Impact of iron associated to organic matter on remote sensing estimates of lake carbon content

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ARTICLE INFO

ABSTRACT

There is a strong need to develop remote sensing methods for mapping lake carbon content on regional to global scales. The use of in situ methods is impractical for monitoring lake water quality over large geographical areas, which is a fundamental requirement to understand the true role of lakes in the global carbon cycle. The coloured component of dissolved organic carbon (DOC), called CDOM, absorbs light strongly in the blue part of the visible spectrum and can be used as a proxy for mapping lake DOC with remote sensing. However, iron associated to organic matter can cause extra browning of waters. Consequently, the remote sensing signal we interpret as DOC may partially be attributed to the presence of iron associated to organic matter, potentially hampering our ability to estimate carbon concentrations.

A thorough analysis of biogeochemical parameters was carried out on Lake Mälaren on August 23, 2010, and a MERIS full resolution image was acquired simultaneously. MERIS standard, Case 2 Regional, and Boreal processors were used to calculate remote sensing products, which were compared with different lake water characteristics.

The carbon to iron ratio was different from the rest of the lake in one of the basins. MERIS standard and Case 2 Regional processors were sensitive to this difference as the correlation between MERIS CDOM product and DOC was low ($R^2 = 0.43$) for all sampling stations and increased to 0.92 when the one basin was excluded. The Boreal Lakes processor results were less disturbed by the different carbon–iron ratios found in one basin and produced reasonably good results ($R^2 = 0.65$).

We found MERIS products (e.g. total absorption) that provided good correlation ($R^2 = 0.80$) with DOC-specific absorbance at 254 nm, called SUVA, which is a metric commonly used to assess drinking water treatability. However, none of the MERIS products were suitable for mapping the total organic carbon in Lake Mälaren. MERIS total suspended matter product was a good ($R^2 = 0.73$) proxy for particulate iron, meaning that the particulate iron content in Mälaren can be mapped from space.

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1. Introduction

Recent studies indicate that lakes play an important role in the global carbon cycle (IPCC, 2013; Tranvik et al., 2009). In addition, over recent decades there has been an increase in the amount of dissolved organic matter (DOM) and browning of many surface waters, at least in boreal and hemiboreal zones for which long time data series exist (Weyhenmeyer, Prairie, & Tranvik, 2014). DOM is an important substrate for microorganisms including bacteria and algae (Tranvik, 1992), and hence in some cases can promote fouling of water, causing problems of taste, odour, and hygiene. Moreover, disinfection of water still containing DOM may result in the formation of carcinogenic chlorinated organic by-products (McDonald & Komulainen, 2005). The need for higher doses of chlorine can enhance the risk of bladder and rectal cancers (Koivusalo, Pukkala, Vartiainen, Jaakola, & Hakulinen, 1997). Likewise, excess DOM in source water results in the need to add higher doses of costly flocculants (Eikebrokk, Vogt, & Liltved, 2004; Matilainen, Vepsalainen, & Sillanpää, 2010).

Despite efforts to remove DOM, the efficiency of DOM removal is highly variable between drinking water treatment plants, which is largely attributed to the varying qualities of DOM (Valade, Becker, & Edzwald, 2009). An easy to measure proxy for DOM quality is the carbon specific UV absorbance (SUVA), which is a useful way of predicting the general chemical characteristics of DOM, particularly the aromatic content of DOM (Weishaar et al., 2003). For several decades, water treatment plants have routinely monitored the SUVA of source waters to

detect changes in its treatability, particularly the potential ease of DOM removal (Edzwald, Becker, & Wattier, 1985). For these reasons, developing a means of estimating the SUVA of surface waters remotely would be highly valuable to the drinking water industry.

Lake monitoring programmes have detected increasing DOM content over the past several decades (Weyhenmeyer et al., 2014). However, lake monitoring is expensive and requires large field crews and the extent of field sampling is limited, both spatially and temporally. There is a strong need to develop remote sensing methods for mapping lake carbon content at larger regional and global scales. Current estimates on the role of lakes in the global carbon cycle (Tranvik et al., 2009) were obtained by upscaling in situ measurements from a few thousand lakes to a statistical estimate of the global distribution of lakes. However, Seekel and Pace (2011) have shown that the Pareto distribution used to produce the global lake abundance estimates (Downing et al., 2006; Lehner & Döll, 2004) contains very large uncertainty, especially in the case of small lakes that comprise the majority of the lakes on Earth. To determine the true role of lakes at a global scale, one needs more accurate numbers on both the abundance of lakes in the world, and better estimates of lake carbon concentrations. Mapping tens of millions of small lakes and collection of in situ data about carbon content in majority of them is not feasible. Recently, mapping of lakes on a global scale was achieved. Verpoorter, Kutser, and Tranvik (2012) developed a methodology to recognise water bodies from 14.25 m spatial resolution Landsat GeoCover mosaics covering practically the whole Earth "land" surfaces and a map of all water bodies greater than 0.2 ha (Verpoorter, Kutser, Tranvik, & Seekel, 2014). Developing more reliable carbon retrieval algorithms is also a work in progress (Brando, Dekker, Park, & Schroeder, 2012; Kallio et al., 2001; Kallio et al., 2008; Kutser, Pierson, Kallio, Reinart, & Sobek, 2005; Kutser, Tranvik, & Pierson, 2009; Kutser et al., 2005; Shuchman et al., 2013). However, there is a need to validate the developed algorithms before the global lake carbon estimate can be produced. There are potentially confusing factors for lake carbon remote sensing (like high concentration of phytoplankton or strongly absorbing sediment) that remote sensing scientists are aware of, but one of the unknown factors is the presence of iron associated to organic matter in lake waters. Our aim was to address this issue in the present study.

The MEdium Resolution Imagining Spectrometer, MERIS, was the best sensor to be used in large lake monitoring over the previous decade, with a 300 m spatial resolution, nearly daily coverage in higher latitudes, and some spectral bands designed for remote sensing of optically complex coastal and inland waters. MERIS was launched on March 1, 2002 and was operational until April 8, 2012. A follow-up instrument OLCI (Ocean and Land Colour Instrument) with a few extra spectral bands is due to be launched on Sentinel-3 in 2015. MERIS had several processors (standard Ground Segment — MEGS, Case 2 Regional, Boreal Lakes, etc.) and each of them with products (yellow substances (CDOM), the diffuse attenuation coefficient of light at 490 nm — $K_d(490)$, turbidity index, etc.) that may be suitable for mapping lake carbon content.

In many areas of the world, 90–95% of organic carbon in lakes is in the dissolved form as DOC (Wetzel, 2001). Therefore, both determining the true role of lakes in the global carbon cycle and monitoring water quality require reliable estimates of lake DOC. Only the visible part of electromagnetic radiation can penetrate the water surface and provide us with information about water properties. Consequently, the parameter we want to measure from space or airborne sensors must affect optical water properties (e.g. reflectance), or correlate directly with water characteristics that affect the optical water properties. For example, suspended matter concentration in lakes can be measured with remote sensing (Kallio et al., 2001) because it has direct impact on reflectance whereas optically "invisible" total phosphorus concentration has been estimated from remote sensing data due to close correlation between the phosphorus and water transparency (Kutser, Arst, Miller, Käärmann, & Milius, 1995) in the studied lake.

DOC contains a coloured component called yellow substances or CDOM (Coloured (or Chromophoric) Dissolved Organic Matter). There is typically a strong correlation between DOC and CDOM in boreal lakes, as well as in many other water bodies (Kallio, 1999; Tranvik, 1990; Yacobi, Alberts, Takacs, & McElvaine, 2003; Zhang, Qin, Zhu, Zhang, & Yang, 2007). For example, a study including 983 boreal lakes distributed across Sweden found that absorbance at 254 or 420 nm was very good predictors of DOC concentration, with R^2 values of 0.95 and 0.96, respectively (Erlandsson, Futter, Kothawala, & Köhler, 2012). However, there is generally a lack of data about the CDOM–DOC relationship around the world. DOM absorbance properties tend to change in lakes with longer retention time (Dillon & Molot, 1997; Köhler, Kothawala, Futter, Liungman, & Tranvik, 2013; Kothawala et al., 2013; Meili, 1990). Validating existing algorithms in some of the more complicated systems is thus potentially a challenge for existing MERIS CDOM products. Furthermore, there may be other MERIS products that are better proxies for DOC than CDOM. For example, characteristics that describe the total effect of phytoplankton, CDOM and TSM on the reflectance (like Secchi depth, beam attenuation coefficient, diffuse attenuation coefficient) or the effect of just two components (like turbidity) may perform better than the algorithms that have been designed to retrieve concentration of just one optically active substance. Water transparency, turbidity and other similar characteristics are robust parameters that are relatively straightforward to estimate from remote sensing data (Kallio et al., 2001; Kutser et al., 1995; Olmanson, Bauer, & Brezonik, 2008). It may happen that remote sensing algorithms are wrong in partitioning the signal caused by the phytoplankton, CDOM and TSM, but perform much better in estimating their sum — transparency/turbidity. If a parameter under investigation (e.g. DOC) is in correlation with one of the transparency/turbidity products, then these products may provide better information about lake DOC concentrations than CDOM products. For example, we have found that MERIS total absorption coefficient product may be a better predictor of DOC and TOC than MERIS CDOM absorption product (Kutser, Verpoorter, Paavel, & Tranvik, 2014). There may be good correlations between some of the water characteristics and some remote sensing products that do not have direct cause–result relationships as far as we know. Therefore, it is worth studying all possible correlations between the water characteristics under investigation and different MERIS products.

The absorbance of filtered water, usually considered as a measure of CDOM concentration, depends also on the amount of iron associated to organic matter in water (Köhler et al., 2013; Weishaar et al. (2003); Xiao, Sara-Aho, Hartikainen, & Vähätalo, 2013). Iron passing the filter can exist as truly dissolved monomeric inorganic iron complexes, or as one of two colloidal forms, 1) as ferrihydrate and 2) iron that is bound to organic matter (Jensen, Mulder, & Verstraten, 2003; Lofts, Tipping, & Hamilton-Taylor, 2008). Rising Fe concentrations with DOC have been observed recently in some landscapes (Evans, Monteith, & Cooper, 2005), however, it has been noted that this rise in Fe is not proportional to the rise in DOC (Kritzberg & Ekström, 2011). If part of the water colour is due to colloidal iron associated to organic matter and part due to dissolved organic matter itself (Köhler et al., 2013; Xiao et al., 2013) and their relative contributions vary, then it may be difficult to develop remote sensing products for mapping lake carbon content.

The aim of this study is to understand whether the variable iron concentration in lake waters hampers our capacity to estimate lake CDOM and DOC contents by means of remote sensing. We test whether any MERIS products are suitable for mapping lake water characteristics such as SUVA or the iron associated to organic matter concentration in lake waters.

2. Study site and methods

Mälaren is the third largest lake in Sweden (Fig. 1). Its surface area is 1140 km^2 and it provides drinking water to approximately 1.5 million people in Stockholm and surrounding communities. Mälaren has a
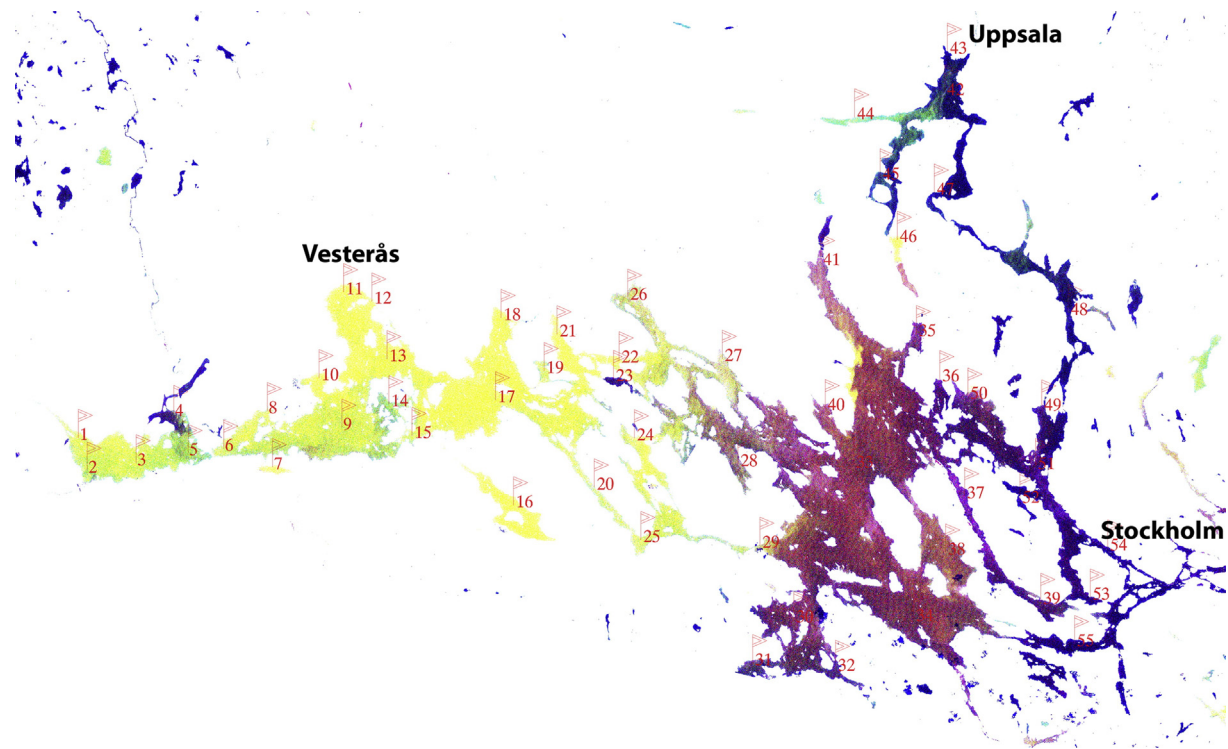
Fig. 1. Location of sampling stations across Mälaren and division of the lake into sub-basins. The map is made from a Landsat image and colours indicate relative water quality from turbid (brighter) to clearer (darker) waters. The division into sub-basins is made according to Köhler et al. (2013).

highly unique geomorphology, being comprised of several hydrologically connected lake basins which flow into each other from west to east, finally draining into the Baltic Sea. Some smaller basins are connected with other parts of the lake by narrows that are only a few metres wide. Many parts of the lake are narrow and elongated resembling rivers rather than lakes. We divided the lake into six major basins as was done by Köhler et al. (2013) and a detailed hydrological study of Mälaren, which defined mean water residence times across the lake (Liungman, Borell Lövstedt, & Moreno-Arancibia, 2010) (Fig. 1). Thus, due to the unique geomorphology of Mälaren, along with the detailed hydrological model of water residence times defined spatially across the lake, we were able to use space as a substitute for water residence time. The basins are quite different from an optical perspective, and changes to the optical properties that have occurred over the last five decades differ from basin to basin (Köhler et al., 2013; Kutser, 2012). For example, the CDOM concentration has increased nearly three times in the westernmost lake basins A and B where the main river inflows drain into, and yet has remained more or less stable during the last fifty years in the easternmost basins C and F (Fig. 1) (Köhler et al., 2013; Kutser, 2012). This can be explained by increasing retention times as both water and DOM age with movement from western to eastern lake basins (Köhler et al., 2013).

The water chemical data used here is identical with the data presented by Köhler et al. (2013). Sampling occurred at 23 lake and 8 river stations (Fig. 1) on August 23, 2010 following the routine monitoring programme (SLU, 2014) as explained in Köhler et al. (2013). The river samples were not used in comparison with MERIS products, as the rivers are too narrow for the MERIS 300 m pixel. However, the river data were taken into account when analysing the behaviour of optical water properties like iron to carbon ratio. From the large number of different chemical parameters measured, only the following subset is used in this manuscript: the absorption coefficient of unfiltered and filtered water samples (a(420) and a_f(420)), total organic carbon (TOC), dissolved organic carbon (DOC using a GF/F filter), the concentration of total suspended solids in solution, total and filtered iron (from the same water sample as DOC using a GF/F filter). The latter is solely composed of iron in colloidal form bound to either organic matter or

as ferrihydrate as explained and discussed in detail in Köhler et al. (2013). Subsequently we refer to this iron as colloidal iron or iron associated to organic matter depending on whether we want to highlight apparent size or the contribution to lake water colour. Particulate iron was calculated as the difference between total and dissolved iron.

In the marine remote sensing community, CDOM is usually defined through the absorption coefficient of light at a particular wavelength by dissolved organic matter that passes a 0.2 μm filter (Mitchell, Kahru, Wieland, & Stramska, 2003). In freshwater systems the use of 0.45 μm filters has been standard for many decades. For example, SLU monitoring data starts from 1965 (SLU, 2014) and the absorbance measurements have always been made with the 0.45 μm filters (5 cm cuvette). Experiments carried out in boreal lakes show that the correlation between the absorption of water samples filtered through 0.2 μm and 0.7 μm filters is very high ($R^2 = 0.99$) and the absorption measured with 0.7 μm filters is higher by 4% on average (Reinart, Paavel, & Tuvikene, 2004). Therefore, we may assume that the difference between 0.2 μm and 0.45 μm filters is even smaller and our absorption coefficient values do not differ from those that could have been measured with the 0.2 μm filters used as a standard in ocean colour community. Thus, the amount of CDOM is characterised in our study as the absorption coefficient of water filtered through 0.45 μm filter and measured at 420 nm.

While the concentration of organic matter is quantified based on the carbon content (DOC), spectral analyses are on whole DOM, and thus we use the term DOM when describing optical results, and DOC when expressing the concentration of organic matter.

A MERIS full resolution (300 m spatial resolution) image of 23 August 2010 was used in the study. Visual inspection revealed high number of small *Cumulus* clouds covering a large portion of the image area. However, the Mälaren area was mostly cloud free. This situation is typical for summer periods where *Cumulus* clouds are formed over land but the sky is clear over large enough water bodies due to downwelling fluxes in the lower atmosphere, and consequent dissipation of the small clouds that occurs over water. Detailed analysis revealed later that there were potentially some cloud shadows affecting the signal measured in one or two stations.

The L1b image (IPF 6.04) was first pre-processed with a Radiometry processor (Bourg, D'Alba, & Colagrande, 2008) to remove the smile-effect, and then with the Improved Contrast between Ocean and Land processor (ICOL v.2.7.4.) to remove the adjacency effect from water pixels close to land. For level 2 processing, the neural networks and bio-optical models of three different processors were used: 1) MERIS standard (MEGS) and 2) Case-2 Regional (C2R, version 1.5.3, Doerffer & Schiller, 2008) and Boreal Lakes. The image processing was done in BEAM 4.9 (Brockmann Consult) and in ODESA CFI software, which provides the MERIS Ground Segment development platform, MEGS®.

For validation, classification flags were first applied on each match-up pixel to exclude cloud pixels. Secondly, each match-up pixel was checked visually for thin *Cirrus* clouds or cloud shadows that were not detected by flags using MERIS L1b images. Thirdly, various confidence and science flags were applied on the data in order to find the most effective approach to eliminate invalid pixels. For MEGS the confidence flags PCD1_13 (which tests if the 13 water-leaving reflectance values are all positive rather than negative) and science flag BPAC_ON (this flag is raised when the Bright Pixels Atmospheric Correction is successful) were applied. For C2R, and Boreal Lakes processors all the quality flags were insensitive (always zero).

All water quality products from all processors were used in the analysis. The obvious product to use in our study was a MERIS CDOM product called yellow substances. However, sometimes it is possible to estimate water characteristics that have no direct impact on reflectance using some other water characteristic as a proxy. Sometimes an algorithm designed for retrieving one water variable may also work in estimating another variable. Inherent optical water properties were also calculated from the MEGS products using Reference Model for MERIS Level 2 Processing: Ocean branch (2011). This study has a quite narrow focus and therefore, we present only the results that are relevant to the main topic.

3. Results and discussion

Concentrations of dissolved and total organic carbon as well as CDOM absorption at 420 nm varied substantially across Lake Mälaren. For example DOC concentration varied between 7.4 mg/l and 15.1 mg/l, TOC varied between 8.8 mg/l and 16.7 mg/l and the CDOM absorption coefficient (at 420 nm) varied between 1.7 m^{-1} and 7.3 m^{-1}. It must be noted that we have carried out another study in Lake Mälaren a year later where CDOM values were between 2.16 m^{-1} and 8.06 m^{-1}, while the DOC and TOC variability was slightly lower than in the present study (Kutser et al., 2014). No iron measurements were carried out in the 2011 field campaign, and therefore that data cannot be used in the present study. The concentration of colloidal iron varied between 14 μg/l and 370 μg/l. Other parameters affecting lake colour, that were not used in this particular study, but worth mentioning due to their affect on remote sensing signal were the concentration of chlorophyll-*a*, and Secchi depth, which varied between 6.5 mg/l and 58.5 mg/l, and 0.9 m to 4.6 m, respectively.

The underlying in-lake processes resulting in observed variability of optical properties namely CDOM absorption, carbon content and colloidal iron in Mälaren are described in detail in Köhler et al (2013). A summary of relevant relationships between optical properties of the lake water, namely CDOM absorption and the carbon content is presented in Figs. 2 and 3. It is seen in Fig. 2C that there is good correlation between laboratory measured CDOM and DOC, with the exception of sampling stations located in basin D (Fig. 2C, samples that fall on the hyphenated line). There was strong correlation between DOC and TOC ($R^2 = 0.88$, river and lake stations together). However, CDOM was not a good predictor of TOC in Mälaren, as is seen in Fig. 2D.

Lake water colloidal iron was predominantly in the organic form rather than as inorganic Fe, as determined from a previous laboratory study (Köhler et al., 2013) using the technique of Kopacek, Klementova, and Norton (2005). Thus, the iron present in lake samples was primarily in colloidal form associated with organic matter. Therefore, it is not surprising that colloidal iron was well correlated to DOC ($R^2 = 0.80$, after removing basin D and half of the river stations) as seen in Fig. 2B, and to CDOM ($R^2 = 0.77$) across the lake in Fig. 2A. It is worth noting that the CDOM to colloidal iron relationship (Fig. 2A) is the same for most of the river and lake stations (except basin D) while the DOC to colloidal iron relationship for basin D and half of the river stations differs from that of most lake stations (Fig. 2C). This sample group has less coloured DOC caused by the lower associated
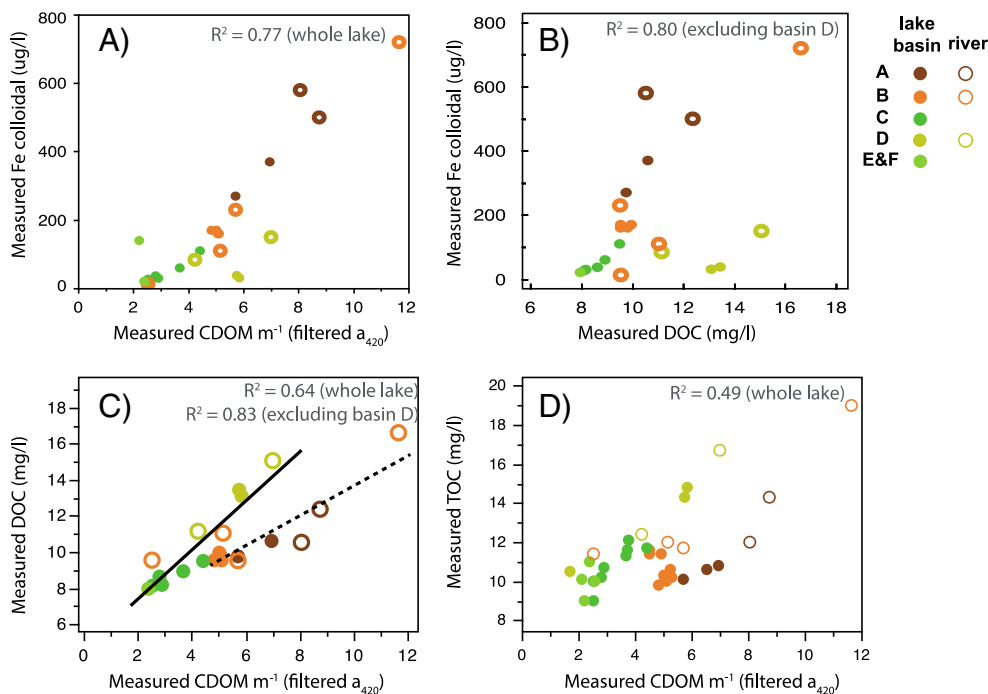

Fig. 2. Relationships between the laboratory measured concentrations of colloidal iron and CDOM (a_{420} filtered) (A), colloidal iron and DOC (B), DOC and CDOM (C), and (D) total organic carbon (TOC) and CDOM in Mälaren lake sites and several rivers draining into the lake basins. Samples in panel (C) that fall on the hyphenated line all have colloidal iron per DOC above 2.5 μM Fe per mMol DOC. Letters in the legend indicate lake basins corresponding to Fig. 1.
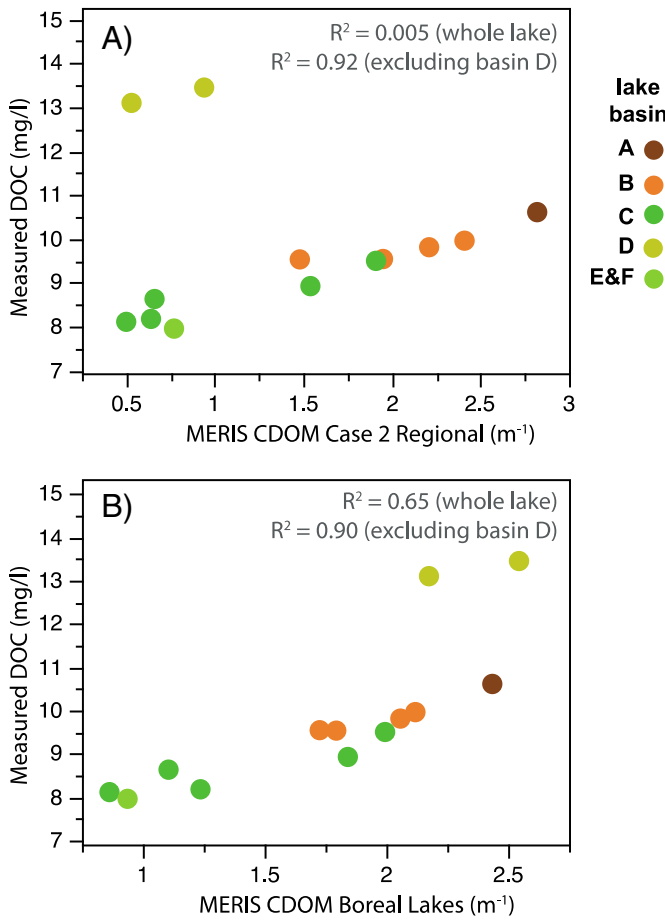
Fig. 3. Measured dissolved organic carbon (DOC) as a function of MERIS estimated CDOM with (A) Case 2 Regional and (B) Boreal Lakes processors.

first obvious proxy for mapping lake carbon from space is CDOM (yellow substance) product obtained from different processors. The correlation between measured and estimated from MERIS data CDOM was low for MEGS and Case 2 Regional processors (R^2 was 0.43 and 0.42 respectively, Table 1). The Boreal Lakes processor performed much better ($R^2 = 0.70$, Table 1). It must be noted that we used absorption coefficient at 420 nm as a measure of CDOM while the MERIS products are given as yellow substance absorption coefficient at 443 nm.

It was already noted that basin D and some of the inflowing rivers differed from the rest of the lake. These differences also emerged in the analysis of the remote sensing results (Fig. 3). However, the results are different when comparing different processors. For instance, both MEGS and Case 2 Regional processors produce the results shown in Fig. 3A, whereby the correlation between DOC and MERIS CDOM is very good for all stations except basin D. In fact, the correlation coefficient between measured DOC and MERIS CDOM was $R^2 = 0.92$, when the basin D points were excluded, but dropped to 0.005 when the basin D points are included (Fig. 3A).

The Boreal Lakes processor works better as shown in Fig. 3B. Basin D sampling stations are still outliers, but the correlation between measured DOC and MERIS CDOM product values is far stronger ($R^2 = 0.65$, Table 1) than for MEGS and Case 2 products, even when all measured stations are included (Fig. 3B). The MEGS and Case 2 Regional processor's bio-optical model are based on North Sea data. In contrast, the Boreal Lakes processor was trained using data from CDOM-rich Finnish lakes. It seems that the training data from Finnish lakes likely contained lakes with variable DOC to iron ratios, as the Boreal Lakes processor coped better with this issue than other processors.

None of the tested MERIS products showed good correlation with TOC in Mälaren ($R^2 < 0.19$). This result was surprising because there is good correlation between TOC and DOC ($R^2 = 0.76$, river stations excluded), and the correlation between CDOM and DOC was $R^2 = 0.58$ even when clear outliers (basin D stations) were included. It must be noted that the number of stations where DOC was measured was smaller than the number of stations where both CDOM and TOC were measured. The CDOM–TOC relationship was worse for the stations where DOC was not measured. This explains why the CDOM–TOC relationship was poor. This is unfortunate as TOC is the standard parameter being measured in the Swedish Monitoring programme and in most drinking water plants.

Analysis of the collected data showed that MERIS total suspended matter product is a very good proxy for estimating lake particulate iron content (Fig. 4A) and measured suspended matter (Fig. 4B). In Mälaren both are closely related. This applies also to basin D where the carbon retrieval algorithms provided results that differ from the rest of the lake. This opens a possibility to improve DOC retrievals, as according to Fig. 2, low colloidal iron content per unit of carbon differentiates basin D from the rest of the lake. Combining the results of MERIS particulate iron and CDOM estimates will potentially allow us to get a more reliable DOC product. In addition, being able to estimate suspended matter concentrations itself is crucial for drinking water

colloidal iron concentrations. Erlandsson et al. (2012) report that CDOM per TOC varies more than one order of magnitude and is closely connected to organically bound iron per TOC and pH. The observed variation of CDOM per TOC in Mälaren (Fig. 2D) is thus not an exception, but rather the rule in the boreal landscape. It is our understanding that the combination of lower incoming colloidal iron concentrations, high pH (>8) and long retention times in basin D (1.2 years) leads to a faster iron removal and that these landscape driven variations may in some cases lead to systematic deviations in prediction of colour and DOC from remote sensing products.

Different products were available in the MERIS standard, Case 2 Regional, and Boreal Lakes processors, which were calculated and compared with parameters measured from water samples (Table 1). The

Table 1
List of MERIS products used in this study and related lake water chemical parameters.

Measurement			Model	
MERIS product name	Parameter	Range	RMSE	R^2
(a_total_443)	SUVA	2.7–4.0	0.18	0.80
Boreal Lake processor (a_ys_443)	DOC	8–14	0.34	0.65
Boreal Lake processor (a_ys_443)	DOC (without basin D)	8.11	0.3	0.90
Boreal Lake processor (a_ys_443)	Absorption coefficient at 420 nm	1.7–7.3	0.81	0.71
Case 2 regional processor (c2r_a_ys_443)	DOC	8–14	n.s.	n.s.
Case 2 regional processor (c2r_a_ys_443)	DOC (without basin D)	8.11	0.3	0.92
Case 2 regional processor (c2r_a_ys_443)	Absorption coefficient at 420 nm	1.7–7.3	1.13	0.42
MERIS TSS	Colloidal iron	25–380	53	0.75
MERIS TSS	Lab measured suspended matter	5–30	1.7	0.94

Fig. 5. Relationship between the MERIS derived total absorption coefficient product and the laboratory measured carbon specific UV absorption at 254 nm (SUVA).
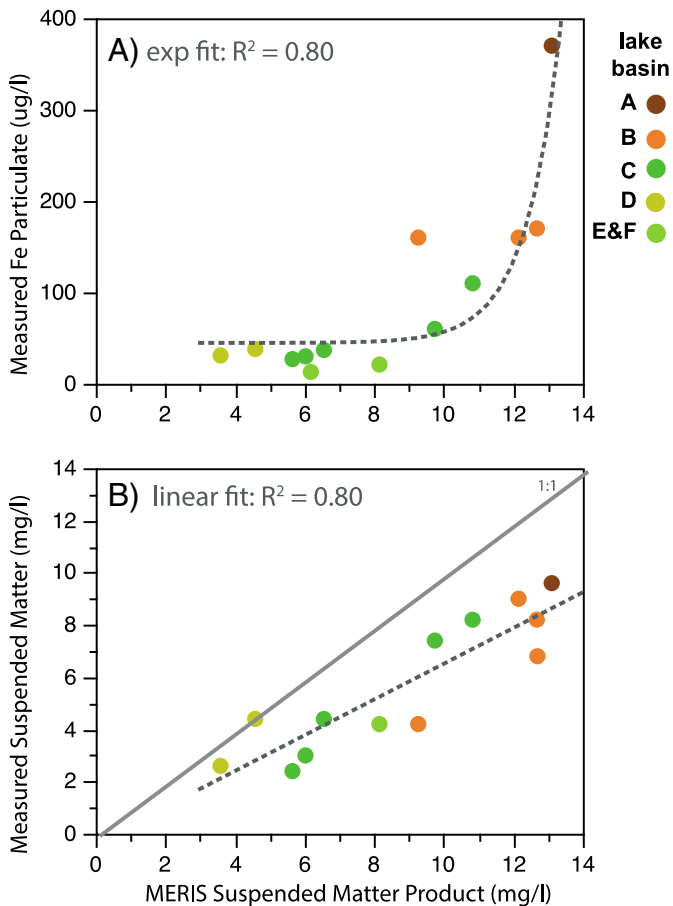
Fig. 4. Correlation between MERIS suspended matter product (A) and the measured concentration of particulate iron, and (B) the measured concentration of suspended matter across the lake. The solid line in panel (B) indicated the expected 1:1 line. Colours in legend correspond to lake basins in Fig. 1.

production as suspended matter may act as a potential transport vector for microbiota.

High colloidal iron, observed in the western part of the basin D, increases SUVA and CDOM (Köhler et al., 2013). Excluding samples with colloidal iron/DOC ratio above 2.5, i.e. samples that fall on the hyphenated line in Fig. 2C, homogenizes the data set such that the specific absorbance is the same across lake and stream water samples. Colloidal iron is known to interfere with the determination of SUVA (Weishaar et al., 2003) and may even influence CDOM (A420 in Köhler et al., 2013). We propose that the effect of the presence of colloidal iron on predicted lake colour is evaluated more systematically both using MERIS but even more when the MERIS follow-up sensor OLCI on Sentinel 3 will be in operation.

The presence of colloidal and particulate iron is strongly dependant on pH (Lofts 2010, Neubauer, Köhler, von der Kammer, Laudon, & Hofmann, 2013). In more alkaline systems (pH > 7.5) iron is predominantly occurring as particulate iron and thus interferences due to varying colloidal iron per DOC would be minimal. MERIS products for lakes in the pH range 5.5 to 7.0 however might be affected by the relative distribution of particulate and colloidal iron (Neubauer et al., 2013). We recommend additional lake specific calibrations in those cases.

A strong correlation was observed between SUVA and the MERIS total absorption coefficient product (at 443 nm) (R^2 = 0.80, Fig. 5). These results are highly promising for further use of remote sensing algorithms to monitor lake water SUVA, and treatability, at unmonitored sites across Mälaren. Currently, water utilities have limited insight into the timing and intensity of abrupt changes to raw water quality since most intensive monitoring is limited to the inlet site. Early
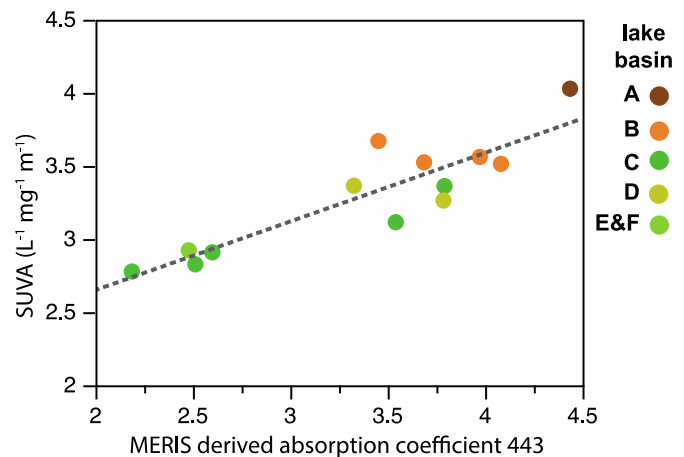
warning of potentially abrupt changes to water quality stimulated by algal blooms, high winds or large precipitation events, would allow water utilities to prepare and adjust treatment strategies, or alternatively shift their source of raw water. For instance, Stockholm water utilities may be mostly interested in abrupt changes to lake basins C and E (Fig. 1), yet would find it advantageous to monitor the full lake surface area particularly when the water residence times are extremely short. With existing hydrological models (Liungman et al., 2010) specific to Mälaren, it now appears more feasible to model the extent and timing of future changes to water quality.

Brezonik, Olmanson, Finlay, and Bauer (in press) studied the correlation between SUVA and in situ measured CDOM in Minnesota and Wisconsin lakes. It occurred that the relationship was hyperbolic. We observed linear relationship between remotely sensed total absorption coefficient and SUVA in Mälaren. The difference in the results can be explained by the SUVA range. In the US lakes SUVA reached values up to 5.45 while it was below 4.5 in Mälaren. Fig. 7b in Brezonik et al. (in press) indicates that the relationship between SUVA and CDOM is almost linear for the SUVA range observed in Mälaren. Thus we showed that SUVA in lake water can be mapped from space, but the in situ data from Brezonik et al. (in press) indicates that this relationship is non-linear for higher values. It is hard to predict how satellite remote sensing will perform in estimating SUVA in very dark lakes, like some of those observed by Brezonik et al. (in press), as the water leaving signal becomes very low in these lakes.

The general trend in Mälaren and many other boreal lakes is that CDOM is highest after ice melts, decreases during summer and increases in the autumn due to higher precipitation (Kutser, 2012). This study was carried out during summer. To evaluate the MERIS CDOM and DOC algorithms properly it would be desirable to have data from different lakes and a slightly wider concentration range of CDOM and DOC. Statistics of lake CDOM in some boreal regions of Finland, Sweden, USA and Canada shows that the highest number of lakes have CDOM between 2 m^{-1} and 7 m^{-1} (Erlandsson et al., 2012; Kutser et al., 2009). Thus, the concentration range observed in Lake Mälaren during our study is close to the typical range for boreal lakes and the results may be applicable more widely than can be assumed from data collected just in a single lake.

4. Conclusions

MERIS standard processor products and the Case 2 Regional processor products were not suitable for mapping lake CDOM and were highly sensitive to differences in carbon–iron ratios. However, the MERIS Boreal Lakes processor was better adopted to the lakes with variable carbon–iron ratio as the correlation between MERIS CDOM product

and measured DOC concentration was reasonably good ($R^2 = 0.65$). Our results also showed that there was good correlation between MERIS suspended matter product and particulate iron, as well as measured suspended matter concentration in the study lake, Mälaren. MERIS total absorption coefficient product was a good proxy for SUVA ($R^2 = 0.80$). This is especially promising for drinking water industry that SUVA and suspended matter could be estimated from remote sensing imagery.

The amount of colloidal iron has significant impact on the lake water colour. Further systematic studies should be undertaken to test whether OLCI (the MERIS follow-up) products differ for lakes with varying colloidal iron per DOC.

Unfortunately, none of the tested MERIS products were suitable for estimating TOC in Mälaren. In situations where DOC, and not TOC, is of major interest such as for estimating the coagulant dose for drinking water production, we strongly recommend to regularly measure and calibrate against DOC and not TOC.

Acknowledgements

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