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Retrieving Chl-a and total suspended solids in in-land waters using EnMAP simulated data

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Abstract

The Environmental Mapping and analysis program (EnMAP) is a new Earth observation satellite which will use imaging spectroscopy to obtain a diagnostic characterisation of the Earth's surface and record changes. Since we hypothesis that imaging spectroscopy can significantly improve the accuracy of predicting and assessing water quality traits of small in-land waters, our study investigates the capability of the simulated EnMAP data to predict chlorophyll-a (Chl-a) and total suspended solids (TSS) as two of the most crucial water quality indicators. Three machine learning (ML) approaches(i.e., The methods used were Principal Component Regression(PCR), Partial Least Square Regression (PLSR) and Random Forest (RF)) were employed to establish links between the simulated image spectra and the above-mentioned water attributes of the samples collected from several in-land water reservoirs

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within the southern part of the Czech Republic. Additionally, an airborne hyperspectral image likewise was used for developing a model to compare its performance with models developed based on simulated EnMAP data. According to the results, adequate prediction accuracy was obtained for Chl-a (RF: $R^2 = 0.89$, RMSE = 43.06, and LCCC = 0.91) and TSS (RF: $R^2 = 0.91$, RMSE = 17.53, and LCCC = 0.94), which was close enough to those obtained for the airborne hyperspectral image. Chl-a and TSS showed a correlation with around 550 and 650 nm and from 700 nm to 800 nm of the red and near-infrared (NIR) regions. The spatial distribution maps derived from the simulated EnMAP were comparable to those obtained by the source image, particularly in water bodies with relatively high and low contents of the water attributes. Overall, it can be concluded that the simulated EnMAP image was successful and reliable in the prediction and spatial mapping of the selected biophysical properties of the small in-land water bodies.

Keywords: Remote sensing, Satellite imagery, Hyperspectral imagery, Machine learning, Biophysical properties, Water quality

1. Introduction

In-land waters (i.e., water bodies with no direct sea or ocean connection) supply essential and diversified natural environment and ecological community services and support biodiversity while providing necessary water for various human applications (Stendera et al., 2012; Carvalho et al., 2013; Palmer et al., 2015; Dörnhöfer & Oppelt, 2016). However, human activities such as water extraction, wastewater discharge, spreading the invasive species, and source water interference have threatened the in-land water quality (Palmer

9 et al., 2015; Maier & Keller, 2019).

10 Developing rapid, low-priced, and precise water quality monitoring and
11 assessment schemes to avert destructive changes through timely treatments is
12 essential. However, conventional point-based in-situ water monitoring plans
13 have limited spatial and temporal variability coverage. In addition, they
14 are time, cost, and labour demanding (Schaeffer et al., 2013) and yield non-
15 representative and inaccurate water quality maps as a result of unevenly
16 distributed single measurements (Van Puijenbroek et al., 2015).

17 Remote sensing (RS) has shown a remarkable ability for monitoring and
18 assessment of in-land water bodies by extracting the water spectral infor-
19 mation and transforming them into some quality parameters such as total
20 suspended solids (TSS) (Guimarães et al., 2019; Saberioon et al., 2020; Du
21 et al., 2022), turbidity (Keller et al., 2018; Cui et al., 2022; Rodríguez-López
22 et al., 2021), microbiological properties such as chlorophyll a (Chl-a) (Keller
23 et al., 2018; Saberioon et al., 2020; Silveira Kupssinskü et al., 2020; Gupana
24 et al., 2021; Maier et al., 2021), and organic properties including dissolved
25 organic carbon (DOC) and colored dissolved organic matter (CDOM) (Cao
26 et al., 2018; Keller et al., 2018; Ross et al., 2019; Li et al., 2022), allowing
27 exhaustive monitoring of in-land water bodies. These advantages have made
28 RS an efficient water monitoring technique which can complement in-situ
29 measurements.

30 Due to the finer spectral resolution of hyperspectral data, significant at-
31 tention has been directed toward the hyperspectral RS. Based on acquisition
32 platforms, three types of hyperspectral RS data have been used for in-land
33 water quality monitoring: (i) satellite data such as Hyperion (Giardino et al.,

2007) and PRecursores IperSpettrale della Missione Applicativa (PRISMA) (Bresciani et al., 2022), (ii) airborne data such as HyMap (Thiemann & Kaufmann, 2002), Airborne Imaging Spectrometer for Applications (AISA) (Pyo et al., 2018; Vinciková et al., 2015), Airborne Spectrographic Imager (CASI) (Beck et al., 2016), and Airborne Prism Experiment (APEX) (Knaeps et al., 2015), and (iii) low altitude platforms acquired data (e.g., unmanned aerial vehicles (UAV)) (Guimarães et al., 2019; Cillero Castro et al., 2020). Most airborne- and UAV-based sensors record very high spatial resolution images without being affected by atmospheric distortions, but they lack temporal continuity since they usually do not operate regularly (Trançon et al., 2018). On the contrary, satellite data is recorded automatically, regularly, and frequently with proper repetitive temporal coverage. However, due to some constraints such as high instrumental imaging and computation cost and low signal-to-noise ratio (SNR), the number of satellite missions with hyperspectral sensors is significantly lower than those carrying the multispectral ones (Govender et al., 2007). Launching new orbital hyperspectral satellites with higher spectral, spatial, temporal and radiometric resolution sensors will lead to more reachable and accurate water quality parameters retrieval and mapping.

The hyperspectral imager (HSI) Environmental Mapping and Analysis Program (EnMAP) is a German satellite mission for global scale monitoring of severe environmental challenges caused by climate change and human activities (Guanter et al., 2015). It was launched on 1st April 2022 with a swath width of 30 km, spatial resolution of 30 m, a radiometric resolution of 14 bits and four days of minimum temporal resolution using tilt angle obser-

59 vations. EnMAP products will consist of 218 bands covering a spectral range
60 from 420 nm to 2450 nm, which we hypothesise that it has ability to detect
61 Chl-a or other pigments in various circumstances (Saberioon et al., 2020).
62 Furthermore, EnMAP covers both red and near infrared (NIR) regions with
63 a relatively high SNR, making it an appropriate choice for remote estimation
64 of water physicochemical properties (Ruddick et al., 2016).

65 Although empirical models developed for quantifying water quality traits
66 through inversion of the nonlinear correlative relationship between water
67 quality parameters and reflectance spectra within the red and NIR portion of
68 the electromagnetic spectrum (Choubey, 1992; Goodin et al., 2008; Ouillon
69 et al., 2008; Chen et al., 2007), they are vulnerable to seasonal and spatial
70 differences. Therefore, Machine Learning (ML)-based approaches including
71 Support Vector Machine (SVM) (Keller et al., 2018; Maier & Keller, 2019),
72 Cubist (Saberioon et al., 2020), Random Forest (RF) (Silveira Kupssinskü
73 et al., 2020; Rubin et al., 2021) , Artificial Neural Networks (ANN) (Sil-
74 veira Kupssinskü et al., 2020; Maier & Keller, 2019), and Extreme Ma-
75 chine Learning (Peterson et al., 2018), became popular for developing semi-
76 empirical models. They provide intelligent ways of eliminating irrelevant
77 spectral wavelengths while unravelling the complex relationship between re-
78 sponse and predictor variables with limited assumption and prior knowledge
79 (Saberioon et al., 2020; Chen et al., 2022).

80 In this context, this study aims to assess the capacity of spectral infor-
81 mation provided by EnMAP for quantifying and mapping Chl-a and TSS, as
82 two important in-land water quality traits. Additionally, Results are com-
83 pared with those Chl-a and TSS values obtained directly by airborne image

84 spectra. The investigation also includes the development of ML models for
85 assessing Chl-a and TSS, which may offer critical information on these water
86 quality metrics in a more accurate, rapid, and less computational-demanding
87 manner than the existing methods.

88 **2. Materials and Methods**

89 *2.1. Test sites, water sampling, and variable measurements*

90 The area of interest is located in the Třeboň Basin Biosphere Reserve,
91 South Bohemia, Czech Republic. It is a historical area that is relatively flat,
92 with a large number of ponds and artificial water reservoirs. These cover
93 up to 15 % of the area. The history of some of the ponds goes back several
94 centuries. The altitude is around 420 m above sea level. The mean annual
95 temperature varies by about 7.8 °C, and the annual sum of precipitation is
96 circa 650 mm. The ponds are shallow turbid reservoirs primarily intended
97 for the commercial breeding of carp (*Cyprinus carpio* L.) or other freshwater
98 fish. The depth of the ponds does not usually exceed 3 m; the area varies
99 from hundreds of square metres up to 648 ha (Rožmberk fishpond). Most
100 of the ponds in the area have eutrophic to hypertrophic character with high
101 turbidity and low water transparency (tens of centimetres). There are also
102 oligotrophic to mesotrophic reservoirs in the area with low turbidity and high
103 water transparency (approx. 1 m). These are mainly sandpits with depths of
104 up to 30 m. These lakes are currently used mostly for recreation and partly
105 for mining. A map of the area of interest is shown in Figure 1.

106 Water samples for laboratory analyses were collected during the aerial
107 imaging campaign on July 11, 2010. Water samples were collected at reser-

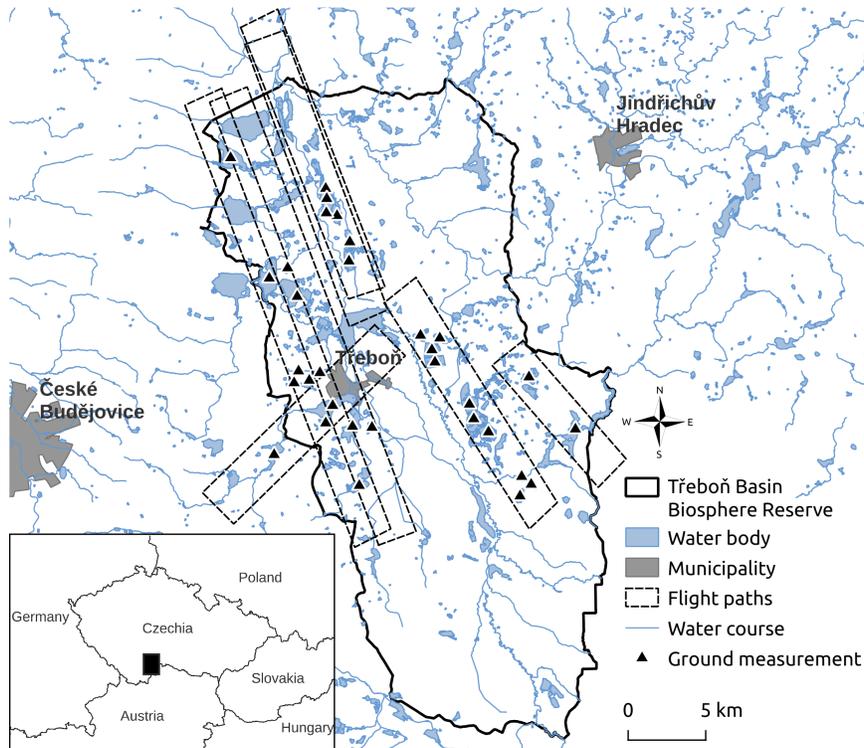


Figure 1: Area of interest map with highlighted flight paths and water sampling points. Aerial hyperspectral imaging was performed on 11 July 2010.

108 voirs with different trophic levels, i.e., hypertrophic ponds and sandpit lakes
 109 with oligotrophic-mesotrophic water types. Each sampling point was recorded
 110 using a GPS tracker. The samples collected were analysed in the laboratory
 111 immediately after collection. Chl-a values were estimated by reading of ab-
 112 sorbance with double beam UV-Vis spectrophotometer Helios Alpha (Uni-
 113 cam, GB) at 664 nm after extraction with a mixture of 90 % acetone:methanol
 114 (Pechar, 1987). TSS was determined as dry weight of seston captured on
 115 pre-weighed Whatman GF/C filters and dried to constant weight at 60 °C
 116 (Vinciková et al., 2015).

117 *2.2. Hyperspectral airborne imaging spectrometers data acquisition and pre-*
118 *processing*

119 Aerial measurements were performed using the AISA Eagle airborne hy-
120 perspectral imaging system (Specim Ltd, Finland). The spectral range was
121 400 to 1000 nm with a spectral resolution of 2.2 nm. Within the seven flight
122 paths, 260 spectral bands were acquired (see Figure 1). The spatial resolution
123 of the hyperspectral images was 5.5 m. The hyperspectral data were acquired
124 between 09:30 and 11:30 central Europe time (CET) on 11 July 2010. The
125 ASD FieldSpec-3 spectroradiometer was used to measure the optical prop-
126 erties of the reference surfaces. These supportive data were used for images
127 calibration and validation. Microtops II Sunphotometer measurements were
128 used to estimate the current atmospheric conditions, aerosol optical thick-
129 ness (AOT) and water vapour (WV). Preprocessing of the AISA Eagle data
130 acquired during the flight campaign was performed in CaliGeo (radiometric
131 corrections), PARGE (orthorectification) and ATCOR-4 (atmospheric cor-
132 rections) software. The hyperspectral image data were georeferenced to the
133 WGS84/UTM Zone 33N (EPSG 32633) coordinate system. For further de-
134 tails see (Hanuš et al., 2008).

135 *2.3. Simulation of EnMAP spaceborne hyperspectral image*

136 EnMAP data and associated radiance and reflectance products (Level
137 1B/1C/2A) were generated using the EnMAP end-to-end simulation software
138 EeteS (Segl et al., 2012). EeteS is an instrument simulator developed to
139 support EnMAP mission preparatory activities. The sequential processing
140 chain of the software consists of four independent modules - the atmospheric,
141 spatial, spectral and radiometric modules, in which hyperspectral reflectance

142 data is used to calculate top-of-atmosphere radiance and subsequently digital
143 numbers (L0). This forward simulator is coupled with a backward simulation
144 branch consisting of sensor calibration modules and a complete L1/L2 pre-
145 processing chain. As a result, a realistic EnMAP scene with 30 m pixel
146 resolution and 242 spectral bands ranging between 420 nm and 2450 nm was
147 generated.

148 *2.4. Quantitative modeling and prediction assessment*

149 Three modeling approaches were used to predict the water parameters:
150 Principal Component Regression (PCR), Partial Least Square Regression
151 (PLSR) and RF. All techniques are appropriate when observations are limited
152 and more predictors are available and they have been reportedly used in the
153 analysis of the hyperspectral RS data water properties (Song et al., 2012;
154 Sudduth et al., 2015; Wang et al., 2020; Flores et al., 2021).

155 PCR is a linear regression model obtained by combining the multiple lin-
156 ear regression (MLR) and principal component analysis (PCA) to suppress
157 the problem of MLR methods facing the multicollinearity between variables
158 (Liu et al., 2003). PLSR is another linear regression method that projects
159 independent variables (X) as predictors and dependent variables (Y) as re-
160 sponses into a set of orthogonal latent factors while maximising the covari-
161 ance between X- and Y-scores (Wold et al., 2001). In RF, as an ensemble
162 learning method, decision trees are trained and then a voting procedure is
163 employed to combine the result obtained by each tree. Unlike the noise sen-
164 sitivity of every single tree’s prediction outcome, uncorrelated trees combina-
165 tion will not yield that much noisy results. Furthermore, training data will
166 be created by bagging approach –drawing sample subsets with replacement–

167 which may cause improved model performance (Belgiu & Drăguț, 2016).

168 Water samples were divided into calibration and testing (75 % and 25 %
169 respectively) sets randomly. Prediction models were trained on the calibra-
170 tion set using 5-repeated 10-fold cross-validation, while their generalisation
171 capability was evaluated on the test set. The coefficient of determination
172 (R^2), root mean square error (RMSE), Lin’s concordance correlation coeffi-
173 cient (LCCC) and bias were used to assess the performance of the models in
174 calibration, validation and testing steps.

175 *2.5. Chl-a and TSS spatial distribution mapping*

176 The best prediction models were applied to both image pixels’ spectra
177 and Chl-a and TSS distribution maps of water bodies were produced by
178 linear Triangulated Irregular Network (TIN) interpolation with grid 10 m
179 in QGIS 3.22 environment. Finally, the spatial patterns of water properties
180 obtained by AISA Eagle hyperspectral airborne and simulated EnMAP data
181 were compared.

182 **3. Results**

183 *3.1. Statistical description of Chl-a and TSS*

184 The water properties box-plots and QQ-plots are shown in Figure 2. As
185 can be seen, one Chl-a value was considered as outlier, while TSS contents
186 of the samples did not include any outlier.

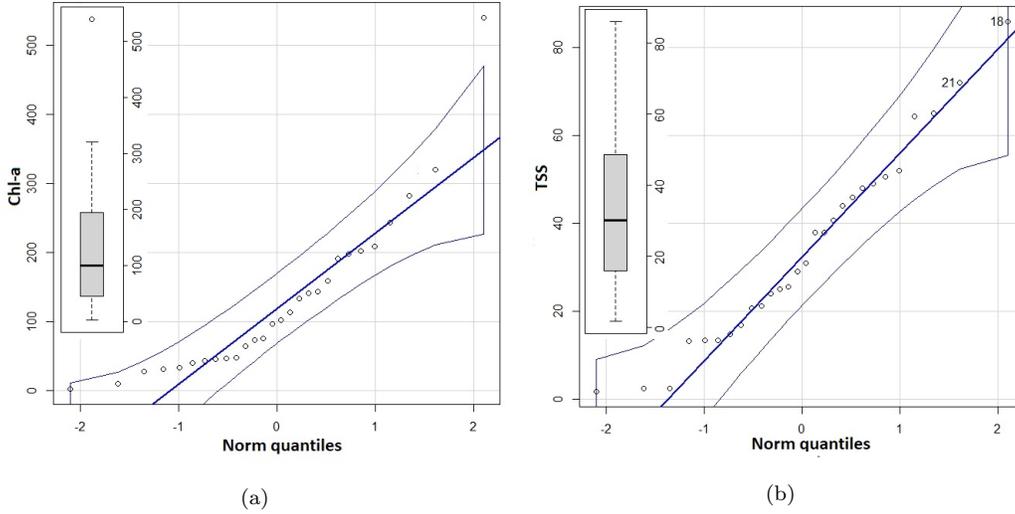


Figure 2: QQ-plots and box-plots of (a) Chl-a and (b) TSS

187 General statistics of Chl-a and TSS contents of water samples, namely
 188 minimum (Min), maximum (Max), mean, standard deviation (SD), coeffi-
 189 cient of variation (CV), and skewness, were calculated after removing the
 190 sample with outlier value of Chl-a (Table 1). Accordingly, compared to TSS,
 191 Chl-a showed more variability due to the wider range of data, which was
 192 reflected in its coefficient of variation value (76.96%), which indicates a more
 193 heterogeneous distribution of Chl-a in comparison to the TSS.

Table 1: Descriptive statistics of Chl-a ($\mu\text{g/L}$) and TSS (mg/L)

Parameter	Min	Max	Mean	SD	Skewness	CV (%)
Chl-a	2.23	320.44	114.08	86.66	1.62	76.96
TSS	1.75	86	33.88	21.52	0.46	63.5

194 3.2. Correlation of Chl-a and TSS with reflectance spectra

195 Pearson correlation analysis was used to explore the correlation between
 196 Chl-a and TSS contents in the in-land water and the spectra of both hy-

197 perspectral images (i.e., AISA Eagle airborne hyperspectral imaging system
 198 and simulated EnMAP) in the range between 420 nm and 980 nm. It can be
 199 observed (Figure 3) that both Chl-a and TSS highly correlated with spectral
 200 wavelengths around 550 nm, 660 nm and also in the red and NIR region
 201 from 700 nm to 800 nm. The maximum correlation values relating to Chl-a
 202 were obtained with the spectra from simulated EnMAP at about 710 nm,
 203 while TSS content and airborne image spectra had their highest correlation
 204 at about 800 nm.

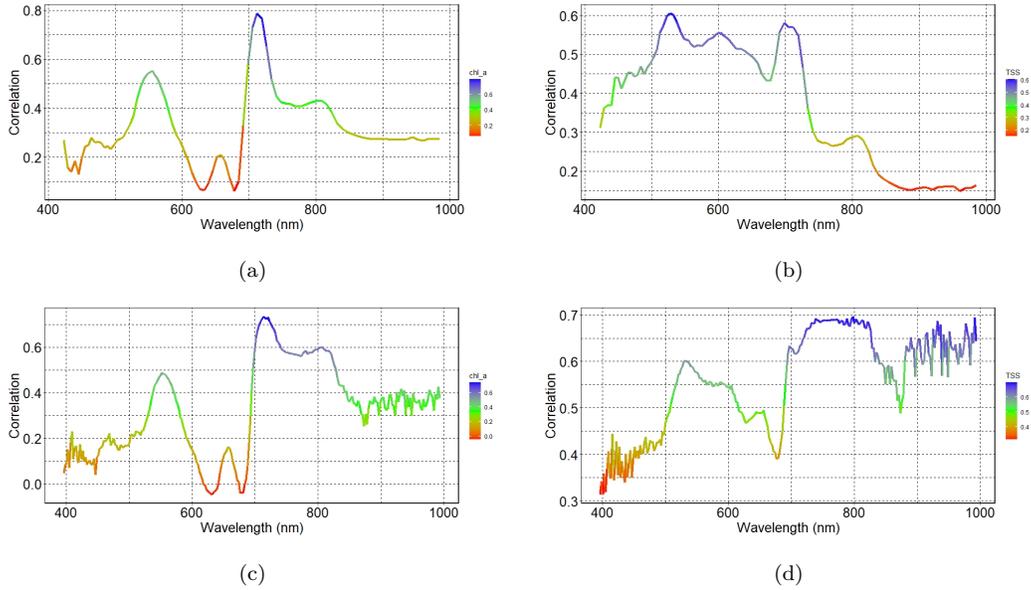


Figure 3: Correlation between the simulated EnMAP pixels spectra and (a) Chl-a, (b) TSS and AISA Eagle airborne hyperspectral image pixels spectra and (c) Chl-a and (d) TSS

205 *3.3. Performance of Chl-a and TSS prediction models*

206 Chl-a and TSS prediction results using both types of RS data (AISA
 207 Eagle airborne and simulated EnMAP) are presented in Table (2).

Table 2: Performance of Chl-a and TSS prediction models developed by PCR, PLSR, and RF

Properties	Method	Dataset	Airborne				EnMAP			
			R ²	RMSE	LCCC	bias	R ²	RMSE	LCCC	bias
Chl-a	PCR	Calibration	0.96	26.24	0.97	-1.55	0.90	56.3	0.93	-3.11
		Validation	0.88	31.95	0.91	-13.71	0.85	59.11	0.89	-18.43
		Test	0.79	53.76	0.84	23.44	0.64	64.67	0.68	40.43
	PLSR	Calibration	0.94	33.08	0.95	0.3	0.92	47.09	0.95	-1.05
		Validation	0.89	48.63	0.92	-12.16	0.87	54.15	0.91	21.05
		Test	0.83	50.34	0.87	25.28	0.69	62.99	0.74	34.72
	RF	Calibration	0.95	29.53	0.98	0.1	0.92	39.88	0.96	2.05
		Validation	0.93	31.82	0.96	-5.36	0.89	40.75	0.95	19.82
		Test	0.91	34.23	0.93	-10.97	0.89	43.06	0.91	33.01
TSS	PCR	Calibration	0.90	8.89	0.91	-0.07	0.88	9.72	0.91	-1.81
		Validation	0.83	11.54	0.88	-10.45	0.81	20.48	0.85	21.05
		Test	0.77	13.39	0.81	-16.32	0.71	29.92	0.72	37.38
	PLSR	Calibration	0.93	7.48	0.95	0.08	0.86	10.94	0.92	-0.56
		Validation	0.87	11.92	0.90	-5.81	0.85	16.22	0.89	9.63
		Test	0.81	18.17	0.84	-7.41	0.75	21.39	0.78	23.44
	RF	Calibration	0.97	8.37	0.99	0.43	0.95	9.16	0.97	1.05
		Validation	0.96	10.36	0.97	3.49	0.93	14.92	0.96	-8.34
		Test	0.94	13.76	0.96	-5.12	0.91	17.53	0.94	11.43

208 Regarding the applied ML method, different results were obtained for
209 different Chl-a and TSS. The best Chl-a prediction was obtained using RF
210 with $R_p^2 = 0.91$, $RMSE_p = 34.23 \mu\text{g/L}$, $LCCC = 0.93$ and $\text{bias} = -10.97$ on
211 the AISA Eagle airborne data (Figure 4a) and $R_p^2 = 0.89$, $RMSE_p = 43.06$
212 $\mu\text{g/L}$, $LCCC = 0.91$ and $\text{bias} = 33.01$ for the simulated EnMAP (Figure
213 4c). Similarly, TSS was best predicted by RF ($R_p^2 = 0.94$, $RMSE_p = 13.76$
214 mg/L , $LCCC = 0.96$ and $\text{bias} = -5.12$) applied on the AISA Eagle airborne
215 image (Figure 4b). The simulated EnMAP and RF estimated TSS with R_p^2
216 $= 0.91$, $RMSE_p = 17.53 \text{ mg/L}$, $LCCC = 0.94$ and $\text{bias} = 11.43$ (Figure 4d).

217 The results highlights that though both water properties were acceptably
218 assessed, TSS was predicted with a higher accuracy than Chl-a.

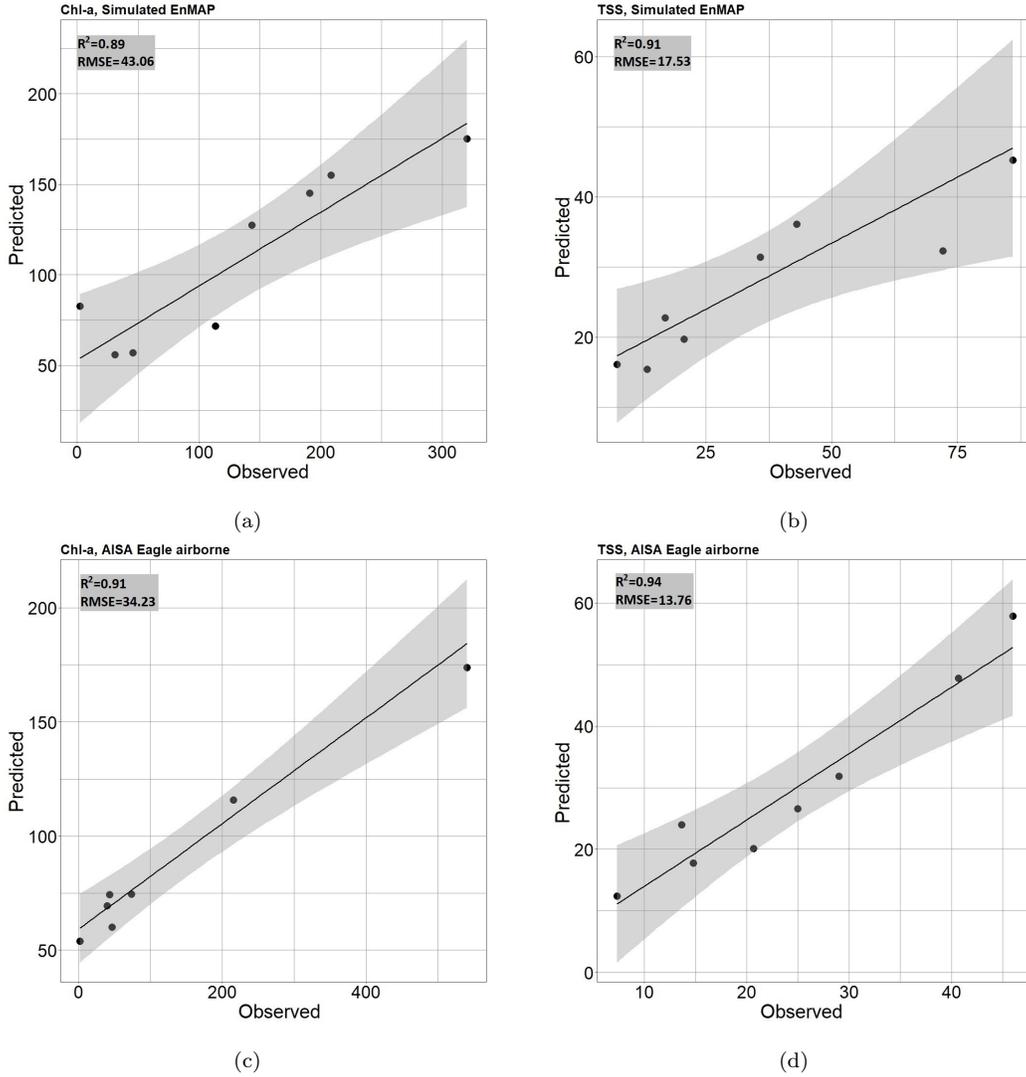


Figure 4: The measured versus RF-predicted values of Chl-a using (a) simulated EnMAP and (c) AISA Eagle airborne images, and TSS using (b) simulated EnMAP and (d) AISA Eagle airborne images (test dataset)

219 As Expected, regardless of the water parameter, all prediction methods
220 (PCR, PLSR, and RF) yielded better results for the AISA Eagle airborne
221 image. This superiority was achieved for calibration, validation, and test
222 datasets. Conversely, the prediction results derived from the simulated En-
223 MAP were acceptable too (Table 2). This highlights that the images from
224 simulated EnMAP were suitable for predicting Chl-a and TSS in this study
225 area.

226 *3.4. Spatial distribution maps of Chl-a and TSS*

227 The spatial distribution maps of the water quality indicators estimated
228 using the AISA Eagle airborne hyperspectral and EnMAP simulated images
229 are shown in Figure 5. Both images yielded similar patterns for Chl-a and
230 TSS in the water bodies under study. The spatial distribution of Chl-a
231 content is similar for both data types (5 a) and c)). The AISA image shows
232 relatively lower values of Chl-a content than the image from the simulated
233 EnMAP data. The images also show that the AISA sensor data show more
234 detail, which is due to the spatial resolution of the original data. The high
235 Chl-a values at the edges of the reservoirs marked by green vegetation belong
236 to the littoral vegetation.

237 The TSS values also have the same spatial distribution in both images
238 (5 b) and d)). The values obtained from the simulated EnMAP data are
239 slightly higher.

240 Within the study area, there are differences in Chl-a and TSS content
241 between the different reservoirs. This is mainly due to the management of
242 each reservoir and nutrient inputs from the catchment.

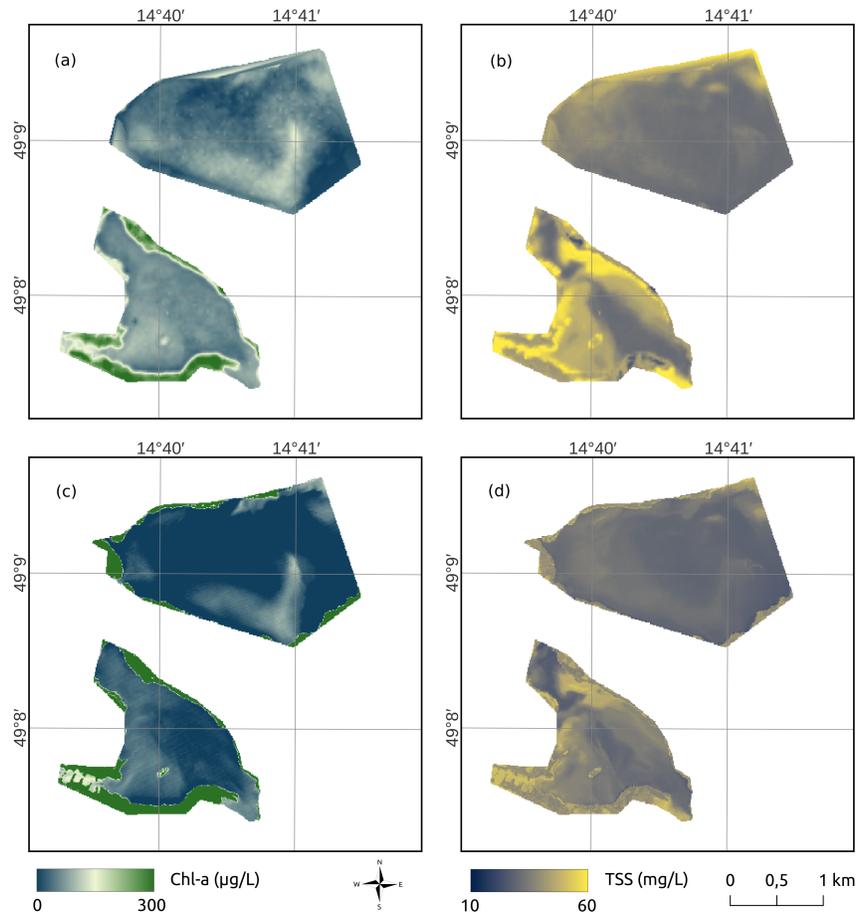


Figure 5: Spatial distribution of Chl-a and TSS in selected fishponds obtained from simulated EnMAP (top row) and AISA Eagle airborne hyperspectral imagery (bottom row)

243 **Discussion**

244 To study ecological, environmental and hydrological processes, it is es-
 245 sential to estimate water dynamics and quality of inland waters; however, it
 246 is challenging as they are complex, dynamic and heterogeneous. Despite the
 247 significant progress made in remote sensing of water bodies and the promis-
 248 ing performance of satellite data for estimating water quality traits, there are

249 still some limitations, such as low spectral, the spatial or temporal resolution
250 of current available multispectral sensors prevent us from taking advantage of
251 remote sensing data fully. However, emerging new sensors such as EnMAP,
252 which have higher resolutions, permit us to accurately monitor water dynam-
253 ics and water qualities for the long term. The results of this study show that
254 Chl-a and TSS contents of in-land water bodies can be quantitatively pre-
255 dicted (Table 2) and mapped (Figure 5) using the simulated EnMAP spectra.
256 In other words, EnMAP can provide enough data to reasonably predict and
257 visualize spatial distribution of Chl-a and TSS in small inland waters. The
258 strong correlation of the Chl-a and TSS with the red and NIR wavelengths
259 of 660 nm and 700–800 nm (Figure 3), which was seen in this study, is in
260 a good agreement with several other literature. Kim et al. (2020) reported
261 three key wavelengths (i.e., 662 nm, 702 nm, and 752 nm) with the highest
262 correlation to estimate Chl-a concentration in a pond. A very high corre-
263 lation of about 0.8 has also been reported between Chl-a content of a lake
264 and in-situ hyperspectral data at 719 nm in a study conducted by Jiao et al.
265 (2006). Similarly, a high correlation between Chl-a and hyperspectral data
266 was found at about 700 nm in the study of retrieving Chl-a concentrations
267 in coastal waters readlized by Ryan & Ali (2016). Saberioon et al. (2020)
268 also reported that both Chl-a and TSS had the highest correlations with
269 Sentinel-2 band 5 (698–713 nm, Central wavelength 703 nm) for inland
270 waters. In addition, Sentinel-2 band 5 also showed the highest correlation
271 with turbidity of lakes water in northeastern China (Ma et al., 2021). These
272 strong correlations can be attributed to chlorophyll absorbance at 670 nm
273 and other plant pigment absorption peaks at 593 and 620nm (Gitelson et al.,

274 1996; Sagan et al., 2020).

275 In terms of TSS, Wu et al. (2014) showed that NIR region (750–900 nm)
276 could yield the best relationship for the prediction of TSS and turbidity
277 in fresh water rivers. Bhargava & Mariam (1990) demonstrated that 700
278 nm to 900 nm was the optimal wavelength range for measuring suspended
279 sediment concentrations. Furthermore, several other studies reported high
280 correlation values between TSS and similar spectral regions (Novo et al.,
281 1991; Han & Rundquist, 1994; Ma & Dai, 2005; Cao et al., 2021). These
282 strong correlations can be ascribed to scattering peak in the red and NIR
283 range of phytoplanktons and other organic and inorganic suspended materials
284 at 700 nm (Olmanson et al., 2013; Sagan et al., 2020).

285 Few studies have explored the relationships between Chl-a and TSS con-
286 centrations and optical properties using details wavelengths other than the
287 spectra in red and NIR ranges, similar to what we have conducted in this
288 study by employing a whole VIS-NIR range hyperspectral data. Using the
289 simulated EnMAP spectra, better results were obtained for both Chl-a (R_p^2
290 =0.89 , $RMSE_p = 43.06$) and TSS ($R_p^2 = 0.91$, $RMSE_p = 17.53$) (Table
291 2) than those of shown in an earlier study by Saberioon et al. (2020) on the
292 same study area using the combination of Sentinel-2A bands and spectral
293 indices (i.e., Chla: $R_p^2 = 0.85$, $RMSE_p = 49.63$; TSS: $R_p^2 = 0.8$, $RMSE_p =$
294 19.55). This can be mainly linked to higher spectral resolution and contri-
295 bution of other effective wavelengths in prediction model. The supremacy of
296 hyperspectral data over multispectral Sentinel-2 images has been reported in
297 other studies too ((Awad, 2014; Sagan et al., 2020; Chen et al., 2022)).

298 Considering (Figure 4), RF performed well in determination of Chl-a and

299 TSS using both AISA eagle airborne hyperspectral and simulated EnMAP
300 spectra. Furthermore, Table 2 highlights that RF outperformed PCR and
301 PLSR in prediction of both Chl-a and TSS. This can principally be attributed
302 to ability of RF to extract variables and interpret nonlinear relationship
303 compared to PLSR and PCR (Ma et al., 2021). In addition, RF has the
304 capability to handle data with small number and high dimensionality. The
305 superiority of RF over other ML methods of predicting water quality traits
306 from inland waters has also been reported in some other studies (Ma et al.,
307 2021; Silveira Kupssinskü et al., 2020).

308 A visual comparison of the calculated Chl-a and TSS images shows similar
309 values for the EnMAP simulated data and the AISA Eagle sensor (5). In the
310 case of the AISA Eagle sensor, the high and low Chl-a values are highlighted.
311 Lower values are likely underestimated in the AISA image, whereas the values
312 from the simulated EnMAP data correspond better to typical Chl-a levels for
313 this type of reservoirs. The calculated TSS values differ slightly, higher values
314 were observed in case of EnMAP simulated data. The spatial pattern of the
315 calculated values is similar for both sensors. More spatial heterogeneity is
316 evident in the case of the AISA Eagle data. The different spatial patterns
317 are mainly due to the spatial resolution of the data used.

318 **Conclusions**

319 This study evaluate the ability of EnMAP simulated data coupled with
320 machine learning algorithms to predict two critical water quality properties
321 for inland waters (i.e., Chl-a and TSS). To this end, Water samples were
322 collected from several lakes and ponds in the south of the Czech repub-

323 lic concurrent to the hyperspectral AISA Eagle airborne imaging campaign.
324 EnMAP simulation data also was generated based on the AISA Eagle air-
325 borne data using EeteS. As it demonstrated, the enhanced spectral resolu-
326 tion of EnMAP permitted the prediction of biochemical properties of small
327 inland waters with acceptable accuracy. Additionally, results indicating that
328 Vis/NIR hyperspectral imaging from orbit combined with machine learning
329 algorithms has the potential to be used as a rapid and accurate method for
330 predicting and mapping the water quality traits in small inland waters. From
331 the point of view of practical applications (e.g. water resources managers,
332 fishponds managers, nature conservation authorities etc.), the EnMAP sim-
333 ulated data provide sufficiently accurate information, both in terms of the
334 accuracy of the determination of values and their spatial characteristics.

335 As actual EnMAP data will be available soon, the subsequent study will
336 examine actual data's capacity for predicting water quality traits in small
337 inland waters from orbit. Furthermore, evaluating the application of dif-
338 ferent spectral unmixing to decompose the optical water components seems
339 necessary for small inland waters practically when we are dealing with hy-
340 perspectral data (Alcantara et al., 2009; Kwon et al., 2022).

341 Other ML algorithms, in general and deep learning algorithms ,in particu-
342 lar, can be applied to hyperspectral data to predict the water quality param-
343 eters with better accuracy and performance using orbital hyperspectral data.
344 The number and spatial distribution of the samples, as well as influence of
345 different atmospheric correction algorithm (Vanhellemont & Ruddick, 2021)
346 are among important parameters that should be noticed in all future studies
347 to create a representative dataset and make a ML-based model with accept-

348 able generalisation (Menezes de Souza et al., 2020). As ML methods are
349 prone to over-fitting and the curse of dimensionality, decreasing the feature
350 space dimension using intelligent feature selection techniques can be another
351 interesting topic of study. Furthermore, Increasing the number of trees does
352 not cause over-fitting of the RF models (Breiman, 2001), which means bet-
353 ter generalizability. Since the capability of our obtained model has not been
354 proved yet, future studies can dedicate to testing it in other areas.

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