
Lutein	139	33	45	23	-7.39	0.85	0.17	36	50	0.95	0.10
Viola	139	95	185	125	-6.72	1.51	0.14	97	226	1.66	0.07
no Neo											
no PE											

e) MERIS 3x3 matchup data set

Pigment	N	*MDPD*	*MPD*	*PB*	*a*	*RMSE*	R^2	$MDPD_{cv}$	MPD_{cv}	$RMSE_{cv}$	R^2_{cv}
TChla	155	28	36	10	-0.47	0.52	0.74	29	47	0.65	0.64
TChlb	155	75	1402	1314	-3.81	2.07	0.28	77	1.E+04	2.18	0.25
PSC	155	36	67	32	-0.76	0.72	0.73	38	72	0.83	0.67
PPC	155	24	35	10	-1.23	0.44	0.50	27	48	0.52	0.49
MVChla	155	36	54	21	-0.58	0.62	0.74	39	59	0.73	0.67
DVChla	155	52	1190	1126	-3.19	1.77	0.15	59	1.E+05	2.17	0.08
MVChlb	155	89	1047	960	-4.16	2.15	0.32	90	5.E+05	2.32	0.26
DVChlb	155	120	205	150	-7.29	1.80	0.09	137	5214	2.10	NA
$Chlc_{1/2}$	155	53	957	894	-2.75	1.46	0.41	56	1170	1.58	0.37
$Chlc_3$	155	89	701	612	-6.16	2.31	0.00	89	9704	2.44	NA
But	155	46	305	249	-2.17	1.21	0.55	50	338	1.33	0.51
Hex	155	41	477	428	-1.76	1.16	0.52	45	530	1.23	0.52
Fuco	155	44	1177	1122	-2.61	1.45	0.45	49	1604	1.66	0.37
Peridin	155	78	609	529	-4.24	1.74	0.35	81	766	1.84	0.31
Allo	155	78	149	107	-6.34	1.46	0.24	78	281	1.59	0.18
Diadino	155	50	282	234	-2.40	1.16	0.48	54	305	1.31	0.40
Diato	155	92	318	242	-6.82	1.79	0.06	93	7.E+05	2.09	NA
Zea	155	25	388	360	-2.02	0.71	0.26	29	778	0.80	0.23
Caro	155	53	574	510	-3.30	1.47	0.31	54	754	1.59	0.22
Lutein	155	36	45	23	-6.72	0.83	0.24	38	50	0.91	0.16
Viola	155	186	198	132	-7.47	1.57	0.05	138	336	1.75	NA
no Neo											
no PE											

f) MERIS 5x5 matchup data set

Pigment	N	*MDPD*	*MPD*	*PB*	*a*	*RMSE*	R^2	$MDPD_{cv}$	MPD_{cv}	$RMSE_{cv}$	R^2_{cv}
TChla	160	27	36	10	-0.47	0.52	0.74	28	48	0.66	0.62
TChlb	160	75	1400	1313	-3.83	2.06	0.28	77	6.E+04	2.14	0.26
PSC	160	33	66	31	-0.78	0.72	0.73	38	74	0.83	0.66
PPC	160	22	34	10	-1.21	0.43	0.51	24	44	0.50	0.48
MVChla	160	35	53	21	-0.59	0.62	0.74	38	58	0.74	0.66
DVChla	160	54	1186	1120	-3.19	1.75	0.14	58	1.E+05	2.08	0.09
MVChlb	160	89	1030	941	-4.28	2.16	0.30	90	2448	2.27	0.27
DVChlb	160	137	211	156	-7.39	1.79	0.08	145	3451	2.12	NA
$Chlc_{1/2}$	160	52	916	854	-2.79	1.44	0.41	54	1088	1.56	0.36
$Chlc_3$	160	90	681	592	-6.20	2.31	<0.01	90	3642	2.43	NA
But	160	48	333	279	-2.23	1.21	0.54	51	390	1.34	0.49
Hex	160	42	488	438	-1.81	1.20	0.51	45	530	1.25	0.52
Fuco	160	45	1138	1082	-2.67	1.46	0.45	50	1580	1.70	0.36
Peridin	160	79	601	522	-4.28	1.74	0.35	82	801	1.85	0.30
Allo	160	77	146	104	-6.39	1.45	0.23	79	376	1.57	0.19
Diadino	160	45	282	234	-2.40	1.15	0.48	52	312	1.31	0.40
Diato	160	91	317	241	-6.58	1.74	0.10	92	9.E+05	2.05	0.4NA
Zea	160	26	389	360	-2.01	0.70	0.26	29	736	0.78	0.25
Caro	160	50	567	505	-3.28	1.47	0.31	53	832	1.60	0.23
Lutein	160	35	44	22	-6.77	0.83	0.23	36	48	0.93	0.16
Viola no Neo no PE	160	193	195	129	-7.53	1.57	0.04	145	427	1.70	NA