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A WATER QUALITY MODEL FOR THE CZECH PART OF THE RIVER ELBE

Abstract: Low water quality is an enduring problem in water management and has global importance due to the increasing use of water by the world's growing population. Based on climate change trends, the availability of water of acceptable quality will increasingly be a hot topic. The main objective of this work was the compilation and validation of a water quality model for the river Elbe (Czech: Labe) for the prediction of water quality under different scenarios (impact of point and nonpoint sources; effect of climate change). The assessment of water quality in the Elbe catchment is extremely important because the Elbe is one of the most important rivers in Europe. We focused on the water quality in the Czech part of the river Elbe, which was simulated and analysed with the QSim water quality simulation model. The model was applied from the Srnojedy weir to the Hrensko at the Czech-German border (river km 961 to km 726), comprising a cascade of 23 impoundments. Based on the measured input parameters for 2010-2015, the water residence time, oxygen conditions, and nutrients were simulated and validated. The model's results strongly agree with the measured data from the monitored period. The proposed model can, therefore, be used to simulate the development of pollution or climate change effects in this watercourse, allowing for the prediction of water quality under different scenarios.

Keywords: water quality modelling, Elbe catchment, QSim model, dissolved oxygen concentration, nutrient concentration, discharge

Introduction

Low water quality poses a persistent challenge in water management globally, gaining significance as water usage continues to rise. Numerous studies have delved into water quality issues not only in European rivers [1-5] but also worldwide. For example, Velazquez-Chavez's study highlights the significant impact of wastewater treatment plants on water quality in the Guadiana Valley, Mexico, leading to high concentrations of phosphates, total dissolved solids, and coliform bacteria [6]. In contrast, a study by Fekrache and Boudeffa addresses the impact of mining activities in Algeria and emphasises the influence of acid drainage [7]. These situations underscore the critical need for effective water resource management strategies to implement measures to mitigate environmental impacts. In Czechia, water quality constitutes a significant ecological concern. With the anticipated climate change, the availability of water of acceptable quality is becoming an increasingly hot topic, particularly regarding water temperature and discharge [8].

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Over the past three decades, surface water quality in Czechia has improved. This improvement is primarily attributed to the restriction of pollution sources, including the closure of numerous factories, the reconstruction and modernisation of industrial technologies, and the construction or modernisation of sanitation and wastewater treatment plants (WWTPs). Langhammer [9] addressed this improvement in the Czech Elbe river basin. The long-term monitoring of selected parameters for the German part of the Elbe, mainly concerning low flows, was handled by Hubner and Schwandt [10]. At the beginning of the 20th century, the Elbe's high water quality allowed for the versatile use of its waters. However, water quality experienced a drastic decline in the second half of the 20th century. Only after the political and economic changes initiated in 1989 (i.e. the Velvet Revolution and the end of communism) did the water quality of the Elbe show signs of improvement. However, these improvements did not reach all parts of the extensive river basin. Rural areas in the Czech Republic, particularly on smaller watercourses, continue to grapple with long-term issues related to surface water quality [11-13]. Importantly, the issues of these local water bodies have subsequent impacts on major European rivers.

Surface water quality models can help simulate and predict chemical pollutants' levels, distribution, and risk in a water body. Water quality data are typically limited; therefore, model validation is important, especially for evaluating compliance with water quality assessment standards [15]. Modelling results from models under different pollution scenarios are important components of environmental impact assessments. They can provide the technical basis for environmental management agencies to make data-driven decisions [16, 17]. Water quality modelling is essential for assessing the impacts of anthropogenic activities on aquatic ecosystems. As highlighted by Ejigu [18], mathematical models are beneficial for evaluating changes in water quality due to wastewater discharges. Various models have been applied globally to address such challenges. These applications demonstrate the critical role of models in understanding how pollutants interact with aquatic environments and affect overall water quality. The increasing demand for river water quality models underscores the necessity of creating river basin management plans in the European Union. Moreover, water quality models are used worldwide for problems regarding eutrophication and drinking water sources [19-23]. Long-term monitoring and tracking of the concentrations of pollutants and their indicators in extensive watersheds is time-consuming and financially demanding, so modelling pollution evolution in streams can significantly facilitate watercourse dynamics monitoring.

The main objective of this study is the compilation and validation of a water quality model for Czech part of the river Elbe for the prediction of water quality under different scenarios (impact of point and nonpoint sources; effect of climate change) using the QSim water quality simulation model. QSim is an instrument for simulating and forecasting the dynamics of oxygen, nutrients, and plankton in running waters [24]. Previous studies have employed the QSim model to assess the Elbe river, however, they only investigated the German part of the river and the estuary [25-28]. A one-dimensional (1D) model approach was employed, simplifying systems by assuming a thoroughly mixed cross-section and neglecting lateral and vertical differences. Despite these simplifications, this technique has proved successful for large scales, where dominant longitudinal gradients exist, especially in global change studies [28-30]. However, 1D approach has limitations since the model mainly captures average water quality conditions [21]. Creating a functional model for the territory of the Czech Republic enables the future connection of models and simulations to cover the entire Elbe river [31]. This paper outlines a numerical modelling approach to water quality, specifically focusing on water temperature, oxygen conditions, and nutrients.

Materials and methods

Description of the study area

The Elbe river is one of Europe's largest rivers and waterways - the Elbe springs origins in the Giant Mountains north of the Czech Republic at an altitude of 1378 m. The Elbe runs through Germany and flows into the North Sea with the estuary. It is 1,094 km long (370.74 km in the Czech Republic) and drains an area of 148,268 km² (49,933 km² in the Czech Republic). This study pursues only the part of the river basin located in the Czech Republic (Fig. 1). The long-term average flow at the state border with Germany (profile Schmilka) is 320 $m^3 \cdot s^{-1}$ (294 $m^3 \cdot s^{-1}$ at the reference period 2010-2015). An important site is river km 837 - the largest tributary on the territory of the Czech Republic; Vltava (Moldau) flows into the Elbe, and the river's total flow is more than doubled. The Elbe itself has a long flow rate of 100 $m^3 \cdot s^{-1}$ (87 $m^3 \cdot s^{-1}$; at the reference period) and the Vltava 152 $m^3 \cdot s^{-1}$ (168 $m^3 \cdot s^{-1}$; at the reference period). The flow is influenced by agricultural and industrial activities (chemical plants, mining). Over 60 % of the catchment area is agricultural land.

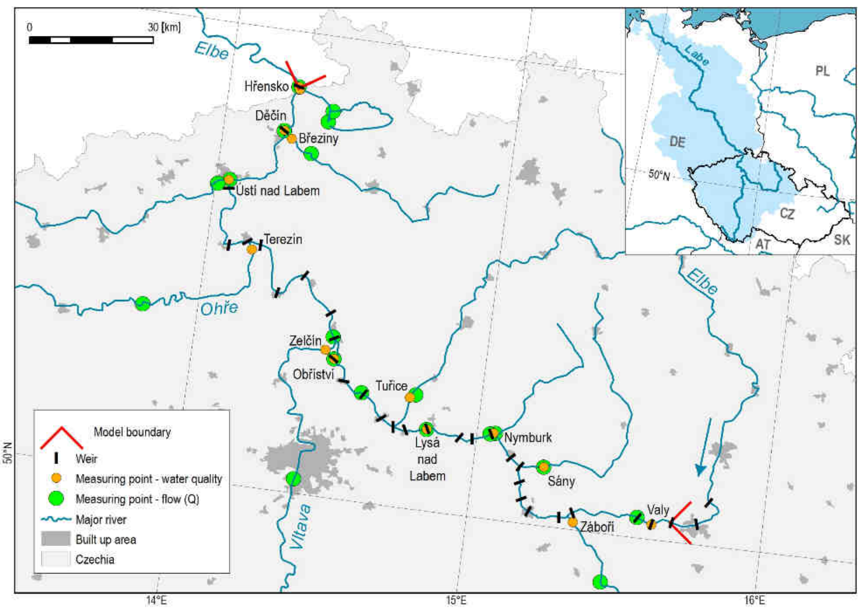

Fig. 1. Model area of water quality modelling in the Elbe (from Srnojedy to Schmilka/Hrensko)

The upper boundary of the model is located below the Srnojedy weir (km 960.8) (1, red arrow). The lower boundary is delineated by the Czech-German border (km 726.6). The total distance of the model section is 234 km and consists of 23 impoundments, which are further divided into segments in spatial resolution of 0.5 km to 2 km. The boundary conditions of the model also include the nine largest tributaries of the Elbe (from the right - Cidlina, Mrlina, Jizera, Ploucnice, Kamenice, from the left - Doubrava, Vltava (Moldau), Ohre (Eger), Bilina).

The modelling part is impounded by 23 navigation dams, which increase the water level for shipping purposes (Fig. 1, black bars). These weirs impact the flow time of the water and thus affect all processes in the water column. The model part of the flow begins at the Srnojedy at an altitude of 209.19 meters. The end of the model on the Schmilka/Hrensko profile is at 118 m a.s.l. (above sea level). In Figure 2, you can see the longitudinal profile of the modelled parts, including individual flow weirs.

The average river depth based on the model grid is 3.02 m. The largest depths are in front of the weirs Roudnice nad Labem and Strekov, where the depth exceed 7 m at mean flow and about 10 m at higher flow. On the contrary, the lowest water depths are just below the weirs, an example being the Strekov weir, which has a depth of about 0.66 m in the case of lower flows.

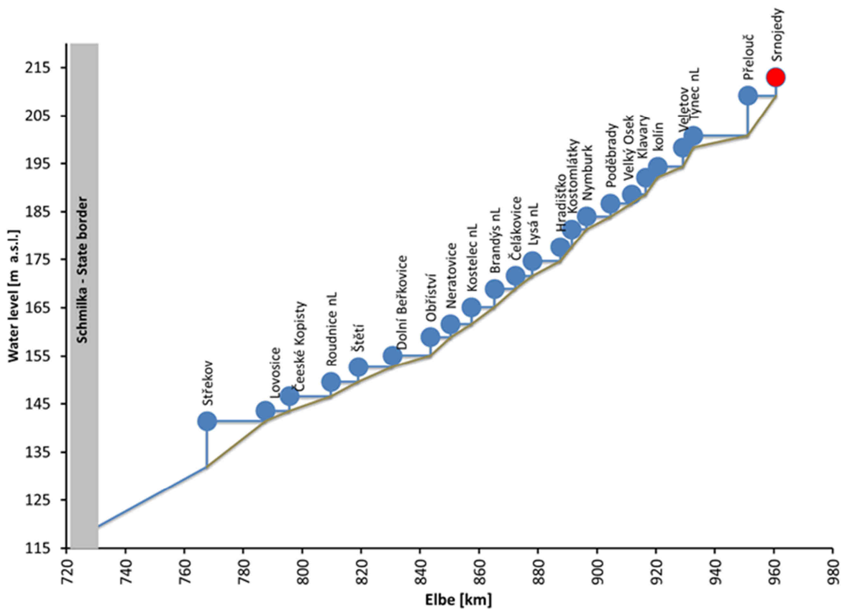

Fig. 2. The longitudinal profile of the modelling part of the river

QSim model

The Qsim water quality model is a tool for simulating and predicting running waters' material balance and plankton dynamics [1, 32, 33]. The current version (version 13.30) results from 30 years of continuous development. The QSim describes mathematically, based on differential and algebraic equations without any stochastic effects, the complex chemical and biological processes in running waters. A key feature of this model is the combination of the hydraulic model HYDRAX, which simulates the discharge, with the QSim model, which includes various water quality and biological model components [31]. The structure of the model and the link between the modules are shown in Figure 3.

The modules can be divided into the following groups: one temperature module, seven biogeochemical modules, three biological modules, and a sediment module. Meteorological, morphological and hydraulic parameters such as water depth and flow velocity are also output as mean values for each cross profile. The modelling results of the physical, chemical and biological state variables are daily mean values at each kilometre along the river axes. The model is suitable for calculating the processes in the main flow of a river [32]. The calculation time step was set to one hour.

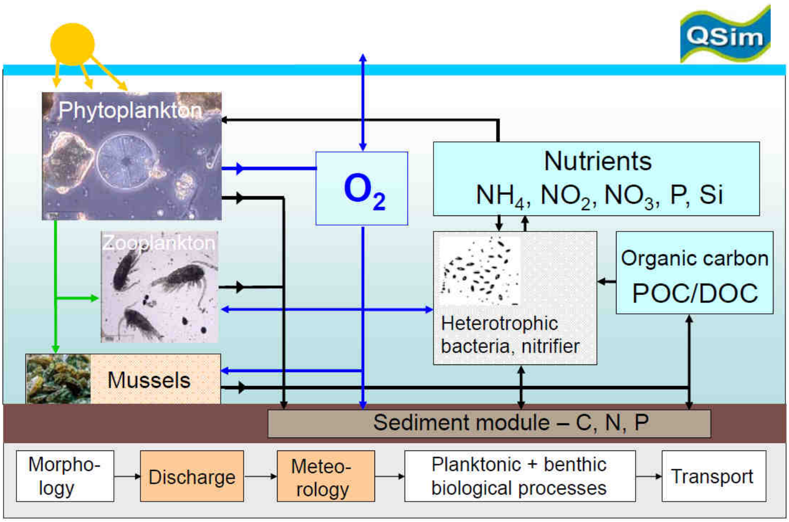

Fig. 3. Module structure and functionality of QSim

The model operates under GERRIS's graphical user interface containing the HYDRAX and QSim program systems [34]. A model editor is used to enter and process morphological and hydrological data. The resulting morphological model is then supplemented in HYDRAX by the input variables discharge and water level. The run-off and water level hydraulic modelling results and parameters such as the mean water depth and flow velocity are then used in an offline coupling for ecological modelling in QSim. Then, meteorological data, including temperature and global radiation data are supplemented in QSim.

Input data (boundary conditions)

Data regarding the river's morphology, discharge, water level, water quality and meteorology (air temperature and global radiation) are required to define the model's boundary conditions. The morphological conditions were derived from river cross-sections every 500 m to 2,000 m. The selected discharge (daily mean) and water quality monitoring stations and the available water quality parameters (most frequent monthly values, discrete sample) for the reference period (2010-2015) are presented in Figure 1. List of available water quality parameters is in Table 1. These data were provided by the Elbe River Basin Authority (PLA), the Ohre River Basin Authority (POH), the Vltava River Basin Authority (PVL), and the Czech Hydrometeorological Institute (CHMI). QSim also requires input water quality data from the tributaries for the upper boundary.

Table 1

List of input data (water quality parameters)

Parameter	Unit
Water temperature (*WT*)	[°C]
Dissolved oxygen (O_2)	[mg·L^{-1}]
Chemical Oxygen Demand (COD)	[mg·L^{-1}]
Amonium nitrogen (NH_4-N)	[mg·L^{-1}]
Nitrite nitrogen (NO_2-N)	[mg·L^{-1}]
Nitrate nitrogen (NO_3-N)	[mg·L^{-1}]
Total nitrogen (TN)	[mg·L^{-1}]
Total phosphor (TP)	[mg·L^{-1}]
Orthophosphores (PO_4-P)	[mg·L^{-1}]
Silicate (SiO_2)	[mg·L^{1}]
pH value	[-]
Alkalinity	[mmol·L^{-1}]
Suspended matter	[mg·L^{-1}]
Calcium (Ca)	[mg·L^{-1}]
Conductivity	[µS·L^{-1}]
Biochemical Oxygen Demand (BOD_5)	[mg·L^{-1}]
Chlorophyll - α	[µg·L^{-1}]

Model validation

Even with a large body of literature on model calibration and validation, comparing modelling results from different studies is challenging because there are no universally accepted guidelines, and users utilise different calibration and validation methods [35].

This study used quantitative statistics for model evaluation, comprising three components. The first component is a standard regression, including the slope *S* and the coefficient of determination R^2. The coefficient of determination measures the collinearity between the modelled and measured data and ranges from 0 (no correlation) to 1 (optimum correlation). Relevant model results have an R^2 value higher than 0.5. The slope shows how well the model data match the measured data provided that the estimated data are error-free. In practice, measured data are rarely without errors. A slope of 1 indicates a perfect match between the model values and the measured values [36]. These two methods, together with the associated illustrations, can indicate the quality of the model.

The second component, relative model evaluation, is dimensionless. For this evaluation, the Nash-Sutcliffe efficiency *(NSE*) was used. *NSE* determines the relative magnitude of the residual variance compared to the measured data variance and indicates how well the plot of observed versus simulated data fits the 1 : 1 line. *NSE* is ideal for use in continuous long-term simulations, allowing assessment of the extent to which the model reproduces trends in the observed output responses [36]. The results can range between $-\infty$ and 1; $NSE < 0$ indicates unacceptable model performance. *NSE* is widely utilised and is considered the optimal objective method for assessing the overall fit of a hydrograph model [33]. Additionally, a simplified form yields the relative error (*REL*), which, under optimal alignment with the data, assumes a value of 0 [37].

The third component is the error index method, which considers the error deviation in the data. An example is the per cent bias (*PBIAS*). The *PBIAS* quantifies the average tendency of simulated data to deviate from observed counterparts, either overestimating or underestimating and describes the deviation of the data expressed as a percentage. A *PBIAS* of 0 indicates that the conformity between the measured and modelled values is optimal;

positive *PBIAS* values indicate model underestimation compared to the estimated data [38]. Relevant model results have *PBIAS* values between ±25 %.

The model results about discharge (HYDRAX) are validated on three profiles - Kostelec nad Labem (nL.). (km 857), Melnik (km 837) and Schmilka/Hrensko (lower boundary of the model - km 726). Model results QSim are validated with two profiles on the Elbe. These are profile Lysá nL. (km 878) and profile Schmilka/Hrensko. In validation results, the variable *N* represents the dataset's cardinality, denoting the total number of data pairs or observations subjected to the validation procedure.

Results and discussion

Flow

Flow plays a significant role in water quality modelling. This section describes the discharge, flow velocity, and residence time. The model works with two extreme flow situations: floods in June 2013 and drought throughout 2015.

Discharge is reproduced with a good fit between the measured and modelled data. Figure 4 compares the discharge for the whole reference period in the monitoring profile Schmilka/Hrensko. The measured values are green; the modelled values are blue. The figure shows a significant match between the values.

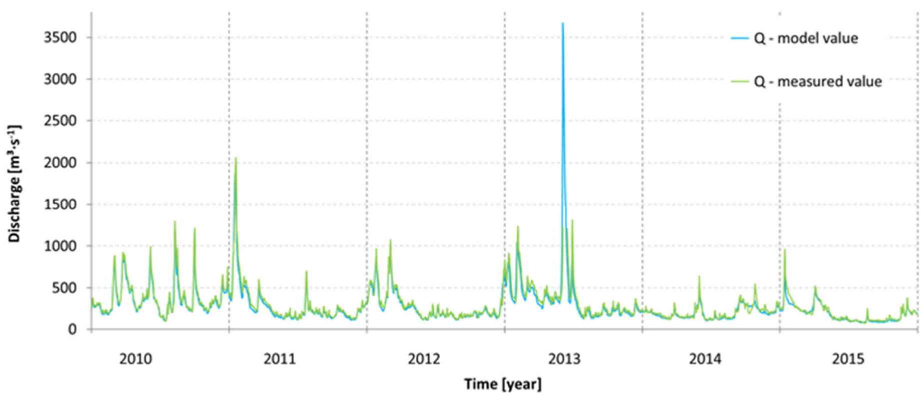

Fig. 4. Comparison of the measured and modelled daily discharge [Q] values for the Schmilka/Hrensko profile

The HYDRAX model accurately replicated discharge dynamics, demonstrating a good fit between the measured and modelled data, particularly in the Schmilka/Hrensko profile. The results of the statistical parameters also indicate perfect model results. Based on the *PBIAS* values, the model slightly underestimated the resulting flow rate. The *NSE* values for all profiles range from 0.520 to 0.980; the lowest value was reached in 2013. This result is caused by the floods in the summer of 2013, which were not limited to the Elbe basin (CHMI 2013). On days 5-14.6, the Schmilka/Hrensko profile flow reached unmeasurable values above 3,000 $m^3 \cdot s^{-1}$. In addition to 2013, the results of the model are significantly better. The comparable *NSE* values with models of other rivers, such as the Danube and the Rhine, underscore the QSim model's aptness for simulating the Elbe's discharge conditions given appropriate boundary conditions. For example, *NSE* values in the range of

0.893-0.956 for 2007-2009 were found in the Danube [39]. In the Rhine, the Bimmen profile 2000 had an *NSE* value of 0.94, or 0.96 in 2008 [25]. The HYDRAX model is very well suited to model the discharge conditions of the Elbe.

The total length of the modelled Elbe section is 234 km. At the top of the model, the average flow rate for the reference period is 52.89 $m^3 \cdot s^{-1}$. The flow is significantly increased by the tributaries: at the lower border of the model, the average flow rate is 294.14 $m^3 \cdot s^{-1}$. Figure 5 shows the longitudinal flow development, including the average flows of all tributaries. The graph shows the influence of all flows on the Elbe. Tributaries with higher flow rates, such as Jizera and Ohre, have the most significant effect on Elbe's flow rate. The river's flow increases the most at the mouth of the Vltava river (km 837). At this point, the average flow of the Elbe was 87.22 $m^3 \cdot s^{-1}$ in the monitored period, whereas the average flow of the Vltava river was 168.3 $m^3 \cdot s^{-1}$. After the mouth of the Vltava River, the discharge of the Elbe is roughly tripled. The considerable influence of the Vltava on the Elbe justifies the monitored parameters described in the following sections.

Residence (flow) time is another parameter that significantly affects the concentrations of substances, plankton, and the processes occurring in the water. Figure 6 shows the average flow time (day) from the upper border of the model (km 960) to the Vltava mouth (km 836, red line) and the lower boundary of the model, i.e. the Schmilka/Hrensko profile (km 726, dashed red line). As shown in the graph, the mean flow time increases from the beginning of the year and peaks at the end of summer and in autumn. The average maximum, reached in November, exceeded 11 days. The average flow time through the model in 2010-2015 was between 5 and 12 days depending on the season. However, extreme situations also occurred. The overall maximum was reached during the spring of 2015 when the flow took more than 22 days. Conversely, the shortest duration was 42 hours, just below two days, during the summer flood event in June 2013.

Table 2

Validation results - discharge

Year	***N***	***NSE***	***PBIAS***	***REL***	**SLOPE**	R^2
Kostelec nL. (km 857)						
2010	365	0.90	8.38	0.11	0.90	0.91
2011	365	0.93	8.22	0.11	0.90	0.94
2012	366	0.94	7.63	0.10	0.91	0.95
2013	365	0.77	9.57	0.14	0.72	0.79
2014	365	0.89	7.57	0.09	0.87	0.92
2015	365	0.94	6.53	0.08	0.91	0.95
Melnik (km 837)						
2010	365	0.96	4.95	0.06	0.93	0.97
2011	365	0.98	6.82	0.07	0.92	0.99
2012	366	0.97	5.28	0.06	0.93	0.98
2013	365	0.96	6.11	0.09	0.94	0.96
2014	365	0.75	1.27	0.12	0.73	0.76
2015	365	0.85	4.07	0.12	0.73	0.88
Schmilka/Hrensko (km 726)						
2010	365	0.93	6.79	0.10	0.89	0.95
2011	365	0.93	8.58	0.13	0.89	0.95
2012	366	0.93	5.00	0.11	0.92	0.96
2013	365	0.52	5.15	0.20	1.11	0.73
2014	365	0.76	7.35	0.12	0.74	0.80
2015	365	0.88	8.47	0.12	0.78	0.92

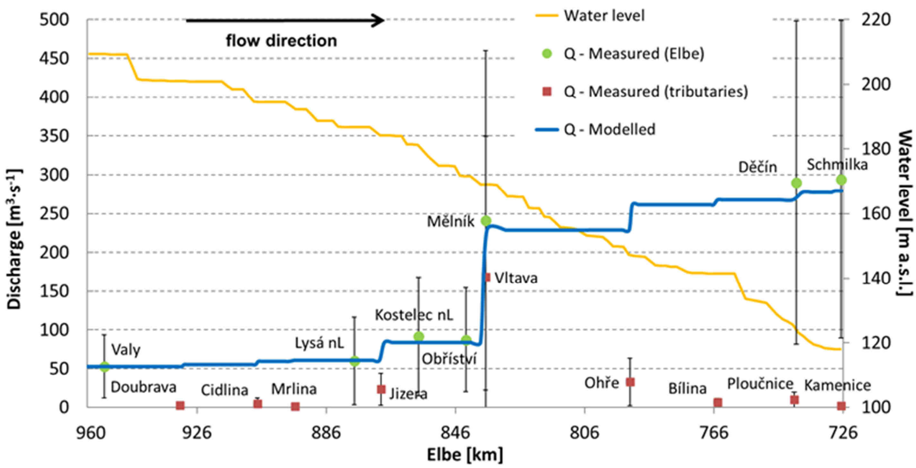

Fig. 5. Longitudinal profile of the measured (green point and line, tributaries, purple point) and modelled (blue line) average discharge [Q] and average water level (orange line) from Srnojedy (km 960) to Schmilka/Hrensko (km 726). The average values are for the reference period 2010-2015. The standard deviations of the measurements are reflected by bars

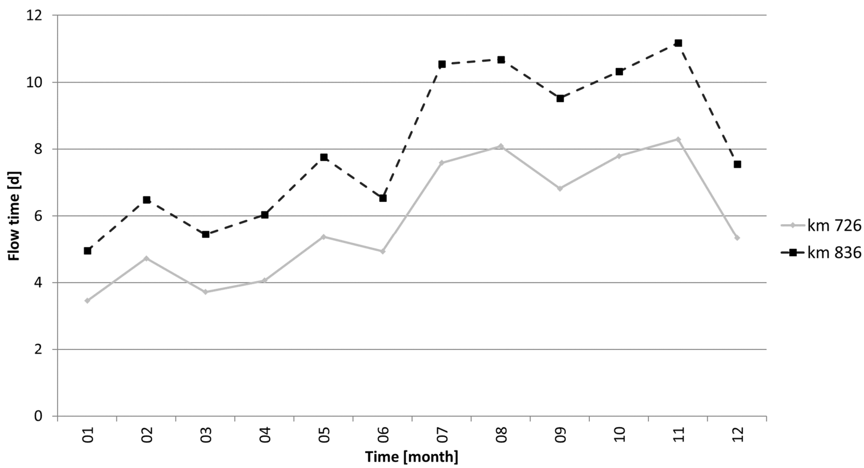

Fig. 6. The average flow time of the reference period 2010 to 2015 for the river stretch from the upper border of the model at Srnojedy (km 961) to the mouth of the Vltava (km 836) and to the lower border of the model at Schmilka/Hrensko (km 726)

Water temperature

Surface water temperature is very important because it affects the solubility of oxygen, the rate of all biochemical processes and, thus, the self-cleaning function of the water stream [40]. Generally, the amount of oxygen in the water decreases with increasing water temperature.

The QSim results for water temperature showed a good fit between the measured and modelled data. At both validation stations, Lysa and Schmilka, the NSE values are higher than 0.9, indicating the model's high accuracy. In the case of the lower section of the Elbe (km 629), Hein [27] reported an NSE value of 0.967, which is quite comparable to the result reported in this study. The agreement among results also occurs with the larger deviation in the winter months due to the release of heat from power plants and chemical plants, which were not included in the model, with the greatest impact occurring in the winter period. Despite the model's slight tendency to underestimate the water temperature, its overall accuracy is high. The statistical results are reported in Table 3. Other results support the suitability of the model. For example, the correlation coefficients are close to 1 yearly, which also indicates a strong match. However, the *PBIAS* values show that the model slightly underestimates water temperature values. Model validation only considered two stations; differences are expected between stretches depending on their water depth and in the case of free-flowing and impounded stretches.

Table 3

Validation results - water temperature

Year	*N*	*NSE*	*PBIAS*	*REL*	SLOPE	R^2
Lysa nL. (km 878)						
2010	12	0.99	–2.84	0.04	1.01	1.00
2011	12	0.95	2.82	0.11	1.05	0.96
2012	12	0.96	7.39	0.11	1.00	0.97
2013	12	0.98	0.69	0.07	1.00	0.98
2014	12	0.96	2.72	0.09	1.11	0.98
2015	19	0.94	10.46	0.11	0.95	0.98
Schmilka/Hrensko (km 726)						
2010	12	0.99	1.87	0.06	1.03	0.99
2011	19	0.96	1.14	0.07	1.05	0.97
2012	18	0.94	6.03	0.10	1.07	0.96
2013	18	0.97	1.15	0.07	0.96	0.97
2014	19	0.93	0.00	0.09	1.14	0.96
2015	20	0.91	8.35	0.11	1.06	0.96

The influence of the tributaries is evident in Figure 8 for all years in the reference period. These graphs show changes in the water temperature during the year in the longitudinal profile of the Elbe. The lowest temperatures, around 0 °C, were reached in January; the highest temperatures, up to 26 °C, were reached in summer. The Vltava has the most significant influence on the temperature of the Elbe. This river warms the Elbe in winter and cools it in summer by several degrees Celsius. This is caused mainly by many deep reservoirs in the Vltava from which the bottom water flows at a more constant temperature. The graphs show that the changes in water temperature vary from year to year. Water temperatures below 10 °C in the Elbe, shown in blue shadowgraphs, occur roughly from the end of October to April. Water temperatures exceeding 20 °C (shades of red) occur in June and are held in mid-September.

The influence of colder tributaries on the Elbe is also visible in the graph in Figure 7, which shows the changes in water temperature on the hottest modelled day for most profiles: 4 August 2014 (daily mean). The modelled water temperature in front of Jizera's mouth is 26 °C. After the mouth of the Jizera and the Vltava River, the temperature in Elbe is lower than 23 °C. Average daily depths in selected profiles are also shown in this chart. As can be seen, a significant dependence of changes in the average water temperature on average daily depths was not confirmed.

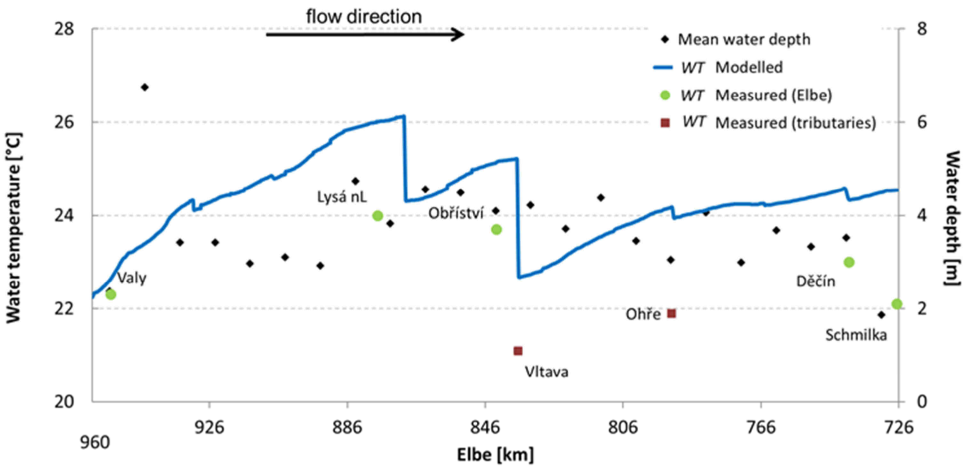

Fig. 7. Longitudinal profile of the measured (green point, tributaries - purple point) and modelled (blue line) daily mean water temperature (*WT*) and daily mean water depth (black point) from Srnojedy (km 960) to Schmilka/Hrensko (km 726). Values for 4.8.2014 - warmest water over the reference period

In the case of water temperature, extremes are critical. The maximum temperatures were measured at the Decin station, where the temperature of the Elbe's water reached 26 °C. The warmest tributary is Cidlina (max. 25.9 °C), while Kamenice is the coldest (max. 17.9 °C). The average measured water temperature in the longitudinal profile increases across the river. The average water temperature in the reference period is 12.15 °C at the upper edge of the model (Valy station). At the lower edge of the model (Schmilka/Hrensko), the average water temperature is 13.31 °C. Besides the value of these maximum temperatures, their frequency and duration are also important. Figure 9 shows the average number of days per year in the longitudinal flow profile at selected stations where the water temperature exceeds 23 °C (blue) and 25 °C (red). It can be seen from this chart that most days with a temperature above 23 °C are at km 878 (Lysa nL.) - a total of 20 days a year, with four days exceeding 25 °C. In July 2014, the most extended temperature wave above 25 °C lasted 13 days and was recorded at this station according to the model's results. Interestingly, in 2011 and 2015, not one day with a temperature above 25 °C was modelled in the profiles. However, this does not mean that this temperature was not exceeded in the whole longitudinal profile of the model. Further downstream, the days with high water temperatures decrease due to the colder inflows from Jizera and Vltava.

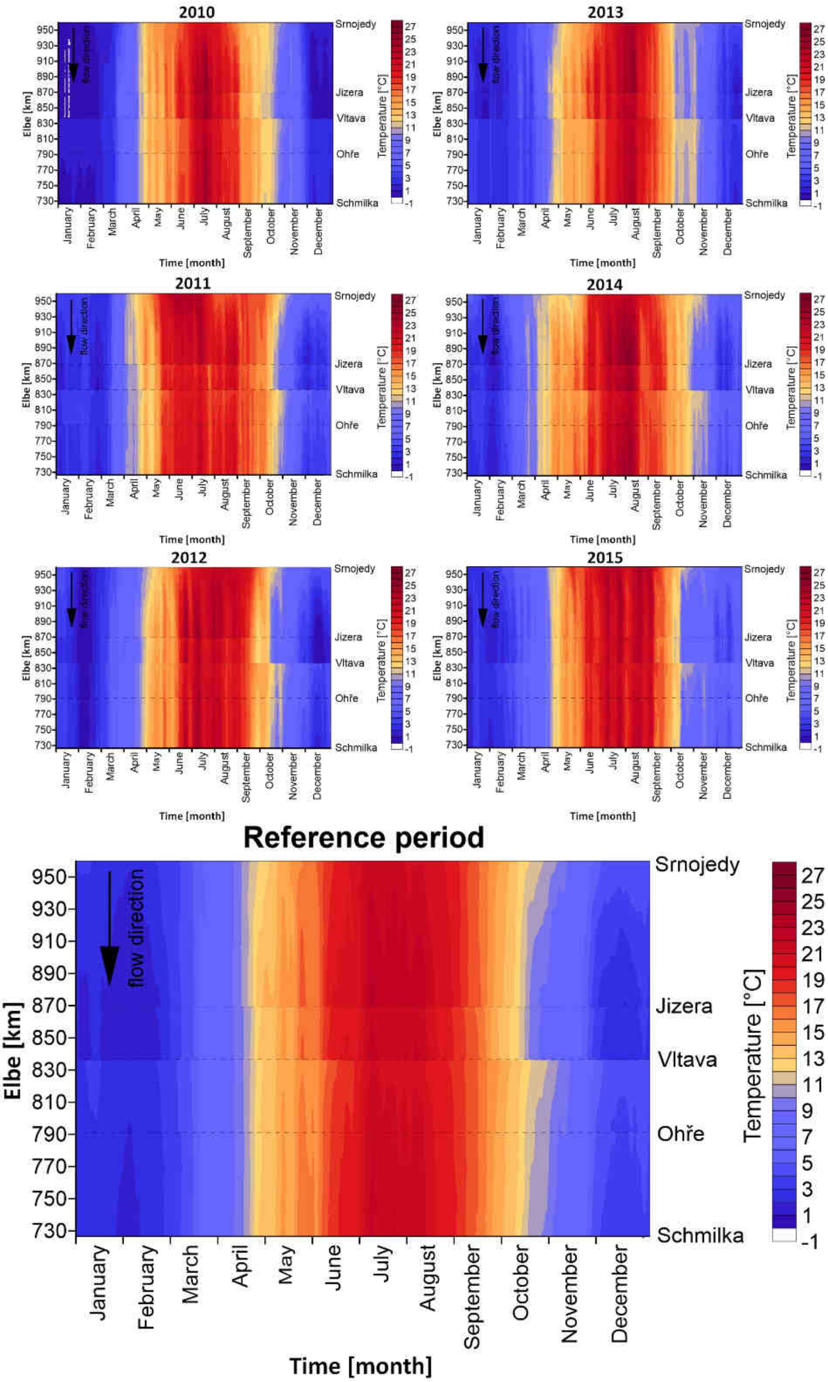

Fig. 8. Development of the modelled water temperature (*WT*) during the year in the Elbe longitudinal profile

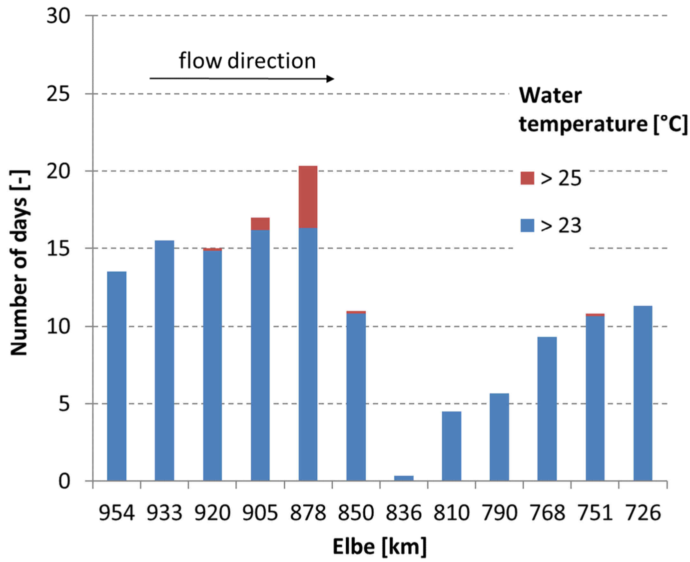

Fig. 9. Longitudinal profile of the modelled water temperature (*WT*). The average number of days per year with temperatures higher than 23 °C (blue) and above 25 °C (red) in the reference period

Oxygen concentration

The outputs from the QSim model regarding oxygen content, which is one of the components of physicochemical water quality assessment, are the concentration of dissolved oxygen, BOD_5, and TOC. The oxygen concentration values were used to validate the model results. Figure 10 shows the oxygen concentration for 2013. The y-axis scale starts at 5 $mg \cdot L^{-1}$ to provide a more detailed illustration. Since May, the model's outputs were overestimated, which is consistent with the *PBIAS* values equal to 8. The most overvalued values are in 2014 and 2015 in the case of the Lysa nL. profile, and 2013 (Table 4). The problematic model results are mainly in 2015. This outcome is related to the drought period that affected the river basin in that year (CHMI 2015).

Comparison with other studies suggests the model adequately represents oxygen concentrations, accounting for variations in different river systems. Comparing statistical validation results with other studies indicated that QSim can model oxygen concentrations relatively well. For example, a 2004 study comparing over 150 studies reported an average R^2 value of 0.7 [37]; one study based on a 1D model concerning the Dez River (Iran) reported an R^2 value higher than 0.9 [19]. This value is close to the average R^2 value for the Elbe from QSim, 0.66 (range: 0.234-0.893). For comparison, studies based on the same model reported R^2 values in the range of 0.499-0.940 for the Danube [39] and 0.51-0.77 for the Rhine [25].

The difference between measured and model values may not necessarily be a model error. The average daily oxygen concentration is calculated based on hourly values. The oxygen budget is also highly influenced by phytoplankton dynamics [17]. The availability of relevant input data for the model also plays a role in its accuracy. By contrast, field measurements are performed every 14 days in best cases. Also, the measurement time can affect the concentration of oxygen in the morning measurements. The oxygen consumption influences the results during the night. On the other hand, in the afternoon, the oxygen concentration is higher due to the phytogenic entry of oxygen into the water [39]. The impact of the drought in 2015 is evident in the model's results, emphasising the model's sensitivity to environmental conditions.

Table 4

Validation results - oxygen concentration

Year	***N***	***NSE***	***PBIAS***	***REL***	**SLOPE**	R^2
Lysa nL. (km 878)						
2010	12	0.74	–2.47	0.09	0.82	0.76
2011	12	–0.70	–13.83	0.17	0.55	0.23
2012	12	0.60	–4.83	0.10	0.75	0.66
2013	13	0.35	–1.51	0.14	0.64	0.44
2014	12	–0.13	–13.28	0.15	0.76	0.52
2015	19	0.17	–13.46	0.22	0.68	0.47
Schmilka/Hrensko (km 726)						
2010	12	0.81	–5.21	0.06	0.84	0.89
2011	19	0.55	–9.62	0.11	0.74	0.77
2012	18	0.50	–11.53	0.13	0.73	0.83
2013	18	0.47	–7.54	0.10	0.98	0.76
2014	19	0.40	–14.84	0.17	0.70	0.83
2015	20	0.00	–20.71	0.21	0.64	0.76

The oxygen concentrations were measured for five Elbe profiles: the two model boundaries and the stations Lysá nL., Obristvi, and Decin. At the upper boundary of the model (Valy profile), the average value of oxygen concentration during the reference period was 9.6 $mg \cdot L^{-1}$. The other profiles in the Elbe had similar values; the concentration at the closing boundary of the model was 9.8 $mg \cdot L^{-1}$. These mean values are shown in green in Figure 11. The minimum measured value in the Elbe (3.8 $mg \cdot L^{-1}$) was measured in June 2015 at km 877 (Lysa nL. profile). Conversely, the maximum concentration of 16.6 $mg \cdot L^{-1}$ was measured in May 2015 at km 954 (Valy profile). In the case of tributaries, whose average values are reported in the same graph in purple, the average values are considerably more varied. The highest and lowest average oxygen concentrations were found in the Kamenice and Mrlina, respectively. The highest concentration was measured in the Vltava river (17 $mg \cdot L^{-1}$) in January 2013. A minimum concentration of 2.6 $mg \cdot L^{-1}$ occurred in January 2010 in Doubrava.

The modelled average values are shown in Figure 11 (blue line). These values indicate a more pronounced increase in the longitudinal profile than the measured data. At the upper boundary of the model, the average value is 9.6 $mg \cdot L^{-1}$. In the Schmilka/Hrensko profile (lower boundary of the model), the average oxygen concentration is 11.3 $mg \cdot L^{-1}$. Again, the concentration of the Vltava river had the largest influence on the Elbe's concentration, increasing the modelled concentrations by 1 $mg \cdot L^{-1}$ on average. The positive impact of the Vltava River can also be seen in the graphs in Figure 13. Except for May and June 2011, the Vltava increased the dissolved oxygen concentration in the Elbe. The influence of other tributaries was not too pronounced. The highest model values were reached in May 2011: at km 870, the oxygen concentration reached 18.9 $mg \cdot L^{-1}$. Conversely, the modelled minimum (5.72 $mg \cdot L^{-1}$) occurred in June 2011 at the upper limit of the model. These values are shown in the Figure 12, where the minima are shown in orange and the maximum concentration at km 870 is shown in dark blue. Overall, oxygen conditions can be considered reasonable since there was no significant oxygen deficiency in the Elbe in the reference period.

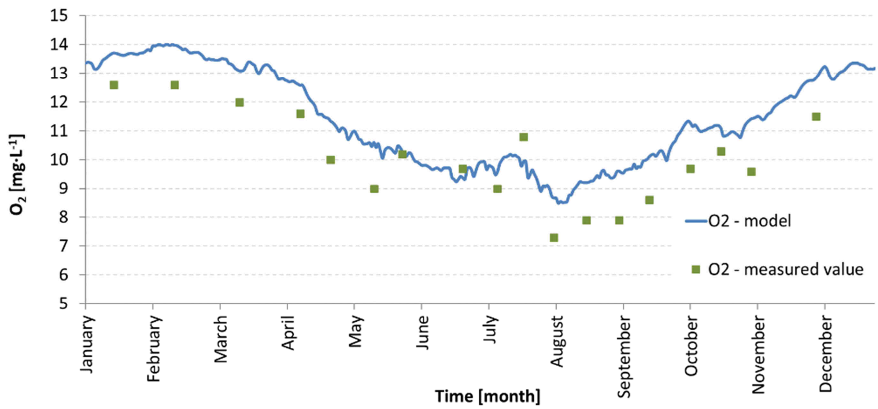

Fig. 10. The measured (green) and daily average modelled values of dissolved oxygen (blue) in Schmilka/Hrensko (km 726) in 2013

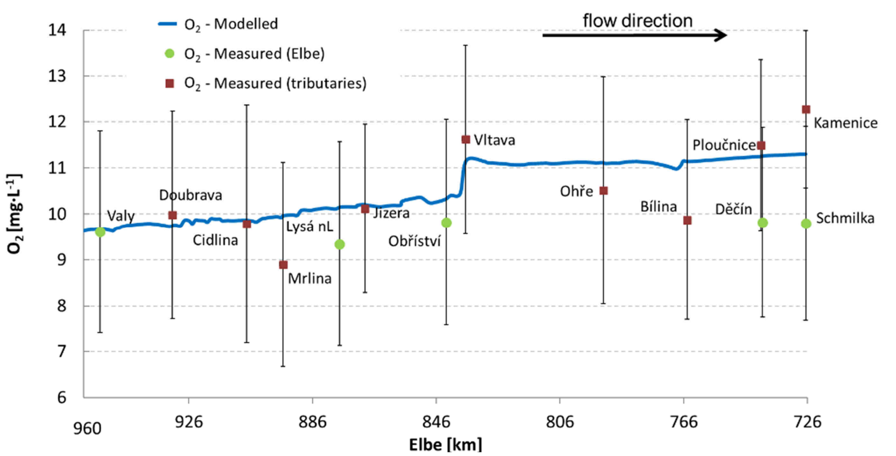

Fig. 11. Longitudinal profile of the measured (green point and line, tributaries - purple point) and modelled (blue line) dissolved oxygen concentrations (O_2) from Srnojedy (km 960) to Schmilka/Hrensko (km 726). The average value for the reference period 2010-2015. The standard deviations of the measurement are reflected by bars

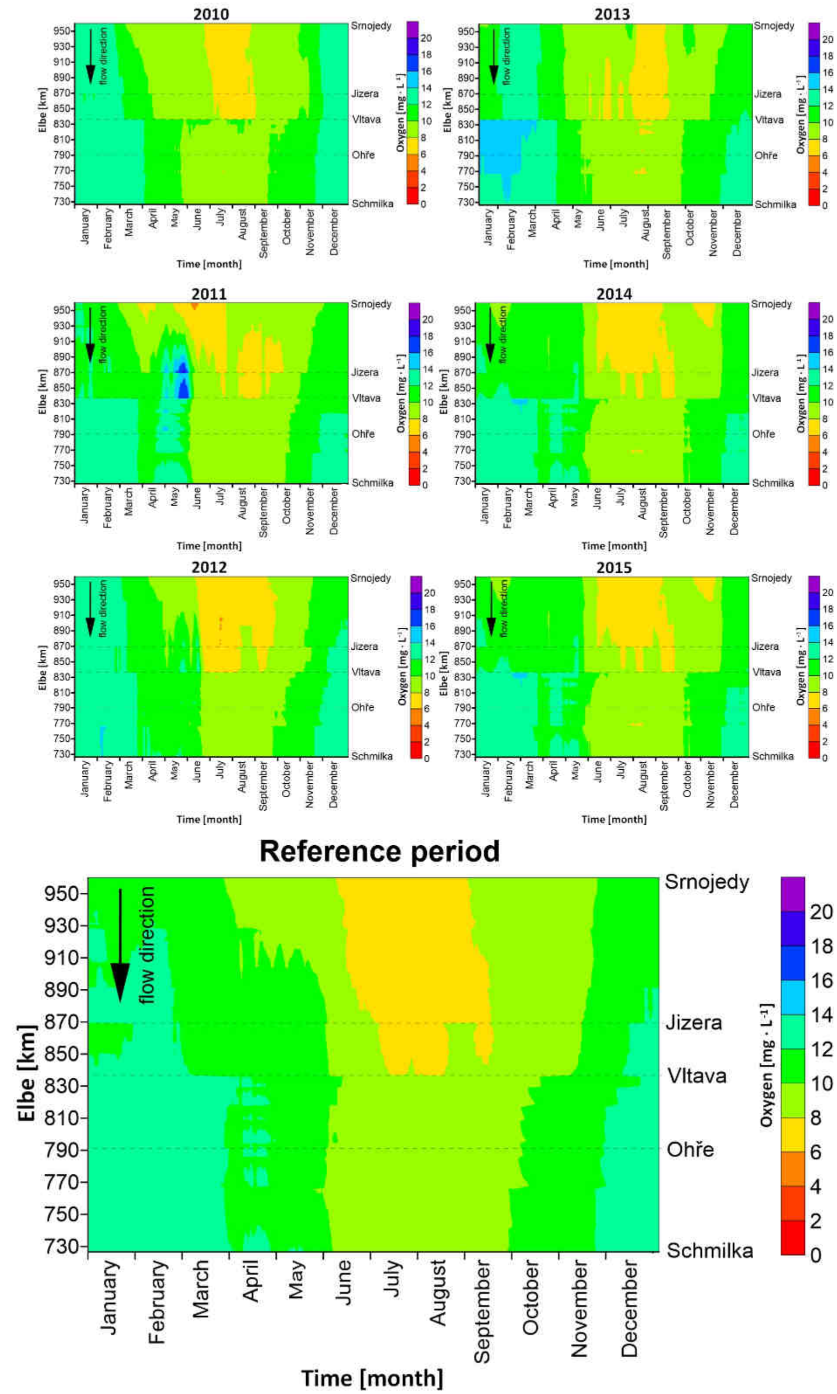

Fig. 12. Development of the modelled oxygen concentration in the Elbe longitudinal profile during the year

Nutrients: total phosphorus and total nitrogen

Two parameters were used to evaluate nutrient ratios in the reference period: total phosphorus (TP) and total nitrogen (TN). Nitrogen and phosphorus were chosen because these two compounds play an essential role in the eutrophication process in the surface water.

The model's TP validation results are more accurate for the Lysa nL. profile than the Schmilka/Hrensko profile. Based on the *PBIAS* results, it can be said that the QSim model underestimates the TP results in the Lysa nL. profile. Concerning the Schmilka profile, such a clear conclusion cannot be made as the model overestimated the results in 2011-2013. This may be caused by the Vltava River, which significantly influences the lower half of the Elbe model. Moreover, it is necessary to consider that measurements take place roughly each month, so the data may not reflect all the changes that occur in the river throughout the year.

The compliance of the model's TN values with the measured TN concentrations is very good, as indicated by the statistical validation results in Table 5. The *PBIAS* value shows that the validated model produces a slight overvaluation. Generally, it can be stated that models perform the complete longitudinal profile of the flow with highly accurate results for the total nitrogen concentration.

The satisfactory validation results for the TP and TN concentrations, with small variations between the Lysa nL. and Schmilka profiles, showcase the QSim model's reliability. Other studies employing the same QSim version achieved similar results. The average *NSE* for the Berlin water model was –1.15. In the case of the Elbe model, the *NSE* was 0.688. The average R^2 was 0.566 for the Berlin [25]; for the Czech part of the Elbe, it was 0.857. As with all result comparisons, each value is the average value over the entire monitored period for all validated stations. Arhonditdisi and Brett [37], comparing more than 150 studies, reported median R^2 values from 0.40 to 0.60 for nutrients.

Table 5

Validation results - total phosphorus, total nitrogen

Total phosphorus								**Total nitrogen**						
Year	***N***	***NSE***	***PBIAS***	***REL***	**SLOPE**	R^2		***Year***	***N***	***NSE***	***PBIAS***	***REL***	**SLOPE**	R^2
Lysa nL. (km 878)														
2010	12	0.83	–4.46	0.10	0.89	0.86		2010	12	0.93	5.63	0.06	0.96	0.97
2011	12	0.56	3.80	0.19	0.54	0.57		2011	12	0.80	8.38	0.10	1.07	0.91
2012	12	0.61	3.61	0.12	0.58	0.64		2012	12	0.73	10.22	0.12	0.77	0.84
2013	12	0.67	4.51	0.11	0.63	0.72		2013	12	0.56	11.02	0.14	0.86	0.81
2014	10	0.78	6.80	0.08	0.88	0.89		2014	10	0.46	14.55	0.15	0.70	0.87
2015	12	0.60	5.33	0.15	0.75	0.64		2015	12	0.76	11.82	0.14	0.93	0.90
Schmilka/Hrensko (km 726)														
2010	12	0.28	8.13	0.15	0.24	0.38		2010	12	0.75	4.25	0.10	0.65	0.79
2011	12	0.45	–10.85	0.17	0.79	0.62		2011	12	0.68	8.91	0.11	1.02	0.87
2012	12	0.11	–1.39	0.19	0.35	0.21		2012	12	0.80	–0.22	0.07	0.84	0.80
2013	11	0.71	–10.81	0.16	0.70	0.50		2013	11	0.98	0.91	0.04	1.12	0.95
2014	12	0.09	0.00	0.15	0.20	0.13		2014	12	0.35	10.26	0.11	0.81	0.76
2015	12	–0.25	11.97	0.26	0.21	0.09		2015	12	0.46	7.00	0.10	1.19	0.81

The dynamics of total phosphorus in the Elbe longitudinal profile are shown in Figure 13. It can be seen from the graph that, on average, there is a slight decrease in the phosphorus concentration downstream. This decline may be due to a lower input of nutrients into the recipient. The reduction may also be due to the increased assimilation of dissolved nutrients by the algae in the Elbe [41]. The measured data's average value is 0.123 mg·L^{-1} at the model's upper boundary and 0.113 mg·L^{-1} at the lower boundary (profile Schmilka/Hrensko). In the Elbe, the highest concentration of 0.22 mg·L^{-1} was measured in the Lysa nL. profile in June 2011 and August 2012. Conversely, the lowest concentration of 0.03 mg·L^{-1} was measured across multiple profiles between 2010 and 2011.

The effect of the inflows is also apparent from the graph in Figure 14. The modelled concentrations decrease mainly in the rivers Jizera and Ohre. On the other hand, the Vltava and Bilina inlets increase the Elbe's concentration. The highest average concentration was 0.23 mg·L^{-1} in the Bilina river, whereas the highest observed concentration, 0.57 mg·L^{-1}, was measured in Mrlina in July 2010. In these two flows, the highest standard deviation is in the estimated data. The lowest average concentration of 0.047 mg·L^{-1} was recorded in the river Kamenice.

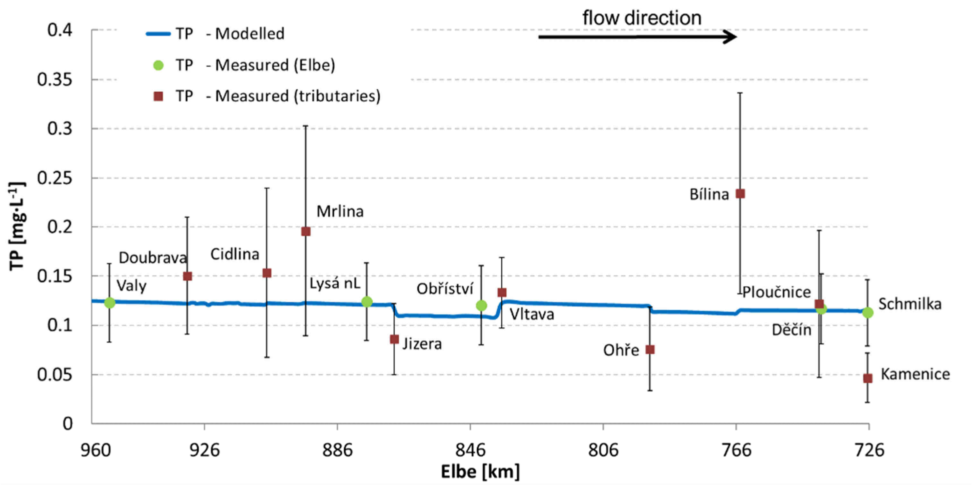

Fig. 13. Longitudinal profile of the measured (green point and line, tributaries - purple point) and modelled (blue line) total phosphor (TP) from Srnojedy (km 960) to Schmilka/Hrensko (km 726). The average value for the reference period 2010-2015. The standard deviations of the measurement are reflected by bars

Regarding total nitrogen in the Schmilka profile, the light blue line in Figure 14 shows a decreasing trend in the concentration. The measured values in the profiles shown in this graph range from about 3 mg·L^{-1} to 9 mg·L^{-1}. However, higher concentrations were measured at the beginning of the reference period (2010 and 2011). Regarding the longitudinal profile, the average measured concentration in the Valy profile (km 954) was 4.35 mg·L^{-1}. This concentration dropped to 4.04 mg·L^{-1} at the lower boundary of the Elbe model. Some tributaries have a significant influence on the TN concentration in the longitudinal profile. The Jizera and Vltava rivers have the most significant influence. The Jizera reduces the total nitrogen concentration by 0.27 mg·L^{-1} on average. Conversely, the Vltava increases the average concentration by 0.38 mg·L^{-1}. The other tributaries have lower impacts on the Elbe's nitrogen concentration. The lowest average concentration is found in Kamenice (2.29 mg·L^{-1}), whereas the highest average was measured in Bilina (6.48 mg·L^{-1}). The maximum value of 12.5 mg·L^{-1} across the monitored profiles was measured in the Mrlina in March 2010. Concerning model values, the lowest concentration was found on 8 August 2015, around km 870. The average values confirmed this result: the lowest average concentration of the entire longitudinal profile was at this kilometre of the river Elbe. Conversely, the maxima were modelled around the river km 894, reaching a concentration of 10.04 mg·L^{-1} in March 2010. These values correspond to the measured values at the nearest profile, Lysa nL. (km 877), where a concentration of 10 mg·L^{-1} was measured in the same month.

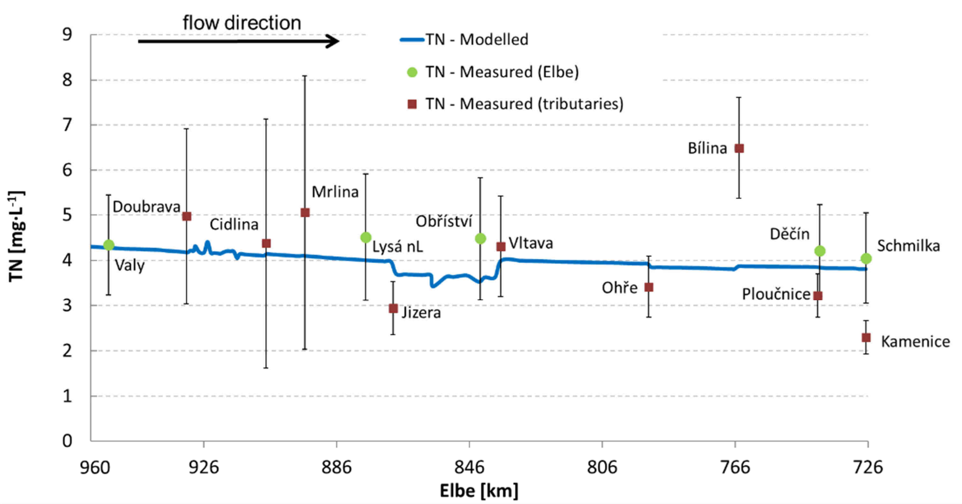

Fig. 14. Longitudinal profile of the measured (green point and line. tributaries - purple point) and modelled (blue line) total nitrogen (TN) from Srnojedy (km 960) to Schmilka/Hrensko (km 726). The average value for the reference period 2010-2015. The standard deviations of the measurement are reflected by bars

Conclusion

A crucial consideration is the accuracy of the proposed model's results. This study focused on validating the model's results, analysing the deviations that occur, and eliminating errors in the boundary conditions (the input values) and the model's setup. The comprehensive evaluation of the QSim model's performance in simulating water quality parameters in the Czech section of the Elbe river yielded valuable insights across multiple dimensions. The findings significantly contribute to better mapping the monitored parameters in the river's longitudinal profile and interactions within the river's ecosystem, offering a foundation for making informed decisions in water resource management. Generally, the QSim model's outputs capture the entire longitudinal profile of the Czech part of the Elbe river, adeptly incorporating the influence of tributaries and presenting accurate results for nutrient concentrations, dissolved oxygen, and water temperature.

The water residence time and flow dynamics are well-represented, including in extreme flow situations like the 2013 floods and the 2015 drought.

The QSim model was validated using hydrological and water quality data collected for five years for the Czech part of the Elbe river, which is highly affected by weirs that complicate the model's setup. The validation results demonstrate the model's ability to reproduce critical parameters, including discharge, water temperature, dissolved oxygen, and nutrient concentrations (total phosphorus and total nitrogen), allowing us to draw meaningful conclusions about the water quality of the Elbe river. To enhance the model's accuracy, significant point sources such as wastewater treatment plants and chemical plants should be incorporated into the model. As the volume of data grows, the model's accuracy is also expected to improve for other water quality parameters. This validated model enables water quality prediction for various scenarios including climate change and changes in pollution sources.

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