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Validation of Envisat MERIS algorithms for chlorophyll retrieval in a large, turbid and optically-complex shallow lake

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ABSTRACT

The 10-year archive of MEdium Resolution Imaging Spectrometer (MERIS) data is an invaluable resource for studies on lake system dynamics at regional and global scales. MERIS data are no longer actively acquired but their capacity for global scale monitoring of lakes from satellites will soon be re-established through the forthcoming Sentinel-3 Ocean and Land Colour Instrument (OLCI). The development and validation of in-water algorithms for the accurate retrieval of biogeochemical parameters is thus of key importance if the potential of MERIS and OLCI data is to be fully exploited for lake monitoring. This study presents the first extensive validation of algorithms for chlorophyll-*a* (chl-*a*) retrieval by MERIS in the highly turbid and productive waters of Lake Balaton, Hungary. Six algorithms for chl-*a* retrieval from MERIS over optically complex Case 2 waters, including band-difference and neural network architectures, were compared using the MERIS archive for 2007–2012. The algorithms were locally-tuned and validated using in situ chl-*a* data ($n = 289$) spanning the five year processed image time series and from all four lake basins. In general, both band-difference algorithms tested (Fluorescence Line Height (FLH) and Maximum Chlorophyll Index (MCI)) performed well, whereas the neural network processors were generally found to much less accurately retrieve in situ chl-*a* concentrations. The Level 1b FLH algorithm performed best overall in terms of chl-*a* retrieval ($R^2 = 0.87$; RMSE = 4.19 mg m^{-3}; relative RMSE = 30.75%) and particularly at chl-*a* concentrations of ≥10 mg m^{-3} ($R^2 = 0.85$; RMSE = 4.81 mg m^{-3}; relative RMSE = 20.77%). However, under mesotrophic conditions (i.e., chl-*a* < 10 mg m^{-3}) FLH was outperformed by the locally-tuned FUB/WeW processor (relative FLH RMSE < 10 mg m^{-3} = 57.57% versus relative FUB/WeW RMSE < 10 mg m^{-3} = 46.96%). An ensemble selection of in-water algorithms is demonstrated to improve chl-*a* retrievals.

1. Introduction

The optical complexity inherent to lakes and other inland waters poses many challenges to the accurate retrieval of biogeochemical parameters using satellite remote sensing (IOCCG, 2000, 2006). Many standard chlorophyll-*a* (chl-*a*) retrieval algorithms originally developed for open ocean waters (optically dominated by phytoplankton and their breakdown products) tend to fail when applied to more turbid inland and coastal waters whose optically properties are strongly influenced by non-covarying concentrations of non-algal particles (NAP) and coloured dissolved organic matter (CDOM) (IOCCG, 2006; Matthews, 2011). In addition, the continentality of the atmospheres overlying inland and coastal waters and the proximity of the adjacent land surface means that standard approaches to atmospheric correction over ocean waters are not always reliable. In view of these challenges, there is a clear need to develop and validate atmospheric (Moore, Aiken, & Lavender, 1999) and in-water (Doerffer & Schiller, 2007, 2008; Matthews, 2011; Odermatt, Gitelson, Brando, & Schaepman, 2012) algorithms specifically for use in highly turbid inland and coastal waters.

The MEdium Resolution Imaging Spectrometer (MERIS) collected data from aboard the European Space Agency's (ESA) Envisat satellite from March 2002 until April 2012 and provided observations at spectral (15 bands from 412.5 to 900 nm), radiometric (16-bit), spatial (300 m at full resolution) and temporal (three day revisit cycle at the equator) resolutions unprecedented by other satellite sensors which allows for improved insights into the concentrations of optically active substances in large lakes, and thereby into the dynamics of these lakes more generally (Koponen et al., 2008; Matthews, Bernard, & Winter, 2010; Odermatt,

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Gitelson, Brando, & Schaepman, 2012). Although MERIS is no longer active, a wealth of archive data remains yet to be fully exploited. Furthermore, the forthcoming Ocean and Land Colour Instrument (OLCI) to be operated on the ESA Sentinel-3 satellites will provide continuity to and to improve upon the data collected by MERIS (Aschbacher & Milagro-Pérez, 2012; Donlon et al., 2012). The continued validation of MERIS products for lakes will strongly inform algorithm development for Sentinel-3 OLCI because of its MERIS heritage.

In recent years, a number of constituent retrieval algorithms for use over coastal and lake waters have been developed. Some are intended specifically for use with or are compatible with MERIS data, and are automated and made available as part of the Basic ERS & ENVISAT (A)ASTER MERIS (BEAM) toolbox (Fomferra and Brockmann, 2005). These include artificial neural network approaches trained to varying parameter concentration and optical property ranges (e.g., the Case 2 Regional (C2R) (Doerffer & Schiller, 2007), the FUB/WeW (Schroeder, Schaale, & Fischer, 2007), the Eutrophic Lake (EUL) and Boreal Lake (BL) (Doerffer & Schiller, 2008) processors), and the band ratio, height-above-baseline Maximum Chlorophyll Index (MCI) and Fluorescence Line Height (FLH) algorithms (Gower, Doerffer, & Borstad, 1999, Gower, King, Borstad, & Brown, 2005). Many of these same, or similar, algorithms will be adaptable to the forthcoming OLCI sensor on Sentinel-3. However, these algorithms have not been widely validated across the continuum of optical water types found in lakes, particularly in highly turbid phytoplankton- or sediment-dominated waters. Prior to their operational use in research, monitoring and management activities, rigorous validation analyses are required to understand the associated performance and uncertainty, to then select the optimal algorithm or combination of algorithms to apply to a given water body in order to achieve the most robust retrieval of the parameter(s) of interest. It has been widely demonstrated that an algorithm performing well in one lake or type of lake may not prove transferable to another lake or another type of lake and vice versa (Kallio et al., 2001; Matthews, 2011; Odermatt, Gitelson, Brando, & Schaepman, 2012), and site-specific and regional validation is therefore very important.

Several of the algorithms listed above have been evaluated individually and in various combinations in terms of their retrieval performance for a number of parameters and for diverse lake conditions. Binding, Greenberg, Jerome, Bukata, and Letourneau (2010) applied the C2R, FLH, and MCI algorithms, with and without the "smile effect" (caused by slight variation in centre wavelength for a given band across the MERIS field-of-view (Bourg, D'Alba, & Colagrande, 2008)) correction and Improved Contrast between Ocean and Land (ICOL) processors applied, to evaluate chl-*a* retrieval from MERIS imagery of Lake of the Woods (Canada/USA) during an intense algal bloom, and also compared these with the standard MERIS algal_2 product. A validation of the C2R, EUL and BL processors' atmospheric correction, IOPs and water quality constituents (chl-*a*, gelbstoff absorbance, and total suspended matter) was carried out over several European and African lakes by Koponen et al. (2008) and Ruiz-Verdú et al. (2008). Alikas and Reinart (2008) evaluated chl-*a* retrieval from Lakes Peipus (Estonia/Russia), Vattern and Vanern (Sweden) using the MERIS standard Case 1 (algal_1) and Case 2 (algal_2) chl-*a* products, in addition to related total suspended matter and yellow substance retrievals. C2R and ICOL were evaluated in application to perialpine lakes (Odermatt, Giardino, & Heege, 2010) and to Lake Trasimeno (Italy; Giardino, Bresciani, Villa, & Martinelli, 2010). Odermatt, Pomati, et al. (2012) report validation results of C2R, EUL and FUB WeW with ICOL applied for Greifensee (Switzerland), including the consideration of in situ measurements at various depths and locally-tuned coefficients relating neural network retrieved pigment absorption to chl-*a* concentration. Gege and Plattner (2004) investigated the performance of MERIS standard L2 products over Lake Constance (Germany), and Matthews et al. (2010) applied C2R and EUL processors, in addition to a suite of empirical algorithms, to Lake Zeekoevlei (South Africa). From such studies, a range of results was found to arise, whereby a given algorithm or processor having performed well in some instances and/or locations, failed in others due to the specific local conditions and limitations of the various algorithms. Lake Balaton (Hungary) itself encompasses a broad range of conditions, and it is expected that some of the algorithms listed above would perform well in some instances and vice versa. Therefore, a validation of algorithms intended for optically-complex waters and available within the BEAM image processing toolbox was undertaken.

In this study, we present the first comprehensive algorithm validation exercise over Lake Balaton. Six algorithms of differing architecture for application to optically complex waters were assessed: the C2R, BL, EUL, FUB/WeW, and MCI/FLH processors. The lake is well suited to satellite validation activities because of its large size, complex optical water types encompassing waters with high and varying concentrations of chl-*a*, total suspended matter (TSM) and CDOM and the availability of existing in situ data from long-term monitoring programmes. With few exceptions (e.g., Alikas & Reinart, 2008; Giardino et al., 2010; Odermatt et al., 2010), many previous validation studies have focused on a specific event or a limited time period. Likewise, validation of Landsat chl-*a* retrievals was previously carried out for Lake Balaton over a short time period (Tyler, Svab, Preston, & Kovacs, 2006). In this study, we used measurements of chl-*a* from the monitoring programmes spanning all seasons for all years of study and covering the full spatial extent of Balaton to investigate differences in MERIS algorithm performance across space and time. The ultimate aim of this study is to evaluate and compare the performance of these algorithms under the range of optical conditions presented by Lake Balaton so as to identify the most appropriate algorithm(s) for MERIS processing and to inform future Sentinel-3 OLCI work.

2. Study site

Lake Balaton, in western Hungary (46°50 N, 17°40 E; Fig. 1), is the largest lake in central Europe by surface area, covering 596 km^2 (Herodek, Lackó, & Virág, 1988; Szabó et al., 2011). Its very shallow depth means that Balaton is a unique system, as both a habitat and a recreational resource, but also in terms of its optical properties. The lake has a mean depth of 3.3 m (max. 10.4 m), and is polymictic in that it does not undergo permanent or seasonal stratification. Its fine, calcareous bottom sediment is easily resuspended causing its characteristically turbid waters with high particulate inorganic matter concentrations (Istvánovics et al., 2007). Secchi depth generally ranges between 0.2 and 1.8 m, depending largely on wind conditions and resulting sediment resuspension, and is highly variable both spatially and temporally (György, Tátrai, & Specziár, 2012; Herodek et al., 1988). Phytoplankton composition also exhibits distinct seasonal trends with diatoms dominant during the spring bloom and cyanobacteria dominant during the summer–fall bloom (Mózes et al., 2006). The phytoplankton community also varies spatially within the lake. Nitrogen-fixing bacteria tend to dominate in all basins during the summer period, but the abundance of chlorophytes and dinophytes increases significantly towards the more mesotrophic conditions encountered in the eastern basin.

There is a gradient in total phytoplankton biomass along the main NE–SW longitudinal axis of the lake, resulting from the fact that the south-westernmost basin, Basin 1 (*Keszthely*), tends to be the most nutrient enriched (eutrophic to hypertrophic) and the northeasternmost basin, Basin 4 (*Siofok*), is least nutrient enriched (generally classified as mesotrophic). The trophic status of the middle basins, Basin 2 (*Szigliget*) and Basin 3 (*Szemes*), falls somewhere in between (Mózes et al., 2006; Présing et al., 2008). This gradient is related to nutrient loading from the Zala River, which flows into the westernmost basin and is the lake's main tributary. The lake has endured major problems with eutrophication and algal blooms, especially in the 1970s and 1980s, but water quality has improved in recent years due to improved management of nutrient inputs.

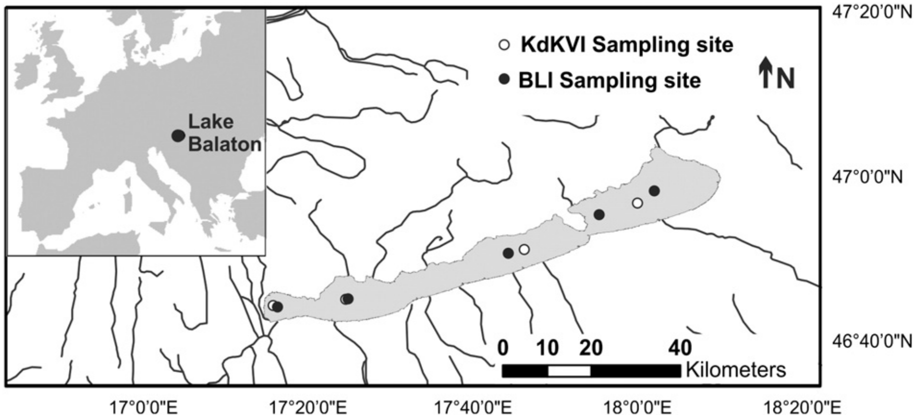

Fig. 1. Locations of Lake Balaton in western Hungary (inset), and the regularly sampled points at the centres of each of its four main basins of the Balaton Limnological Institute (BLI) and the Central Transdanubian (Regional) Inspectorate for Environmental Protection, Nature Conservation and Water Management (KdKVI), in situ data used in this study.

3. Methodology

3.1. MERIS chlorophyll-a algorithms

The C2R processor was developed to compliment the retrieval algorithm designed for use with MERIS data over clear ocean waters, as the latter would often fail in more optically complex conditions (Doerffer & Schiller, 2007). A neural network (NN) inversion approach was adopted to achieve the dual requirements of accuracy and efficiency for operational processing as part of the MERIS ground segment, consisting of coupled forward and backward neural networks. A separate neural network module first performs atmospheric correction, using geometric and reflectance data of L1b input imagery. Reflectance of eight MERIS spectral bands, post-atmospheric correction, and three angles are then used as input into the in-water algorithm and result in the output of three inherent optical properties (IOPs) at MERIS band 2 (443 nm) (particle scattering (b_tsm), absorption coefficient of phytoplankton pigments (a_pig) and absorption coefficient of gelbstoff (a_gelb); Doerffer & Schiller, 2007). The derived IOPs are then converted to constituent concentrations based on measured mass-specific IOP (SIOP) coefficients. As IOPs are also provided as output, the user retains the option of specifying their own SIOP set to suit their particular region (Doerffer & Schiller, 2007).

IOP and in-water constituent concentration data from cruises in optically complex coastal waters, mainly in the North Sea, as well as in the North Atlantic, Baltic Sea and Mediterranean Sea, were used to establish the bio-optical model, followed by HydroLight™ simulation of a large radiance reflectance dataset to train the coupled inverse and forward NNs. Concentration ranges within which the C2R processor has been trained are 0.016–43.18 mg m^{-3} chl-*a*, 0.0086–51.6 g m^{-3} TSM and 0.005–5 m^{-1} gelbstoff (a_gelb (443)) (Doerffer & Schiller, 2007; Table 1). Both the EUL and the BL processors replicate the atmospheric correction and coupled inverse/forward neural network architecture of the C2R processor, making use of the same MERIS spectral and angular inputs, but unlike C2R are trained using bio-optical data from eutrophic Spanish and boreal Finnish lakes (Doerffer & Schiller, 2008; Koponen et al., 2008). The training ranges for chl-*a* were 0.5–50 mg m^{-3} and 1–120 mg m^{-3}, 0.1–20 g m^{-3} and 0.42–50.9 g m^{-3} for TSM, and 0.25–10 m^{-1} and 0.1–3 m^{-1} for CDOM ($a_{CDOM}(442)$) for the BL and EUL processors respectively (Doerffer & Schiller, 2008; Table 1).

The FUB/WeW processor is also based on artificial neural network architecture trained using radiative transfer simulations. Unlike the C2R, EUL and BL algorithms, however, the FUB/WeW processor uses MERIS TOA radiances as input into four separate NNs used to simultaneously derive concentrations of gelbstoff/yellow substance absorbance at 443 nm, chl-*a*, and TSM directly, as well as atmospherically corrected water-leaving reflectance for MERIS bands 1–7 and 9, and Aerosol Optical Thickness at four wavelengths (Schroeder et al., 2007). Concentration ranges used in the NN training were 0.05–50 mg m^{-3} chl-*a*, 0.05–50 g m^{-3} TSM, and 0.005–1 m^{-1} CDOM ($a_{CDOM}(443)$) (Schroeder et al., 2007; Table 1).

The MCI/FLH processor makes use of the height of a peak related to chl-*a* concentration above a baseline (Gower, Brown, & Borstad, 2004, 1999, 2005, Gower et al., 1999, 2005). Because red and near-infrared wavelengths are used, the masking of pigment spectral features by CDOM and TSM, most strong in the blue and green spectral regions, is largely avoided (Gower et al., 1999). Both algorithms take the general form presented in Eq. (1),

$$\mathrm{FLH/MCI} = \mathrm{L2} - k * [\mathrm{L1} + (\mathrm{L3} - \mathrm{L1})((\lambda 2 - \lambda 1)/(\lambda 3 - \lambda 1))] \quad (1)$$

whereby L2 is the radiance or reflectance (depending on the use of L1b or L2 input data) measured in the peak wavelength, λ2, and L1 and L3 are the radiance or reflectance of the baseline wavelengths, λ1 and λ3. *k* is a constant with the default value in BEAM = 1.005, set differently from one so as to reduce the effect of thin cloud (adapted from Gower et al., 1999; Brockmann Consult, Hamburg). However, whereas the MCI uses the peak of MERIS band 9 (708 nm) above bands 8 (680.5 nm) and 10 (753 nm), the FLH algorithm uses the peak of MERIS band 8 (680.5 nm; associated with solar-induced chl-*a* fluorescence) above bands 7 (664 nm) and 9 (708 nm) (Gower et al., 2005). The exact bands used in either algorithm are adjustable and can be defined by the user. The most appropriate choice of peak wavelength has been found to generally co-vary with chl-*a* concentration level (Matthews, Bernard, & Robertson, 2012). Here, the original band settings are used. The coefficients of the relationship between either FLH or MCI and chl-*a* can then be determined empirically for the study region and applied to retrieve chl-*a* concentrations from L1b or atmospherically corrected L2 MERIS data (Gower et al., 1999, 2005; Matthews et al., 2012).

Table 1
Chl-*a*, TSM and CDOM training ranges of the neural network processors.

Processor	chl-*a* (mg m^{-3})	TSM (g m^{-3})	CDOM (a440 m^{-1})
C2R	0.016–43.18	0.0086–51.6	0.005–5
EUL	1–120	0.42–50.9	0.1–3
BL	0.5–50	0.1–20	0.25–10
FUB/WeW	0.05–50	0.05–50	0.005–1

3.2. MERIS processing

All images within the archive of L1b MERIS 300 m full resolution, full swath, georeferenced (FSG) data available for Lake Balaton from January

2007 until April 2012 were processed using the PHenology And Vegetation Earth Observation Service (PHAVEOS) developed through the Value Adding Element of ESA's Earth Observation Market Development programme (Lankester, Dash, Baret, & Hubbard, 2010). Although originally intended to facilitate the extraction of terrestrial vegetation biophysical parameters (Normalized Differential Vegetation Index, fraction of Absorbed Photosynthetically Active Radiation, Leaf Area Index, etc.) from large volumes of data, the main steps comprising the PHAVEOS processing chain are equally applicable to the retrieval of optically active water constituents when appropriate algorithms are included in the processing chain.

MERIS image tiles containing Lake Balaton were extracted from the archive via a vector-based region of interest mask in PHAVEOS. The MERIS data were then geolocated using Accurate MERIS Ortho-Rectified Geo-location Operational Software (AMORGOS (Bicheron et al., 2008)) prior to further processing. The code for the C2R, EUL and BL processors, including their atmospheric correction NN modules, and the MCI/FLH processors was adapted for PHAVEOS and the AMORGOS corrected L1b MERIS FSG imagery were provided as inputs into the processing chain. The outputted IOPs and constituent concentrations were then resampled to a 250 m grid (Fig. 2). The FUB/WeW processor was implemented separately through Visat BEAM v.4.10 (Brockmann Consult, Hamburg) but using the same AMORGOS-corrected L1b MERIS FSG imagery inputted into PHAVEOS.

The mean of each retrieved parameter was extracted from a 3 × 3 pixel kernel (approximately 0.56 km^2 surface area) corresponding to the geographic location of the in situ chl-*a* data. This included the chl-*a* concentration and a_pig(443) (absorption by pigment at 443 nm) from the C2R, EUL and BL processors, algal_2 ($\log_{10}$ (chl-*a* concentration)) from the FUB/WeW processor, and MCI and FLH indices from the MCI/FLH processor. In this study we restricted the matchups to the same day as the MERIS overpass assuming that the chl-*a* concentration would not change significantly in this time period. Samples were typically acquired within three hours of image acquisition.

A total of 1409 MERIS images acquired between January 2007 and April 2012 with full or partial coverage of Lake Balaton were identified by PHAVEOS. Of these, 68 coincided with matchup in situ data measured on the same day as image acquisition. This resulted in a total of 289 in situ matchups across the four basins, although the final number of matchups for each processor differed due to flagging (see reported *n* in Table 4). All Level 1 flagged matchups corresponding with pixels identified as “invalid”, “coastline”, land (“land_ocean”), “bright”, “suspect” or at risk of glint (“glint_risk”), as well as those flagged by the given neural network at the Level 2 were excluded. Level 2 C2R, EUL and BL processor flags excluded were land, cloud or ice pixels (“land”, “cloud_ice”, determined by default expressions of specific bands' reflectance greater or lesser than defined thresholds or the reflectance of another band), atmospheric correction, top-of-standard-atmosphere and top-of-atmospheric reflectance in band 13 out of the training range (“atc_oor”, “tosa_oor” and “toa_oor”), large solar zenith angle (“solzen”), water leaving reflectance out of scope (“wlr_oor”), concentration out of training range (“conc_oor”), spectrum out of training range (“ootr”; set by default as chi square greater than 4.0), wind speed greater than 12 m s^{-1} (“whitecaps”) and “invalid”. Level 2 FUB/WeW processor flags excluded were “Level 1b_masked”, and input (in) or output (out) retrieval failure of chlorophyll-a (chl), yellow substance (yel), total suspended matter (tsm) and atmospheric correction (atm) (“chl_in”, “chl_out”, “yel_in”, “yel_out”, “tsm_in”, “tsm_out”, “atm_in” and “atm_out”). Remaining matchups were used in algorithm calibration and validation.

The matchup dataset was randomly divided, using 70% of the matchups for algorithm calibration, followed by validation using the remaining 30%. For calibration, the derived MCI/FLH indices and a_pig(443) values from C2R, EUL and BL processors were related to the measured concentration of chl-*a* via ordinary least squares regression. The absorption of particulate matter at 440 nm ($a_{pl}(440)$) was calculated from the retrieved FUB/WeW algal_2 product, using the equation and coefficients from Schroeder (2005) and Bricaud, Morel, Babin, Allali,

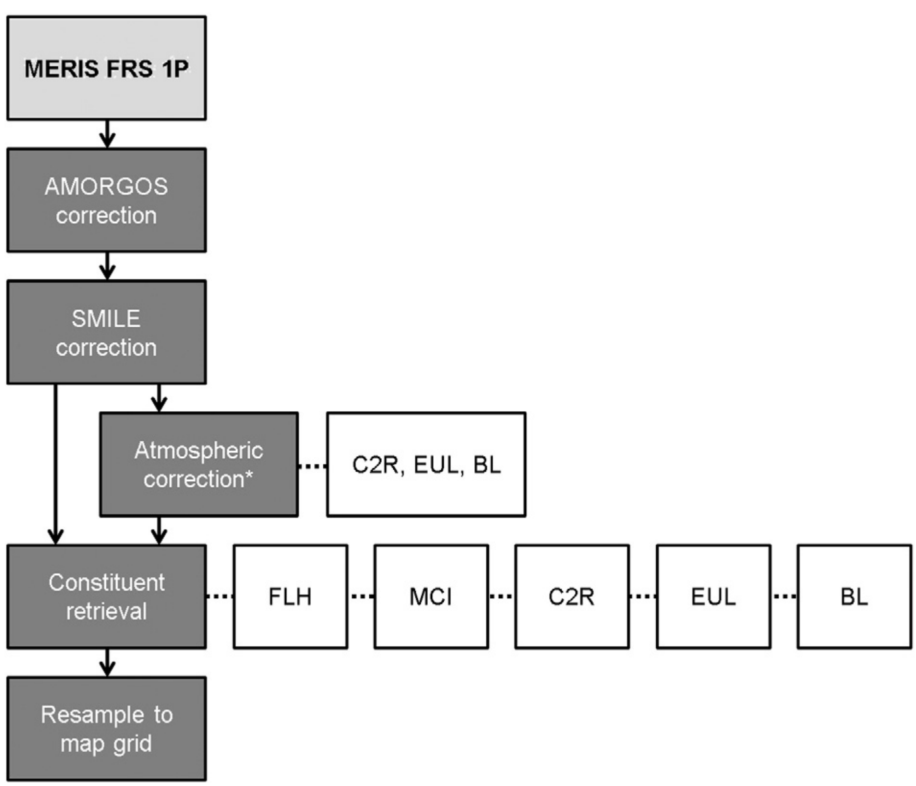

Fig. 2. The PHAVEOS image processing chain employed, including geometric correction, optional atmospheric correction, constituent retrieval using the selected algorithms, and resampling to the 250 m map grid.

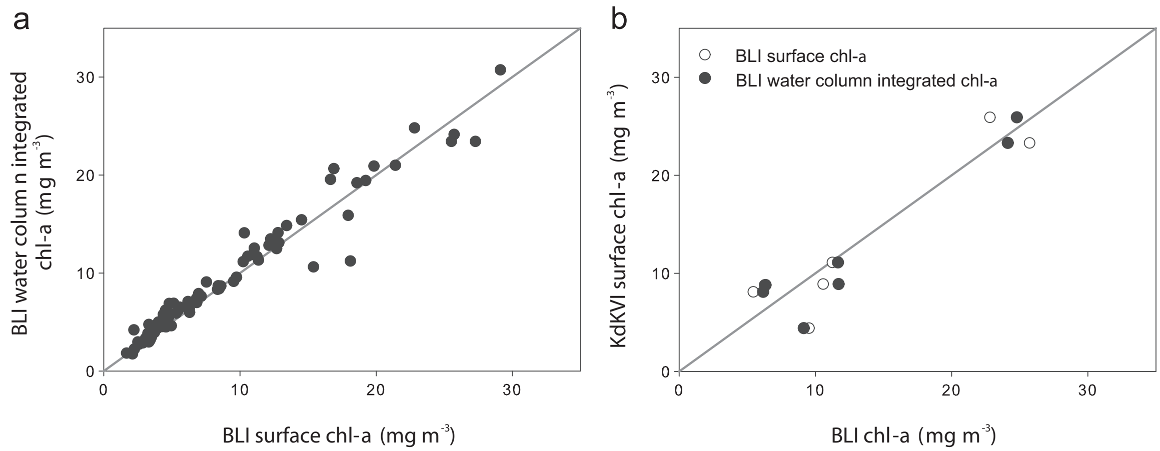

Fig. 3. Chl-*a* concentrations from coinciding surface and water column integrated samples collected and measured by the BLI (a), and from surface samples collected by the water authority (KdKVI) and BLI surface and water column integrated samples (b).

and Claustre (1998) (Table 3), and ordinary least squares regression between $a_{pl}(440)$ and in situ chl-*a* concentrations was then used to locally tune the algorithm as for the other processors. For all algorithms, linear, exponential and power relationships were tested and the relationship producing the highest resulting coefficient of determination (R^2) was selected. The validation of all the algorithms was evaluated in terms of R^2, absolute and relative root mean standard error (RMSE), and bias, calculated via comparison of retrieved chl-*a* against the in situ chl-*a* concentrations. Algorithm performance was assessed for all basins combined, as well as per lake basin, and the potential to optimise chl-*a* concentration retrievals through the application of different algorithms under different conditions (e.g., per basin) was explored.

3.3. In situ validation data

In situ data for MERIS validation was obtained from two routine monitoring programmes on Lake Balaton by the Balaton Limnological Institute (BLI) of the Hungarian Academy of Sciences Centre for Ecological Research and the Central Transdanubian (Regional) Inspectorate for Environmental Protection, Nature Conservation and Water Management (Közép-dunántúli Környezetvédelmi, Természetvedelmiés Vízügyi Felügyeloség (KdKVI)). KdKVI samples are collected at four locations, at the centre of each of the four main basins of the lake. BLI samples are collected from five locations across the lake, also at the centres of each of the main basins as well as to the east of the Tihany Peninsula (Fig. 1). A total of 692 chl-*a* measurements were available from the period January 2007 to April 2012, coinciding with the period for which MERIS image data used in this study were also available. Chl-*a* was determined by spectrophotometry following sample filtration using Whatman GF/C filters (1.2 μm), extraction in hot methanol (in the case of the BLI; Iwamura, Nagai, & Ishimura, 1970) or ethanol (in the KdKVI laboratory) and clarification by centrifugation.

KdKVI samples are taken from the surface layer (top < 0.5 m), whereas the BLI collects bulk samples integrated over the total water column depth of the sampling location. An experiment carried out biweekly over the full ice-free period of 2012 compared the concentrations derived from coinciding surface and water column integrated samples. Samples were collected and analysed by the BLI ($n = 80$ comparisons), and a non-parametric Mann–Whitney *U*-test applied, given the non-normal distribution of the measured concentrations. BLI and KdKVI samples taken from the centre of the same basin on the same date and analysed in the laboratories of the two institutions following their standard protocols were similarly compared ($n = 7$). This was undertaken to reveal any systematic differences between the two archive datasets and to determine whether both sets of archive data would be suitable for use as satellite retrieval matchups.

In all cases – BLI water column integrated and BLI surface, BLI surface and KdKVI surface, and BLI water column integrated and KdKVI surface – coinciding samples were found to resemble closely (Fig. 3). The *U*-test (Mann–Whitney rank sum test) applied to chl-*a* concentrations of coinciding BLI surface and BLI water column integrated pairs of samples confirmed that no significant difference exists between the medians of the two groups ($P = 0.501$). Likewise, no significant difference was found between the medians of the BLI surface samples and KdKVI surface samples ($P = 0.902$), or BLI water column integrated samples and KdKVI surface samples ($P = 0.710$). Any difference between the datasets is therefore expected to be due to random variability and not systematic effects of the different methods. This is likely a result of the relatively well-mixed nature of Balaton, and the two datasets were thus combined for use in all analyses.

4. Results

4.1. Chlorophyll-a retrieval performance

Descriptive statistics for the in situ matchup subset used here are found in Table 2, for the full lake and per basin. The full range of in situ chl-*a* concentrations from this study is 1.50–57.0 mg m^{-3}, with decreasing concentrations generally from west to east (basins 1 to 4), as per the well-known trophic gradient of Lake Balaton, described in Section 2. Matchups where in situ chl-*a* concentrations exceeded the training range of a neural network-based algorithm were excluded from calibration and validation of that particular algorithm.

C2R, EUL, and BL matchups were flagged similarly at the Level 2 (remaining $n = 166$, 168 and 130 respectively), mainly as a result of invalid pixels and atmospheric correction and water leaving radiance out of the training range ("atc_oor", "wlr_oor"), with all additional matchups flagged by BL, and not by C2R or EUL, associated with water leaving radiance reflectance out of range ("wlr_oor"). The FUB/WeW processor was found to exclude more matchups than any of the other three neural network algorithms due to Level 2 flags being raised

Table 2
Descriptive statistics of the in situ matchup data used in this study (chl-*a* (mg m^{-3})).

Basin	n*	Min.	Max.	Mean	Med.	St. Dev.
Full lake	201	1.50	57.00	12.75	8.90	11.14
1	59	3.30	57.00	17.37	12.69	12.65
2	47	4.40	46.48	16.09	11.92	11.34
3	38	2.20	41.45	12.87	9.21	10.57
4	57	1.50	13.62	5.14	4.30	2.72

* Number of matchup points after removing those flagged at Level 1.

(remaining $n = 108$), including all matchups where in situ chl-*a* exceeded 30 mg m^{-3} (Fig. 4d, Fig. 5d). After Level 1 flagged matchups were excluded, approximately 70% of the Level 2 flags raised by the FUB/WeW processor were due to atmospheric correction failure ("atm_in" and "atm_out"), with the others resulting from constituent retrieval failure (various combinations of "chl", "yel" and "tsm" "in" and "out"). Because no Level 2 flags are raised by FLH or MCI, these present a larger number of matchups than for the neural network processors ($n = 201$ after L1 flags are removed).

Coefficients of determination (R^2), equations and tuning coefficients relating FLH and MCI indices and neural network a_pig(443) (C2R, EUL and BL) and $a_{pl}(440)$ (FUB/WeW) to chl-*a* concentrations, retrieved by regression against the unflagged in situ matchups using a randomly selected 70% of the matchup data, can be found in Fig. 4 and Table 3. Power functions were found to produce the highest correlation between neural network retrieved pigment absorption and in situ chl-*a* concentrations in all cases ($R^2 = 0.46$ for C2R; $R^2 = 0.42$ for EUL; $R^2 = 0.48$ for BL; and $R^2 = 0.36$ for FUB WeW), and linear relationships optimised the chl-*a* retrieval of both MCI and FLH algorithms ($R^2 = 0.62$ and 0.78 respectively). The neural network processors' default equations and coefficients are also presented in Table 3 for comparison.

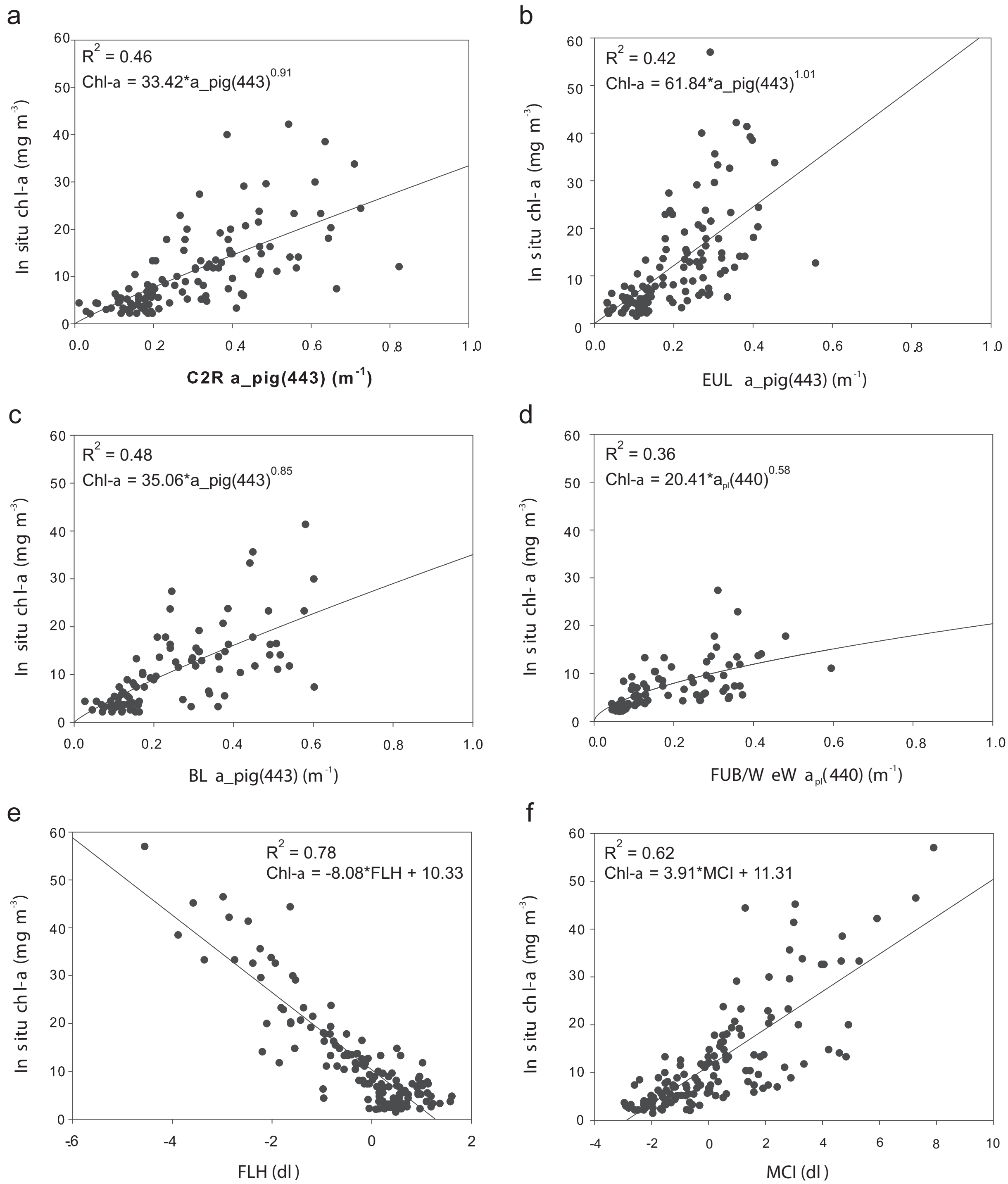

Fig. 4. Calibration of the selected algorithms (C2R (a), EUL (b), BL (c), FUB/WeW (d), FLH (e), and MCI (f)) through regression between a_pig(443) (C2R, EUL, BL processors), $a_{pl}(440)$ (FUB/WeW processor), MCI/FLH indices and matchup in situ chl-*a* concentrations. 70% of the matchup datasets was used for the calibration step.

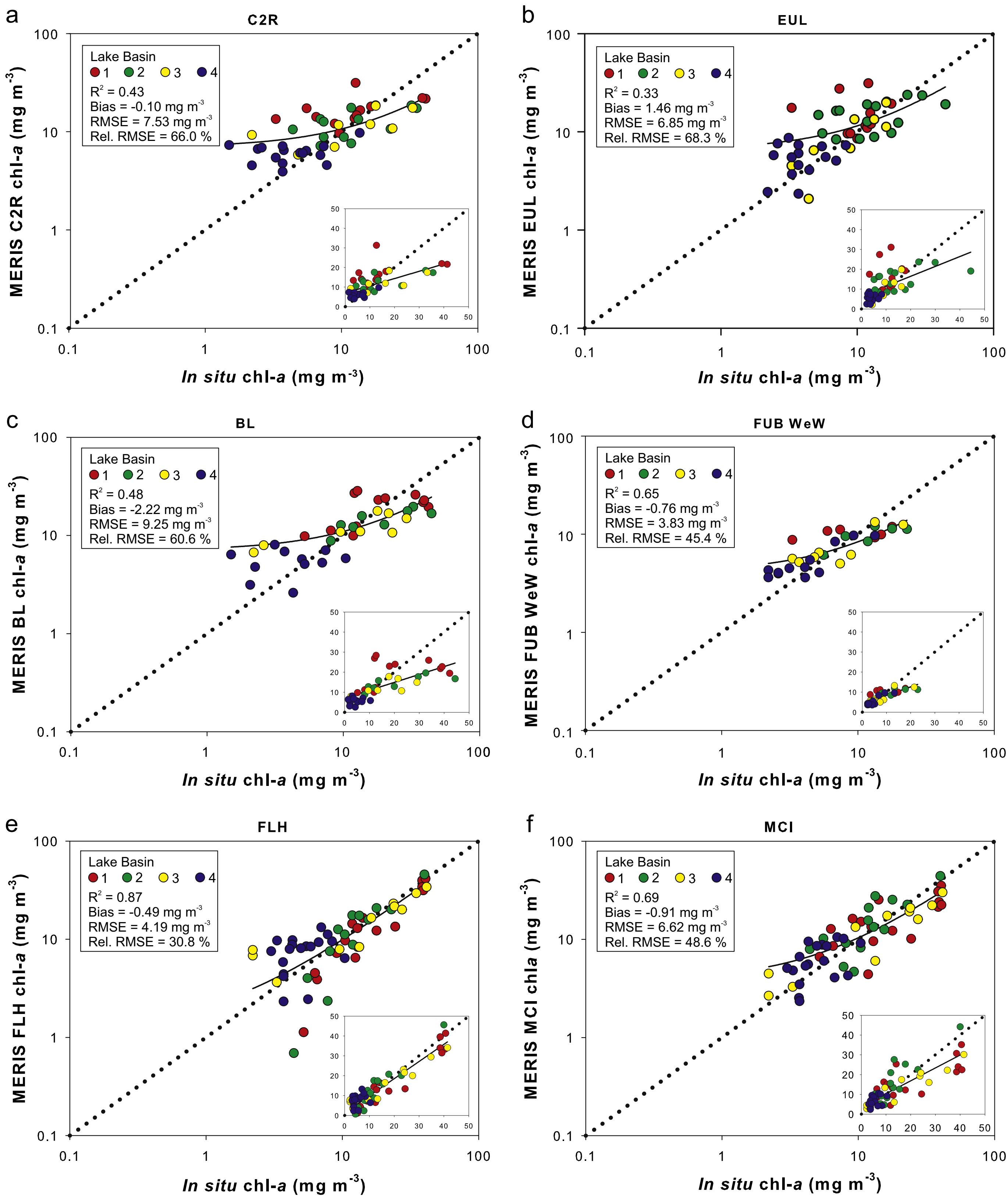

Fig. 5. Chl-*a* retrieval performance of the six selected and locally calibrated algorithms (C2R (a), EUL (b), BL (c), FUB/WeW (d), FLH (e), and MCI (f)) relative to matchup in situ data. Performance statistics reported in the insets are for all basins combined. Individual basin matchups are indicated by colour-coding and further per basin matchup statistics are reported in Table 4. 30% of the full matchup datasets was used for this validation step.

The remaining 30% of the matchup dataset was used to compare validation results of all six locally tuned algorithms. Validation retrieval performance of each is presented in Fig. 5, with additional performance indicators found in Table 4. The FLH algorithm was found to perform best in terms of R^2 (0.87) and RMSE (4.19 mg m^{-3}; 30.75%) for the full lake (Table 4; Fig. 5e), although relative RMSE ranges from 23.25

Table 3
Local tuning of algorithms using 70% of the in situ Lake Balaton chl-*a* data and a_pig(443), $a_{pl}(440)$ or MCI/FLH indices.

Processor	*n*[a]	R^2	Locally tuned equation	Original equation
C2R	116	0.46	Chl-*a* = 33.42 ∗ a_pig(443)$^{0.91}$	Chl-*a* = 21 ∗ a_pig(443)$^{1.04}$[b]
EUL	118	0.42	Chl-*a* = 61.84 ∗ a_pig(443)$^{1.01}$	Chl-*a* = 31.45 ∗ a_pig(443)[c]
BL	91	0.48	Chl-*a* = 35.06 ∗ a_pig (443)$^{0.85}$	Chl-*a* = 62.61 ∗ a_pig(443)$^{1.29}$[c]
FUB/WeW	76	0.36	Chl-*a* = 20.41 ∗ $a_{pl}(440)^{0.58}$	Chl-*a* = 105.21 ∗ $a_{pl}(440)^{1.58}$[d]
L1b FLH	141	0.78	Chl-*a* = −8.08 ∗ FLH + 10.33	n.a.
L1b MCI	141	0.62	Chl-*a* = 3.91 ∗ MCI + 11.31	n.a.

[a] 70% of number of matchup points after removing those flagged by the processor.
[b] Doerffer and Schiller (2007).
[c] Doerffer and Schiller (2008).
[d] Schroeder (2005), Bricaud et al. (1998).

to 68.86% when considered per basin. In general, an underestimation of in situ chl-*a* concentrations is observed for all neural network processors and MCI above approximately 10 mg m^{-3} (Fig. 5). MCI relative RMSE for the full lake is 48.63%, ranging from 40.73 to 49.18% for each individual basin. Relative RMSE of the neural networks is more variable; 65.98% for the full lake and ranging from 54.11 to 66.23% in the case of C2R, 68.31% for the full lake and ranging from 30.20 to 82.12% for EUL, 60.61% and ranging from 39.78 to 61.47% for BL, and 45.43%, ranging from 32.17 to 46.63% for FUB/WeW.

The mapped products from the six locally-tuned processors are compared in Fig. 6, during a bloom event in the westernmost basins which took place in early August 2010. At the time of the image acquisition presented here, same day in situ chl-*a* concentrations were measured as 38.5 and 7.0 mg m^{-3} in basins 1 and 4 respectively. Here, FLH is found to quite accurately retrieve chl-*a* concentrations during the bloom event, and reveals bloom extent and detail of spatial features, although low concentrations in basin 4 are overestimated by the algorithm. All the other algorithms do capture a SW–NE trending trophic gradient, however bloom concentrations are not accurately retrieved by any. These are slightly underestimated in MCI mapping, and greatly underestimated in that of FUB/WeW, with C2R, EUL and BL processor mapping falling between. Over the full five years analysed in this study, FLH is found to consistently and accurately capture bloom events as well as timing of onset and decline (Fig. 7).

Evaluating the algorithms in terms of performance for each of the four main lake basins independently (Table 4), it can be observed that although FLH is the best performing overall and for the three westernmost basins (relative RMSE < 30%) (basins 1–3; Fig. 1), its performance is relatively poor in Basin 4 (relative RMSE > 68%). Considering Fig. 5, it is clear that most FLH retrievals from Basin 4 are characterised by chl-*a* concentrations less than approximately 10 mg m^{-3}. Although fewer in number, Basin 1–3 chl-*a* retrievals less than approximately 10 mg m^{-3} in concentration (i.e., from non-bloom periods) are also poorly retrieved by FLH (Fig. 5e). Considering only retrievals of >10 mg m^{-3} from all basins, overall FLH performance improves by almost 10% (relative RMSE 20.77% compared with 30.75% including the full concentration range of matchups, and relative RMSE of retrievals for concentrations <10 mg m^{-3} = 57.57%) (Table 5). An ensemble approach was then applied, whereby chl-*a* concentrations retrieved by the FLH algorithm as chl-*a* concentration of <10 mg m^{-3} were then

Table 4
Chl-*a* retrieval performance parameters of each selected algorithm for the full lake and each Lake Balaton basin separately. R^2 > 0.7 and relative RMSE < 40% are highlighted in bold.

Basin	Processor	*n*[a]	Slope	Intercept	R^2	Bias (mg m^{-3})	RMSE (mg m^{-3})	Rel. RMSE (%)
Full lake	C2R	50	0.38	7.02	0.43	−0.10	7.53	65.98
	EUL	50	0.50	6.49	0.33	1.46	6.85	68.31
	BL	39	0.39	7.02	0.48	−2.22	9.25	60.61
	FUB/WeW	32	0.43	4.09	0.65	−0.76	3.83	45.43
	L1b FLH	60	0.85	1.52	**0.87**	−0.49	4.19	**30.75**
	L1b MCI	60	0.65	3.83	0.69	−0.91	6.62	48.63
1	C2R	13	0.22	13.80	0.21	1.71	10.21	66.23
	EUL	12	0.20	13.92	0.01	5.01	9.09	82.12
	BL	12	0.22	14.94	0.18	−1.60	11.79	55.62
	FUB/WeW	6	0.08	9.39	0.16	−0.17	4.86	46.63
	L1b FLH	16	0.93	−1.51	**0.92**	−2.91	4.77	**23.25**
	L1b MCI	16	0.48	6.79	0.58	−3.80	9.69	47.18
2	C2R	12	0.24	8.75	0.40	−2.11	8.39	58.67
	EUL	15	0.25	10.86	0.27	−0.53	8.89	58.32
	BL	8	0.21	10.15	0.59	−6.70	11.96	56.36
	FUB/WeW	6	0.26	6.29	0.56	−3.47	5.66	42.75
	L1b FLH	14	1.19	−2.48	**0.91**	0.05	3.64	**26.58**
	L1b MCI	14	1.06	1.67	**0.77**	2.54	5.65	41.29
3	C2R	8	0.31	6.97	0.53	−3.05	7.88	54.11
	EUL	8	0.93	0.72	0.72	0.09	2.90	**30.20**
	BL	8	0.37	7.20	0.56	−2.81	5.91	**39.78**
	FUB/WeW	8	0.47	3.53	**0.74**	−1.02	3.63	42.61
	L1b FLH	12	0.79	1.41	**0.91**	−2.10	4.65	**27.76**
	L1b MCI	12	0.68	1.31	**0.86**	−4.06	6.82	40.73
4	C2R	17	0.23	5.04	0.23	1.32	2.81	58.53
	EUL	15	0.22	4.61	0.04	1.33	2.58	61.62
	BL	11	0.09	5.09	0.02	0.80	2.90	61.47
	FUB/WeW	12	0.63	2.34	**0.81**	0.48	1.61	**32.17**
	L1b FLH	18	0.48	5.08	0.11	2.30	3.67	68.86
	L1b MCI	18	0.62	3.11	0.23	1.08	2.62	49.18

[a] 30% of number of matchup points after removing those flagged by the processor.

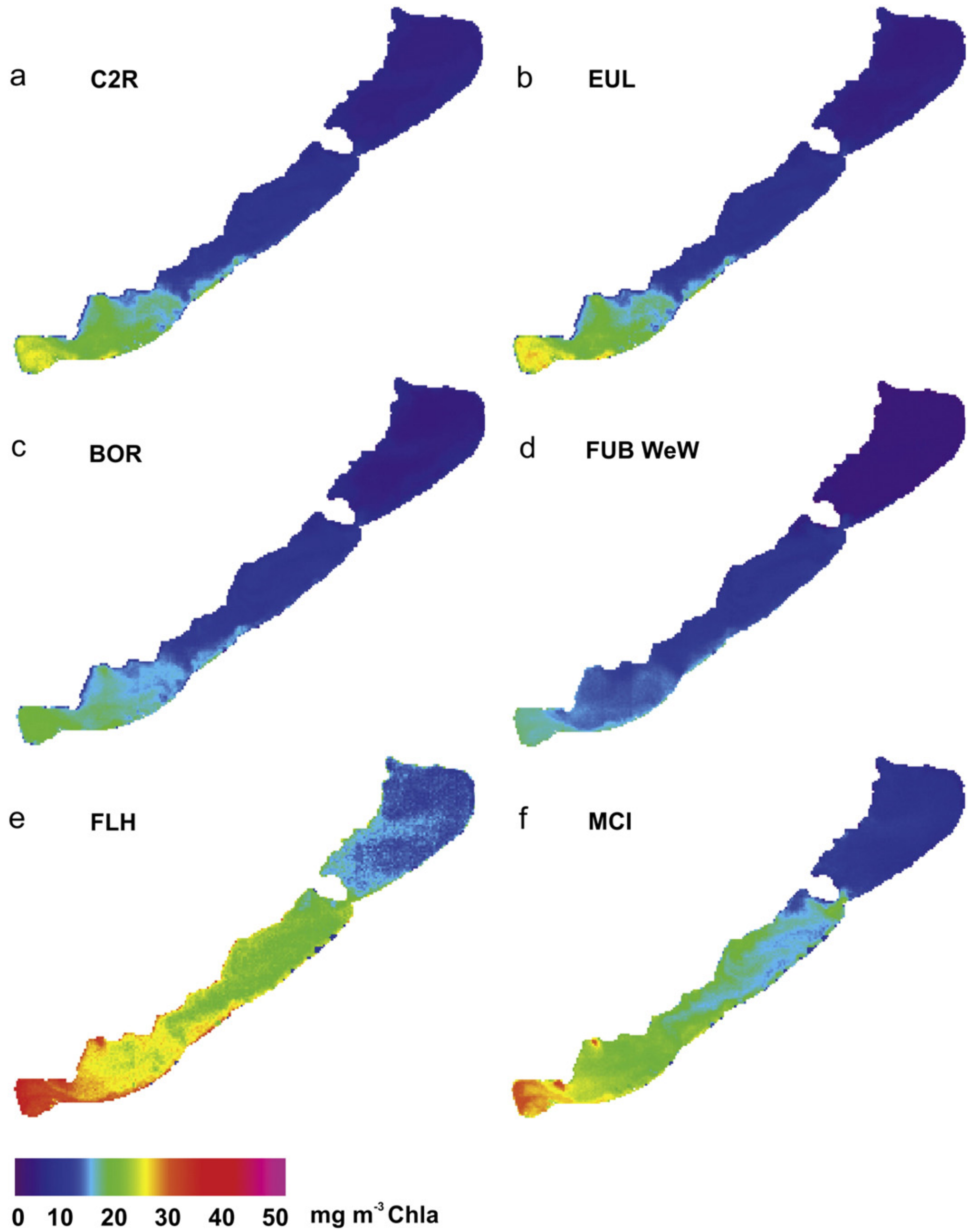

Fig. 6. Chl-*a* concentration mapping by the different processors (C2R (a), EUL (b), BL (c), FUB/WeW (d), FLH (e), and MCI (f)) during a bloom event in August 2010.

processed instead by the FUB/WeW processor. Relative RMSE of FUB/WeW retrievals of <10 mg m^{-3} $= 46.96\%$, an improvement of almost 11% over FLH at low concentrations, although the number of matchups decreases from $n = 34$ to $n = 22$ due to the more extensive flagging of the FUB/WeW processor. The two datasets (FLH $>$ 10 mg m^{-3}, FUB/WeW $<$ 10 mg m^{-3}) were then combined, resulting in a 4.3% improvement to the overall retrieval performance above the application of the FLH algorithm alone, as measured by the relative RMSE (Table 5).

5. Discussion

The overall inaccuracy of chl-*a* concentration retrievals by the neural network algorithms used in this study is apparent in the mapped products (Fig. 6), initial algorithm calibration (Fig. 4; Table 3) and matchup validation statistics alike (Fig. 5; Table 4), highlighting that the application of these algorithms to monitoring Lake Balaton phytoplankton blooms would not be appropriate. Results are consistent with validation results for the EUL processor chl-*a* retrievals over a similar concentration range in Spanish lakes, whereby concentrations were greatly underestimated above approximately 10 mg m^{-3} (Koponen et al., 2008). Validation of the C2R processor in the Canadian/American Lake of the Woods revealed a similarly limited range of retrieved chl-*a* concentrations, 10–15 mg m^{-3} over much of the lake surface compared to the 2–70 mg m^{-3} range of in situ sampled concentrations (Binding et al., 2010). However, whereas Binding et al. (2010) and others (Odermatt et al., 2010; Ruiz-Verdú et al., 2008) report an overestimation of chl-*a* for concentrations of $<$20 mg m^{-3}, no systematic overestimation is found at any concentration level for either the C2R or EUL processors in the current work (Fig. 5a, b), and only 1–2 outlying points are found to

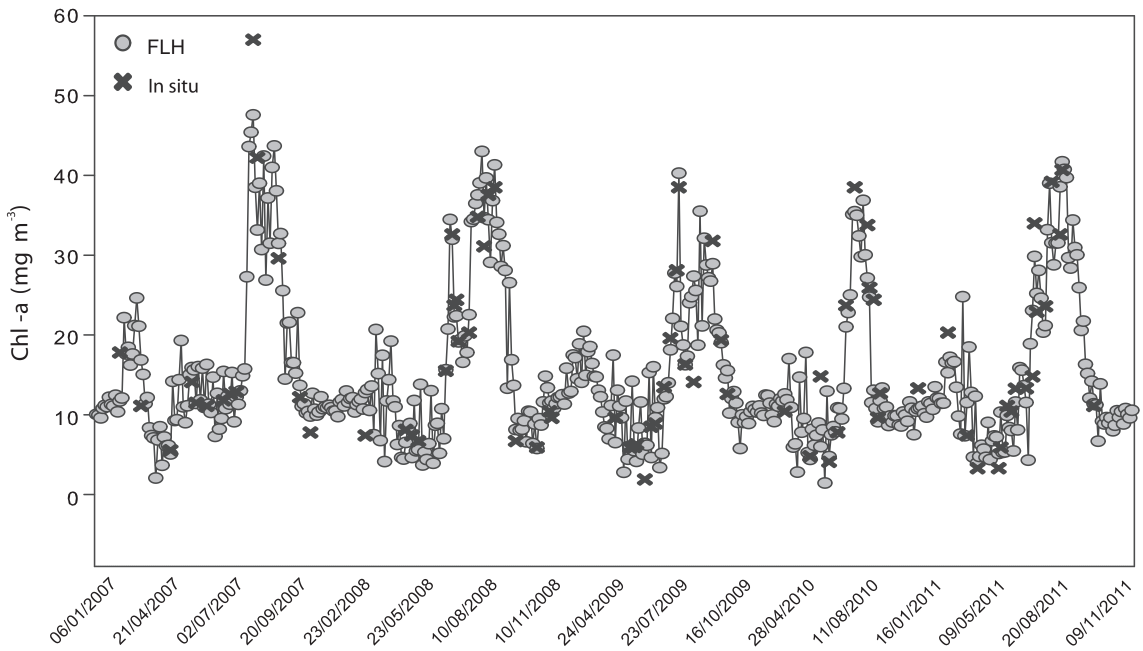

Fig. 7. January, 2007 to December, 2011 time series comparing FLH chl-*a* retrievals and in situ chl-*a* measurements from Basin 1 (Fig. 1).

significantly overestimate chl-*a* at concentrations less than approximately 15 mg m^{-3}.

Both band-difference algorithms (FLH, MCI), and especially FLH, were found to generally outperform all neural network type processors investigated here. Although the specific relationship between the FLH or MCI values and chl-*a* concentration found here performs well for Lake Balaton, this is not directly transferable to other lake systems, rather local tuning would again be required. For example, application of the L1 MCI slope and intercept coefficients found by Binding et al. (2010) (6.166 and 6.347 respectively; Table 6) results in the underestimation of chl-*a* concentrations of the current study (bias $= -5.06$ mg m^{-3}, relative RMSE $= 70.28\%$, compared with bias $= -0.91$ mg m^{-3}, relative RMSE $= 48.63\%$ achieved through local tuning (Table 4)). Similarly, local tuning applied to the selected NN processors here would not be expected to be transferable to other sites. The relationships obtained between chl-*a* concentrations retrieved by some of the investigated algorithms (using default SIOPs in the cases of neural networks) and in situ chl-*a* concentrations reported for other sites, elsewhere in the literature and over similar chl-*a* concentration ranges as Balaton are reported in Table 6, and are compared with relationships obtained for Balaton between in situ concentrations and the processors' default chl-*a* products (prior to local tuning using a_pig(443) so as to be comparable with the other studies). Although chl-*a* retrievals from the C2R, EUL, BL and FUB/WeW processors were partially locally tuned in the current work through modification of SIOP coefficients used to convert a_pig(443) or $a_{pl}(440)$ retrieved by the algorithm to chl-*a* concentrations, overall performance remains relatively poor. This suggests that the retrieval of a_pig(443) and $a_{pl}(440)$ over Lake Balaton by the neural networks was itself not accurate and that the band difference algorithms are more reliable in this case.

An important difference between the two algorithm types investigated here – band-difference and neural network-based – is that, whereas the FLH and MCI algorithms use top-of-atmosphere radiance data without atmospheric correction for chl-*a* retrieval, the neural network processors all perform an atmospheric correction, whether in a separate module prior to deriving constituent concentrations or concurrent with constituent retrieval. In the case of the neural network type processors, the relative contributions of potentially unreliable atmospheric correction and IOP or constituent retrieval itself to the poor overall performance are not known, but can each play an important role. For example, in validating the EUL processor over largely eutrophic Spanish lakes, Koponen et al. (2008) report a significant improvement to chl-*a* retrievals when in situ measured reflectance is input directly into the constituent retrieval module of the processor, bypassing the atmospheric correction module. Although an underestimation of chl-*a* at high concentrations remained, it was much less pronounced.

The strong, negative relationship found here between the FLH algorithm and the in situ chl-*a* dataset for Lake Balaton (Fig. 4) suggests that rather than fluorescence underpinning the physical basis of the algorithm in this instance, that chl-*a* absorption and/or phytoplankton backscattering are dominant, as has been reported elsewhere for meso-, eu- and hypertrophic waters (Binding et al., 2010; Matthews et al., 2012). The algorithm is nonetheless found to robustly retrieve chl-*a* concentrations (Fig. 5e; Table 4). This negative relationship may also indicate cyanobacteria dominance, as suggested by Binding et al. (2010) as well as Wynne et al. (2008) and Matthews et al. (2012), although information on phytoplankton species composition is lacking in the current investigation. This is due to the majority of cyanobacteria chl-*a* being contained within the non-fluorescing Photosystem I, and therefore not contributing to the fluorescence signal (Johnsen & Sakshaug, 1996; Matthews et al., 2012; Mimuro & Fujita, 1977).

The chl-*a* retrieval performance of the FLH algorithm generally improves with higher chl-*a* concentration, over the ranges investigated

Table 5
Improvement to chl-*a* concentration retrievals of <10 mg m^{-3} and overall using an ensemble FLH–FUB/WeW processor approach over retrievals using FLH alone.

Processor	n	R^2	Bias (mg m^{-3})	RMSE (mg m^{-3})	Rel. RMSE (%)
<10 mg m^{-3}					
FLH	34	0.11	−0.19	3.64	57.57
FUB/WeW	22	0.26	0.85	2.97	46.96
Improvement	−12	0.15	−0.66	0.67	10.61
Full data range					
FLH	60	0.87	−0.49	4.19	30.75
FLH–FUB/WeW ensemble	48	0.90	−0.09	4.07	26.47
Improvement	−12	0.03	0.40	0.12	4.28

Table 6
Comparison of relationships between in situ measured chl-*a* and MCI or neural network derived chl-*a* reported in the literature over similar concentration ranges as Lake Balaton, and those for Lake Balaton.

Study	Model	Chl-*a* range ($mg\ m^{-3}$)	R^2	Current model[c]	Current R^2
Alikas and Reinart (2008)	0.86 * C2R chl-*a*	~0–35	0.52	1.63 * C2R chl-*a* + 1.09	0.46
Binding et al. (2010)	6.17 * L1b MCI + 6.35	1.9–70.5	0.77	3.91 * L1b MCI + 11.31	0.62
Binding et al. (2010)	0.66 * C2R chl-*a* + 7.13		0.16	1.63 * C2R chl-*a* + 1.09	0.46
Binding et al. (2010)	−0.13 * EUL chl-*a* + 17.68		0.19	2.01 * EUL chl-*a* − 0.57	0.42
Binding et al. (2010)	0.44 * BL chl-*a* + 7.57		0.21	0.65 * BL chl-*a* + 3.25	0.46
Koponen et al. (2008)[a]	2.86 * EUL chl-*a* − 1.15	1.2–53.2	0.97	2.01 * EUL chl-*a* − 0.57	0.42
Koponen et al. (2008)[b]	0.62 * EUL chl-*a* + 3.13	4–19	0.92	2.01 * EUL chl-*a* − 0.57	0.42
Odermatt, Pomati, et al. (2012)[d]	7.87 * C2R chl-*a* − 2.92	~5–40	0.40	1.63 * C2R chl-*a* + 1.09	0.46
Odermatt, Pomati, et al. (2012)[d]	12.20 * EUL chl-*a* − 3.17	~5–40	0.41	2.01 * EUL chl-*a* − 0.57	0.42
Odermatt, Pomati, et al. (2012)[d]	1.27 * WeW chl-*a* + 4.70	~5–40	0.39	0.30 * WeW chl-*a* + 4.63	0.32

[a] Spanish lakes.
[b] Lake Victoria.
[c] Relationship between in situ chl-*a* and MERIS MCI or uncalibrated mean chl-*a* of neural network processors, using calibration dataset.
[d] Obtained using 5 m depth averaged fluorescence profile in situ measurements.

here, with best performance in basin 1, decreasing towards basin 4. Basin 4 is distinct from the other three basins in that it is considered to be mesotrophic, instead of eutrophic (Mózes et al., 2006). This finding is comparable to other studies where the use of red-NIR band combination algorithms only retrieved valid chl-*a* concentrations above a certain chl-*a* concentration threshold, typically between 8 and 20 mg m^{-3} (Domínguez Gómez, Alonso Alonso, & Alonso Garcia, 2011). In contrast, the neural network type processors generally performed better at lower chl-*a* concentrations (basin 4 vs. basins 1–3), as measured by the relative RMSE of each (Table 4). The potential overall improvement to be gained from applying the FUB/WeW where relatively low, mesotrophic (<10 mg m^{-3}) chl-*a* concentrations have been identified by FLH, and FLH elsewhere is demonstrated in Table 5. Although overall improvement is limited (a 4.28% reduction in relative RMSE was obtained through the ensemble approach as compared with applying only FLH), improvement to retrievals of <10 mg m^{-3} was more substantial (a 10.61% reduction in the relative RMSE). In considering high chl-*a* concentration bloom events alone, the application of only FLH can be considered reliable for the onset detection and monitoring of bloom events for lake management. On the other hand, such a stepwise, ensemble FLH-FUB/WeW processor approach could be considered to optimise chl-*a* concentration retrievals, including at low concentrations.

An important point to note is that although attention was paid to apply algorithms only within the range of chl-*a* concentrations used in their training in the case of the neural network processors, and to exclude flagged pixels which may also be beyond training ranges, validation data are lacking regarding TSM concentrations, water leaving spectra and IOPs. Should these be beyond the training ranges, they would be expected to adversely impact the chl-*a* retrievals. This is necessary to consider for the application of algorithms where in situ data are less available than would be ideal. Knowledge and consideration of conditions, if not validation of all constituents and IOPs, are recommended where possible. Although CDOM measurements are not routinely available, concentrations typically range from 0.3 m^{-1} in the westernmost basin to 0.01 m^{-1} in the easternmost basin. TSM concentrations are highly variable in Lake Balaton and typically ranged from 2 to 70 g m^{-3} over the five year period, although concentrations between 90 and 115 g m^{-3} were measured on several occasions, exceeding the ranges of the neural network algorithms. Such high and variable TSM concentrations may also influence the specific FLH and MCI coefficients found for Lake Balaton, as they would affect the baseline above or below which the given index is calculated.

6. Conclusions

MERIS satellite data have been demonstrated here to be effective, not only in detecting the occurrence of bloom events in Lake Balaton through archive imagery, but also in accurately retrieving chl-*a* concentrations during both algal bloom events and non-bloom periods, across all seasons over a five-year time series and across the spatial extent of the lake. The results suggest the potential for valid time series analysis using MERIS imagery. A locally-tuned FLH model was found to result in the best chl-*a* retrievals from the six algorithms tested, although the negative relationship between the derived FLH index and in situ chl-*a* suggests a physical basis related to chl-*a* absorption and/or phytoplankton backscattering rather than fluorescence. The transferability of this algorithm to forthcoming Sentinel-3 OLCI data and the improved channel configuration of this sensor for atmospheric correction and water constituent retrievals over turbid waters support the feasibility of applying similar approaches in the future. This will be key to the generation of consistent satellite time series and to the development of operational water quality products for lakes globally. The realisation of operational products for lakes will substantially support the requirements of the ongoing basis towards meeting European Commission Water Framework Directive for spatially cohesive water quality monitoring, including the concentration of phytoplankton biomass.

The variable performance of the algorithms tested underlines that atmospheric and in-water models must be carefully selected and validated prior to reliable use for a given site or optical water type. Widely variable results using the same processors have been found from lake to lake, and caution must be taken when applying unvalidated algorithms. Likewise, within-lake variability in optical properties may necessitate the use of two or more different algorithms for optimal retrievals, as has been demonstrated here for Lake Balaton.

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