Communications

Mathematical description of vertical algal accessory pigment distributions in oceans – a brief presentation*

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Abstract

A straightforward mathematical expression for describing the vertical distributions of algal accessory pigments in oceans is presented. To this end ca 1500 empirical datasets of accessory pigment depth profiles gathered during some 200 research

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cruises in different oceanic regions were analysed. These data were retrieved from the bio-optical databases of SeaBASS and U.S. JGOFS published on the Internet.

The statistical relationships were analysed between the concentrations of accessory pigments and the trophic indices of waters, as measured by the surface concentrations of chlorophyll *a* and the optical depths in different oceanic regions. A mathematical expression was established and formulas based on it were found, approximating the relations between the vertical distributions of accessory pigments and the chlorophyll *a* concentration. These formulas can be used to model the species composition of algae in different parts of the ocean and in remote sensing algorithms.

1. Introduction

The variability in the vertical distributions of accessory pigments in seas and oceans was investigated already in the latter half of the 20th century (see e.g. Margalef 1967, Koblentz-Mishke 1971, Woźniak & Ostrowska 1990, Brunet et al. 1993, Claustre et al. 1994, Bricaud et al. 1995, Majchrowski & Ostrowska 1999), and also more recently (Brunet et al. 2003, 2006, Oubelkheir et al. 2005, Woźniak & Dera 2007, Uitz et al. 2008, 2009). Accessory pigments are divided into two main groups according to their functions in the photosynthetic apparatus: photosynthetic pigments (PSP) and photoprotecting pigments (PPP) (Babin et al. 1996). The intensive research being carried out by various marine research centres around the world and the availability on the Internet of empirical data on the concentrations of these accessory pigments in marine algae have made it possible to perform statistical analyses to determine the vertical distributions of these pigments in different regions of the ocean.

The objective of this work was to find a straightforward mathematical description of the vertical distributions of algal accessory pigments in case 1 waters[1]. The analysis focused on the vertical distributions of pigments often treated as markers enabling groups of algal species to be defined (Jeffrey et al. 1997, Wright & Jeffrey 2006): chlorophyll *b* – *chl b*, chlorophyll *c* – *chl c*, fucoxanthin – *fuco*, 19'-butanoyloxyfucoxanthin – *but*, 19'-hexanoyloxyfucoxanthin – *hex*, diadinoxanthin – *diadino*, diatoxanthin – *diato*, alloxanthin – *allo*, peridinin – *perid*, and zeaxanthin – *zea*.

2. Methods and empirical material

The material for this analysis was drawn from the empirical database accessible on the Internet websites of The SeaWiFS Bio-optical Archive and Storage System SeaBASS (seabass.gsfc.nasa.gov) (Werdell & Bailey 2002)

[1]The classification of sea water according to Morel & Prieur 1977.

and the U.S. Joint Global Ocean Flux Study – U.S. JGOFS Data System (usjgofs.whoi.edu) (Bidigare 1995, 2002a, b, c, Goericke 2001a, b, c, d).

The analysis covered a total of 1460 profiles, consisting of around 11 500 sets of empirical data on pigment concentrations at different depths. The datasets were gathered during 203 research cruises in different oceanic regions: North Atlantic (739 profiles), South Atlantic (221 profiles), Mediterranean Sea (256 profiles), North Pacific (41 profiles), Equatorial Pacific (157 profiles) and South Pacific (46 profiles). Phytoplankton pigment concentrations were determined by HPLC (High Performance Liquid Chromatography), whereas optical depths were determined approximately for each pigment profile using the MCM model (the multi-component marine photosynthesis model – Woźniak et al. 2003) on the basis of the real depth z [m] and the surface concentration of chlorophyll a $C_a(0)$.

The first step in the analysis was to subdivide the vertical distributions of the algal accessory pigments in accordance with the trophic index[2]. This was followed by an analysis of the relationships between the relative concentrations of the pigments (referred to the chlorophyll a concentration C_a) and the optical depth τ defined as $\tau(z) = -\ln(T(z))$, where $T(z)$ is the PAR energy transmittance in the sea. After a good number of attempts, we were able to derive a general mathematical expression adequately describing the vertical profiles of the relative concentrations of different pigments, that is, the dependence of these concentrations on the optical depth for all trophic indices:

$$\frac{C_{pigm}(\tau)}{C_a(\tau)} = a \times \exp(-b\tau) + c \times \exp(-(d - e\tau)), \tag{1}$$

where C_a – concentration of chlorophyll a, C_{pigm} – concentration of the relevant accessory pigment (*pigm* stands for *chl b*, *chl c*, *fuco*, *but*, *hex*, *diadino*, *diato*, *zea*, *allo*, *perid*, as appropriate); a, b, c, d, e – empirical parameters of this dependence.

For the statistical analyses the data sets were divided into three groups, according to geographical zone and climate. The first, 'tropical' group contained ca 5500 datasets for latitudes 35°N–35°S; the second, 'mid-latitudes' group had ca 5050 datasets for latitudes 55°N–35°N and 35°S–55°S; the third, 'polar' group consisted of some 950 data sets from the

[2]In accordance with the convention used by our research team, the trophic index (trophicity) is defined as the surface concentration of chlorophyll a $C_a(0)$. Depending on the concentration $C_a(0)$ [mg tot. chl m^{-3}], the following trophic types of waters can be distinguished: oligotrophic: O1 – $C_a(0) = 0.02$–0.05; O2 – $C_a(0) = 0.05$–0.10; O3 – $C_a(0) = 0.10$–0.20; mesotrophic: M – $C_a(0) = 0.2$–0.5; intermediate: I – $C_a(0) = 0.5$–1.0; eutrophic: E1 – $C_a(0) = 1$–2; E2 – $C_a(0) = 2$–5.

Antarctic region. In addition, each of these groups was subdivided according to trophic index. Table 1 lists the numbers of profiles for the various pigments and the trophic index subgroups.

Table 1. Number of vertical profiles for the different pigments and trophic subgroups. Geographical and climatic denotations: t – tropical, m-l – mid-latitudes, p – polar. The symbols O1, O2, O3, M, I, E1 and E2 denote trophic types (see footnote 2)

	diadino			*diato*			*zea*			*allo*			*perid*		
	t	**m-l**	**p**	**t**	**m-l**	**p**	**t**	**m-l**	**p**	**t**	**m-l**	**p**	**t**	**m-l**	**p**
O1	101	19	7	97	19	0	54	20	7	98	19	7	98	19	7
O2	116	149	20	112	148	20	64	149	20	116	149	20	116	149	20
O3	192	102	34	184	100	34	159	102	34	192	102	34	192	102	34
M	150	139	26	147	138	26	124	138	26	150	139	26	150	139	26
I	9	137	32	8	136	32	7	137	32	9	137	32	9	137	32
E1	13	73	45	13	73	45	14	73	45	13	73	45	13	73	45
E2	17	58	18	0	58	18	17	58	18	17	58	0	17	58	18
	chl b			*chl c*			*fuco*			*but*			*hex*		
	t	**m-l**	**p**	**t**	**m-l**	**p**	**t**	**m-l**	**p**	**t**	**m-l**	**p**	**t**	**m-l**	**p**
O1	101	10	4	72	15	4	101	19	7	101	20	7	101	20	7
O2	109	53	3	79	93	3	116	149	20	116	149	20	116	149	20
O3	172	60	12	145	44	12	192	102	34	192	102	34	192	102	34
M	139	27	15	113	96	15	150	139	26	150	139	26	150	139	26
I	2	16	10	3	103	10	9	137	32	9	137	32	9	137	32
E1	4	7	10	4	14	10	13	73	45	13	73	14	13	73	45
E2	10	17	0	7	4	0	17	58	18	17	58	18	0	0	0

3. Results and discussion

The mean profiles of the relative concentrations of accessory pigments in all the subgroups were determined first. These analyses were carried out with reference to the upper layer of waters delimited by an optical depth of $\tau = 7$ (i.e. down to about 1.5 times the thickness of the euphotic layer). Then, using non-linear methods of regression, these mean profiles were approximated with the aid of equation (1). All the coefficients for the various subgroups are listed in the Appendix.

Figures 1 and 2 show the results of the successive stages of the analysis. Figure 1 illustrates the results concerning the photoprotecting pigments (PPP) – *diadino*, *allo*, *diato*, *perid* and *zea*. Figure 2 presents the results for the photosynthetic pigments (PSP) – *fuco*, *chl c*, *but*, *hex* and *chl b*. The top rows of plots in both figures show the mean, empirical depth profiles of the relative pigment concentrations for the different trophic indices. The

Table 2. Errors in calculating pigment concentrations using equation (1)

	Arithmetic statistics		Logarithmic statistics			
	Systematic error	Statistical error	Systematic error	Standard error factor	Statistical error	
	$< \varepsilon >$ [%]	σ_ε [%]	$< \varepsilon >_g$ [%]	x	σ_- [%]	σ_+ [%]
1	2	3	4	5	6	7
diadino – tropical	32.2	81.4	12.8	1.75	−43.0	75.4
diadino – mid-lat.	16.4	55.8	4.28	1.61	−37.9	61.0
diadino – polar	24.7	76.3	9.22	1.64	−39.2	64.5
diato – tropical	3.22	110	−21.2	2.26	−55.9	126
diato – mid-lat.	−7.68	80.1	−30.4	2.10	−52.4	110
diato – polar	54.5	140	15.6	2.07	−51.7	107
zea – tropical	55.3	154	18.0	1.96	−49.0	95.9
zea – mid-lat.	101	226.4	31.8	2.39	−58.2	139
zea – polar	26.9	99.9	−0.65	1.99	−49.8	99.1
allo – tropical	5.40	137.5	−31.8	2.68	−62.6	168
allo – mid-lat.	37.5	218	−11.5	2.35	−57.5	135.3
allo – polar	75.3	154	26.8	2.21	−54.7	120
perid – tropical	20.8	130.7	−15.7	2.21	−54.8	121.2
perid – mid-lat.	13.5	112.2	−15.5	2.07	−51.8	107
perid – polar	78.7	189.7	24.3	2.26	−55.9	126
chl b – tropical	44.3	165	7.13	2.01	−50.2	101
chl b – mid-lat.	17.8	74.0	1.52	1.70	−41.1	70.0
chl b – polar	80.9	153	33.6	2.28	−56.2	128
chl c – tropical	38.6	135	2.47	2.20	−54.6	120
chl c – mid-lat.	8.66	39.5	2.41	1.41	−29.1	41.0
chl c – polar	12.5	87.0	−0.15	1.58	−36.6	57.7
fuco – tropical	49.6	103	21.3	1.94	−48.4	93.8
fuco – mid-lat.	53.2	102	22.2	2.00	−50.1	100
fuco – polar	13.5	54.6	2.7	1.56	−36.0	56.2
but – tropical	24.3	94.1	5.84	1.68	−40.7	68.5
but – mid-lat.	30.2	111.3	8.71	1.71	−41.5	70.9
but – polar	47.0	1.13	17.0	1.92	−47.9	92.0
hex – tropical	19.6	73.2	7.7	1.51	−33.8	51.1
hex – mid-lat.	38.0	155	12.4	1.71	−41.5	71.0
hex – polar	61.6	131	20.6	2.21	−54.7	121

where:
$\varepsilon = (C_{i,\,mod} - C_{i,\,meas})/C_{i,\,meas}$ – relative error,
$< \varepsilon >$ – arithmetic mean of errors,
σ_ε – standard deviations of errors (statistical error),
$< \varepsilon >_g = 10^{<\log(C_{i,\,mod}/C_{i,\,meas})>} - 1$ – logarithmic mean of errors,
$< \log(C_{i,\,mod}/C_{i,\,meas}) >$ – mean of $\log(C_{i,\,mod}/C_{i,\,meas})$,
$\sigma_{\log}$ – standard deviation of $\log(C_{i,\,mod}/C_{i,\,meas})$,
$x = 10^{\sigma \log}$ – standard error factor,
$\sigma_- = \frac{1}{x} - 1$ and $\sigma_+ = x - 1$,
where $C_{i,\,meas}$ – measured values, $C_{i,\,mod}$ – estimated values (subscript $meas$ = measured; subscript mod = modelled).

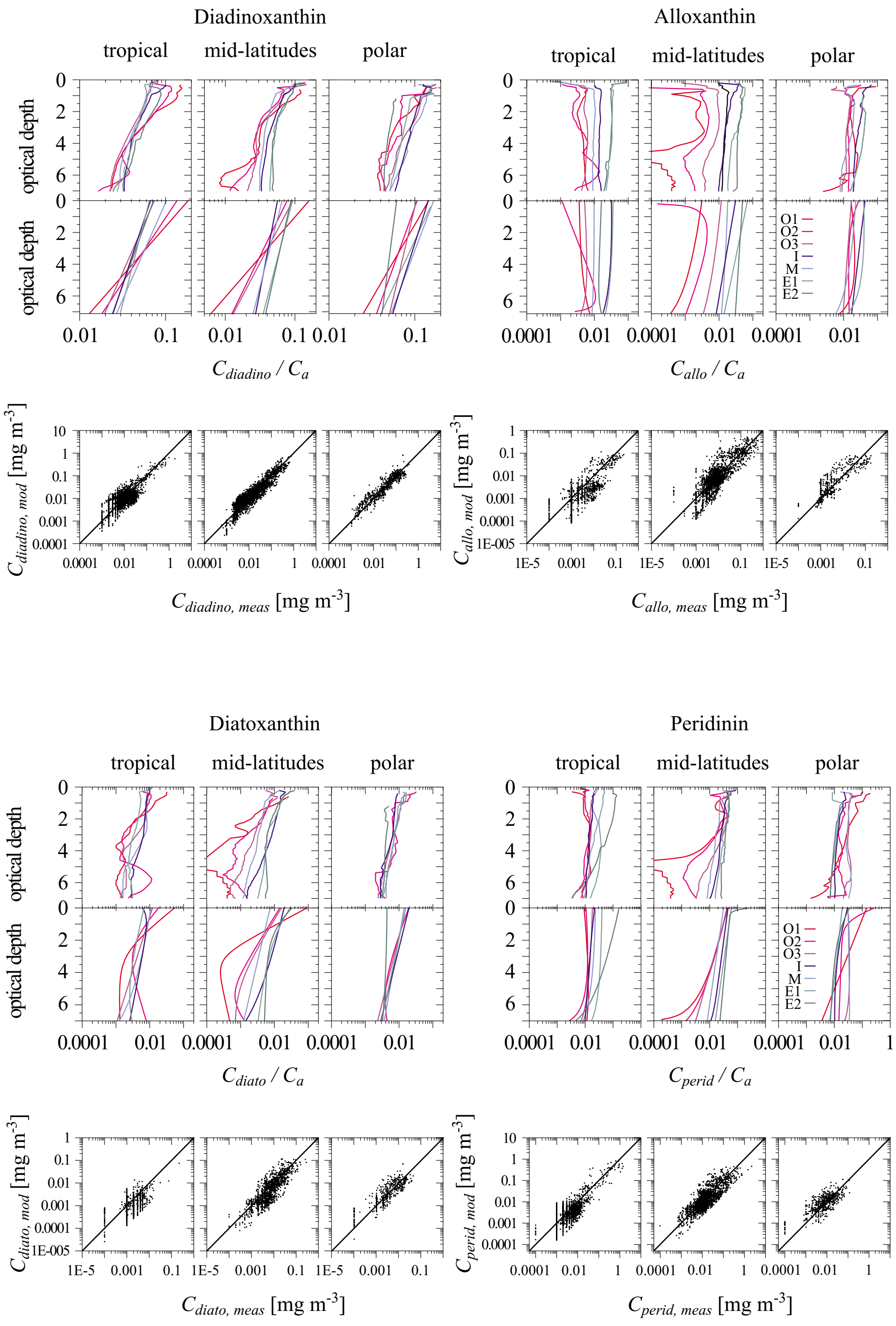

Figure 1. (*continued next page*)

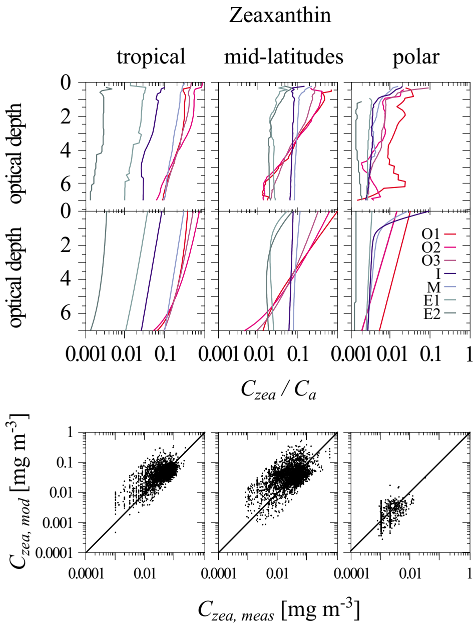

Figure 1. Mean empirical (top rows) and modelled (middle rows) depth profiles of the relative concentrations of photoprotecting pigments – diadinoxanthin, alloxanthin, diatoxanthin, peridinin and zeaxanthin. The columns represent the various geographical-climatic zones. Bottom rows – comparison of empirical and modelled pigment concentrations (for description – see text). The symbols O1, O2,... stand for the trophic type for which the profile was determined (see footnote 2)

middle rows show the depth profiles of the relative pigment concentrations approximated using equation (1) for the various trophic types. The bottom rows compare the empirical and modelled pigment concentrations, where $C_{pigm, meas}$ – the measured pigment concentration and $C_{pigm, mod}$ – the pigment concentrations determined using equation (1).

Figure 1 shows that the relative concentrations of PPPs are usually the greatest at the surface and decrease with increasing optical depth. This trend is particularly conspicuous in the case of diadinoxanthin and zeoxanthin. The highest relative concentrations of these two pigments are found in oligotrophic waters (types O1, O2, O3). These relationships for the other PPPs are more complex.

The relative concentrations of PSPs (Figure 2) increase with depth, particularly in oligotrophic waters. This increase is practically monotonic; only in the case of *chl b*, *chl c* and *but* do their relative concentrations diminish below an optical depth of ca 5.

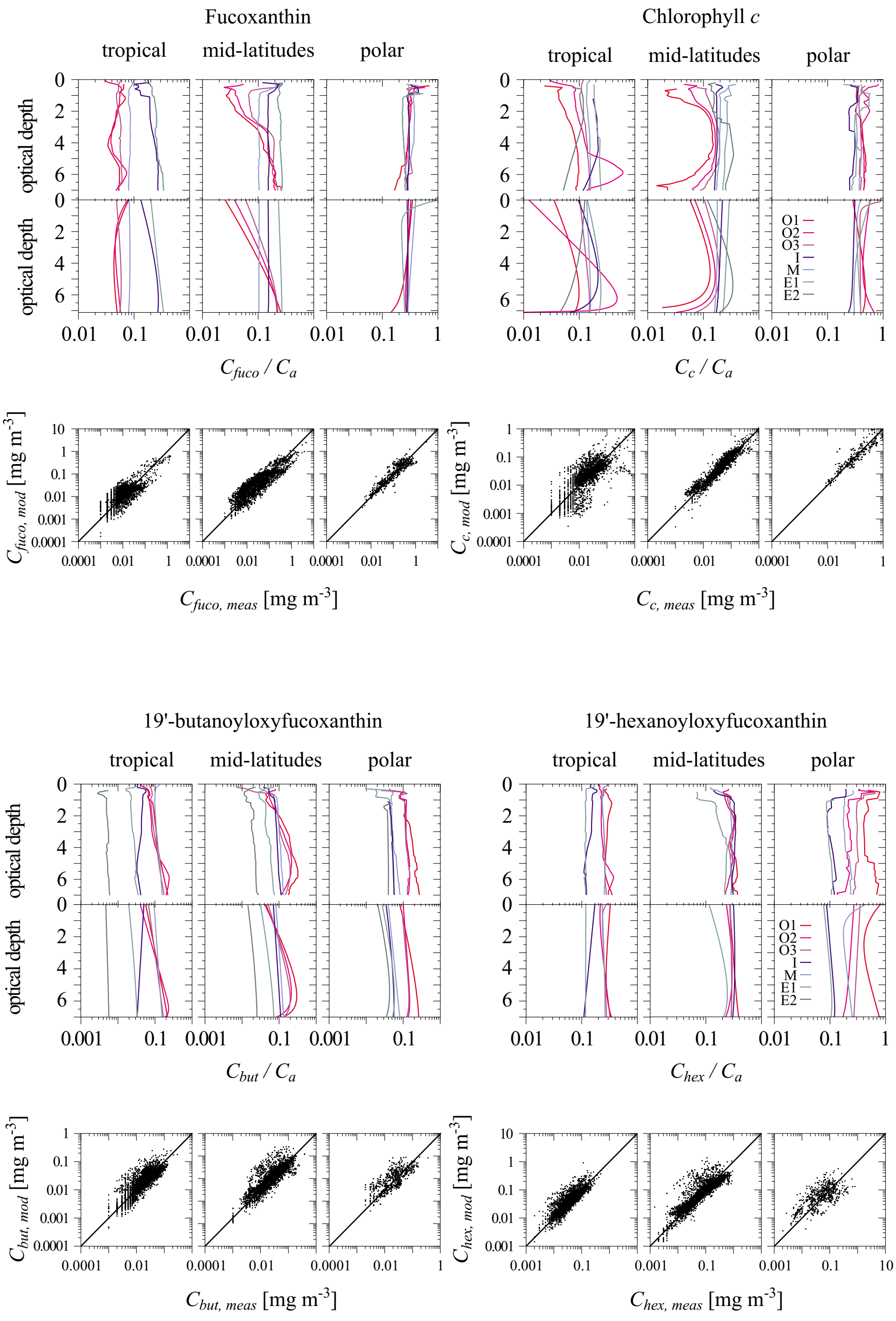

Figure 2. (*continued next page*)

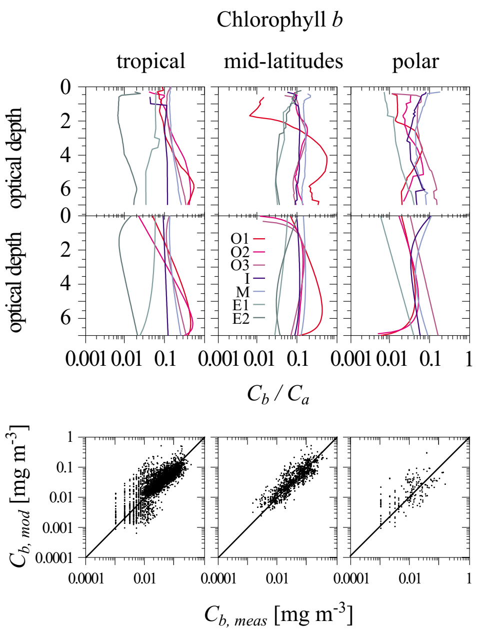

Figure 2. Mean empirical (top rows) and modelled (middle rows) depth profiles of the relative concentrations of photosynthetic pigments – fucoxanthin, chlorophyll *c*, 19'-butanoyloxyfucoxanthin, 19'-hexanoyloxyfucoxanthin, and chlorophyll *b*. The columns represent the various geographical-climatic zones. Bottom rows – comparison of empirical and modelled pigment concentrations (for description – see text). The symbols O1, O2,... stand for the trophic type for which the profile was determined (see footnote 2)

The dependence of the relative pigment concentration on the Deep Chlorophyll Maximum layer (DCM) was also analysed, but no clear relationship could be found.

Clearly, the nature of all these tendencies is complex, and a detailed elucidation for all the PPPs and PSPs covered here goes beyond the scope of the present article; in any case it requires further study.

The next step was to assess the precision of the various pigment concentrations calculated using the empirical formulas worked out here. Perusal of Table 2 (see page 565), which gives the errors in these estimates for all the pigments, shows that the errors are relatively small and in most cases comparable with the errors inherent in the empirical methods for determining pigment concentrations. Evidence for this is provided, for example, by the values of the standard error factor x (see column 5 of Table 2), which in the majority of cases are relatively low, that is, $x \leq 2$. Only in a small number cases was x larger than 2.

4. Final remarks

The empirical formulas based on equation (1), which describe the vertical distributions of algal accessory pigments, have relatively small errors and have a variety of potential applications. Knowledge of these vertical distributions can be used (i) to determine the species composition of algae, (ii) in the bio-optical modelling of the transmission of light in water and its role in photosynthesis and other processes in the marine ecosystem, and (iii) in remote sensing applications.

The search will continue to find formulas that will give a better precision of calculations. Future studies will do well to take seasonality into consideration as a factor governing the resources and composition in the sea of various PPPs and PSPs. Because of the relative paucity of the relevant empirical data, this problem was not addressed in the present work.

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References

Babin M., Morel A., Claustre H., Bricaud A., Kolber Z., Falkowski P. G., 1996, *Nitrogen- and irradiance-dependent variations of the maximum quantum yield of carbon fixation in eutrophic, mesotrophic and oligotrophic marine systems*, Deep-Sea Res. Pt. I, 43 (8), 1241–1272.

Bidigare R., 1995, *tt007 pigments*, U.S. JGOFS Data System, http://usjgofs.whoi.edu/jg/serv/jgofs/eqpac/tt007/pigments.html0.

Bidigare R., 2002a, *tt008 pigments*, U.S. JGOFS Data System, http://usjgofs.whoi.edu/jg/serv/jgofs/eqpac/tt008/pigments.html0.

Bidigare R., 2002b, *tt011 pigments*, U.S. JGOFS Data System, http://usjgofs.whoi.edu/jg/serv/jgofs/eqpac/tt011/pigments.html0.

Bidigare R., 2002c, *tt012 pigments*, U.S. JGOFS Data System, http://usjgofs.whoi.edu/jg/serv/jgofs/eqpac/tt012/pigments.html0.

Bricaud A., Babin M., Morel A., Claustre H., 1995, *Variability in the chlorophyll-specific absorption coefficients of natural phytoplankton: Analysis and parameterisation*, J. Geophys. Res., 100 (C7), 13 321–13 332.

Brunet C., Brylinski J. M., Lemoine Y., 1993, *In situ variations of the xanthophylls diadinoxanthin and diatoxanthin: photoadaptation and relationships with a hydrodynamical system of the eastern English Channel*, Mar. Ecol.-Prog. Ser., 102, 69–77.

Brunet C., Casotti R., Aronne B., Vantrepotte V., 2003, *Measured photo-physiological parameters used as tools to estimate vertical water movements in the coastal Mediterranean*, J. Plankton Res., 25 (11), 1413–1425.

Brunet C., Casotti R., Vantrepotte V., Corato F., Conversano F., 2006, *Picophytoplankton diversity and photoacclimation in the Strait of Sicily (Mediterranean Sea) in summer. I. Mesoscale variations*, Aquat. Microb. Ecol., 44 (2), 127–141.

Claustre H., Kerhervé P., Marty J.-C., Prieur L., 1994, *Phytoplankton photoadaptation related to some frontal physical processes*, J. Marine Syst., 5 (3–5), 251–265.

Goericke R., 2001a, *rr-kiwi6 HPLC pigments*, U.S. JGOFS Data System, http://usjgofs.whoi.edu/jg/serv/jgofs/southern/rr-kiwi_6/HPLC_pigments.html0.

Goericke R., 2001b, *rr-kiwi7 HPLC pigments*, U.S. JGOFS Data System, http://usjgofs.whoi.edu/jg/serv/jgofs/southern/rr-kiwi_7/HPLC_pigments.html0.

Goericke R., 2001c, *rr-kiwi8 HPLC pigments*, U.S. JGOFS Data System, http://usjgofs.whoi.edu/jg/serv/jgofs/southern/rr-kiwi_8/HPLC_pigments.html0.

Goericke R., 2001d, *rr-kiwi9 HPLC pigments*, U.S. JGOFS Data System, http://usjgofs.whoi.edu/jg/serv/jgofs/southern/rr-kiwi_9/HPLC_pigments.html0.

Jeffrey S. W., Mantoura R. F. C., Wright S. W., 1997, *Phytoplankton pigments in oceanography: Guidelines to modern methods*, UNESCO Publ., Paris, 661 pp.

Koblentz-Mishke O. I., 1971, *Same ecological and physiological properties of phytoplankton*, [in:] *Functioning of pelagic plankton communities in the tropical regions of the ocean*, M. E. Vinogradov (ed.), Nauka, Moskva, 80–87, (in Russian).

Majchrowski R., Ostrowska M., 1999, *Modified relationships between the occurrence of photoprotecting carotenoids of phytoplankton and Potentially Destructive Radiation in the sea*, Oceanologia, 41 (4), 589–599.

Margalef R., 1967, *Some concepts relative to the organisation of plankton*, Oceanogr. Mar. Biol. Ann. Rev., 5, 257–289.

Morel A., Prieur L., 1977, *Analysis of variations in ocean color*, Limnol. Oceanogr., 22 (4), 709–722.

Oubelkheir K., Claustre H., Sciandra A., Babin M., 2005, *Bio-optical and biogeochemical properties of different trophic regimes in oceanic waters*, Limnol. Oceanogr., 50 (6), 1795–1809.

Uitz J., Huot Y., Bruyant F., Babin M., Claustre H., 2008, *Relating phytoplankton photophysiological properties to community structure on large scales*, Limnol. Oceanogr., 53 (2), 614–630.

Uitz J., Claustre H., Garcia N., Griffiths F. B., Ras J., Sandroni V., 2009, *A phytoplankton class-specific primary production model applied to the Kerguelen Islands region (Southern Ocean)*, Deep-Sea Res. Pt. I, 56 (4), 541–560.

Werdell P. J., Bailey S. W., 2002, *The SeaWiFS Bio-optical Archive and Storage System (SeaBASS): Current architecture and implementation*, NASA Tech. Memo. 2002-211617 , G. S. Fargion & C. R. McClain (eds.), NASA Goddard Space Flight Center, Greenbelt, MD, 45 pp.

Woźniak B., Dera J., 2007, *Light absorption in sea water*, Atmos. Oceanogr. Sci. Libr., 33, Springer, New York, 454 pp.

Woźniak B., Dera J., Ficek D., Majchrowski R., Ostrowska M., Kaczmarek S., 2003, *Modelling light and photosynthesis in the marine environment*, Oceanologia, 45 (2), 171–245.

Woźniak B., Ostrowska M., 1990, *Composition and resources of photosynthetic pigments of the sea phytoplankton*, Oceanologia, 29, 91–115.

Wright S. W., Jeffrey S. W., 2006, *Pigment markers for phytoplankton production*, [in:] *Marine organic matter: Biomarkers, isotopes and DNA*, J. K. Volkman (ed.), Springer-Verlag, Berlin, 71–104.

Appendix

Values of coefficients a, b, c, d, e for equation (1) for the various pigments and trophic subgroups

Tropical					
	Chlorophyll *b*				
	a	*b*	*c*	*d*	*e*
O1	5.420E − 02	−4.960E − 01	−4.783E − 03	−1.858E − 01	7.808E − 01
O2	2.136E − 02	−5.606E − 01	−1.041E − 04	3.360E + 00	1.753E + 00
O3	6.278E − 02	9.117E − 01	1.409E − 03	−3.842E + 00	2.357E − 01
M	6.563E − 02	2.785E − 01	1.415E − 03	−3.854E + 00	1.838E − 01
I	8.892E − 02	−4.089E − 02	1.680E − 04	−1.752E + 00	3.783E − 02
E1	4.159E − 01	−1.086E − 01	−3.093E − 03	−4.755E + 00	1.257E − 01
E2	9.699E − 03	1.600E + 00	3.430E − 04	−2.537E + 00	2.203E − 01
	Chlorophyll *c*				
	a	*b*	*c*	*d*	*e*
O1	1.428E − 01	−3.704E − 01	−2.032E − 02	−1.668E + 00	4.043E − 01
O2	1.233E − 02	−6.761E − 01	−1.370E − 04	3.272E + 00	1.786E + 00
O3	1.025E − 01	−7.146E − 02	−5.184E − 05	3.916E + 00	1.401E + 00
M	1.362E − 01	−3.098E − 02	−7.679E − 05	3.454E + 00	1.204E + 00
I	1.241E + 00	−3.871E − 01	−6.462E − 02	−2.874E + 00	3.981E − 01
E1	1.152E + 00	−2.537E − 01	−6.002E − 02	−2.825E + 00	2.673E − 01
E2	8.008E − 01	−6.378E − 02	−4.961E − 02	−2.610E + 00	8.310E − 02
	Fucoxanthin				
	a	*b*	*c*	*d*	*e*
O1	5.378E − 02	5.501E − 01	6.259E − 03	−1.449E + 00	8.526E − 02
O2	4.313E − 02	8.510E − 01	7.034E − 04	−3.883E + 00	7.374E − 02
O3	4.907E − 02	−6.229E − 02	−3.395E − 04	−9.045E − 01	4.566E − 01
M	2.067E − 01	−7.027E − 02	−3.850E − 03	−3.481E + 00	1.034E − 01
I	5.885E − 01	−2.644E − 01	−5.125E − 03	−4.489E + 00	2.902E − 01
E1	2.008E − 01	−6.805E − 02	6.621E − 06	−4.163E + 00	5.276E − 01
E2					
	19'-butanoyloxyfucoxanthin				
	a	*b*	*c*	*d*	*e*
O1	2.761E − 01	−2.493E − 01	−1.124E − 02	−2.974E + 00	2.606E − 01
O2	4.009E − 02	−2.853E − 01	−1.335E − 08	5.924E + 00	3.120E + 00
O3	2.437E − 01	−1.327E − 01	−1.636E − 03	−4.683E + 00	1.327E − 01
M	2.550E − 01	−7.095E − 02	−1.406E − 02	−2.438E + 00	7.096E − 02
I	5.376E − 02	6.069E − 02	−1.697E − 05	−5.311E + 00	−6.193E − 02
E1	6.376E − 02	−1.551E − 01	−8.267E − 04	−3.978E + 00	1.802E − 01
E2	8.846E − 02	−6.162E − 02	−4.905E − 03	−2.838E + 00	6.331E − 02

Appendix (*continued*)

Values of coefficients a, b, c, d, e for equation (1) for the various pigments and trophic subgroups

Tropical					
	19'-hexanoyloxyfucoxanthin				
	a	*b*	*c*	*d*	*e*
O1	3.227E − 01	5.383E − 02	3.405E − 04	−5.841E − 01	7.514E − 01
O2	3.547E − 02	8.150E − 01	2.722E − 02	−1.901E + 00	8.221E − 02
O3	6.568E − 02	3.028E + 00	2.869E − 03	−4.364E + 00	3.124E − 02
M	2.670E − 01	−4.653E − 02	−6.556E − 03	−1.671E + 00	1.612E − 01
I	2.124E − 01	6.628E − 02	−6.789E − 03	−1.753E + 00	−6.719E − 02
E1	1.211E − 01	1.795E − 03	−4.008E − 03	4.769E − 01	−3.676E − 03
E2	*	*	*	*	*
	Diadinoxanthin				
	a	*b*	*c*	*d*	*e*
O1	1.844E − 01	3.795E − 01	0	0	0
O2	1.364E − 01	2.876E − 01	0	0	0
O3	7.414E − 02	1.908E − 01	0	0	0
M	7.255E − 02	1.573E − 01	0	0	0
I	6.702E − 02	1.444E − 01	0	0	0
E1	6.501E − 02	1.124E − 01	0	0	0
E2	1.026E − 01	1.917E − 01	0	0	0
	Diatoxanthin				
	a	*b*	*c*	*d*	*e*
O1	5.431E − 02	1.362E + 00	1.066E − 03	−5.255E − 03	2.714E − 02
O2	1.767E − 02	9.358E − 01	3.476E − 04	−7.453E − 01	3.384E − 01
O3	1.207E − 02	3.450E − 01	−2.116E − 04	4.960E + 00	−4.798E + 00
M	2.303E − 02	9.662E − 02	−8.878E − 04	−2.627E + 00	−2.282E − 02
I	1.137E − 02	2.127E − 01	−6.452E − 04	−2.148E + 00	−1.454E + 00
E1	6.668E − 03	2.567E − 01	2.771E − 04	1.392E + 00	4.703E − 01
E2	*	*	*	*	*
	Zeaxanthin				
	a	*b*	*c*	*d*	*e*
O1	3.511E + 00	−4.570E − 02	−1.041E − 01	−3.412E + 00	5.908E − 02
O2	1.078E + 01	7.547E − 02	−8.655E − 03	−7.061E + 00	−6.705E − 02
O3	4.467E + 00	7.626E − 02	−5.621E − 03	−6.563E + 00	−6.477E − 02
M	2.835E − 01	1.567E − 01	−4.894E − 07	2.692E + 00	1.556E + 00
I	1.375E − 01	1.697E − 01	−6.883E − 03	−2.124E + 00	−1.697E − 01
E1	1.069E − 01	1.037E − 01	−9.799E − 03	−1.991E + 00	−7.692E − 02
E2	5.585E − 02	−5.767E − 02	−8.400E − 03	−1.833E + 00	6.417E − 02

Appendix (*continued*)

Values of coefficients a, b, c, d, e for equation (1) for the various pigments and trophic subgroups

Tropical

	Alloxanthin				
	a	b	c	d	e
O1	3.679E − 05	−6.402E − 01	4.328E − 01	4.814E + 00	1.794E − 02
O2	1.072E − 03	−4.287E − 01	−2.907E − 06	4.292E + 00	1.888E + 00
O3	5.201E − 03	−6.646E − 02	−1.724E − 04	6.189E − 01	5.464E − 01
M	1.166E − 02	−3.547E − 02	−6.960E − 04	−1.031E + 00	1.704E − 01
I	1.155E − 01	−1.107E − 01	−4.818E − 03	−2.856E + 00	1.460E − 01
E1	7.770E − 02	−6.621E − 02	−3.510E − 03	−2.486E + 00	1.264E − 01
E2	1.613E − 02	4.084E − 02	5.151E − 05	4.466E + 00	1.258E + 00

	Peridinin				
	a	b	c	d	e
O1	4.520E − 02	−2.074E − 01	−3.212E − 03	−2.418E + 00	2.310E − 01
O2	4.526E − 02	−2.032E − 01	−2.887E − 03	−2.482E + 00	2.397E − 01
O3	1.850E − 02	4.240E − 02	−2.605E − 04	2.813E − 01	5.023E − 01
M	1.117E − 01	−8.184E − 02	−4.283E − 03	−3.027E + 00	1.090E − 01
I	1.952E − 02	9.618E − 02	1.023E − 03	−9.126E − 01	−7.466E − 01
E1	4.093E − 02	1.715E − 02	−2.938E − 04	−8.669E − 01	4.735E − 01
E2	1.489E + 00	1.690E − 01	−1.952E − 02	−4.217E + 00	−1.537E − 01

Mid-latitudes

	Chlorophyll b				
	a	b	c	d	e
O1	3.669E + 00	−5.980E − 01	−1.776E − 01	−3.010E + 00	6.005E − 01
O2	1.967E − 01	9.534E − 02	−4.897E − 03	−3.634E + 00	−9.434E − 01
O3	4.771E − 01	2.689E − 01	−1.561E + 00	1.091E + 00	−6.835E − 01
M	6.191E − 01	−1.514E − 01	−4.391E − 01	−8.466E − 02	1.782E − 01
I	4.913E − 01	−1.729E − 01	−4.182E − 01	5.556E − 02	1.963E − 01
E1	6.281E − 02	1.218E − 01	−4.463E − 02	1.744E + 00	−9.459E − 01
E2	2.204E − 03	−3.689E − 01	2.067E − 01	7.427E − 01	−3.728E − 01

	Chlorophyll c				
	a	b	c	d	e
O1	6.486E − 01	−4.174E − 01	−4.691E − 02	−2.534E + 00	4.310E − 01
O2	6.591E − 01	−3.958E − 01	−4.717E − 02	−2.524E + 00	4.115E − 01
O3	7.846E − 01	−3.324E − 01	−5.105E − 02	−2.590E + 00	3.514E − 01
M	1.781E − 01	−3.607E − 03	−1.706E − 03	7.974E − 01	5.004E − 01
I	2.198E − 01	2.809E − 02	−1.186E − 05	3.768E + 00	1.505E + 00
E1	2.927E − 01	3.420E − 02	−3.581E − 06	6.066E + 00	1.943E + 00
E2	1.137E + 00	−4.146E − 01	−6.215E − 02	−2.797E + 00	4.290E − 01

Appendix (*continued*)

Values of coefficients a, b, c, d, e for equation (1) for the various pigments and trophic subgroups

Mid-latitudes					
	Fucoxanthin				
	a	*b*	*c*	*d*	*e*
O1	1.299E − 01	−4.814E − 01	−3.064E − 03	−3.529E + 00	5.027E − 01
O2	2.777E − 01	−4.524E − 01	−3.425E − 02	−1.949E + 00	4.682E − 01
O3	4.374E − 01	−3.609E − 01	−3.866E − 02	−2.279E + 00	3.759E − 01
M	1.154E − 01	1.566E − 03	−7.220E − 03	−4.458E − 01	−2.548E − 03
I	1.515E − 01	−4.707E − 03	−1.876E − 05	4.225E + 00	1.403E + 00
E1	2.319E − 01	−2.406E − 02	−1.198E − 04	2.586E + 00	9.520E − 01
E2					
	19'-butanoyloxyfucoxanthin				
	a	*b*	*c*	*d*	*e*
O1	2.799E − 01	−6.026E − 01	−8.225E − 03	−3.368E + 00	6.245E − 01
O2	3.026E − 01	−5.302E − 01	−8.584E − 03	−3.405E + 00	5.517E − 01
O3	5.138E − 02	−2.896E − 01	−2.503E − 04	5.446E − 02	9.970E − 01
M	1.267E − 01	−9.884E − 02	−3.592E − 03	−2.529E + 00	1.414E − 01
I	1.182E − 01	−8.356E − 02	−3.724E − 03	−2.564E + 00	1.066E − 01
E1	9.719E − 02	−2.284E − 01	−4.344E − 03	−2.716E + 00	2.611E − 01
E2	9.131E − 02	−1.949E − 01	−4.702E − 03	−2.795E + 00	2.089E − 01
	19'-hexanoyloxyfucoxanthin				
	a	*b*	*c*	*d*	*e*
O1	2.684E − 01	−4.632E − 02	7.530E − 05	2.256E + 00	1.095E + 00
O2	1.905E + 00	−1.942E − 01	−4.404E − 02	−3.636E + 00	2.086E − 01
O3	2.769E − 01	−1.096E − 02	−1.744E − 05	3.826E + 00	1.526E + 00
M	1.053E + 00	−8.411E − 02	−3.048E − 02	−3.249E + 00	1.027E − 01
I	1.886E + 00	−9.524E − 02	−3.923E − 02	−3.691E + 00	1.089E − 01
E1	8.116E − 01	−3.101E − 01	−3.719E − 01	−6.286E − 01	3.275E − 01
E2	*	*	*	*	*
	Diadinoxanthin				
	a	*b*	*c*	*d*	*e*
O1	1.576E − 01	4.639E − 01	0	0	0
O2	7.668E − 02	2.610E − 01	0	0	0
O3	9.245E − 02	2.817E − 01	0	0	0
M	5.583E − 02	1.035E − 01	0	0	0
I	6.514E − 02	1.373E − 01	0	0	0
E1	9.150E − 02	1.381E − 01	0	0	0
E2	8.728E − 02	1.196E − 01	0	0	0

Appendix (*continued*)

Values of coefficients a, b, c, d, e for equation (1) for the various pigments and trophic subgroups

Mid-latitudes	Diatoxanthin				
	a	*b*	*c*	*d*	*e*
O1	9.000E − 02	2.045E + 00	4.308E − 02	6.223E + 00	2.449E − 01
O2	1.419E − 02	6.699E − 01	2.926E − 05	2.295E + 00	8.550E − 01
O3	1.568E − 02	6.804E − 01	8.316E − 03	3.583E + 00	1.270E − 01
M	7.206E − 03	2.531E − 01	6.537E − 04	1.104E + 00	−7.426E − 01
I	3.276E − 02	1.908E − 01	−2.869E − 03	−1.563E + 00	−9.126E − 02
E1	1.989E − 02	9.130E − 01	1.276E − 03	−1.909E + 00	−1.402E − 01
E2	2.576E − 02	1.275E + 00	1.676E − 03	−1.389E + 00	−4.145E − 02
	Zeaxanthin				
	a	*b*	*c*	*d*	*e*
O1	9.826E − 01	7.174E − 01	3.431E − 03	5.969E − 01	1.866E − 01
O2	6.112E + 00	3.726E − 01	−2.297E − 03	−7.778E + 00	−3.586E − 01
O3	2.303E + 00	2.444E − 01	−1.602E − 03	−7.119E + 00	−2.260E − 01
M	1.026E − 01	1.194E − 01	1.185E − 03	−2.273E + 00	1.489E − 01
I	1.413E − 01	1.582E − 03	−3.224E − 04	−5.310E + 00	2.921E − 02
E1	3.718E − 02	1.488E + 00	5.481E − 04	−3.412E + 00	5.697E − 02
E2	6.141E − 02	9.940E − 01	2.354E − 03	−1.640E + 00	5.882E − 02
	Alloxanthin				
	a	*b*	*c*	*d*	*e*
O1	6.490E − 03	6.640E − 02	−9.225E − 04	−1.300E + 00	1.338E − 02
O2	2.967E − 01	5.403E − 01	−6.618E − 03	−3.807E + 00	−5.650E − 01
O3	3.637E − 01	1.074E − 02	−7.998E − 03	−3.785E + 00	−7.538E − 03
M	2.291E − 02	8.690E − 03	−4.113E − 03	−1.748E − 01	9.954E − 02
I	3.773E − 01	1.882E − 01	−7.960E − 03	−3.774E + 00	−1.882E − 01
E1	8.059E − 02	2.277E − 01	−5.921E − 03	−6.595E − 01	−2.327E − 01
E2	5.287E − 02	7.130E − 02	−3.146E − 03	−3.532E − 03	−8.185E − 02
	Peridinin				
	a	*b*	*c*	*d*	*e*
O1	4.060E − 01	1.774E − 01	−2.539E − 03	−4.964E + 00	−1.616E − 01
O2	3.124E − 01	1.873E − 01	−6.259E − 03	−3.768E + 00	−1.694E − 01
O3	3.754E − 02	3.806E − 01	1.667E − 01	3.174E + 00	−3.820E − 01
M	3.087E − 02	1.928E − 01	3.987E − 04	3.482E − 01	−2.665E − 01
I	4.486E − 02	1.759E − 01	−9.396E − 06	3.009E + 00	1.220E + 00
E1	5.945E − 02	2.059E − 01	9.639E − 04	1.734E + 00	3.144E − 01
E2	5.513E − 02	1.239E − 01	7.196E − 03	−3.293E + 00	−1.245E + 01

Appendix (*continued*)

Values of coefficients a, b, c, d, e for equation (1) for the various pigments and trophic subgroups

Polar					
	Chlorophyll *b*				
	a	*b*	*c*	*d*	*e*
O1	1.648E − 01	−3.913E − 01	−2.337E − 02	−1.831E + 00	4.085E − 01
O2	7.783E − 02	−4.639E − 01	−1.543E − 02	−1.381E + 00	4.979E − 01
O3	3.295E − 02	−2.322E − 01	−2.366E − 03	4.750E − 01	2.322E − 01
M	1.232E − 02	−2.167E − 02	1.460E − 02	−3.539E − 02	−9.045E − 01
I	8.407E − 02	1.138E + 00	6.340E − 01	3.514E + 00	1.564E − 01
E1	9.155E − 02	−2.769E − 01	−7.186E − 02	−1.788E − 01	2.770E − 01
E2	*	*	*	*	*
	Chlorophyll *c*				
	a	*b*	*c*	*d*	*e*
O1	2.871E − 01	−1.162E − 01	−1.629E − 03	8.203E − 01	8.157E − 01
O2	5.777E − 01	9.335E − 02	8.640E − 04	−6.608E − 01	7.800E − 01
O3	9.526E − 01	5.839E + 00	9.470E − 02	−1.396E + 00	4.902E − 03
M	9.056E − 02	1.244E + 00	2.385E − 02	−2.555E + 00	3.662E − 02
I	3.124E − 01	1.933E − 02	−2.751E − 06	3.864E + 00	1.899E + 00
E1	4.683E − 01	3.271E − 01	3.224E − 02	−1.431E + 00	9.201E − 02
E2	*	*	*	*	*
	Fucoxanthin				
	a	*b*	*c*	*d*	*e*
O1	3.645E − 01	6.182E − 02	−1.550E − 04	2.782E − 01	9.478E − 01
O2	4.233E − 06	−1.263E + 00	9.876E + 00	3.365E + 00	−4.300E − 02
O3	3.161E − 01	−4.416E − 02	−1.871E − 02	−4.522E − 01	2.209E − 01
M	4.178E − 01	4.922E − 02	2.115E − 06	8.187E + 00	2.284E + 00
I	4.609E − 02	7.451E − 03	3.971E − 01	4.295E − 01	−7.627E − 03
E1	2.181E − 01	−2.679E − 02	1.519E − 01	−1.706E + 00	−3.474E + 00
E2					
	19'-butanoyloxyfucoxanthin				
	a	*b*	*c*	*d*	*e*
O1	4.014E − 01	−3.079E − 01	−9.553E − 03	−3.511E + 00	3.292E − 01
O2	1.001E − 01	−7.283E − 02	−4.997E − 06	3.504E + 00	1.753E + 00
O3	8.956E − 02	−9.023E − 02	−2.792E − 05	1.993E + 00	1.340E + 00
M	1.004E − 01	−1.005E − 01	−4.172E − 03	−2.676E + 00	1.005E − 01
I	1.282E − 01	−1.957E − 01	−5.185E − 03	−2.893E + 00	2.240E − 01
E1	1.521E − 01	−3.023E − 01	−5.994E − 03	−3.039E + 00	3.242E − 01
E2	1.166E − 01	−3.107E − 01	−5.251E − 03	−2.906E + 00	3.335E − 01

Appendix (*continued*)

Values of coefficients a, b, c, d, e for equation (1) for the various pigments and trophic subgroups

Polar

19'-hexanoyloxyfucoxanthin

	a	b	c	d	e
O1	5.928E − 01	7.964E − 01	1.082E − 03	−5.237E + 00	1.899E − 01
O2	2.700E − 01	4.701E − 02	−7.581E − 05	2.156E + 00	1.129E + 00
O3	3.449E − 01	3.767E − 02	1.107E − 03	−1.379E + 00	−3.473E − 02
M	2.897E − 01	2.098E + 00	1.055E − 02	−2.625E + 00	7.820E − 02
I	8.679E − 02	−5.725E − 02	−2.193E − 06	3.591E + 00	1.711E + 00
E1	7.683E − 02	−6.825E − 02	−8.449E − 04	3.492E + 00	9.497E − 01
E2	*	*	*	*	*

Diadinoxanthin

	a	b	c	d	e
O1	1.451E − 01	2.517E − 01	0	0	0
O2	1.060E − 01	1.558E − 01	0	0	0
O3	1.641E − 01	2.016E − 01	0	0	0
M	1.652E − 01	1.636E − 01	0	0	0
I	1.425E − 01	1.358E − 01	0	0	0
E1	1.036E − 01	1.025E − 01	0	0	0
E2	6.112E − 02	5.604E − 02	0	0	0

Diatoxanthin

	a	b	c	d	e
O1	*	*	*	*	*
O2	1.888E − 02	4.049E − 01	1.340E − 03	1.764E + 00	3.801E − 01
O3	1.608E − 02	2.782E − 01	2.997E − 03	2.943E + 00	−1.946E + 00
M	−1.186E − 01	1.964E − 01	1.605E − 01	1.897E − 01	−1.963E − 01
I	5.996E − 01	2.744E − 01	−1.072E + 00	6.142E − 01	−2.744E − 01
E1	5.984E − 01	2.354E − 01	−1.075E + 00	6.118E − 01	−2.354E − 01
E2	5.772E − 01	−6.474E − 02	−1.065E + 00	6.206E − 01	6.532E − 02

Zeaxanthin

	a	b	c	d	e
O1	5.404E − 02	2.554E − 01	−5.611E − 03	−1.441E + 00	−2.557E − 01
O2	6.240E − 02	2.888E − 01	−8.072E − 03	−1.794E + 00	−2.886E − 01
O3	6.248E − 02	2.891E − 01	−8.067E − 03	−1.793E + 00	−2.892E − 01
M	2.167E − 02	2.697E + 00	1.276E − 04	−3.636E + 00	−9.428E − 02
I	8.538E − 02	3.847E + 00	2.711E − 05	−4.918E + 00	−5.033E − 02
E1	3.286E − 03	5.685E − 02	1.193E − 04	1.654E + 00	2.827E − 01
E2	1.388E − 03	1.150E − 02	1.699E − 05	3.381E + 00	−3.297E + 00

Appendix (*continued*)

Values of coefficients a, b, c, d, e for equation (1) for the various pigments and trophic subgroups

Polar					
	Alloxanthin				
	a	*b*	*c*	*d*	*e*
O1	3.736E − 02	−2.131E − 01	−8.706E − 03	−8.819E − 01	2.890E − 01
O2	1.232E − 02	−2.167E − 02	1.460E − 02	−3.539E − 02	−9.045E − 01
O3	1.720E − 02	8.252E − 02	−1.390E − 03	8.375E − 01	−1.740E − 01
M	9.341E − 02	−3.509E − 02	−1.549E − 02	−1.523E + 00	6.722E − 02
I	4.649E − 02	1.321E − 01	−3.819E − 03	−1.322E − 01	−1.438E − 01
E1	1.946E − 01	−1.447E − 01	−2.264E − 02	−1.930E + 00	1.731E − 01
E2	*	*	*	*	*
	Peridinin				
	a	*b*	*c*	*d*	*e*
O1	1.322E − 01	5.283E − 01	2.442E − 03	−1.407E + 00	−5.367E − 01
O2	2.441E − 01	3.171E + 00	8.336E − 02	1.409E + 00	−4.939E − 02
O3	3.153E − 02	−4.834E − 02	−2.824E − 04	−1.802E − 01	5.893E − 01
M	3.060E − 02	−2.153E − 02	−1.454E − 07	4.866E + 00	2.039E + 00
I	2.241E − 02	4.850E − 01	1.018E − 01	2.667E + 00	4.124E − 02
E1	1.952E − 02	1.484E − 01	−4.929E − 04	−1.607E − 01	−2.347E − 01
E2	2.297E − 02	1.014E + 00	1.957E − 03	−1.806E + 00	−7.299E − 02

* – no data available.