

Empirical ocean color algorithms and bio-optical properties of the western coastal waters of Svalbard, Arctic

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ARTICLE INFO

Article history:

Received 5 December 2017

Received in revised form 17 March 2018

Accepted 23 March 2018

Available online 2 April 2018

Keywords:

Ocean color algorithms

Svalbard

Coastal waters

Chlorophyll

Total suspended matter

ABSTRACT

Chlorophyll (Chl) concentration is one of the key indicators identifying changes in the Arctic marine ecosystem. However, current Chl algorithms are not accurate in the Arctic Ocean due to different bio-optical properties from those in the lower latitude oceans. In this study, we evaluated the current Chl algorithms and analyzed the cause of the error in the western coastal waters of Svalbard, which are known to be sensitive to climate change. The NASA standard algorithms showed to overestimate the Chl concentration in the region. This was due to the high non-algal particles (NAP) absorption and colored dissolved organic matter (CDOM) variability at the blue wavelength. In addition, at lower Chl concentrations (0.1–0.3 mg m⁻³), chlorophyll-specific absorption coefficients were ~2.3 times higher than those of other Arctic oceans. This was another reason for the overestimation of Chl concentration. OC4 algorithm-based regionally tuned-Svalbard Chl (SC4) algorithm for retrieving more accurate Chl estimates reduced the mean absolute percentage difference (APD) error from 215% to 49%, the mean relative percentage difference (RPD) error from 212% to 16%, and the normalized root mean square (RMS) error from 211% to 68%. This region has abundant suspended matter due to the melting of tidal glaciers. We evaluated the performance of total suspended matter (TSM) algorithms. Previous published TSM algorithms generally overestimated the TSM concentration in this region. The Svalbard TSM-single band algorithm for low TSM range (ST-SB-L) decreased the APD and RPD errors by 52% and 14%, respectively, but the RMS error still remained high (105%).

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1. Introduction

In recent studies, climate models predict that sea ice will disappear in the near future during the Arctic summer (e.g., Stroeve et al., 2012; Overland and Wang, 2013). Rapidly declining Arctic sea ice is changing the Arctic marine ecosystem, including an earlier occurrence of the phytoplankton bloom and increased primary production (Arrigo et al., 2008; Kahru et al., 2011; Vancoppenolle et al., 2013; Ji et al., 2013; Arrigo and Dijken, 2015). Satellite remote sensing is useful for short- or long-term monitoring of these changes in the Arctic Ocean, where direct access is difficult. Chlorophyll (Chl) concentration derived from satellite images has been effectively used to calculate the primary production of the Arctic Ocean (Arrigo et al., 2008; Arrigo and Dijken, 2015). However, several studies have confirmed that the Chl concentrations assessed using the NASA standard algorithms in the Arctic Ocean are different from the in situ measured Chl concentrations (Cota

et al., 2003; Stramska et al., 2003; Matsuoka et al., 2007; Mustapha et al., 2012). The NASA standard Chl algorithms such as OC2S, OC4 (SeaWiFS) and OC3M (MODIS) are mainly based on field data in low and mid-latitude regions. Because the bio-optical properties of the Arctic Ocean are different from those in waters at lower latitude, these algorithms can produce larger errors at high latitudes than at lower latitudes.

The NASA standard Chl algorithms in the Labrador Sea and the north polar region of the Atlantic Ocean generally overestimated Chl at low concentrations and underestimated Chl at high concentrations (Cota et al., 2003, 2004; Stramska et al., 2003). The reason for the underestimation of Chl in this region is known to be the strong packaging effect of large-size phytoplankton (mainly diatoms). On the other hand, the reason that Chl is overestimated at low concentration is due to the high variability in the ratio of colored dissolved organic matter (CDOM) to total non-water absorption versus Chl concentration (Cota et al., 2003). In the western Arctic Ocean including the coastal waters of the Beaufort and Chukchi seas, previous studies have shown that the NASA standard algorithms overestimated the Chl concentration due to the high

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contribution of CDOM and non-algal particles (NAP) (Wang and Cota, 2003; Mustapha et al., 2012; Chaves et al., 2015). To solve these problems in Arctic and Sub-Arctic waters, regionally tuned and semi-analytical algorithms have been proposed (Cota et al., 2003; Mustapha et al., 2012; Chaves et al., 2015). However, most of these studies have evaluated and developed algorithms in the oceans between 70° and 75°N. Studies at high latitudes above 75°N, such as Svalbard, and on coasts with complex optical properties, are very limited, especially in the fjords. Stramska et al. (2003) investigated linkages between ocean color algorithms and bio-optical properties in the north polar region of the Atlantic including the western ocean waters of Svalbard. However, this study excluded fjords and coastal waters of western Svalbard affected by terrestrial input. Shanmugam et al. (2013) evaluated MODIS bio-optical algorithms on the western coastal waters of Svalbard. They identified a significant difference between the Chl algorithm-derived results and in situ data, and speculated that these errors were because of the large-size phytoplankton and CDOM. However, this study did not clearly explain the relationship between the bio-optical properties and these errors.

Consequently, the main objective of this study is to assess the performance of current ocean color algorithms in the western coastal waters of Svalbard including fjords and to develop empirical algorithms to estimate Chl and total suspended matter (TSM) reflecting the regional bio-optical properties (Fig. 1). We will assess statistically the bio-optical properties such as phytoplankton and the NAP and CDOM absorption coefficients in the western Svalbard coastal waters comparatively with other regions. This will help us understand the bio-optical properties of this region and develop empirical ocean color algorithms.

2. Study area

The study area includes coastal waters and two fjords, Kongsfjorden and Krossfjorden surrounded by large tidewater glaciers in its inner parts (Fig. 1). The area shows subarctic environment characteristics due to the West Spitsbergen Current (WSC) that transports warm and saline Atlantic Water (AW) northward. Between the WSC and the Kongsfjorden-Krossfjorden system, colder, less saline Arctic Water (ArW) flows northward in a coastal current. Unlike many Arctic fjords, the Kongsfjorden-Krossfjorden system does not have a sill in its mouth, which makes it easier

for warm waters from the WSC to flow into the fjords (Svendsen et al., 2002). The fjord system normally has the maximum amount of AW during the late summer and the fjord water masses are replaced by the ArW (Cottier et al., 2005).

The warm WSC keeps the west coast of Svalbard ice free. The inner part of Kongsfjorden is usually covered by sea ice between December and March and persisting until June. However, in February 2006, the intrusion of massive AW into the fjord resulted in the fast ice of the Kongsfjorden melting very quickly compared to a normal year (Cottier et al., 2007; Gerland and Renner, 2007). Over the next two winters (2007 and 2008), there was also no fast and drift ice in the fjord and on the coast. This indicates that the fjord water mass is increasingly warmer (Gerland et al., 2007; Hegseth and Tversbeg, 2013).

The biological ecosystem, such as plankton species composition, varies seasonally along with freshwater discharge from snow and glaciers, solar radiation, wind patterns, tidal currents and topographical steering in the Kongsfjorden-Krossfjorden system. The seasonal pattern of phytoplankton in Kongsfjorden shows a marine ecosystem with the main biomass accumulation occurring during the spring and a low-biomass-regenerating system predominating during the summer. Previous studies have shown that the spring blooms appear mainly in April and May (Hop et al., 2002; Hodal et al., 2011; Hegseth and Tversbeg, 2013). Neritic diatom species dominate the phytoplankton assemblage during the spring and are replaced by a regenerating community dominated by smaller flagellates and dinoflagellates during the summer (Lydersen et al., 2014). Particularly during the summer, the suspended sediments caused by glacier calving at the head of fjords become rich, which leads to high turbidity waters. It decreases the depth of the euphotic and impact phytoplankton composition and primary productivity (Piwoz et al., 2009).

3. Materials and methods

3.1. Analysis of water samples

The water samples used in this study were collected from three field campaigns which were conducted from 6 to 11 August 2006, from 12 to 17 June 2007, and from 4 to 11 June 2008. The location of the field data is shown in Fig. 1. For Chl measurements, surface ocean water was collected using a water sampler and filtered through a 47-mm GF/F filter. Filters were stored in 20-ml vials with 10 ml of 90% acetone for 24 h at 4 °C refrigeration. PTFE type syringe filters (25 mm) were used to remove impurities such as cellular debris. The Chl optical density (OD) was measured using a dual-beam spectrophotometer (Perkin Elmer, Lambda 19) and the Chl concentration was calculated using the equation proposed by Jeffrey and Humphrey (1975). For TSM, surface waters were filtered using a 25-mm pre-weighed GF/F filter. The filters were rinsed with distilled water to remove salt remaining on the filter surface. The filters were dried in a 60 °C oven for 4 h and then reweighed using a microbalance. The difference in filter weight before and after filtration was determined as the TSM concentration.

The absorption coefficients of total particles, $a_p(\lambda)$, and nonalgal particles, $a_{NAP}(\lambda)$, were measured following the protocol of Kishino et al. (1985). Surface ocean waters are collected and filtered (25-mm GF/F filter) using the same methods as the process of TSM. After baseline measurement, the OD of particulate matter ($OD_f(\lambda)$) and the OD of the blank GF/F filter ($OD_{bf}(\lambda)$) were measured using a dual-beam spectrophotometer ranging from 350 to 900 nm. The $a_p(\lambda)$ and $a_{NAP}(\lambda)$ were calculated as follows:

$$a_{PorNAP}(\lambda) = \frac{(OD_f(PorNAP)(\lambda) - OD_{bf}(\lambda) - OD_{null}(\lambda)) \times 2.303}{(V/A) \times \beta} \quad (1)$$

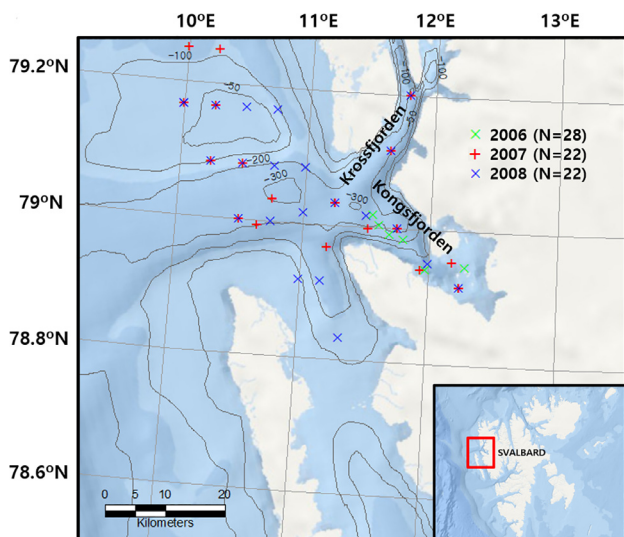


Fig. 1. Sampling locations of the field data are displayed in different colors for 3 field campaigns.

where V is the volume of filtered water, S is the area of filter, and β is the path amplification constant (set to 2) (Roesler, 1998). The mean $OD_f(\lambda)$ in the 10-nm interval 790 nm to 800 nm was used as the null value, OD_{null} , of $a_p(\lambda)$ and $a_{NAP}(\lambda)$ (Mitchell et al., 2003). After measuring $OD_p(\lambda)$, the sample filters were immersed in pure methanol to measure $OD_{fNAP}(\lambda)$ to completely remove the pigment. The absorption coefficients of phytoplankton, $a_p(\lambda)$ is determined as follows:

$$a_p(\lambda) = a_p(\lambda) - a_{NAP}(\lambda) \quad (2)$$

Surface ocean waters for $a_{CDOM}(\lambda)$ analyses were filtered through 25-mm syringe filters and collected into a clean 50-ml glass bottle. The filtered sample waters were used to measure OD spectra using 10-cm quartz optical cell and a dual beam spectrophotometer. The $a_{CDOM}(\lambda)$ was calculated as follows:

$$a_{CDOM}(\lambda) = \frac{(OD_s(\lambda) - OD_{bs}(\lambda) - OD_{null}(\lambda)) \times 2.303}{l} \quad (3)$$

where l is the cuvette pathlength (0.1 m), $OD_s(\lambda)$ is the optical density of the filtrate sample cell, $OD_{bs}(\lambda)$ is optical density of a purified water blank cell, and OD_{null} is the average optical density at the wavelength where absorption by CDOM is assumed to be zero.

3.2. Above-water optical measurements

Above-water reflectance measurements were collected using an ASD FieldSpec 512 channel radiometer covering a spectral range of 350–1050 nm immediately after water sample acquisition. A dual spectrometer unit with two fiber optic cables was used to measure downwelling irradiance (E_d) and total upwelling radiance (L_t) simultaneously from above the water. The L_t and L_s (sky radiance) were measured at a viewing direction of approximately 30° from the nadir and zenith, respectively. The azimuth angle to measure L_t and L_s was maintained at 135° from the Sun. The R_{rs} was calculated according to Eq. (4) as follows:

$$R_{rs} = \frac{L_t - \rho L_s}{E_d} \quad (4)$$

where ρ is the sea surface reflectance factor of sky conditions, wind speed, solar zenith angle, and viewing geometry. If ρ is not estimated accurately, significant errors can occur in the estimated R_{rs} . The aforementioned corrections using a ρ value are often inaccurate due to the residual surface reflection, ε in Eq. (5) as follows:

$$R_{rs} = \frac{L_t - \rho L_s}{E_d} - \varepsilon \quad (5)$$

Ruddick et al. (2005, 2006) proposed an algorithm for the improvement of sky glint correction. They analyzed and tabulated as a similarity spectrum by normalization at 780 nm, and estimated the ε using measurements at 720 nm and 780 nm as follows:

$$\varepsilon = \frac{\alpha(720, 780)R_{rs}(780) - R_{rs}(720)}{\alpha(720, 780) - 1} \quad (6)$$

where $\alpha(720, 780)$ can be read from the tabulated similarity spectrum from Ruddick et al. (2006). In this study, the sky glint effect was corrected using this method.

3.3. Ocean color algorithms

The performance of the NASA Chl standard algorithms (OC3M, OC2S, and OC4) and one Arctic algorithm (OC4L) for Chl estimating was evaluated (Table 1). These algorithms commonly are based on the relationship between the Chl concentration and a blue-to-green band ratio of R_{rs} . The band ratio of each algorithm consists

Table 1

Description of NASA Chl standard algorithms and global and regional TSM algorithms used in this study.

Algorithm	Equation	Reference
OC3M.v6	Chl = $10^{0.2424 - 2.5828R + 1.70578R^2 + 0.3415R^3 - 0.8818R^4}$ $R = \log_{10} \left[\frac{\text{Max}(R_{rs}(443), R_{rs}(448))}{R_{rs}(551)} \right]$	O'Reilly et al. (1998)
OC2S.v6	Chl = $10^{0.2511 - 2.0853R + 1.5305R^2 - 3.1747R^3 + 0.3383R^4}$ $R = \frac{R_{rs}(490)}{R_{rs}(555)}$	
OC4.v6	Chl = $10^{0.3272 - 2.994R + 2.7218R^2 - 1.2259R^3 - 0.5683R^4}$ $R = \log_{10} \left[\frac{\text{Max}(R_{rs}(443), R_{rs}(490), R_{rs}(510))}{R_{rs}(555)} \right]$	
OC4L	Chl = $10^{0.592 - 3.607R}$ $R = \log_{10} \left[\frac{\text{Max}(R_{rs}(443), R_{rs}(490), R_{rs}(510))}{R_{rs}(555)} \right]$	Cota et al. (2004)
EA-SB-H	TSM = $700 \times R_{rs}(645)$	Darlington (2015)
SAA-L	TSM = $\frac{384.11 \times \rho_w(670)}{\left(1 - \frac{\rho_w(670)}{0.1747}\right)} + 1.44$ $\rho_w(670) = \pi \times R_{rs}(670)$	Han et al. (2016)
EA-MB-L	TSM = $10^{0.451 + 22.674R1 - 0.399R2}$ $R1 = R_{rs}(555) + R_{rs}(670), R2 = \frac{R_{rs}(490)}{R_{rs}(555)}$	

of 2 to 4 bands in the spectrum region of 443 to 555 nm depending on the band element of the satellite sensor.

To estimate TSM, we evaluated the Multi-Bands Empirical Algorithm, EA-MB-L, originally developed by Tassan (1994), and the second semi-analytical algorithm, SAA-L, originally developed by Nechad et al. (2010), both of which are new algorithms recently tuned for a global low TSM range (<100 g m⁻³) by Han et al. (2016). The Single Band Empirical Algorithm, EA-SB-H, was also tested. The EA-SB was originally developed by Miller and McKee (2004), and its coefficients were tuned to fit the Kongsfjorden high turbidity waters (>50 g m⁻³) in Svalbard by Darlington (2015).

3.4. Evaluation criteria

The performance of the algorithms was evaluated through error estimation such as the normalized root mean square (RMS, %) error, mean absolute percentage difference (APD, %), and mean relative percentage difference (RPD, %) (e.g. Darecki and Stramski, 2004; Ouillon and Petrenko, 2005; Siswanto et al., 2011; Cui et al., 2014). These errors are defined as follows:

$$\text{RMS} = \text{stdev} \left(\frac{y_{\text{alg}} - y_{\text{is}}}{y_{\text{is}}} \right) \times 100 \quad (7)$$

$$\text{APD} = \text{mean} \left| \frac{y_{\text{alg}} - y_{\text{is}}}{y_{\text{is}}} \right| \times 100 \quad (8)$$

$$\text{RPD} = \text{mean} \left(\frac{y_{\text{alg}} - y_{\text{is}}}{y_{\text{is}}} \right) \times 100 \quad (9)$$

where y_{alg} is the Chl or TSM concentration derived from the algorithm and y_{is} is the concentration value measured in situ. RMS indicates random error, APD provides an accuracy or uncertainty, and RPD denotes systematic error or direction of bias. The squared correlation coefficient and slope between the log-transformed retrieved and measured values were also calculated. Mean and standard deviation are defined as follows:

$$\text{Mean}(x) = \bar{x} = \frac{1}{N} \sum_{i=1}^N x_i \quad (10)$$

$$\text{Stdev}(x) = \left[\frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2 \right]^{1/2} \quad (11)$$

where x is the variable of interest and N is the number of in situ data.

4. Results

4.1. Evaluation of Chl algorithms

Fig. 2a shows a comparison between Chl concentration derived using three NASA Chl standard algorithms and one Arctic algorithm and the in-situ-measured Chl concentration. These algorithms generally overestimated the Chl, especially at low Chl concentrations (Fig. 2b). The uncertainty in estimated Chl concentration from the algorithms was the highest during August 2006 (APD, 561–1622%) and the lowest during June 2007 (APD, 121–209%) (Table 2). All Chl algorithms showed much smaller RMS, APD and RPD and a much higher coefficient of determination (R^2) in the June 2007 data. On the other hand, in the August 2006 data, the algorithm estimates were very inaccurate (RMS, APD and RPD were too high and the R^2 too low). This is closely related to the TSM concentration, and details are given in the next section. The OC3M and OC4 algorithms showed better performance than the other algorithms, except for the 2006 data, which had large errors. The APD (209%) and RPD (203%) errors for OC3M are the lowest among the algorithms used, and the OC4 showed the lowest RMS (211%). The results of the Arctic OC4L algorithm exhibited the highest APD (262%) and RPD (261%) errors.

4.2. Evaluation of TSM algorithms

The TSM algorithms provided better performance (a higher R^2 and a slope close to 1) in August 2006 data than in June 2007 and June 2008 data (Fig. 3a and Table 3). In particular, there was no relationship between the algorithm-derived and field-measured TSM concentrations in the June 2007 data. The EA-SB algorithm provides the lowest RPD (66%) for the whole data set excluding the June 2007 data that has an R^2 that is too low and an inappropriate slope. The EA-MB-L algorithm showed better performance in the RMS (154%) and APD (92%), but it had a higher RPD (86%) than that of the EA-SB. The SAA-L algorithm provides the highest R^2 (0.75) but it overestimates TSM by up to 192% (RPD) for the whole data set excluding the June 2007 data. This algorithm

Table 2

Statistical results for the validation of various Chl algorithms.

Period		OC3M.v6	OC2S.v6	OC4.v6	OC4L
Aug. 2006 (N = 17)	RMS (%)	746	715	974	1921
	APD (%)	594	561	780	1622
	RPD (%)	594	561	780	1622
	R^2	0.11	0.14	0.21	0.21
	Slope	−0.08	−0.08	−0.12	−0.13
Jun. 2007 (N = 18)	RMS (%)	97	114	99	112
	APD (%)	121	143	129	209
	RPD (%)	118	141	129	209
	R^2	0.79	0.77	0.82	0.85
	Slope	0.60	0.55	0.62	0.84
Jun. 2008 (N = 17)	RMS (%)	441	453	513	934
	APD (%)	395	438	419	584
	RPD (%)	385	428	413	583
	R^2	0.43	0.45	0.46	0.42
	Slope	0.31	0.28	0.37	0.52
All (N = 34 ^a or 33 ^b)	RMS (%)	213	235	211	220
	APD (%)	209	242	215	262
	RPD (%)	203	235	212	261
	R^2	0.68	0.69	0.72	0.73
	Slope	0.45	0.41	0.50	0.75

^a In the comprehensive statistical evaluation including all periods, data with an APD greater than 1000% were excluded.

^b The number of samples is 34 (OC3M), 34 (OC2S), 34 (OC4), and 33 (OC4L), respectively.

tended to be more inaccurate in low TSM concentration ($<1.0 \text{ g m}^{-3}$) (Fig. 3b).

Compared to that of June 2007 and June 2008, in the August 2006 data, the TSM algorithms showed relatively high accuracy and the Chl algorithms showed low accuracy (Tables 2 and 3). All data for August 2006 were obtained within the Kongsfjorden, while the data for June 2007 and 2008 included offshore samples (Fig. 1). The shape of the in situ R_{rs} spectra obtained during August 2006 is similar to that of the spectrum with turbid water having a high reflectance near the red wavelength (620–740 nm) (Fig. 4a). In contrast, the R_{rs} spectra of waters measured during June are similar to the spectrum of clean water with low values near the red wavelength (Fig. 4b and c). In fact, the TSM concentrations measured during August 2006 and June 2007 are similar. Nonetheless, the R_{rs} for June 2007 differs in shape from the reflectance spectra typically found in turbid water (Fig. 4a and b). This is probably due to a difference in optical contribution depending on the TSM component. More details are given in Section 4.3.2.

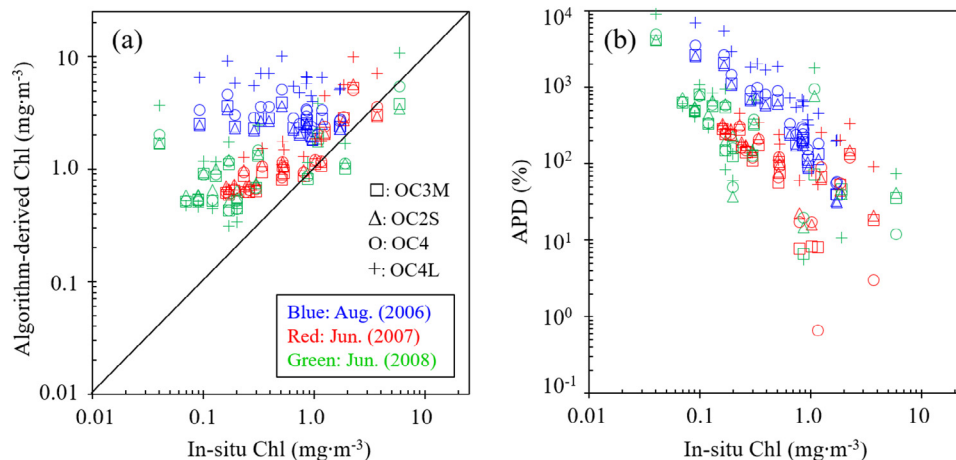


Fig. 2. (a) Comparison between in situ and algorithm-derived Chl concentrations. (b) Variation of APD with Chl concentrations.

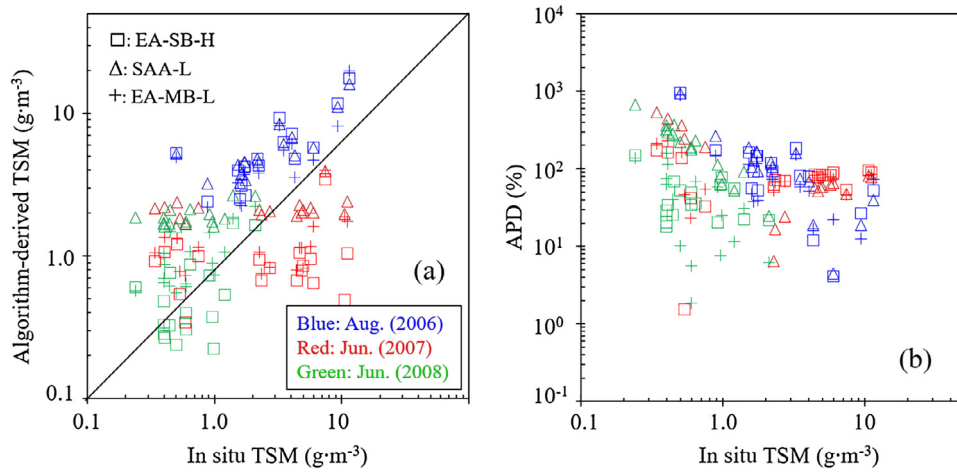


Fig. 3. (a) Comparison between in-situ and algorithm-derived TSM concentrations. (b) Variation of APD according to TSM concentrations.

Table 3
Statistical results for the validation of various TSM algorithms.

Period		EA-SB	SAA-L	EA-MB-L
Aug. 2006 (N = 17)	RMS (%)	215	213	206
	APD (%)	143	156	122
	RPD (%)	142	156	116
	R ²	0.57	0.61	0.49
	Slope	0.51	0.42	0.49
Jun. 2007 (N = 18)	RMS (%)	91	200	107
	APD (%)	83	143	89
	RPD (%)	-26	75	-8
	R ²	0.03	0.07	0.17
	Slope	0.06	0.04	0.14
Jun. 2008 (N = 17)	RMS (%)	56	162	70
	APD (%)	46	228	61
	RPD (%)	-11	228	56
	R ²	0.33	0.49	0.46
	Slope	0.16	0.48	0.52
All (N = 34) ^a	RMS (%)	173	190	154
	APD (%)	94	192	92
	RPD (%)	66	192	86
	R ²	0.70	0.75	0.74
	Slope	1.14	0.56	0.83

^a 34 is the number excluding June 2007 data.

4.3. Bio-optical properties

4.3.1. Phytoplankton absorption

The empirical relationship between $a_{\varphi}(\lambda)$ and Chl concentration in Case 1 waters can be derived by least squares fitting to power functions (Bricaud et al., 1995, 1998) as follows:

$$a_{\varphi}(\lambda) = A_{\varphi}(\lambda)[Chl]^{B_{\varphi}(\lambda)} \quad (12)$$

$$a_{\varphi}^*(\lambda) = A_{\varphi}(\lambda)[Chl]^{B_{\varphi}(\lambda)-1} \quad (13)$$

where $A_{\varphi}(\lambda)$ and $B_{\varphi}(\lambda)$ are wavelength-dependent constants. The relationship between Chl concentration and $a_{\varphi}(443)$ in the region is as follows:

$$a_{\varphi}(443) = 0.0411(\lambda)[Chl]^{0.5681}, R^2 = 0.71, n = 68 \quad (14)$$

The correlation between Chl concentration and $a_{\varphi}(443)$ ($R^2 = 0.71$) was relatively weak compared to that of the other regions (Fig. 5a). This is related to the study region being a coastal area where Case 1 and Case 2 waters are mixed. Previous studies mainly

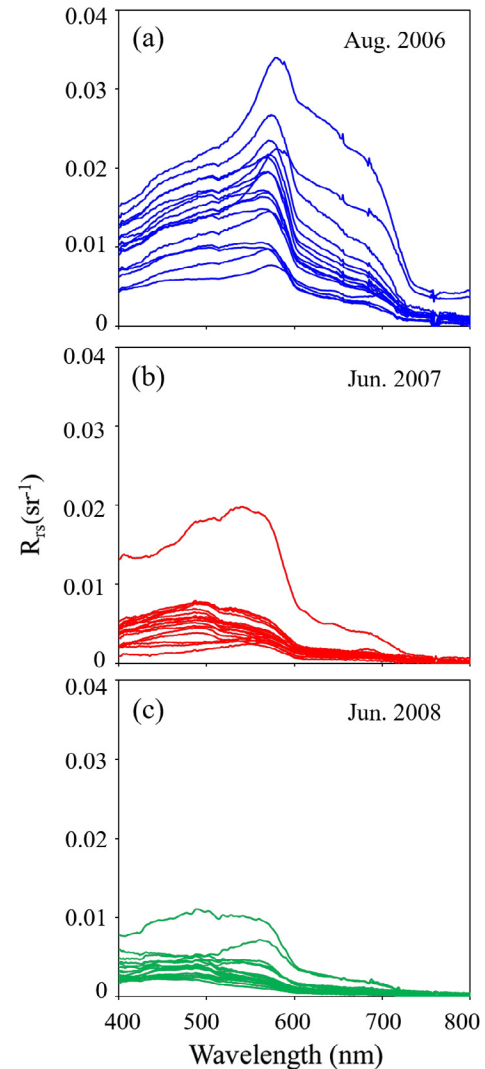


Fig. 4. R_{rs} spectra in the western coastal waters of Svalbard during (a) August 2006, (b) June 2007, and (c) June 2008.

were from Case 1 waters. The trend between the two variables in this study is similar to that of Bricaud et al. (1998) and Cota et al. (2003) investigating in various oceanic waters (Case 1) and

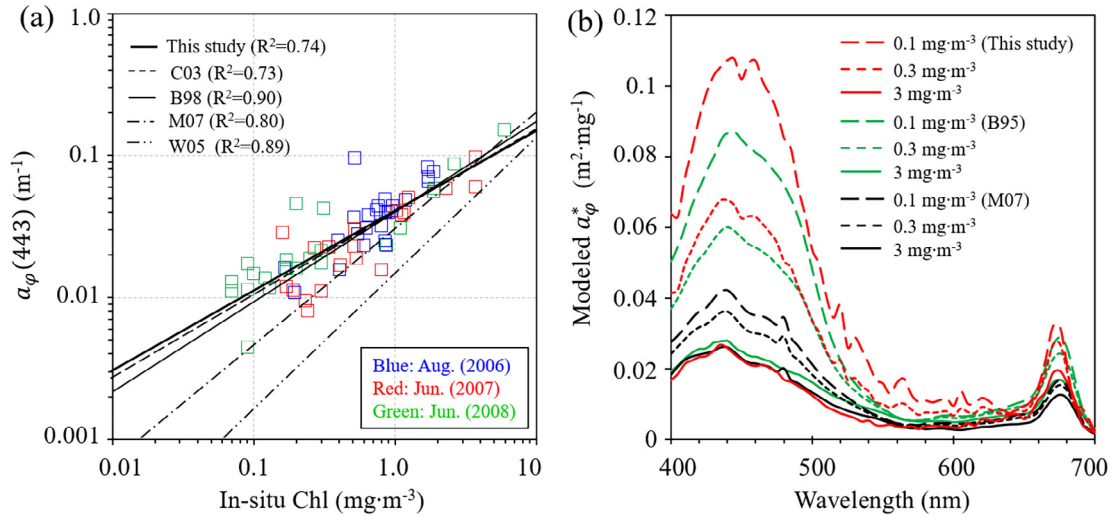


Fig. 5. (a) Relationship between $a_{\phi}(\lambda)$ and Chl concentration at 443 nm. Regression lines of previous studies are illustrated for comparison (C03: Cota et al. (2003), B98: Bricaud et al. (1995), M07: Matsuoka et al. (2007), W05: Wang et al. (2005)). (b) $a_{\phi}^*(\lambda)$ spectra for various values of the Chl concentration (0.1 to 3 mg m⁻³) reconstructed from the power function (Red color). The $a_{\phi}^*(\lambda)$ spectra of Bricaud et al. (1995) and of Matsuoka et al. (2007) are illustrated by the green color (B95) and black color (M07), respectively, for comparison.

in the Labrador Sea, respectively. Our trend line is most similar to the trend of the Labrador Sea. The trend of $a_{\phi}(443)$ versus Chl concentration in this study is also similar to that of Babin et al. (2003) identified on the coastal waters around Europe (not shown in Fig. 5a). In contrast, it is much different from the trends of Wang et al. (2005) and Matsuoka et al. (2007) observed in the western Arctic Ocean. The difference between our trend and the trend of the western Arctic Ocean could be caused by many factors such as accessory pigment composition and concentration, packaging effect, light adaptation, cell size, and etc. (Bricaud et al., 1995; Cota et al., 2003). This difference is more evident through a comparison of the chlorophyll-specific absorption coefficient of phytoplankton, $a_{\phi}^*(\lambda)$.

Fig. 5b presents the “mean” $a_{\phi}^*(\lambda)$ spectra for three values of the Chl concentration (0.1, 0.3, and 3 mg m⁻³) reconstructed by Eq. (13). At low Chl concentrations (0.1 and 0.3 mg·m⁻³), the $a_{\phi}^*(\lambda)$ of the study region is greater than that of the other regions (the lower-latitude oceans and western Arctic Ocean) at the same Chl concentration. This difference mainly occurs due to the packaging effect and the difference in accessory pigment concentration. Assessment of the pigment packaging effect is most effective in the red absorption band near 675 nm that is least affected by accessory pigments (Bricaud et al., 1995). Cota et al. (2003) reported a highly packaged red (670–676 nm) peak of 0.010 m² (mg Chl)⁻¹ for a_{ϕ}^* of large diatoms near the Labrador Sea. Larger cells tend to increase the pigment packaging effect that reduces the absorption of light by the pigments, and do not contain numerous accessory pigments compared with those of pico-sized phytoplankton (Bricaud et al., 1995; Cota et al., 2003). In the western Arctic Ocean, the averaged $a_{\phi}^*(676)$ value was 0.014 m² (mg Chl)⁻¹ suggesting a significant pigment packaging effect (Wang et al., 2005). By contrast, the mean $a_{\phi}^*(675)$ value for our study region is 0.023 m² (mg Chl)⁻¹. This value is within the red peak values between 0.020 and 0.029 m² (mg Chl)⁻¹ reported in polar waters that are dominated by Phaeocystis with no or less pigment-packaging effect (Moisan and Mithchel, 1999; Stuart et al., 2000), which suggests that our study region has a low pigment-packaging effect. To better understand the phytoplankton social structure, we performed size classification. According to the size classification, the proportion of nano- (2–20 μm) and pico- (<2 μm) sized phytoplankton was high (2006: 99%, 2007: 83%, 2008:

61%). At the stations with low Chl concentrations, the standing crops (cells l⁻¹) of unidentified pico-sized phytoplankton were overwhelmingly high. The dominance of these small-sized phytoplankton is closely related to the high $a_{\phi}^*(\lambda)$ at low Chl concentrations in this region (Fig. 5b). Conversely, at high Chl concentrations (3 mg m⁻³), our $a_{\phi}^*(\lambda)$ was similar to $a_{\phi}^*(\lambda)$ in other regions with the packaging effect (Fig. 5b). At the stations with high Chl concentrations (>3 mg m⁻³), we found phytoplankton blooms caused by the dominance of large diatoms or by the colony-forming prymnesiophyte Phaeocystis with large diatoms, which suggests that our region can also have the packaging effect at high Chl concentrations.

4.3.2. Nonalgal particle absorption

The $a_{NAP}(443)$ obtained from three surveys were generally higher than those found in previous studies (Fig. 6a). Particularly, during August 2006, $a_{NAP}(443)$ was higher as the Chl concentration was lower, and the $a_{NAP}(443)$ and Chl concentrations were inversely correlated as follows:

$$a_{NAP}(443) = 0.1195(\lambda)[Chl]^{-0.402}, R^2 = 0.28, n = 28 \quad (14)$$

The relationship between $a_{NAP}(443)$ and Chl during August 2006 [Eq. (14)] is related to the failure of the Chl algorithms in 2006 (blue color in Fig. 2; Table 2). A relatively close relationship [$R^2 = 0.62$ in Eq. (15)] between the $a_{NAP}(443)$ and Chl in June 2008 partially explains why Chl was overestimated in 2008 (green color in Fig. 2; Table 2).

$$a_{NAP}(443) = 0.0299(\lambda)[Chl]^{0.5461}, R^2 = 0.62, n = 22 \quad (15)$$

Fig. 6b shows that the contribution to $a_p(443)$ by $a_{NAP}(443)$ is very large and variable, especially, at low Chl concentrations (<1 mg·m⁻³). Our value range of $a_{NAP}(443)/a_p(443)$ between 0.26 and 0.99 is higher than that between 0.2 and 0.8 observed in global oceanic waters of previous studies (Cleveland, 1995; Bricaud et al., 1998). Therefore, nonalgal particles in our region would have played a larger role in overestimating Chl at low Chl concentrations (Fig. 2).

The absorption spectrum by nonalgal particles can be formulated as an exponential function (Roesler et al., 1989; Bricaud et al., 1998) as follows:

$$a_{NAP}(\lambda) = a_{NAP}(\lambda_0) \exp^{-S(\lambda - \lambda_0)} \quad (16)$$

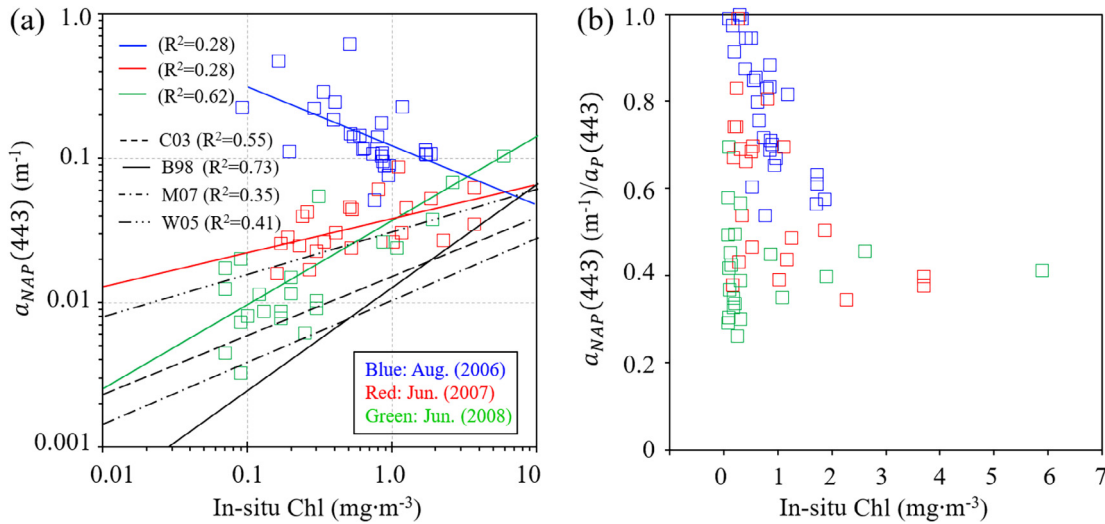


Fig. 6. Relationship between $a_{NAP}(443)$ and Chl concentration. Regression lines of previous studies are illustrated for comparison (C03: Cota et al. (2003), B98: Bricaud et al. (1995), M07: Matsuoka et al. (2007), W05: Wang et al. (2005)). (b) Ratio of $a_{NAP}(443)$ to $a_P(443)$ versus Chl concentration.

where λ_0 is the reference wavelength and 443 nm is used in this study. We used only data ranging between 380 and 730 nm, excluding the 400–480 and 620–710 nm ranges to avoid any residual absorption by pigment when fitting the exponential function (Babin et al., 2003). The slope, S_{NAP} , value estimated from the measured a_{NAP} ranged between 0.007 and 0.014 nm⁻¹, with an average value of 0.010 ± 0.0017 nm⁻¹. The average value is similar to that obtained in previous studies (0.011 ± 0.0017 – 0.0025 nm⁻¹) (Roesler et al., 1989; Bricaud et al., 1998).

Fig. 7 shows examples of representative $a_{NAP}(\lambda)$ spectra obtained from three surveys. These spectra are provided with the reconstructed spectra in exponential form [Eq. (16)]. The values of $a_{NAP}(\lambda)$ spectra during August 2006 and June 2008 are higher as the concentration of TSM is higher (Fig. 7a and c). On the other hand, during June 2007, the values of the $a_{NAP}(\lambda)$ spectra do not change proportionally to the TSM concentration (Fig. 7b), and are very small compared to those of the $a_{NAP}(\lambda)$ spectra with similar TSM concentrations during August 2006 (Fig. 7a and b). During August 2006 and June 2008, the $a_{NAP}(\lambda)$ spectra values are higher than the exponential spectra at 470–570 nm and lower than the exponential spectra at wavelengths shorter than 470 nm (Fig. 7a and c). These features are similar to $a_{NAP}(\lambda)$ which exhibit spectral features near 450–550 nm by inorganic suspended matter (ISM), such as minerals (Babin et al., 2003). These features are not shown in the $a_{NAP}(\lambda)$ spectra of June 2007 (Fig. 7), which may be due to component difference in the TSM concentrations, such as organic suspended matter (OSM). Unfortunately, we cannot definitely prove this because we did not measure ISM and OSM separately. However, despite the high TSM concentration, the low R_{rs} spectra during June 2007 (Fig. 4b) are presumably due to the low backscattering coefficients by OSM, which is why the TSM algorithm failed. Excluding the data of June 2007, we obtained a linear relationship between the TSM concentration and the $a_{NAP}(\lambda)$ ($R^2 = 0.82$), and the trend was very similar to that identified by Babin et al. (2003) (Fig. 8).

4.3.3. CDOM absorption

There is no correlation between the absorption of CDOM at 443 nm and Chl concentration in the Svalbard coastal waters (Fig. 9a). The following equation shows only 2% of the variability of the absorption by CDOM (443), which is the same as that measured in the Labrador Sea by Cota et al. (2003).

$$a_{CDOM}(443) = 0.0751(\lambda)[Chl]^{0.061}, R^2 = 0.02, n = 72 \quad (17)$$

The relationship is meaningless as an error can easily exceed 2%. Variability in CDOM cannot be explained by Chl alone, but rather by the combined effects of many biological, chemical, and physical processes (Wang et al., 2005). The fraction of absorption contribution by CDOM to the total non-water absorption, $a_{CDOM}(443)/a_{t-w}(443)$, in Svalbard coastal waters is significantly lower (33–64%) than that measured in other Arctic waters (65–84%) (Table 4). This means that the contribution of CDOM absorption in the region is not as great as that in other Arctic waters. In addition, in 2006, the contribution of $a_{NAP}(443)$ to $a_{t-w}(443)$ was higher (51%) than that of $a_{CDOM}(443)$ (33%).

The $a_{CDOM}(\lambda)$ spectrum, similar to the $a_{NAP}(\lambda)$ spectrum (equation (16)), shows an exponential decline with increasing wavelength. The S_{CDOM} values estimated from the measured $a_{CDOM}(\lambda)$ spectra range between 0.006 and 0.024 nm⁻¹, with an average value of 0.011 ± 0.0034 nm⁻¹. These values are similar to those reported by previous studies. Our S_{CDOM} values are in a broader range having a slightly lower mean than the values reported by Kirk (1986) who observed S_{CDOM} varying from 0.010 to 0.020 nm⁻¹, with mean values between 0.012 and 0.015 nm⁻¹ in typical seawaters. Cota et al. (2003) reported that the mean value of S_{CDOM} was 0.013 ± 0.002 nm⁻¹ in the Labrador Sea.

The low covariance between CDOM and Chl (Fig. 9a) can degrade the accuracy of Chl retrievals by producing non-systematic errors in the Chl algorithms using blue-to-green ratios (Carder et al., 1989; DeGrandpre et al., 1996). In addition, the fact that the relationship between the ratio of $a_{CDOM}(443)$ to $a_P(443)$ and the Chl concentration is highly variable at low Chl concentrations suggests that the accuracy of the Chl algorithms can be reduced by CDOM at low Chl concentrations, especially as observed during June 2008 (Fig. 9b).

5. Discussion

The Arctic OC4L algorithm was originally designed to replace the NASA Chl standard algorithms that underestimated the Chl concentration in a region with a high packaging effect (see Cota et al., 2004). Therefore, this model was not suitable for our region where the Chl concentration is overestimated. The NASA Chl standard algorithms were designed for Case 1 waters and do not fully

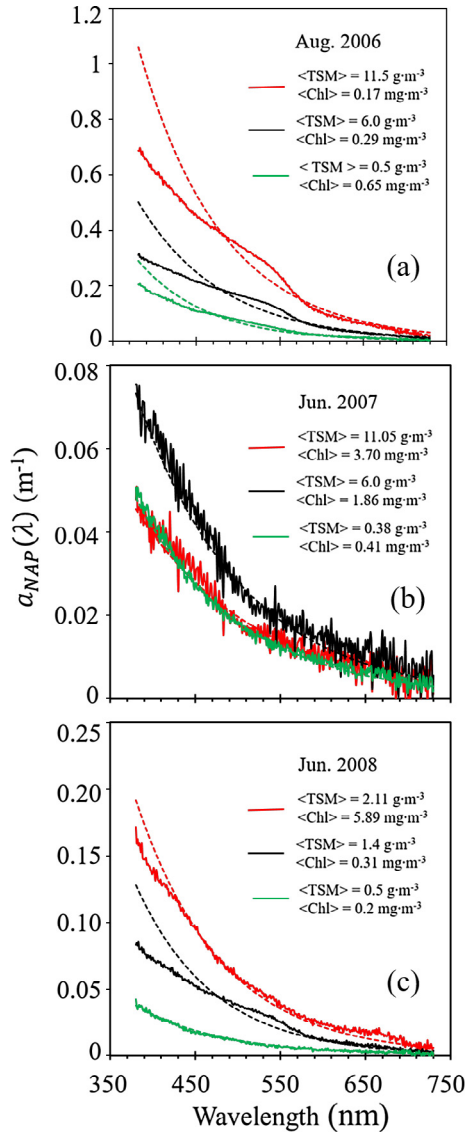


Fig. 7. Examples (a-c) of nonalgal particle absorption spectra (solid lines) and the corresponding exponential fit (dashed lines) from three surveys.

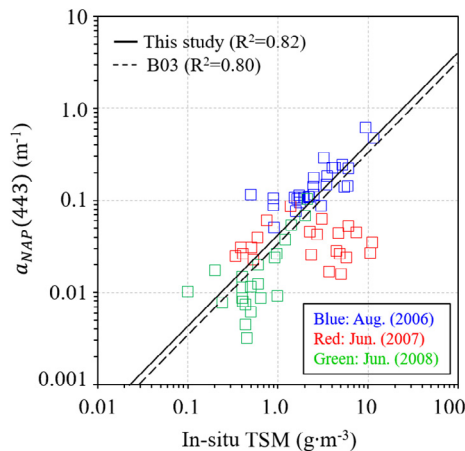


Fig. 8. Scatterplot of $a_{NAP}(443)$ as a function of TSM. Regression line is illustrated for comparison with previous study derived by [Babin et al. \(2003\)](#).

reflect the biological characteristics of the polar oceans because the experimental dataset does not contain much polar data. As previously mentioned (in [Section 2](#)), the western coastal waters of Svalbard are affected by both fresh water from fjord glaciers and seawater from the ArW and AW. This indicates that this area can have Case 1 waters and Case 2 waters separately or together. These regional properties may have led to the poor performance of the NASA Chl standard algorithms.

The total APD and RPD errors of OC3M were 209% and 203%, respectively, except for the 2006 data and the stations with unrealistically high overestimations ($APD > 1000\%$) ([Table 2](#)). The APD error of OC3M in our region is lower than the error ($APD = 284\%$) estimated by a semi-analytical algorithm (GSM01) in the south-eastern Beaufort Sea ([Mustapha et al., 2012](#)). However, the APD and RPD errors are much higher than the errors reported for the Mediterranean Sea (OC4 APD: 92% and RPD: 78%; [Volpe et al., 2007](#)) and around the Korea Peninsula (OC3M APD: 71% and RPD: 46%; [Kim et al., 2016](#)). Our RMS error of 213% (OC3M) is higher than that of 120% in the Gulf of Lions (OC2S; [Ouillon and Petrenko, 2005](#)) and that of 155% in the Baltic Sea (OC4; [Darecki and Stramski, 2004](#)). The level of error in our region is similar to or higher than that shown in previous studies in other coastal regions. This is probably because our region is located at a higher latitude and is situated on more complex coastal environmental conditions (e.g., the tide glacier and mixed water mass in fjord) compared to those of previous studies.

The concentration of TSM within the Kongsfjorden is generally higher than offshore because of sediment laden meltwater originating from the calving of tidewater glaciers ([Svendsen et al., 2002](#)). The decline in velocity of the Kronbreen's glacier, which has the greatest effect on the turbidity of Kongsfjorden, reaches its maximum in July. The speed slows down gradually during August ([Schellenberger et al., 2015](#)). Therefore, the TSM concentration in the Kongsfjorden increases during July and August, and can have a significant impact on the performance of the Chl algorithm.

[Fig. 10a](#) shows the relationship between the measured Chl concentration and the blue-to-green band ratio of R_{rs} calculated using the NASA Chl standard algorithms (OC3M, OC2S, and OC4 in [Table 1](#)). It displays a general pattern in which the band ratio value decreases with increasing Chl concentration. Data affected by strong absorption by NAP (blue in [Fig. 6](#)) and CDOM ($a_{CDOM}(443)/a_P(443) > 4$ in [Fig. 9b](#)) were considered unusual stations and excluded from the development of the empirical Chl algorithms ([Fig. 10a](#)). This strong absorption in the blue band by NAP and CDOM causes a low blue-to-green band ratio value and leads to an abnormal overestimation of the Chl concentration ([Fig. 2](#) and [Table 1](#)).

From the empirical relationship between the measured blue-to-green band ratio and Chl concentration in the coastal waters of Svalbard, we established empirical Chl algorithms derived by power functions ([Fig. 10a](#)). The empirical Chl algorithms, termed Svalbard Chl (SC)-3M, -2S, and -4, are defined as follows:

$$SC3M : Chl = 1.1699 \left[\frac{\text{Max}\{R_{rs}(443), R_{rs}(448)\}}{R_{rs}(551)} \right]^{-3.683}, R^2 = 0.74 \quad (18)$$

$$SC2S : Chl = 1.1663 \left[\frac{R_{rs}(490)}{R_{rs}(555)} \right]^{-3.493}, R^2 = 0.74 \quad (19)$$

$$SC4 : Chl = 1.3608 \left[\frac{\text{Max}\{R_{rs}(443), R_{rs}(490), R_{rs}(510)\}}{R_{rs}(555)} \right]^{-3.8}, R^2 = 0.77 \quad (20)$$

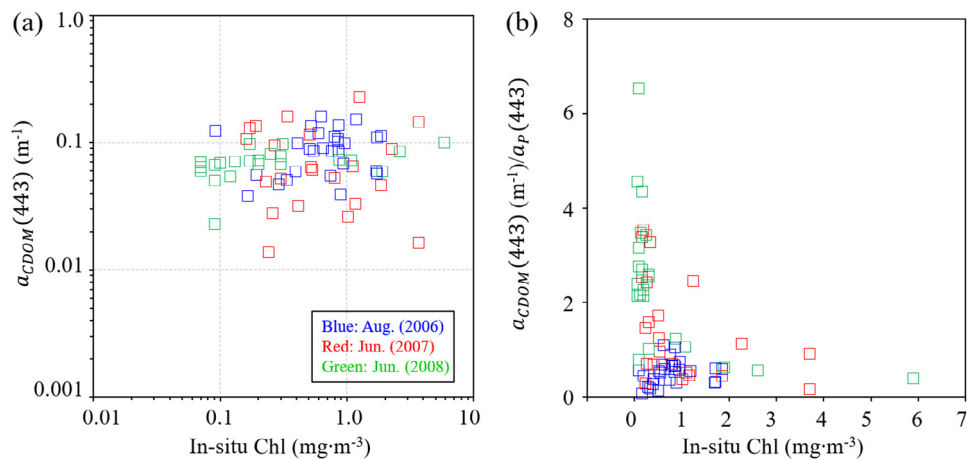


Fig. 9. (a) Relationship between $a_{CDOM}(443)$ and Chl concentration. (b) Ratio of $a_{CDOM}(443)$ to $a_P(443)$ versus Chl concentration.

Table 4
Relative contributions of absorption coefficient for phytoplankton, nonalgal particles, and CDOM to the total non-water absorption at 443 nm.

	Ares	Date (m/y)	n	$a_P(443)/a_{t-w}(443)$	$a_{NAP}(443)/a_{t-w}(443)$	$a_{CDOM}(443)/a_{t-w}(443)$
This study	Coastal waters, western Svalbard	08/06	25	0.16 ± 0.09	0.51 ± 0.17	0.33 ± 0.11
		06/07	21	0.22 ± 0.13	0.28 ± 0.14	0.50 ± 0.19
		06/08	22	0.21 ± 0.09	0.15 ± 0.09	0.64 ± 0.16
Babin et al. (2003)	Coastal waters, Europe	4–9/97–98	317	0.36 ± 0.14	0.22 ± 0.13	0.41 ± 0.14
Matsuoka et al. (2007)	Western Beaufort and Chukchi	9–10/04	183	0.16 ± 0.11	0.08 ± 0.05	0.76 ± 0.13
Matsuoka et al. (2009)	Southeastern Beaufort	9–10/03	50	0.07 ± 0.04	0.09 ± 0.06	0.84 ± 0.08
		10–11/03	102	0.11 ± 0.07	0.15 ± 0.08	0.74 ± 0.09
Brunelle et al. (2012)	Amundsen Gulf	5–7/08	20	0.21	0.07	0.72
		10–11/07	10	0.11	0.21	0.68
	Canadian Archipelago	10–11/07	6	0.21	0.14	0.65
Mustapha et al. (2012)	Southeastern Beaufort	6–8/04	46	0.13 ± 0.09	0.17 ± 0.10	0.70 ± 0.14

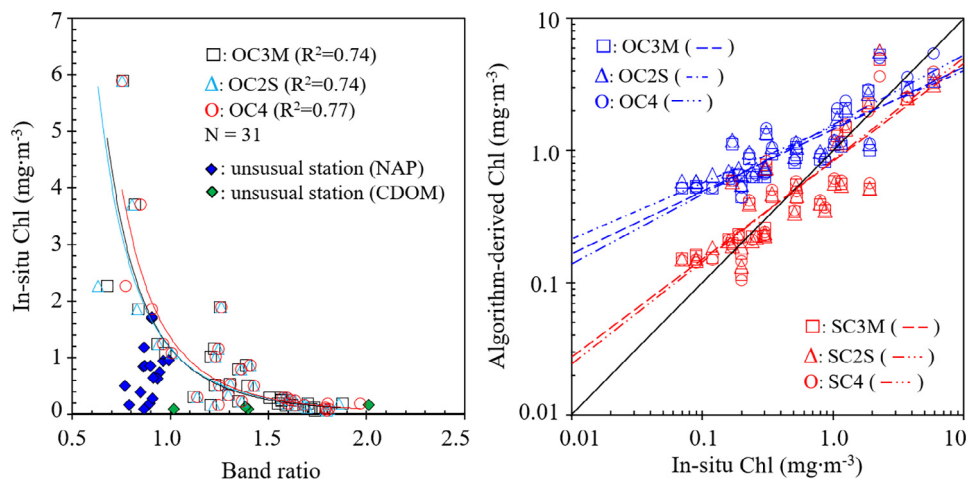


Fig. 10. (a) Relationship between the measured Chl concentration and the blue-to-green band ratio of R_{rs} (OC3M, OC2S, and OC4 in Table 1). Diamonds represent unusual stations by NAP and CDOM. (b) Estimated Chl concentrations using NASA Chl standard algorithms (blue) and empirical Chl algorithms (red).

These empirical algorithms have a greatly reduced error compared with that of the NASA Chl standard algorithms (e.g., the OC3M APD error is 209%, while the SC3M error is 51%, see Table 2 and 5) and are effective in adjusting the overestimation at low chlorophyll concentrations less than $1.0 \text{ mg} \cdot \text{m}^{-3}$ (Fig. 10b). As previously mentioned, this overestimation is associated with high absorption by NAP, CDOM and small-size phytoplankton. The SV4 based on max band ratios of SeaWiFS (OC4) is the best algorithm in the western coastal waters of Svalbard

Table 5
Statistical results for the validation of empirical Chl algorithms.

Period		SC3M	SC2S	SC4
All (N = 31)	RMS (%)	70	71	68
	APD (%)	51	51	49
	RPD (%)	17	17	16
	R^2	0.74	0.74	0.77
	Slope	0.74	0.74	0.77

although systematic error still exists (RPD = 16%). The random error for the SV4 remains high (RMS = 68%), but it is significantly lower than that for the OC4 algorithm (RMS = 211%) (Tables 2 and 5). The slope was also improved from 0.5 to 0.77 and the R^2 was slightly better (0.77 versus 0.72). In fact, the three empirical algorithms (SC3M, SC2S, and SC4) showed no significant difference in the statistical evaluation (Table 5). Therefore, the SV3M and SC2S algorithms can also be used effectively in this region.

The coefficients of the EA-SB-L and EA-MB-L algorithms were regionally tuned using in situ R_{rs} as follows:

$$ST - SB - L : TSM = 420.86[R_{rs}(645)] + 0.1206, R^2 = 0.72 \quad (21)$$

$$ST - MB - L : TSM = 10^{0.088 + 22.369[R_{rs}(555) + R_{rs}(670)] - 0.256\left[\frac{R_{rs}(490)}{R_{rs}(555)}\right]}, R^2 = 0.75 \quad (22)$$

In situ TSM data for 2007, which are not considered to be TSM concentration by NAP (Fig. 7b and 8), were excluded from the data set for empirical TSM algorithm development. These empirical algorithms with retuned coefficients estimate the TSM concentration more precisely than the original algorithm (Fig. 11). The Svalbard TSM-single band algorithm for low TSM range (ST-SB-L) reduces the statistical error values (RMS: 105% instead of 173%, APD: 52% instead of 94%, and RPD: 14% instead of 66%) in estimating the TSM concentration compared to the Darlington algorithm (EA-SB) and makes the slope closer to 1 (from 1.13 to 0.98) (Tables 3 and 6). The Svalbard TSM-multi-band algorithm for low TSM range (ST-MB-L) reduces the error value more than two-fold compared with the EA-MB-L algorithm of Han et al. (2016), but the slope value is rather farther from 1 (from 0.83 to 0.74).

Our results show that in the western coastal waters of Svalbard, very different bio-optical characteristics occur even during the summer of a similar time. This is due to the very complex environ-

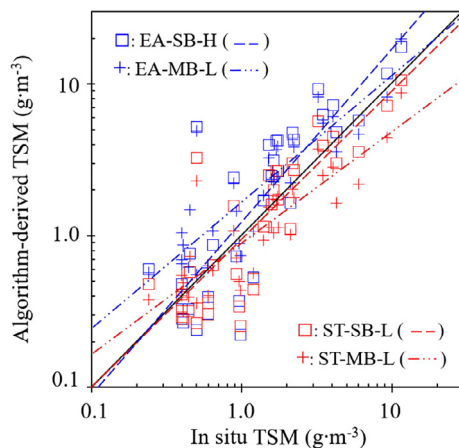


Fig. 11. Estimated TSM concentration using original TSM algorithms (blue) and empirical TSM algorithms (red).

Table 6
Statistical results for the validation of empirical TSM algorithms.

Period		ST-SB-L	ST-MB-L
All (N = 34)	RMS (%)	105	72
	APD (%)	52	40
	RPD (%)	14	–5
	R^2	0.72	0.75
	Slope	0.98	0.74

mental characteristics (fjords, tidal glaciers, etc.) of this region. Therefore, regional algorithms are of particularly needed in this region. We note that the empirical algorithms presented in this study were made using a relatively small data set, therefore, they should be tested and improved using a larger data set from this region. Semi-analytical inversion models (e.g. Carder et al., 1999; Maritorena et al., 2002; Budhiman et al., 2012; Chen et al., 2014; Watanabe et al., 2016) or hybrid algorithm proposed by Matsushita et al. (2015) can also be considered as alternatives in this region, but these methods are not always superior to empirical algorithms (see O'Reilly et al., 1998; Mustapha et al., 2012). Various models have to be further tested to find algorithms that fit the high latitude Arctic coastal environment in future work.

6. Conclusions

We evaluated the performance of the NASA Chl standard algorithms and the published TSM algorithms using in situ data collected during the summer (June and August) from 2006 to 2008 in the western coastal waters of Svalbard, Arctic. The results showed that the standard and published ocean algorithms tended to largely overestimate the Chl and TSM concentrations in the region. In particular, the fraction of absorption contribution by NAP to the total non-water absorption observed in this region, especially during August 2006 (51%), was significantly higher than that of other polar and Europe coastal waters (7–22%). This is caused by the suspended sediments originating from a glacier calving at the head of the fjords. The high $a_{\phi}^*(\lambda)$ due to the dominance of small size (nano and pico) phytoplankton is another reason for the overestimation at low Chl concentrations ($<1 \text{ mg m}^{-3}$) in this region. We found that in low Chl concentrations (0.1 to $0.3 \text{ mg} \cdot \text{m}^{-3}$), the mean $a_{\phi}^*(667)$ with $0.023 \text{ m}^2 (\text{mg Chl})^{-1}$ in Svalbard coastal waters is larger than that with 0.010 – $0.014 \text{ m}^2 (\text{mg Chl})^{-1}$ of other regions such as the lower-latitude oceans and western Arctic Ocean.

In the June 2007 data, the TSM algorithms completely failed to estimate the TSM concentration. The R^2 between algorithm-derived and in situ TSM concentrations was only 0.03 to 0.17. This is probably because the TSM concentrations were mainly OSM rather than ISM. R_{rs} value may not increase in proportion to TSM concentration due to the low backscattering coefficient of OSM (Stavn and Richter, 2008). We found that the values of $a_{NAP}(443)$ measured during June 2007 do not increase in proportion to TSM concentration. Except for 2007, which failed to estimate the TSM concentration, the published TSM algorithms overestimated the TSM concentration because they were developed for high TSM concentrations.

The results from regionally tuned algorithms for the Svalbard coastal waters modifying the standard Chl algorithms significantly reduced errors. The SC4 algorithm for retrieving Chl concentration showed the best result; the RPD decreased from 212% to 16% and the RMS from 211% to 68%. We also obtained regionally tuned coefficients for published TSM algorithms for TSM retrieval. For the ST-SB-L algorithm, the APD and RPD errors were reduced to 52% and 14%, respectively, with a slope closer to 1 (0.98), but the RMS error still remained high (105%).

Acknowledgments

This study was supported by the Korea Polar Research Institute (KOPRI) Grant PE18120 (Research on analytical technique for satellite observation of arctic sea ice). The authors thank Jeong-Eon Moon from Korea Institute of Ocean Science and Technology (KIOST) for his help on field measurements.

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