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Modelling the impact of the agricultural holdings and land-use structure on the quality of inland and coastal waters with an innovative and interdisciplinary toolkit

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Abstract

The changes taking place in the marine coastal zones are extremely important, as about 40 percent of the human population currently lives in the coastal areas (within 100 kilometres of the coastline) increasing anthropogenic pressure on the marine ecosystems. Agriculture is a significant source of nutrients to the marine environment that increase hypoxia, eutrophication and may pose a threat to the services provided by ecosystems. In particular, surface water and submarine groundwater discharge (SGD) are dominant pathways of nutrient loads. The main aim of this study is to present the capabilities and results of an innovative and complex toolkit that enables researchers to identify the sources of nutrient and pesticide pollution, calculate their flux via rivers and SGD, and directly assess the influence of pesticides and nutrient flux on the coastal ecosystem. We combined the in situ sampling of surface water, groundwater, soil, SGD, and seawater with a model study to create a set of tools for assessing the influence of agriculture on the marine environment. The maximum concentrations of nitrates and phosphates were measured in the drainage ditches and were equal to 15.5 mg N-NO_3^- L^{-1} and 7.7 mg P-PO_4^{3-} L^{-1} respectively. The nutrients concentrations varied from 0.1 to 12.9 mg N-NO_3^- L^{-1} and from 0.0 to 0.5 mg P-PO_4^{3-} L^{-1} in all freshwater samples. In contrast, the lowest concentrations were observed in seawater with maximum levels of 0.8 mg N-NO_3^- L^{-1} and 0.1 mg P-PO_4^{3-} L^{-1} respectively. The collected data were used to establish an innovative and interdisciplinary online toolkit in which surface run-off was modelled with Soil and Water Assessment Tool (SWAT), groundwater flow with Modflow, and marine waters using the EcoPuckBay model. Additionally, the tool includes two interactive calculators for calculation of the nutrient balance and nitrogen leaching for single fields on farms.

keywords: coastal management, agriculture, water quality, nutrients, pesticides

1 Introduction

Marine coastal areas are the most productive areas in the world and therefore are extensively and increasingly used for numerous activities. In addition, about 40 percent of the human population currently lives in coastal areas that further increase the anthropogenic pressure and enhance climate change. Anthropogenic activities, such as agriculture and farming, result in freshwater (groundwater and surface water) pollution with many chemical substances, mainly nutrients, but also others such as pesticides. The interaction of groundwater and surface water is a complex process, as contaminated aquifers that discharge into ditches and streams can cause long-term contamination of surface water; conversely, streams can be a major source of contamination to aquifers. Surface water usually is hydraulically coupled to groundwater, but the connections are difficult to observe and quantify, therefore, commonly have been ignored in water management considerations and policies. Enhanced nutrient inputs from land are the main drivers for coastal eutrophication and hypoxia. Therefore, proper understanding of the sources of the pollution, the processes changing their concentrations on the way to the sea, and their impact on the functioning of the marine ecosystem are of the highest importance.

The Baltic Sea, similarly to many inland seas, is an example of the marine environment being under high anthropogenic pressures. The Baltic Sea is one of the most polluted seas in the world due to its geographical and oceanographical characteristics. Its water residence time accounts for 20-25 years and, additionally, Baltic Sea is surrounded by agriculture areas of highly industrialised countries. As a result, nutrients loads, mainly nitrogen and phosphorous, to the Baltic Sea are high. Increased nutrients load to the Baltic Sea results in a declining environmental status of the sea, with widespread eutrophication (Gustafsson et al., 2012). Eutrophication together with physical factors, particularly the frequency and intensity of inflow of saltier water (Markus Meier, 2007; Reissmann et al., 2009) causes hypoxia (Österblom et al., 2007; Zillén and Conley, 2010; Helsinki Commission, 2018), usually defined as oxygen concentrations less than 2 mg L^{-1}. At least 97 per cent of the region was assessed as eutrophicated in 2011–2016 according to the integrated status assessment while large areas in the Baltic Sea suffer from low hypoxic conditions. The occurrence of both eutrophication and hypoxia significantly affect the aquatic life and nutrient cycling (Carstensen et al., 2014). Despite the considerable decrease of total nitrogen and phosphorous loads from anthropogenic sources in the last 20 years, eutrophication of the Baltic Sea still remains one of the major concerns (Baltic Sea Hydrographic Commission, 2013). The Baltic Marine Environment Protection Commission, which is also known as the Helsinki Commission (HELCOM, 2021) — is an intergovernmental organisation that gives a comprehensive overview of the ecosystem health of the entire regional sea. These major assessments assist the region's environmental managers and decision-makers so that they can base their work on sound, up-to-date knowledge of the status of the sea. HELCOM is also responsible for providing the programme to restore the good ecological status of the Baltic marine environment called Baltic Sea Action Plan (BSAP, 2021). BSAP incorporates the latest scientific knowledge and innovative management approaches into strategic policy implementation and stimulates goal-oriented multilateral cooperation around the Baltic Sea region. In order to fulfil the goals of BSAP, innovative approaches for environmental management are necessary. Although there have been many projects conducting the subject of nutrients loads from agriculture, there is still a lack of comprehensive studies merging the land and ocean-based investigations. The Baltic Sea is just an example of the marine environment lacking tools for proper coastal ocean management.

Many earlier studies used Soil and Water Assessment Tool (SWAT) to evaluate watershed-scale hydrological cycle and the associated transport of nutrients and pesticides (Neitsch et al., 2011). Applications related to the Baltic Sea watershed include, among others, Piniewski et al. (2014, 2017); Thodsen et al. (2017); Trolle et al. (2019). However, SWAT uses a simplified representation of groundwater flow, which does not allow quantifying the direct groundwater discharge to the sea (submarine groundwater discharge — SGD) and for this and other reasons may be insufficient for complex post-glacial multi aquifer systems occurring e.g., on the Polish Baltic coast. In order to overcome the limitations of groundwater modelling, several authors used SWAT in combination with dedicated groundwater flow and transport models, usually based on the MODFLOW/MT3D family of computer programs (Harbaugh, 2005; Zheng and Wang, 1999). Application of SWAT-MODFLOW coupled models is described, e.g., in Pulido-Velazquez et al. (2015); Bailey et al. (2016); Ehtiat et al. (2018). However, only few of such studies focus on coastal zone and SGD quantification. Galbiati et al. (2006) estimates nutrient load discharged to an Adriatic coastal lagoon with the use of SWAT, MODFLOW, MT3D, and a stream water quality model. In the work of Welch et al. (2019) the recharge estimates obtained from SWAT were fed to the MODFLOW/MT3D groundwater model to estimate SGD on one of the Samoan Islands. Coupling of land and sea eco-hydrological models to represent water and nutrient cycling in the coastal zone has rarely been undertaken, too. Trolle et al. (2019) applied Mike-SHE and SWAT models to estimate nutrient loads to Odense fiord on the Danish coast under different climate change scenarios. The resulting evolution of ecological state indicators in seawater was calculated with empirical models.

Usually, scientists evaluate anthropogenic pressure by characterizing the flux of contaminants using separate models such as SWAT for surface run-off, Modflow for groundwater flow, and 3D models for presenting complex processes in the marine environment being under contaminants discharge (Neitsch et al., 2011; Ehtiat et al., 2018; Adu and Kumarasamy, 2018; Torres-Bejarano et al., 2013; Dzierzbicka-Glowacka et al., 2018). As far as the authors are concerned up to date there is only one attempt to couple environment observations together with different models in the way that is similar to our approach that is Kimberley Marine Research Program (KMRP) by the Western Australian Marine Science Institution. However, KMRP has not developed an online tool, and therefore we cannot compare with their solution.

This was the main motivation for developing the WaterPUCK project which is an interdisciplinary and innovative approach integrating knowledge of different disciplines into the implementation of the environmental protection policy, sustainable growth and improvement of the competitiveness of the Polish economy (Dzierzbicka-Glowacka et al., 2018; Dzierzbicka-Głowacka et al., 2019). In this project different components and methods such as retrospective analyses of existing monitoring data sets, in situ measures and the application of various models were used to estimate main mechanisms and threats responsible for the pollution transport from the agricultural holdings and land-use structure to the surface and groundwater and potential predictability of environment change of the Baltic Sea coastal area.

The main aim of this study is to present the capabilities and results of the WaterPUCK online toolkit. WaterPUCK is an innovative and complex toolkit that enables researchers to identify the sources of nutrient and pesticide pollution, understand the main mechanisms responsible for the transport of these pollutants in surface and groundwater, calculate their flux via rivers and SGD, and directly assess the influence of pesticides and nutrient flux on the Bay of Puck ecosystem, including the creation of scenarios projecting the effects of changes in land use on chemical loads from the Puck Commune that are transported via surface and groundwater to the Bay of Puck. Additionally, within the service, we present the way the different environmental data such as in situ measures and model outcomes can be operated. The paper focuses on the description of the full modelling framework. Detailed presentation of some components can be found in earlier publications from our group (Dzierzbicka-Głowacka et al., 2019; Dybowski et al., 2019, 2020a,b; Szymkiewicz et al., 2020; Kalinowska et al., 2020; Wielgat et al., 2021).

2 Materials and Methods

2.1 Conceptual scheme of the solution

The method of modelling the impact of farms and land-use structure on the quality of land (surface water and groundwater) and coastal waters was developed and verified as part of the WaterPUCK project. The service is a set of computer models interconnected with each other, operating continuously, forced with meteorological data and combines four main modules (Figure 1):

1. Agricultural holdings — survey system and two calculators for farms as interactive applications,
2. LAND WATER — a comprehensive model of surface water run-off based on SWAT model and a numerical model of groundwater flow based on Modflow which we named GroundPuck,
3. COASTAL WATER — a three-dimensional numerical model of coastal ecosystem consisting of a hydrodynamic and biochemical part with a nutrient spread module based on Community Earth System Model (CESM),
4. MARINE WATER — a three-dimensional numerical model of the marine ecosystem providing boundary condition to COASTAL WATER module.

A schematic flowchart of the modelling system is presented in Figure 2. We coupled the EcoPuckBay model from the land side with two models: SWAT (surface water) and GroundPuck (groundwater). Information about the water volume discharged by rivers is being provided by the hydrological model SWAT that has been implemented as one of the WaterPUCK project's stages (Kalinowska et al., 2020). The SWAT model includes the preparation of the innovative and complex hydrological model coupled with the nutrient concentration module including meteorological data (precipitation, wind, temperature, and atmospheric pressure). The transformation of precipitation data into surface run-off have been achieved with the SCS (Soil Conservation Service) curve number procedure through the accumulated run-off volume and the time of concentration (the time from the beginning of a rainfall event until the entire subbasin area contributes to flow at the outlet) (Kalinowska et al., 2020).

A numerical transport model based on the Modflow code (GroundPuck) allows determining the nitrate load in the groundwater flowing into the Bay of Puck. The MT3DMS numerical code was applied to solve the advection–reaction–dispersion equation (Zheng and Wang, 1999). Transient calculations were performed with the third-order total-variational diminishing (TVD) numerical method for the advective term, while for the steady-state solution, the standard finite difference discretization was applied. This model was calibrated based on actual NO_3^- concentration values and was joined with the EcoPuckBay model through a coupling module.

The results of the 3D EcoPuckBay model are limited to the area of the Bay of Puck. However, the entire model grid covers a wider area (Dybowski et al., 2020b). This is to ensure that boundary conditions are properly simulated. Along the line of the northern border of the 3D EcoPuckBay model, data from the 2.3 km three-dimensional Coupled Ecosystem Model of the Baltic Sea (3D CEMBS) prediction model are transferred to the EcoPuckBay model. Results from 3D CEMBS (Dzierzbicka-Głowacka et al., 2013a,b) are used to provide forcing fields in the EcoPuckBay model through sequential information transfer. The mechanism of this module is to interpolate values from 3D CEMBS to EcoPuckBay model's grids.

2.2 Study area and database

The entire tool has been designed and assembled regardless of geographical location. This means that the application of methods developed within the described solution is possible (after calibration to a specific region) in any coastal area. However, the area of the Puck Commune and the Bay of Puck (Figure 3) was chosen to test and verify the developed methods.

The study area is located in northern Poland, on the southern coast of the Baltic Sea. It includes the Bay of Puck drainage basin located in the Puck Commune with an area of 176 km^2. The Puck Commune is

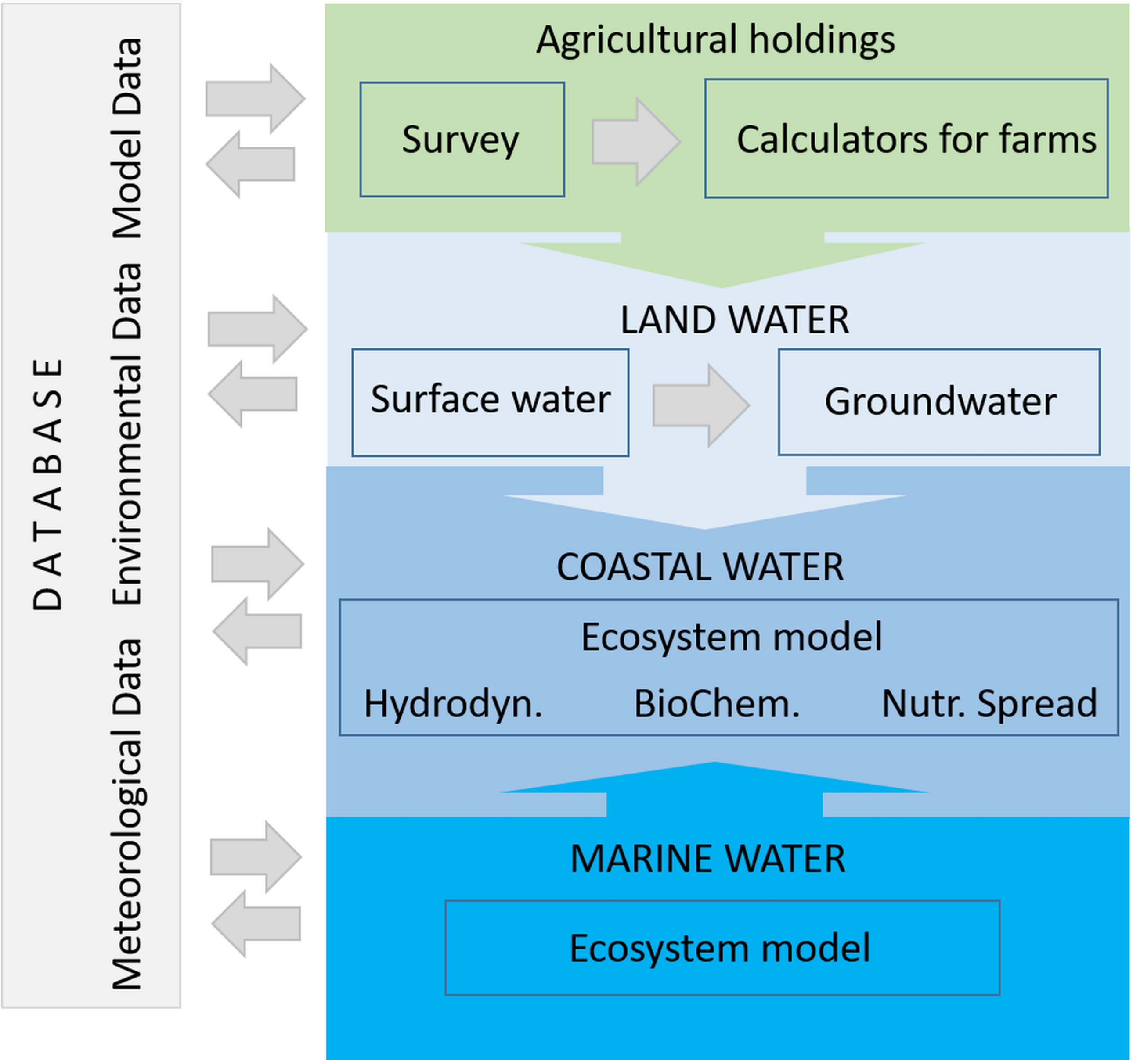

Figure 1: **Structural scheme of the WaterPUCK toolkit.**

of agricultural character. Its area is 57.3% covered by utilised agricultural area (UAA), the vast majority of which is characterised by high yield potential (Witek, 1994; Igras and Pastuszak, 2009). The remaining area of the municipality is covered by forests and areas classified as forest ((33.7%), roads and areas under buildings (7.1%) as well as waterlogged land and unused land (1.9%). Among the agricultural lands, the largest area is occupied by arable land — 77% of UAA, followed by grassland — about 20.5% of UAA. Arable land (AL) is mainly used to grow cereals, such as: rye, winter wheat, spring wheat, spring barley, oat, winter triticale, cereal mixture. Their sowing area occupies more than 2/3 of the AL. Other major crops include ground vegetables, rape, potatoes, and maize (for green fodder). Agricultural activity in the Puck Commune, apart from crop production, also includes milk and pig production. The average livestock density in the municipality is less than 0.5 livestock unit per 1 ha of UAA.

The Puck Commune area represents a typical young postglacial landscape with relatively high relief (from -0.5 to 113.5 m above sea level). It consists of isolated fragments of the moraine plateau separated from each other by deeply cut ice-marginal valleys. The whole area is covered with Quaternary deposits. The Quaternary deposits consist of moraine glacial till with sand and gravel layers, and glacifluvial or river sand and silty sand in the valleys. The dominant soil types are sandy loam (glacial till), sandy loam covered by loamy sand (weathered glacial till), sand (of glacifluvial origin), and peat (in larger river valleys). The thickness of the sediment ranges from 40 m in the east to 95-100 m in the west. Such a significant difference is probably a result of a diversified land surface or large range in altitude of the top of older layers (Jereczek-Korzeniewska and Jegliński, 2011).

Groundwater forms a complex system with several aquifer units (Figure 4). Shallow groundwater occurs in

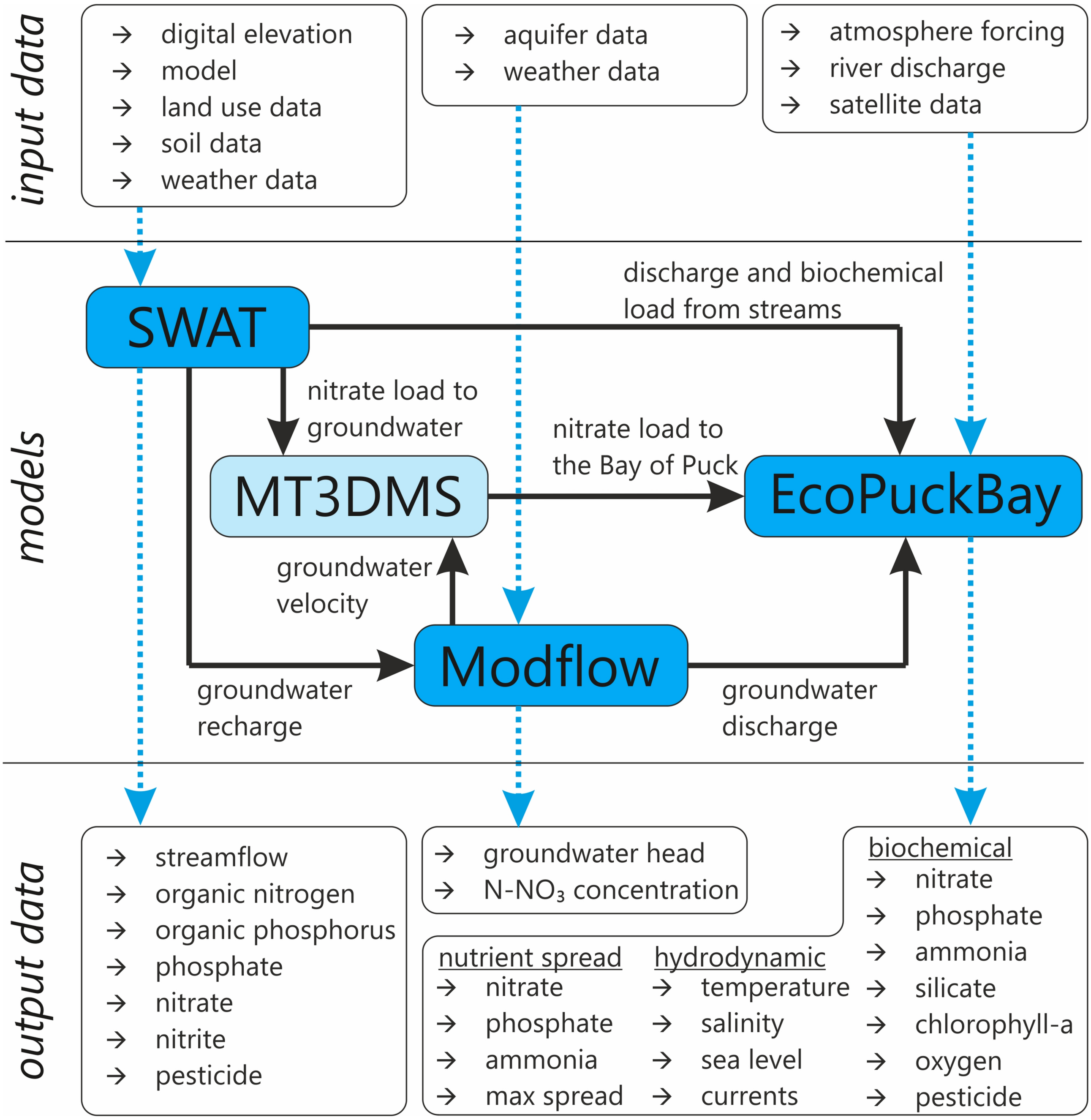

Figure 2: **Schematic flowchart of the modelling system.**
The blue tiles represent the three main models (SWAT, Modflow, and EcoPuckBay) together with SWAT/Modflow combining module - MT3DMS. The blue dotted arrows show the relationship of the models to the Input/Output data. The solid black arrows show flow direction of the specific type of data between the models.

small perched aquifers and in sand lenses enclosed in moraine deposits (Figure 4). These aquifers do not play an important role in water supply, but they are exploited locally by farms and summer houses. Two deeper Quaternary aquifers span most of the area: The upper (inter-moraine) aquifer (Q1) and the lower sub-moraine aquifer (Q2). They were formed in glacifluvial deposits (sand and gravel) separated by a layer of moraine till. These two large aquifers are hydraulically connected. Shallow groundwater is recharged by the infiltration of rainwater. Deeper aquifers are influenced by inflow from the west and take the seepage water from the layers above. The entire hydrosystem is drained mainly by the Baltic Sea (Bay of Puck), either directly via SGD or indirectly via streams and rivers. Aquifers Q1 and Q2 are the main source of water supply in the region (Szymkiewicz et al., 2020).

There are seven streams flowing through the area of Puck Commune: Reda river, Zagórksa Struga, Mrzezino Canal, Gizdepka, Błądzikowski Stream, and Płutnica river together with its inflow — Darżlubie Stream. The streams discharge directly to the Bay of Puck. All stream catchments are covered with a dense hydrographic

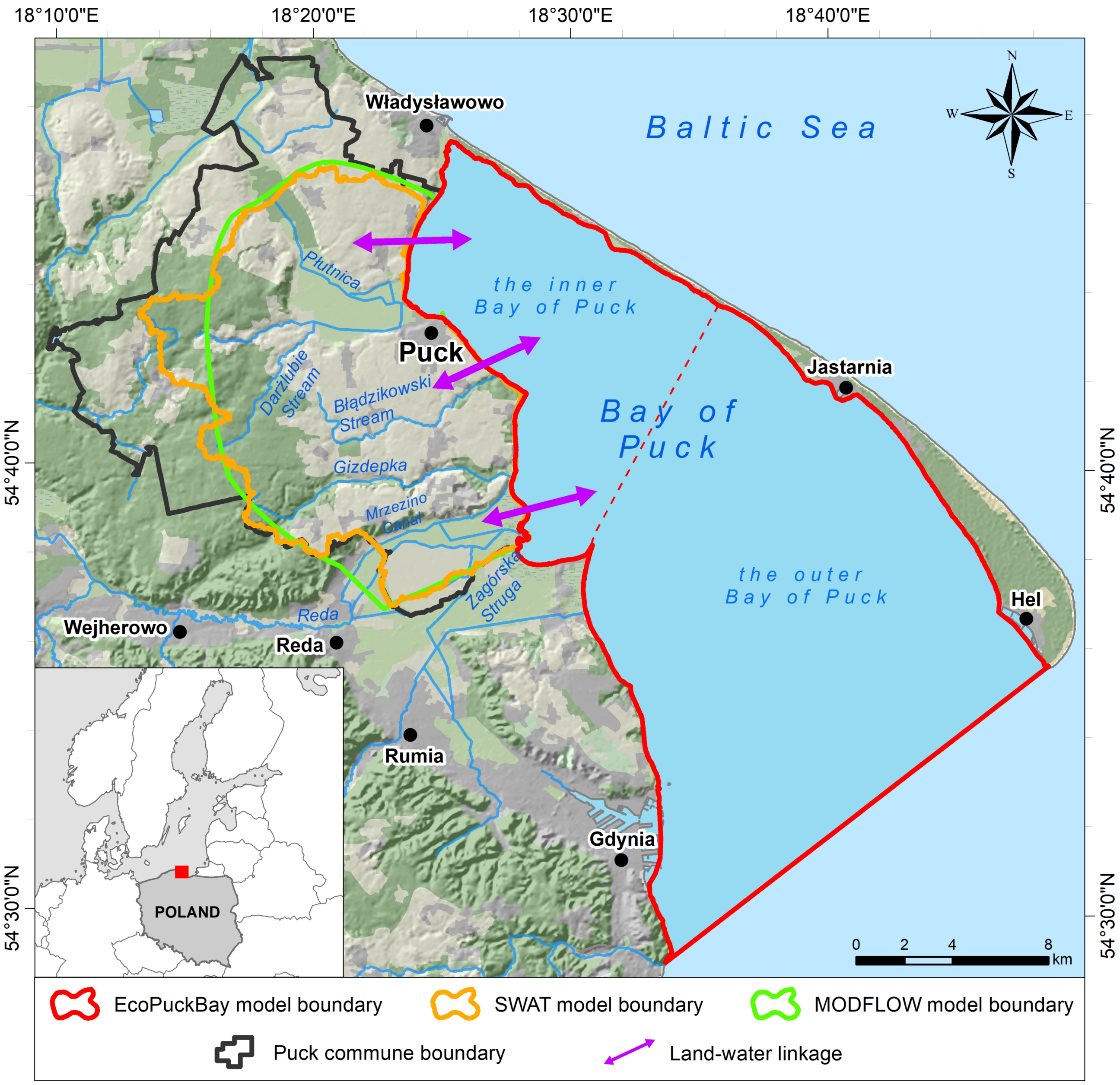

Figure 3: **Map presenting location of the testing area.**
Marked boundaries of the Puck commune (black), SWAT model domain (orange), Modflow model domain (green), EcoPuckBay model effective domain (red) and land-water linkage (purple arrows).

network (drainage ditches, canals) as well as tiles serving regulation of water level for agriculture. Average concentrations of nutrients in the analysed streams flowing through the Puck Commune area: Zagórska Struga, Reda, Mrzezino Canal, Gizdepka, Błądzikowski Stream, Płutnica and Darżlubie Stream generally fulfilled the requirements for the I or the II class of quality according to the Regulation of the Ministry of Marine Management and Inland Navigation of 11th October 2019 concerning classification of ecological status of surface waters and environmental quality classes for priority pollutants (Dz. U. 2019 poz. 2149). The worst quality status was observed in the case of Błądzikowski Stream and Gizdepka which flow through intensively used agricultural terrain. The episodes with elevated nutrients concentrations, especially during summer months. The catchment of Błądzikowski Stream is characterized by predominating agricultural land use, with almost 90% share of agricultural land in the total land area. The relationship between N surplus in the agricultural farms in the Błądzikowski Stream catchment and the elevated concentrations of total nitrogen was proved (Wojciechowska et al., 2019b). Also, for Płutnica river and its tributary — Darżlubie Stream the incidental situations when nutrient concentrations exceeded the requirements of the II class were observed, mostly in summer months or after intensive rainfalls. On the other hand, Reda river and Zagórska Struga were characterized by very good status regarding nutrient concentrations. Average flows in the analysed watercourses are: Gizdepka 0.178 m^3s^{-1}, Błądzikowski Stream 0.035 m^3s^{-1}, Płutnica river 0.718 m^3s^{-1} (Bogdanowicz and Cysewski, 2008).

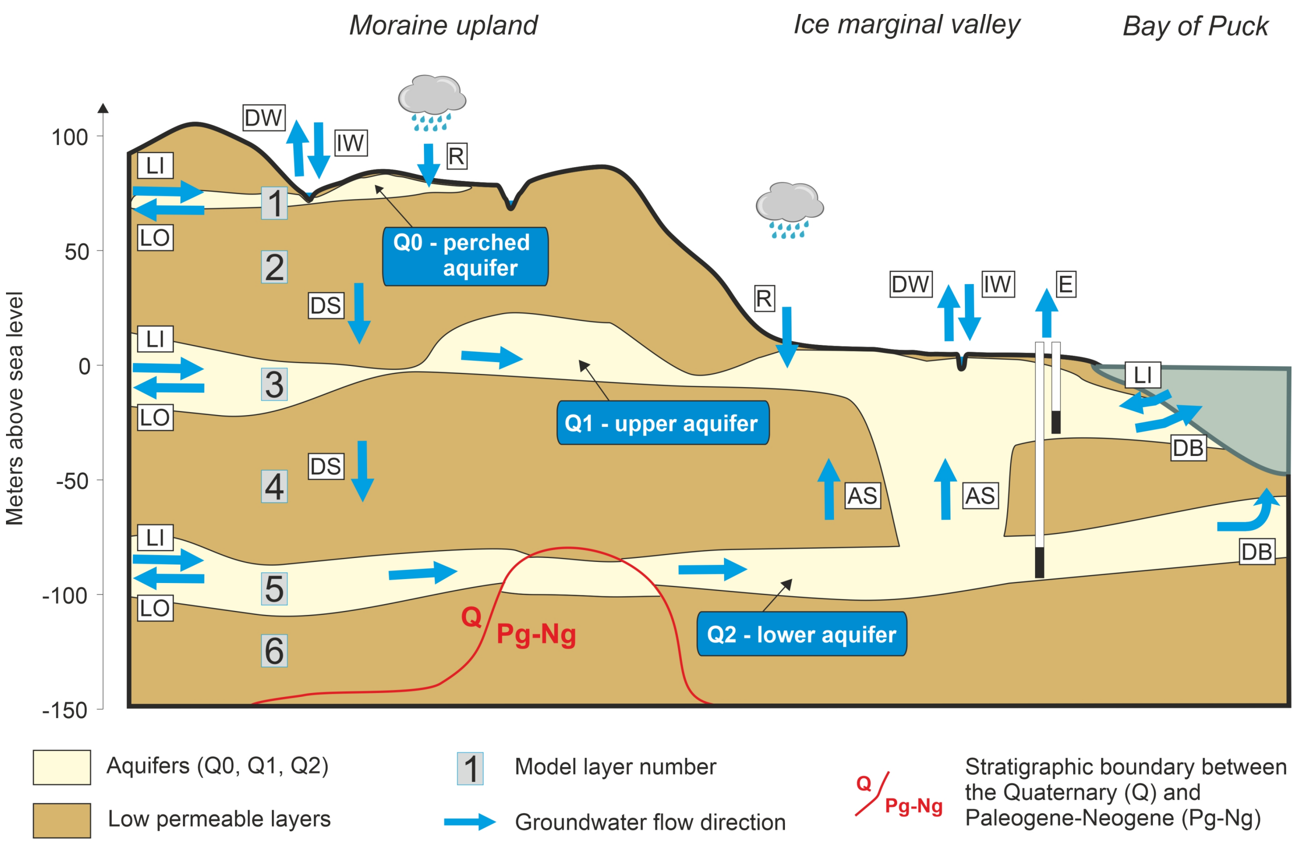

Figure 4: **Conceptual model of groundwater flow in Puck area.**
Explanation of abbreviations: R - groundwater recharge, IW - infiltration from surface water, DW - drainage to surface water, E - groundwater exploitation, DS - descent seepage, AS - ascent seepage, LI - lateral inflow, LO - lateral outflow, DB - discharge to the Bay of Puck.

Water quality in individual rivers varies depending on the season, vegetation intensity, and stage of agricultural practices (Wojciechowska et al., 2019a). Despite intensive agriculture in the catchment area, soils are characterised by low pH. This results in the conversion of phosphate fertilisers into insoluble compounds unavailable to plants and forces the use of increased doses of nitrogen fertilisers. The climate of this region is temperate maritime. In the period 2011-2020, the annual average temperature was about 7.5 °C and the average annual precipitation was 712 mm (the highest precipitation during summer) (Wielgat et al., 2021).

The southern part of the Baltic Sea enclosing the Puck Commune is a popular tourist region that is also heavily influenced by an anthropogenic activity of local residents and farming. This makes the Bay of Puck a natural reservoir for waste deposition of fertilisers and other inputs delivered through the soil, groundwater, rivers, or direct deposition. This region is massively shaped and influenced by several factors that can pressure the state of physical and biochemical parameters. One of the most important factors influencing the region's unique ecosystem is topography. The average depth of the Gulf of Gdańsk is about 50 m, with a maximum depth (Gdańsk Deep) of 118 m. From the northeast, it is surrounded by Hel Peninsula, which serves as a natural barrier for mixing with the open waters of the Baltic Sea, keeping the salinity ranging mostly within the range of 7–8 with a deviation of around 1. Bay of Puck is also heavily influenced by the river discharge from land, resulting in lowered salinity, especially in the coastal surface waters. The largest river in the region is the Vistula, discharging an average of over 1000 m^3s^{-1} of freshwater. Water temperature in the region ranges from over 20 °C at the surface during summer, with the maximum usually in August, to around 2 °C in February. Water stratification is frequent during the warmer months, leading to the occurrence of seasonal thermoclines. During winter, thermocline declines and the water becomes well mixed (Dybowski et al., 2020b). The ecosystem of the Bay of Puck, especially its inner part (called Puck Lagoon) due to the geomorphological separation from the rest of the bay (marked with a dashed line in Figure 3), is very prone to degradation from land-based pollution. The area of the Bay of Puck is equal to 356 km^2, and maximal depth is 55 m. The exchange of water between Puck Lagoon and outer Bay of Puck is very limited, and therefore any contaminants getting directly into Puck Lagoon with watercourses from the Puck Commune pose a real threat to which special attention should be paid. This applies especially to agriculture, which is a dominant land-use type in the Puck Commune.

2.2.1 The pH of the soils and abundance of arable land in macro-nutrients

In the spring of 2018, soil samples from 61 agricultural plots on 22 farms with a total area of 171.05 ha, were taken based on the guidelines included in the Polish standard PN-R-04031 (1997). pH measurement of soil was conducted in suspension of 1 mole KCl L^{-1} solution by the potentiometric method according to the Polish standard PN-ISO 10390 (1997) (pH_{KCl}) (Barszczewki et al., 2000; Sapek, 1979, 1993, 2008). The fraction content below 0.02 mm was determined by the sedimentation (pipette) method according to the Polish standard PN-EN ISO 17892-4 (2016). The concentration of available P forms in mineral soils (in agronomic soil P test — STP) was determined by acid ammonium lactate (pH ca. 3.55) according to the Polish standard PN-R-04023 (1996) (P_{ER}) (Pietrzak et al., 2016, 2020) and by the extract of 0.5 mole HCl L^{-1} according to the Polish standard PN-R-04024 (1997) (P_{HCl}) in organic soils (Sapek, 2008). The concentration of exchangeable K in mineral soils was determined by Egner-Riehm method according to the Polish standard PN-R-04022 (1996). The concentration of exchangeable Mg in mineral soils was determined by Schachtschabl'e method according to the Polish standard PN-R-04020 (1994). The concentrations of exchangeable K and Mg in organic soils were analysed by the extract of 0.5 mole HCl L^{-1} according to the Polish standard PN-R-04020 (1994) (Lityński et al., 1976; Nowosielski, 1974, 1988; Sady et al., 1994).

2.2.2 Nutrients in stream water

Stream water samples were collected between June 2017 and July 2019, in 4 weeks intervals (26 sampling campaigns). Location of sampling points is presented in the Figure 5. Each time, 1 litre of water every 5 min during a 30-min period of time was collected from the midstream course. The samples were immediately placed in a portable cooler (8 °C) and transported to the laboratory. The measurements of ammonium nitrogen (N-NH_4^+), nitrite nitrogen (N-NO_2^-), nitrate nitrogen (N-NO_3^-), total nitrogen (TN), mineral phosphorus (P-PO_4^{3-}) and total phosphorus (TP) concentrations were carried out according to Polish Standards compatible with EU and US-EPA standards. All measurements were carried out in 3 replications.

2.2.3 Nutrients in surface waters from drainage ditches

Water samples were collected once a month from February to September 2018 from drainage ditches surrounding each studied agricultural plot. The determination of nitrate nitrogen residue in water samples has been performed according to Polish Standard PN-EN ISO 10304-1:2009/AC (2012) compatible with EU standard. The measurement of TN, phosphate phosphorus, and TP concentrations were carried out according to the procedures developed and implemented by the accredited Laboratory of Maritime Institute Gdynia Maritime University (respectively: PB-03 edition No. 3, PB-07 edition No. 2, and PB-20 edition No. 1).

2.2.4 Nutrients in SGD

Submarine groundwater discharge samples for nutrient analyses were collected at 10 cm depths by means of push points (e.g., Szymczycha et al. (2012, 2020)) every 1 m along a 5-m-long transect perpendicular to the shoreline at each study site. Samples were brought to the surface by acid-washed Teflon tubing connected to nylon tubing by a peristaltic pump. Several void volumes were pumped before sampling.

2.2.5 Nutrients in groundwater

Groundwater samples were collected between June 2017 and July 2019 in 9 sampling campaigns. Water samples were taken from 60 sampling points, including 12 dug wells (7 in Q0 — perched aquifers, and 5 in Q1 — shallow Quaternary aquifer), 37 drilled wells (21 in Q1 and 16 in deeper Quaternary aquifer Q2), 9 temporary boreholes in Q1 aquifer and 2 springs (one in Q0 and Q1). Location of sampling points is presented in the Figure 5. The measurements of electrical conductivity (EC), pH, redox potential (E_h), and temperature were carried out in field with a multi-parameter portable meter (model MultiLine® Multi 3630 IDS WTW, Xylem Analytics, Weilheim, Germany) using the electrodes with liquid-filled electrolyte with ceramic (model SenTix® ORP-T 900 WTW, Xylem Analytics, Weilheim, Germany) or platinum diaphragm (model SenTix® 950 WTW, Xylem Analytics, Weilheim, Germany) and conductivity electrode cell made of graphite (model TetraCon® 925 WTW, Xylem Analytics, Weilheim, Germany). The nitrogen (NH_4^+, NO_2^-, NO_3^-) and phosphorus (PO_4^{3-}) content was determined using a photometer (model pHotoFlex® STD WTW, Xylem Analytics, Weilheim, Germany). Additionally, 15 selected groundwater samples were also tested in 2 replications in the laboratory. The determination of nutrients (ammonium nitrogen (N-NH_4^+), nitrite nitrogen (N-NO_2^-), nitrate nitrogen (N-NO_3^-), TN, mineral phosphorus (P-PO_4^{3-}) and TP) residue in groundwater samples were made with the same method and in the same laboratory as the stream water tests (2.2.2).

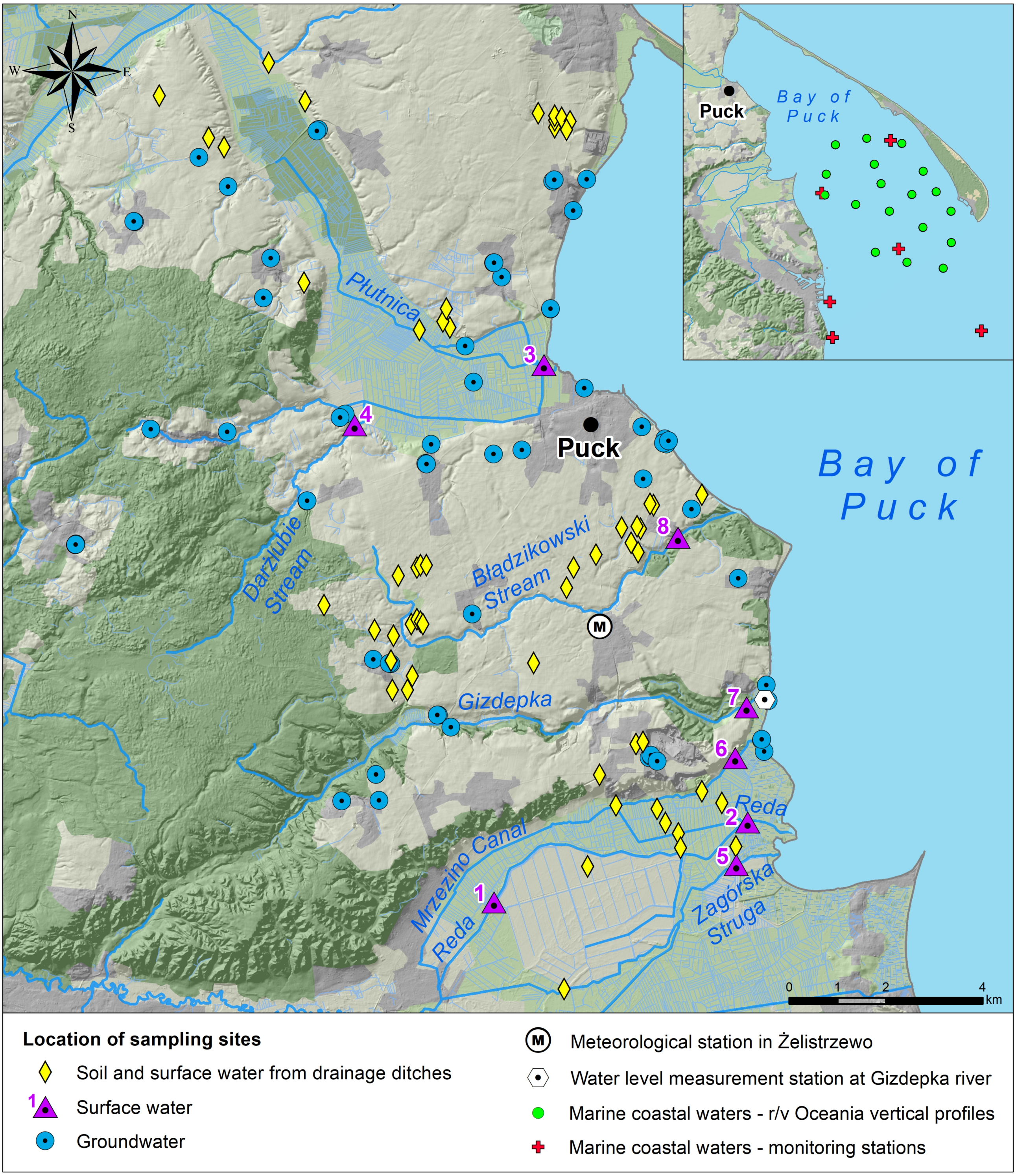

Figure 5: **Locations of sampling sites.**
Locations of soil and surface water form drainage ditches, surface water, groundwater, and marine coastal waters sampling sites as well as meteorological station in Żelistrzewo and water level measurement station at Gizdepka.

2.2.6 Pesticides in waters and soils

The determination of organochlorine pesticides (aldrin, dieldrin, endrin, isodrine, dichlorodiphenyltrichloroethane and its isomers and alpha, beta, gamma, and delta isomers of hexachlorocyclohexane) content in soil samples has been performed according to the procedure PB-45 “Determination of organochlorine pesticides in soil samples”, edition No. 2, developed and implemented by the accredited Laboratory of Maritime Institute Gdynia Maritime University. The examination (in water samples) of the content of 309 active substances classified as pesticides was carried out in accordance with the methodology described in the procedures SOP-LA-GC-033-04 and D. Becker 1.4.2019 developed and implemented by the accredited Eurofins Laboratory (Pazikowska-Sapota et al., 2020). The content of glyphosate and aminomethylphosphonic acid (AMPA) in water samples has been performed according to the procedure SOP-LA-LCMS-039-04 and D. Becker 1.4.2019 implemented and used by the accredited Eurofins Laboratory (Pazikowska-Sapota et al., 2020).

2.3 Toolkit's modules

2.3.1 Interactive online calculators and farm questionnaires

The survey on the farm management on the studied farms in the Puck Commune was composed of 9 parts (with total of 64 questions), entitled as follows:

1. Identification of the farm and farmer;
2. Farm type;
3. Crops;
4. Breeding;
5. Storage of natural fertilisers;
6. Fertilisation management;
7. Plant protection products;
8. Purchased, sold and used products;
9. Comments and remarks.

The survey was carried out on a representative group of 31 farms with a diversified agricultural production profile, and its aim was to determine in detail how farmers in Puck Commune manage their farms. The questionnaires were conducted using a specially prepared online form, which significantly improved the subsequent post-processing and data analysis. In the next step, which was at the same time an element of research and resulted as a support tool for farmers, we developed two interactive calculators to help farmers determine the Nitrogen, Phosphorus and Potassium (NPK) balance on the farm (called CalcGosPuck) and the amount of nitrogen leaching from the field (called CalcNPuck). The calculators were designed to directly use the data from the farmers' surveys. Detailed information on the "At the farm gate method" and the leaching of N from the individual field have been described in detail in the following papers Dzierzbicka-Glowacka et al. (2019) and Dybowski et al. (2020a).

2.3.2 SWAT — surface run-off model

The SWAT model is a tool for complex agricultural catchment area analysis. Based on weather and spatial data such as digital elevation model, land use and soil maps, SWAT model calculates the hydrological response of the basin and water balance. Additionally, based on information about plants, method of cultivation, doses and types of fertilisers and pesticides, it calculates yields, as well as water and soil chemical quality. Depending on meteorological information sources, this model can be used for real-time calculations, forecasting or simulation of archival events. The SWAT model in our configuration uses data from the Institute of Meteorology and Water Management station in Żelistrzewo, marked in Figure 5 (2000-2010 start-up period needed to stabilise soil and water conditions) and Interdisciplinary Centre for Mathematical and Computational Modelling of Warsaw University (ICM) forecast (2011-2019). The meteorological station operating in the years 2018-2019 enabled the verification of data needed for the forecasting model (Kalinowska et al., 2020). In the WaterPUCK toolkit, the surface water run-off model has been set up with 17 sub-basins and 353 HRU (hydrological response units, i.e., areas with the same land development, slope and soil profile) (Wielgat et al., 2021).

2.3.3 GroundPuck – groundwater flow and transport model

Here, we present a brief description of the groundwater model, following Szymkiewicz et al. (2020). Groundwater flow simulations were carried out with MODFLOW-NWT numerical code. The rectangular grid had 6 layers, 410 rows, and 296 columns. The total number of cells was 728,160, of which 340,496 were active. The spacing in the horizontal direction was uniform and equal to 50 m to capture the topographic features and minimize discretization errors. The 6 layers were defined (Figure 4) as follows: (I) Sandy, perched aquifers, occurring locally (Q0), (II) low-permeability till deposits, (III) inter-moraine aquifer in glacifluvial sand (Q1), (IV) low permeable till layer, (V) sub-moraine aquifer in glacifluvial sand (Q2), (VI) low-permeability layer representing Quaternary glacial till and Neogene clay and silt.

2.3.4 EcoPuckBay — ecosystem model of the coastal environment

The marine environment (specifically the coastal zone) is represented by an ecohydrodynamic model of the Bay of Puck called EcoPuckBay (EPB). The EPB is a high-resolution three-dimensional model that originates from the Community Earth System Model (CESM, 2021) developed by National Center for Atmospheric Research (NCAR). The EPB's ecosystem part is based on the nutrient-phytoplankton-zooplankton-detritus (NPZD) approach (Moore et al., 2001). The model predicts nutrient distributions (N, Si, and P), three phytoplankton functional types (diatoms, picophytoplankton/nanophytoplankton, and diazotrophs (nitrogen-fixing organisms)), chlorophyll-a as separate variables, zooplankton, pelagic detritus, dissolved oxygen, and pesticides (glyphosate, diflufenican, metazachlor, chlorpyrifos, and antrachinon). Sources of nutrients include atmospheric deposition and sedimentary sources. Sinking particles can be associated with ballast, and the presence of ballast changes the remineralization length scale assumed for the model. Many, though not all, models can be cast in a general form as a coupled set of time-dependent advection, diffusion, reaction equations (Dybowski et al., 2020b).

2.4 Boundary conditions, calibration, and validation

2.4.1 SWAT

The SWAT model was required to provide data on water balance, water quality, and infiltration (Dzierzbicka-Glowacka et al., 2018, 2019). Due to the lack of sufficient data on water flows and water levels in watercourses, it was decided to perform calibration using the "manual trial and error procedure" (Szymkiewicz et al., 2020). The method of calibration was chosen not only because of the small amount and short time series of measurement data. It also results from the purpose of the model, it was created as part of the larger project. The combination of the 3 models, dependent on the same variable — daily rainfall, was a challenge from the point of view of calibration, because each of the models processes the same parameters in a slightly different way. The authors wanted to maintain consistency in defining the study area (parameters of the basin, soil, watercourses, etc.), thus it was necessary to calibrate 3 completely different models simultaneously. Additionally, some of the calibrated parameters (or their ranges) were limited. In this situation, the simplest solution seemed to be to perform "manual trial-and-error" calibration. Meteorological data from 2000-2009 were used for the calibration. The criteria for calibration and validation represented the components of hydrological budget and biomass, for which reliable estimates were reported in earlier studies (references available in Szymkiewicz et al. (2020); Wielgat et al. (2021); Kalinowska et al. (2020)). Specifically, we aimed to obtain the average annual groundwater recharge in the range between 3% and 30% of the average annual precipitation, depending on soil type and land use (Duda et al., 2013; Jaworska-Szulc, 2015). Moreover, the average annual evaporation calculated by SWAT was required to be in the range 450 to 495 mm, as measured for a location in Poland with very similar climate and land use conditions (Czyżyk and Steinhoff-Wrześniewska, 2017). As the third calibration goal we used the average annual production of biomass in pine forests (Orzeł et al., 2006). In the calibration process, we modified: (i) SCS curve numbers which describe the partitioning between runoff and infiltration (their values were increased to the range 80 to 94), (ii) maximum water storage in canopy (CANMX, increased in forests from 0 to 2 mm), (iii) fraction of water in the shallow aquifer returning to the root zone (REVAP, increased in forests from 0 to 0.06), and (iv) parameters describing growth of pine trees (BLAI = 4.50, FRGRW1 = 0.01, LAIMX1 = 0.01, FRGRW2 = 0.10, ALAI_MIN = 2.99). For a detailed description of these parameters see Arnold et al. (2011).

Validation of SWAT model was performed by comparing the observed and calculated average daily outflow from the Gizdepka river (marked in Figure 5). The Gizdepka river was chosen because it flows through all the land use types existing in the analysed basin, especially through agricultural land used in different ways. To validate the model, monitoring in the years 2018-2019 was used. The monitoring consisted of a water level measurement station. Then the water level was converted into the flow rate using a rating curve based on measurements carried out in the years 2017-2019. We used the following measures (defined in A) to verify the model: mean error (ME), mean-square error (MSE) and root-mean-square error (RMSE).

Additional validation criteria included the weight of the yield of the major crops in the area: winter wheat, rape (canola), and silage corn and hay production on grassland. Model predictions for the period 2000-2009 were compared to data obtained from local farmers (Szymkiewicz et al., 2020). Average crop yields from questionnaires conducted among farmers with crops in the study catchment were used as reference values (Dzierzbicka-Glowacka et al., 2019). Based on information from farmers and agricultural advisors we assumed that the fraction of dry mass in yield is 85% for winter wheat, 90% for rape (canola), 35% for silage corn and 85% for hay (dried).

2.4.2 GroundPuck

The sea boundary was represented by a constant head boundary in the Q1 aquifer (direct hydraulic contact with water in the Bay of Puck) and by a general head boundary (GHB, third type) in the Q2 aquifer, which represented the outflow through a distant outcrop at the sea bottom (the discharge zones are situated in the bottom of the Bay of Puck, at a distance of 2–3 km from the coast). The GHB boundary was also used to simulate the lateral flow across the land part of the boundary in Q1, Q2, and those perched aquifers (Q0), which were intersected by the model boundary. Wells were assumed to be constantly in operation and the pumping rates were identified based on the available reports from groundwater administration. rivers were represented by the third-type boundary conditions (RIVER package). The results obtained from SWAT were processed by scripts written in the Python language using the FloPy library (Bakker et al., 2016), in order to set the recharge values in the MODFLOW model. In steady-state simulations, we used the average values for each HRU from the period of 2000–2009. For transient simulations, monthly averages were calculated for each HRU from SWAT daily results. We followed the approach described by Bailey et al. (2016) to transfer HRU-based SWAT results to the grid-based MODFLOW input. Calibration of the groundwater flow model was based on the steady-state solution, representing the average conditions in the period of 2000–2009. We used groundwater head measurements from 95 points in the area, as shown in Figure 6. To estimate model accuracy we made calculation using standard measures such as mean error (ME), mean absolute error (MAE) and root mean squared error (RMSE) that we described in datail in the A.

Based on the groundwater flow model developed in MODFLOW, a simulation of N-NO_3^- transport was carried out. MT3DMS numerical code was applied to solve the advection-reaction-dispersion equation. Transient calculations were performed with the third-order total-variational diminishing (TVD) numerical method for the advective term, while for steady-state solution, the standard finite difference discretization was applied. Denitrification of nitrates was described with the first-order kinetic reaction. We used a constant reaction rate of biodegradation equal to 1×10^{-5} h^{-1}, which was established by model calibration. In the model, we considered only diffuse sources of nitrates. Concentrations of N-NO_3^- in water reaching the groundwater table were calculated from the results of SWAT simulation for the years of 2000–2009 for each HRU. As in the case of groundwater recharge, the transfer of HRU-based SWAT data to grid-based MT3DMS data was carried out with the aid of Python scripts, making use of the FloPy library. The model of nitrate nitrogen transport was calibrated manually by adjusting the reaction rate in order to obtain a satisfactory agreement between range of the calculated N-NO_3^- concentrations and the results of chemical analysis of the 60 samples taken from the aquifers. Calibration was based on a steady-state flow and transport simulation, using average values of recharge and N-NO_3^- loads from the period 2000–2009 and the current land use and agricultural practices. The land-side pesticide propagation was modelled only in the SWAT surface run-off, but not in the Modflow groundwater flow.

2.4.3 EcoPuckBay

From the land side, the EcoPuckBay model is coupled with SWAT (surface run-off) and Modflow (groundwater flow), while from the open sea side, forcing data from the 3D CEMBS (Dzierzbicka-Głowacka et al., 2013a,b; Nowicki et al., 2019), after the previous interpolation, is delivered to the domain's borders. The EPB model has been validated and runs in operational mode, producing a 60h forecast for physicochemical conditions of the Bay of Puck's environment (Dybowski et al., 2019, 2020b). We used the following standard measures (described in detail in the A) to test the quality of the EcoPuckBay model: Pearson's correlation coefficient (r), root-mean-square error (RMSE), standard deviation (STD), and mean error (ME).

To evaluate EcoPuckBay model, we used several sources of *in situ* samples. That includes measurements taken throughout the monitoring activities of the Voivodship Inspector of Environmental Protection (VIEP) in Gdańsk and vertical profiles of temperature and salinity recorded in 2018 during one of the measurement campaigns of the s/y Oceania along the Southern Baltic coast (Figure 5). In addition, we compared our results with the numerical data of hydrodynamic and biochemical parameters calculated with the ice-ocean model NEMO-Nordic (Nucleus for European Modelling of the Ocean) coupled with the biogeochemical model SCOBI (Swedish Coastal and Ocean Biogeochemical model) acquired from the Marine Copernicus database. The most commonly used pesticides in the studied area, which are glyphosate, diflufenican, metazachlor, chlorpyrifos, and antrachinon, are modelled in the EcoPuckBay model.

3 Results

3.1 Environmental studies

The set of environmental measurement data was divided into two parts. One part of the data was used as a set forcing numerical models (directly, but also for parameterization, calibration). The second part of the environmental data was used to verify and test the correctness of the developed methods implemented in numerical models.

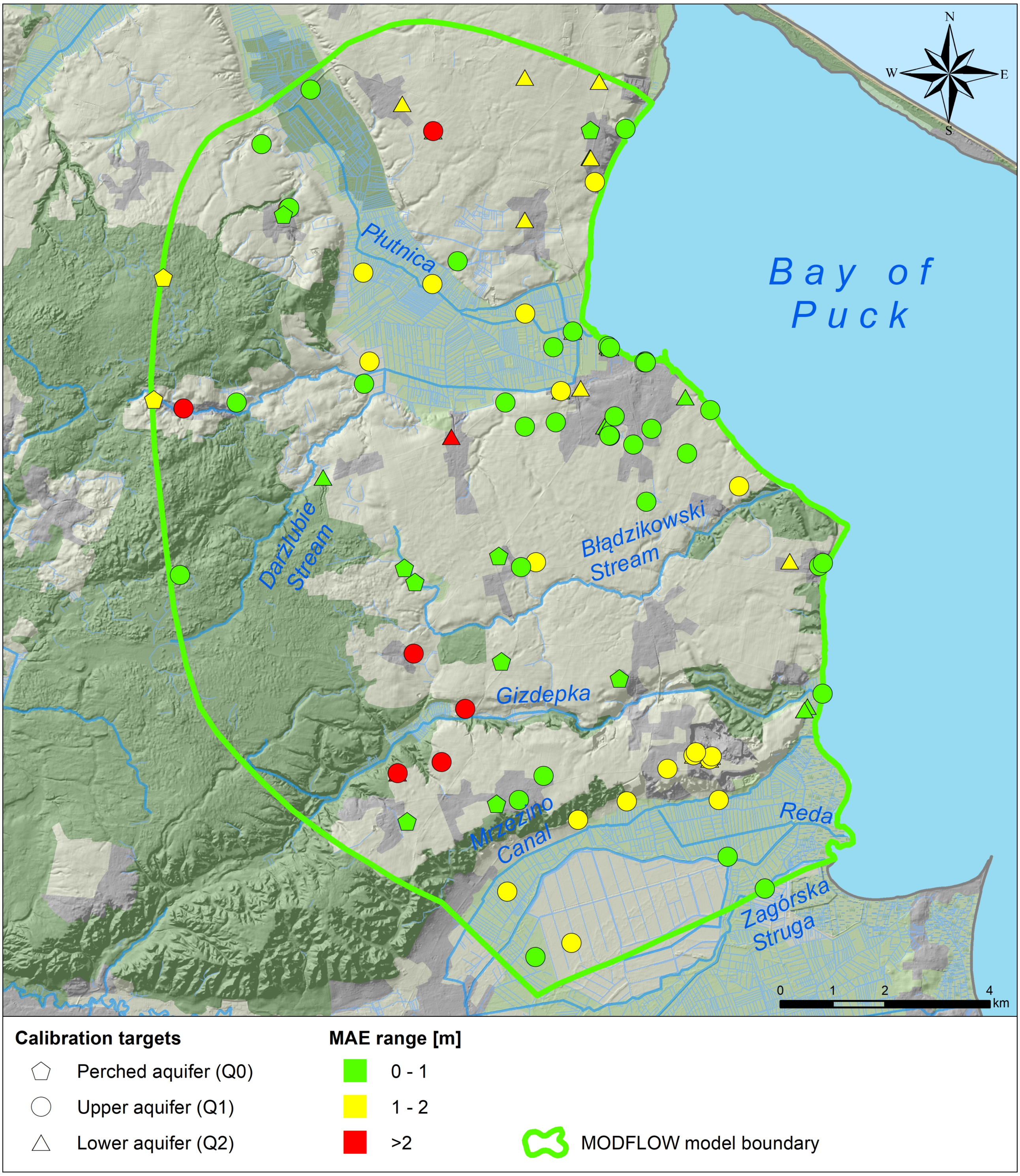

Figure 6: **Calibration results for groundwater flow model (steady state solution).** MAE - mean absolute error of observed and computed groundwater heads.

3.1.1 The pH of the soils and abundance of arable land in macro-nutrients

Based on the results of the granulometric composition, the analysed mineral soils were classified taking into account fraction content below 0.02 mm into agronomic categories of very light (up to 10% of fraction content below 0.02 mm), light (11-20%), medium (21-35%) and heavy (>35%).

Soil acidification was assessed according to the accepted standards and soils were also categorised by their reaction classes as very acidic (measured pH was $\leq$4.5), acidic (4.5–5.5), slightly acidic (5.5–6.5), neutral (6.5–7.2) and alkaline (>7.2).

The studied soils in the 0-30 cm layer had a pH in the range of 4.2-7.2 (average 5.4). The content of available P for plants in the 0-30 cm layer of studied soils ranged from 3.6 to 66.5 mg P_{ER} kg^{-1} (average 33.3 mg P_{ER}

kg^{-1}) in mineral soils and from 171.0 to 707.0 mg P_{HCl} kg^{-1} (average 340.6 P_{HCl} kg^{-1}) in organic soils (Pietrzak et al., 2020).

The mineral soils were characterised by a good abundance of exchangeable potassium ions (from 0.604 to 2.15 mg K kg^{-1} — on average 1.19 mg K kg^{-1}). Over 96% of soil samples had at least an average or higher level of potassium content. All organic soils were characterised by very low content of exchangeable potassium ions. The content of exchangeable magnesium ions in mineral soils ranged from 0.305 to 1.92 mg Mg kg^{-1} (average 0.96 mg Mg kg^{-1}) and was high and very high in 92% of soil samples. While the organic soils of the studied area in terms of exchangeable magnesium ions content were classified as low and very low at level 0.994-5.14 mg Mg kg^{-1} (average 2.04 mg Mg kg^{-1}).

3.1.2 Nutrients in stream water

The concentrations of nutrients and chemical oxygen demand (COD) measured during the study period are presented in Figures 7 and 8, respectively. The TN concentrations ranged from 0.50 mg N L^{-1} to 13.10 mg N L^{-1}. The highest concentrations were measured in Błądzikowski Stream. General observation for Błądzikowski Stream, Mrzezino Canal, Gizdepka river, Płutnica river, and Reda river (in and out) showed lower TN concentrations in the summer and autumn months, followed by a substantial increase in winter and spring (from January to April or May), exceeding the limits of first class or even second class according to Polish standards (Regulation of the Ministry of Marine Development and Inland Shipping).

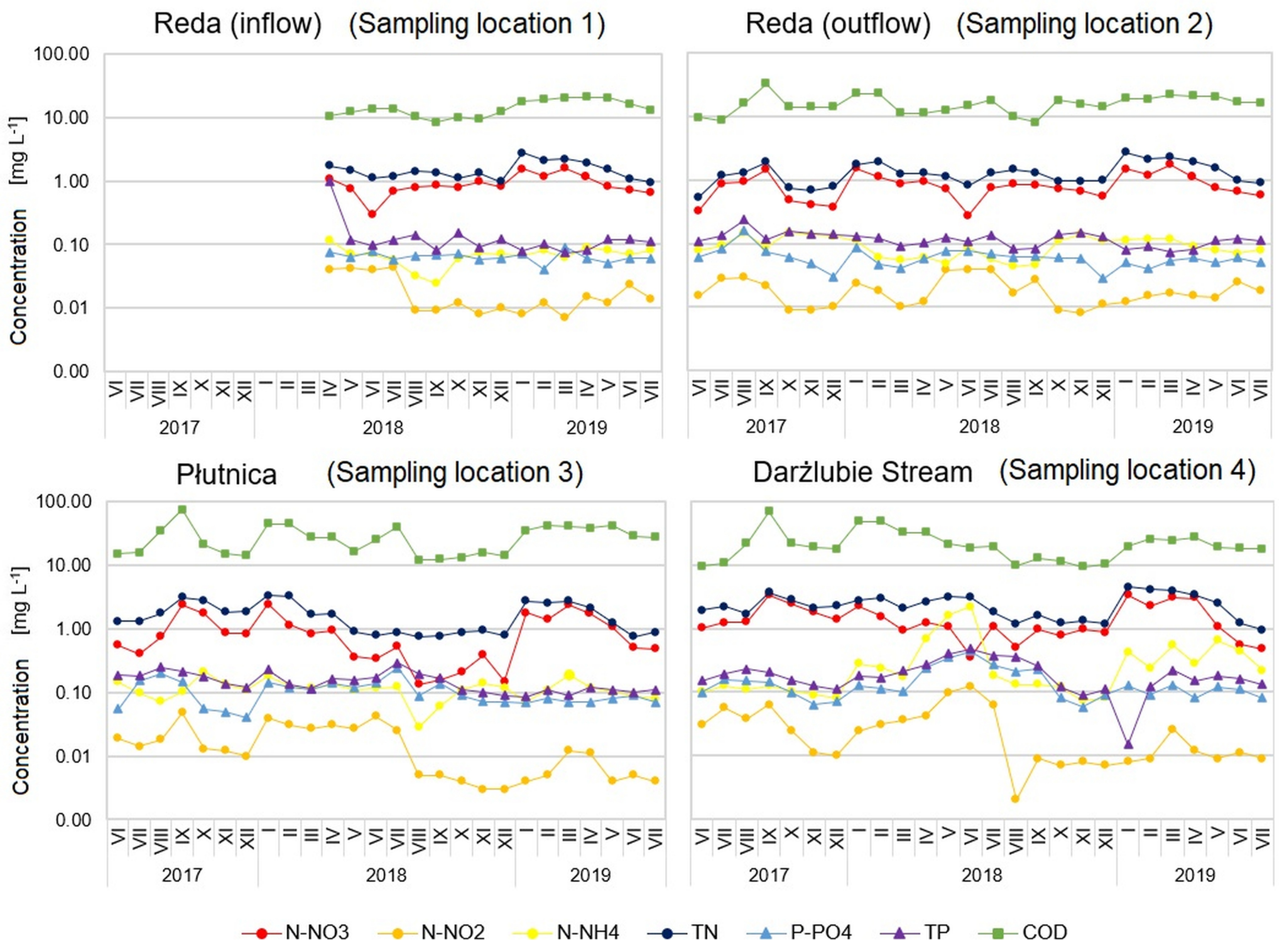

Figure 7: **Concentrations (in mg L^{-1}) of nitrogen and phosphorus compounds in surface water sampling sites in the Puck Commune on the west coast of the Puck Bay (Southern Baltic Sea): Reda river inflow (1) Reda river outflow (2), Płutnica (3), and Darżlubie Stream (4) during the study period VI 2017 – VII 2019.**
Explanation of abbreviations: TN – total nitrogen, TP – total phosphorus; N-NO$_2^-$ - nitrite nitrogen, N-NO$_3^-$ - nitrate nitrogen, N-NH$_4^+$ – ammonium nitrogen, P-PO$_4^3$– – mineral phosphorus, COD – chemical oxygen demand.

The second-class limits for TN occurred first of all in Błądzikowski Stream, but also in Gizdepka and on some occasions in Płutnica river. In comparison, to two main rivers in Poland (Vistula and Oder) the mean concentrations reported by Pastuszak et al. (2018) were in 2016 2.3 and 3.3 mg N L^{-1}, respectively. Regarding many European countries, the TN concentration of 3.6 mg N L^{-1} was normally noted in high proportion, while in catchments intensively used for agricultural purposes the concentration over 5.6 mg N L^{-1} was frequently observed (European Environment Agency, 2018). On the other hand, concentrations below 0.8 mg N L^{-1} are characteristic of unaffected rivers (Scandinavian rivers – Stålnacke et al. (1999)). Analysis of N species shows that in the case of Błądzikowski Stream and Gizdepka, with catchments intensively used by agriculture, $N\text{-}NO_3^-$ constituted the most abundant nitrogen species, which indicates the input of surface run-off from fertilised fields. The adverse trend, with a higher share of $N\text{-}NH_4^+$ was observed in the case of Płutnica river and its inflow Darżlubie stream. Similar tendency was observed by Bączkowska et al. (2021) in Karwianka river located in approx. 20 km distance from the investigated area, which was justified by discharges of untreated wastewater. This could be explained by some manure spills, domestic wastewater discharge, or by the discharge of fish processing industrial plant located in this catchment, which are frequently considered as a sources in polish rivers (Preisner et al., 2021). The impact of an industrial plant can also explain the higher COD concentrations in Płutnica river and Darżlubie Sream in comparison to other watercourses. The lowest N concentrations were observed in Zagórska Struga and Reda river, which flow through meadows, wetlands, and natural reserve area.

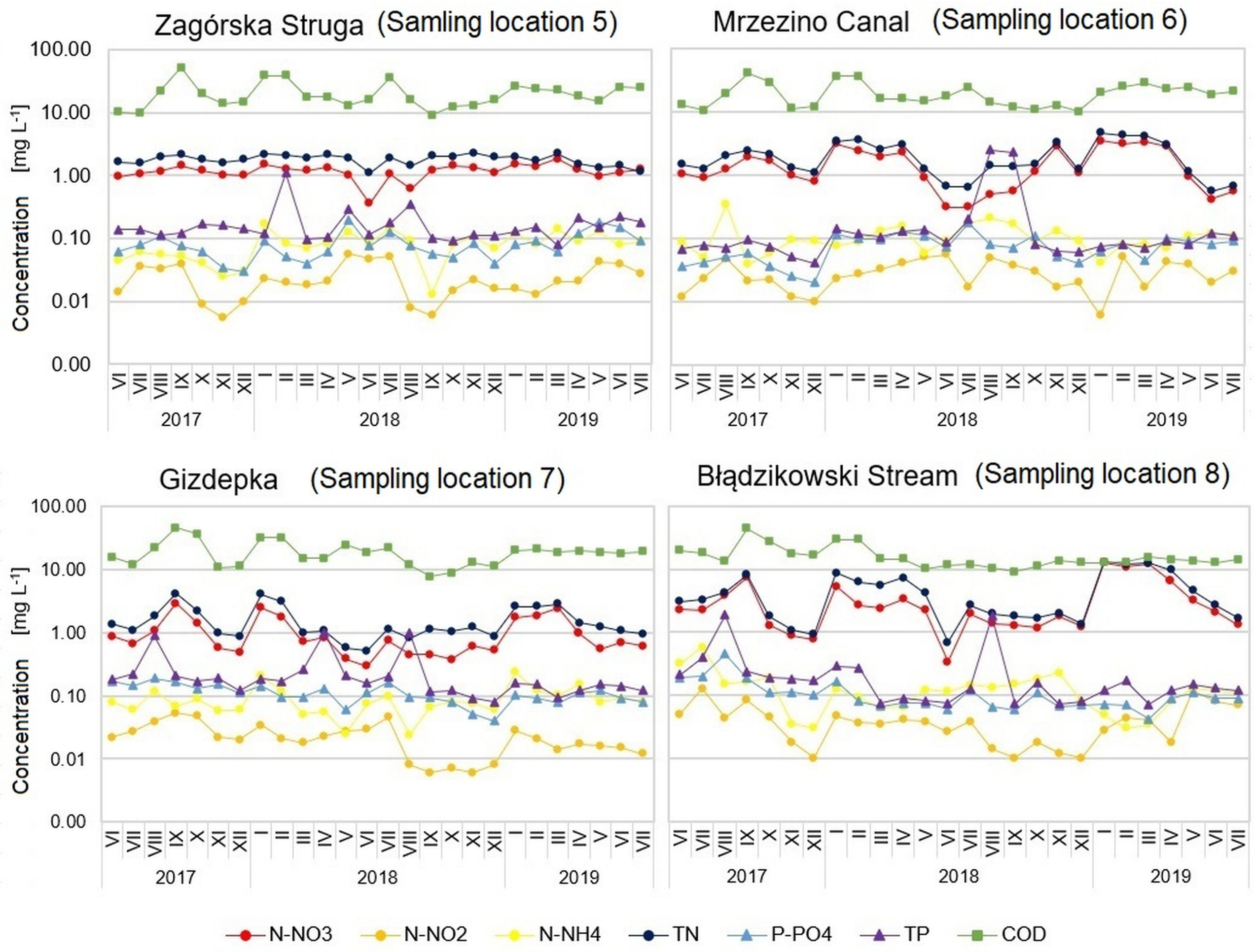

Figure 8: **Concentrations (in mg L^{-1}) of nitrogen and phosphorus compounds in surface water sampling sites in the Puck Commune on the west coast of the Puck Bay (Southern Baltic Sea): Zagórska Struga (5), Mrzezino Canal (6), Gizdepka (7), and Błądzikowski Stream (8) during the study period VI 2017 – VII 2019 (cont.)**
Explanation of abbreviations: TN – total nitrogen, TP – total phosphorus; $N\text{-}NO_2^-$ - nitrite nitrogen, $N\text{-}NO_3^-$ - nitrate nitrogen, $N\text{-}NH_4^+$ – ammonium nitrogen, $P\text{-}PO_4^{3}-$ – mineral phosphorus, COD – chemical oxygen demand.

Regarding TP, the concentrations were generally below 0.2 mg P L^{-1}, the limit concentration of the first quality class according to Polish regulations. The worst situation was observed in Darżlubie Stream, where not only the first class limit was regularly exceeded, but also incidentally the second class limit (0.3 mg P L^{-1}) was exceeded too. According to European Environment Agency (2018) the concentrations above 0.1 mg P L^{-1} are considered as relatively high. The elevated concentrations in the contributory Darżlubie stream influenced also Płutnica river. In Błądzikowski Stream and Gizdepka river, the elevated TP concentrations (reaching the maximum of 1.89 mg P L^{-1} in Błądzikowski Stream) persisted during the first months of the study (June –

September 2017) with only incidental elevations in the later period. In Mrzezino Canal, TP concentrations corresponded to the first-class limit except for summer peak concentrations in summer 2018. In Zagórska Struga and Reda river, the elevated (first-class limit) TP concentrations were observed only incidentally. In water samples of Piaśnica, Karwianka and Czarna Wda rivers located in the northern region of Poland the PO_4^{3-} ions were in the range of 0.11-0.62 mg P L^{-1} (Bączkowska et al., 2021).

3.1.3 Nutrients in surface waters from drainage ditches

The assessment of the state of water pollution was carried out in the scope of nitrate pollution and susceptibility to eutrophication. The assessment of nitrate pollution was done based the population of results falling within the water quality classes: 0–24.99; 25-39,99; 40-50 and > 50 mg NO_3^- L^{-1}, in accordance with the guidelines for preparing reports on the implementation of the Nitrates Directive by the Member States. The assessment of the susceptibility of waters to eutrophication was carried out based on a comparison of the obtained results (nitrate nitrogen, total nitrogen, and total phosphorus) with the limit values of the basic indicators of eutrophication of waters above which eutrophication occurs (according to the Regulation of the Minister of the Environment of December 23, 2002, on the criteria for determining waters sensitive to nitrogen pollution from agricultural sources (Journal of Laws 2002.241.2093) — currently considered repealed).

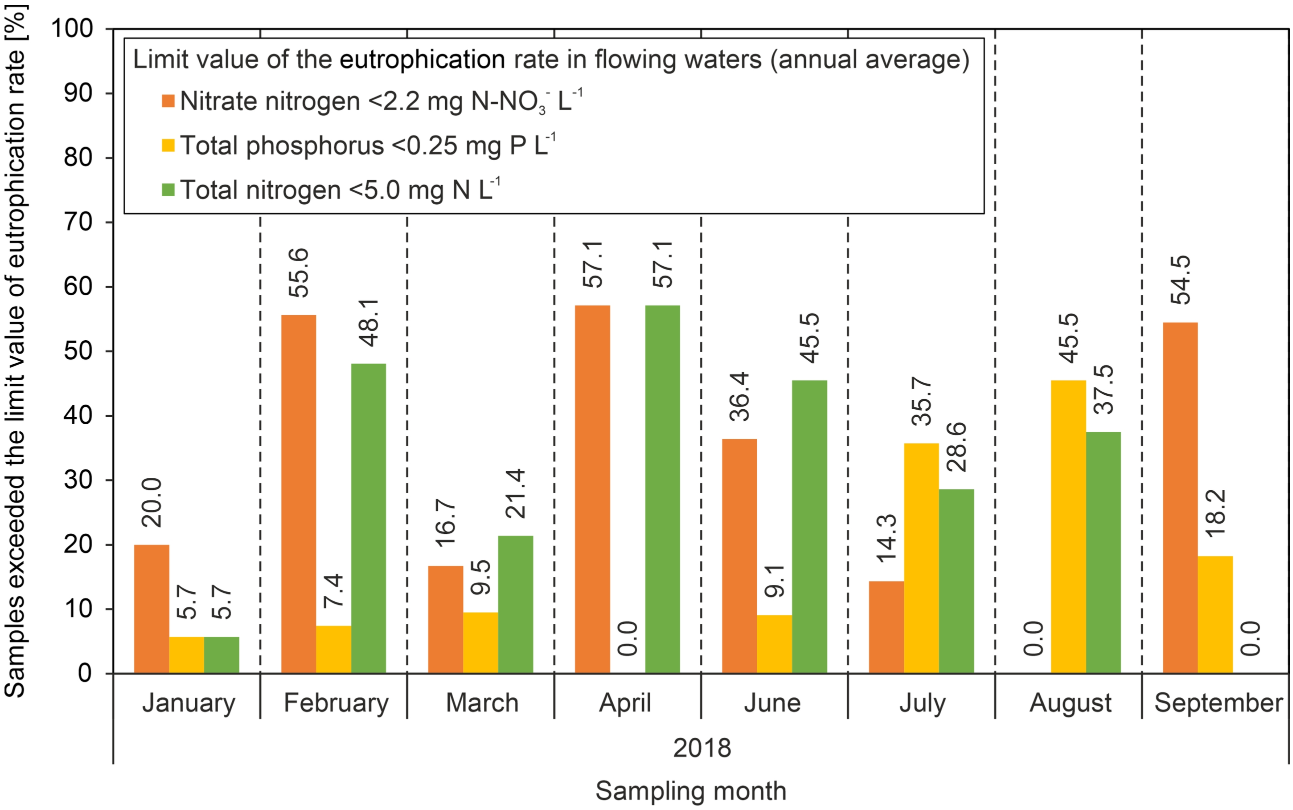

Figure 9: **Distribution of samples exceeded the eutrophication rates in analysed drainage ditches in the Puck Commune in different months of 2018.**
Limit values of the eutrophication rate in flowing waters are 2.2 mg NO_3^- L^{-1}; 0.25 mg P L^{-1}; and 5.0 mg N L^{-1}.

The assessment of the state of water pollution with nutrients in drainage ditches in the Puck Commune showed in particular that:

- only 5.2% of the samples tested had water contaminated with nitrates, or threatened with nitrate contamination;
- due to exceeding the limit values of eutrophication indicators: nitrate, total nitrogen, and total phosphorus, the share of the analysed water samples was relatively small (one eutrophication indicator was exceeded, at most in 29% of the samples — as an annual average) (Figure 9). In comparison, at least one eutrophication rate was found to be exceeded at nearly 70% of the monitoring points located in drainage ditches in the whole country. The limit value of the eutrophication rate in flowing waters (annual average) is as follows:
  - total phosphorus (P_{tot}) — <0.25 mg P L^{-1};

- total nitrogen (N_{tot}) — <5.0 mg N L^{-1};
- nitrate nitrogen — <2.2 mg N-NO_3^- L^{-1}.

However, similar results from the other tests performed in the region are not available in literature. The drainage ditches are located mainly in agricultural areas. The obtained results of nutrient concentrations confirm the seasonal variability typical for agricultural areas (Matej-Lukowicz et al., 2020; Wojciechowska et al., 2019a).

3.1.4 Nutrients distribution and flux via SGD

Details related to the groundwater (SGD) influence on pore water salinity and SGD rate in the Bay of Puck can be found in Kłostowska et al. (2020). Generally, the usual seawater salinity in the Bay of Puck oscillates around 7.0, and, typically, significantly lower surface water salinities indicate the freshwater source, such as precipitation and/or rivers. Within all collected samples, the oxidation-reduction potential (Eh) ranged from -11.6 to 36 mV, the dissolved oxygen concentrations ranged from 0.7 to 9.8 mg L^{-1}, and the pH levels ranged from 4.9 to 8.3. The nutrients concentrations ranged from 0.2 to 45.1 µmol L^{-1} for PO_4^{3-}, from 3.1 to 488.9 µmol L^{-1} for NH_4^+, and from 0.0 to 506.6 µmol L^{-1} for NO_3^- in all collected samples. Szymczycha et al. (2012) obtained similar results for PO_4^{3-} and NH_4^+, apart from the nitrates concentrations observed in autumn that were significantly higher in this study (Szymczycha et al., 2020). In order to estimate the nitrate, ammonium, and phosphate fluxes via SGD we used nutrients concentrations, measured within the salinity gradients and depth profiles, while the SGD was adopted from the previous study by Kłostowska et al. (2020). Firstly, we identified the minimum, maximum, average, and median concentration for each measured nutrient and for each season. The obtained data did not have a normal distribution therefore, we calculated nutrients loads using median concentrations. The seasonal fluxes of nutrients via SGD were calculated by multiplying median concentrations, minimum, and maximum rates. Finally, the obtained nutrients loads corresponded to the average values (± standard deviation). The estimated seasonal and annual loads of both dissolved inorganic nitrogen (DIN 9303 t yr^{-1}) and PO_4^{3-} (950 t yr^{-1}) via SGD were the most significant source of nutrients to the Bay of Puck and remarkably higher than quantified before (fresh SGD nutrients loads, 50 t yr^{-1} and 56 t yr^{-1} for DIN and PO_4^{3-}, respectively). The SGD fluxes reported here show some of the highest rates of sediment-water fluxes reported in the Baltic Sea.

3.1.5 Nutrients in groundwater

There were clear differences in nutrients concentration between shallow aquifers (Q0 and Q1) and deeper aquifer (Q2). The concentrations of nutrients were higher in shallow wells (Figure 10). The nitrate (NO_3^-) concentrations in perched aquifer (Q0) ranged from 2 to 49 mg L^{-1} (median 26 mg L^{-1}) and in the upper Quaternary aquifer (Q1) ranged from <0.1 to 92 mg L^{-1} (median 10 mg L^{-1}). While in contrast, in the deeper Quaternary aquifer (Q2) ranged from <0.1 to 1 mg L^{-1} (median 0.3 mg L^{-1}). The concentrations of ammonium (NH_4^+) were similar in all aquifers, but still slightly higher in shallow aquifers. The obtained values in aquifers Q0, Q1, and Q2 were respectively, from <0.01 to 3.56 mg L^{-1} (median 0.03 mg L^{-1}), from 0.01 to 3.32 mg L^{-1} (median 0.03 mg L^{-1}) and from <0.01 to 0.37 mg L^{-1} (median 0.14 mg L^{-1}). The concentrations of phosphate (PO_4) were clearly higher in the shallow wells. The obtained values were in range from 0.16 to 6.38 mg L^{-1} (median 0.5 mg L^{-1}) in Q0 aquifer, from <0.1 to 3.06 mg L^{-1} (median 0.37 mg L^{-1}) in Q1 aquifer and from 0.09 to 0.49 mg L^{-1} (median 0.14 mg L^{-1}) in Q2 aquifer (Potrykus et al., 2020). Field and laboratory research of groundwater quality, shows a local contamination caused by human activity. The contamination is limited to shallow aquifers and has a local extent. The analysis of groundwater samples indicates agricultural activity and municipal wastes as main reasons of groundwater contamination (Potrykus et al., 2020).

3.1.6 Pesticides in waters and soils

In all analysed water and soil samples the concentrations of organochlorine pesticides (aldrin, dieldrin, endrin, isodrine, dichlorodiphenyltrichloroethane and its isomers and alpha, beta, gamma, and delta isomers of hexachlorocyclohexane) were below the limit of detection of the used methodology (Pazikowska-Sapota et al., 2020). However, in soil samples, surface waters from drainage ditches and watercourses as well as in groundwater samples out of 309 active substances examined, the following pesticides have been detected:

- organophosphatic insecticides: chlorpyrifos-ethyl;
- fungicides: boscalid, epoxiconazole, difenoconazole, fluopicolide;
- herbicides: dimetachlor, diflufenican, metazachlor, glyphosate and its metabolite AMPA;
- repellents: anthraquinone.

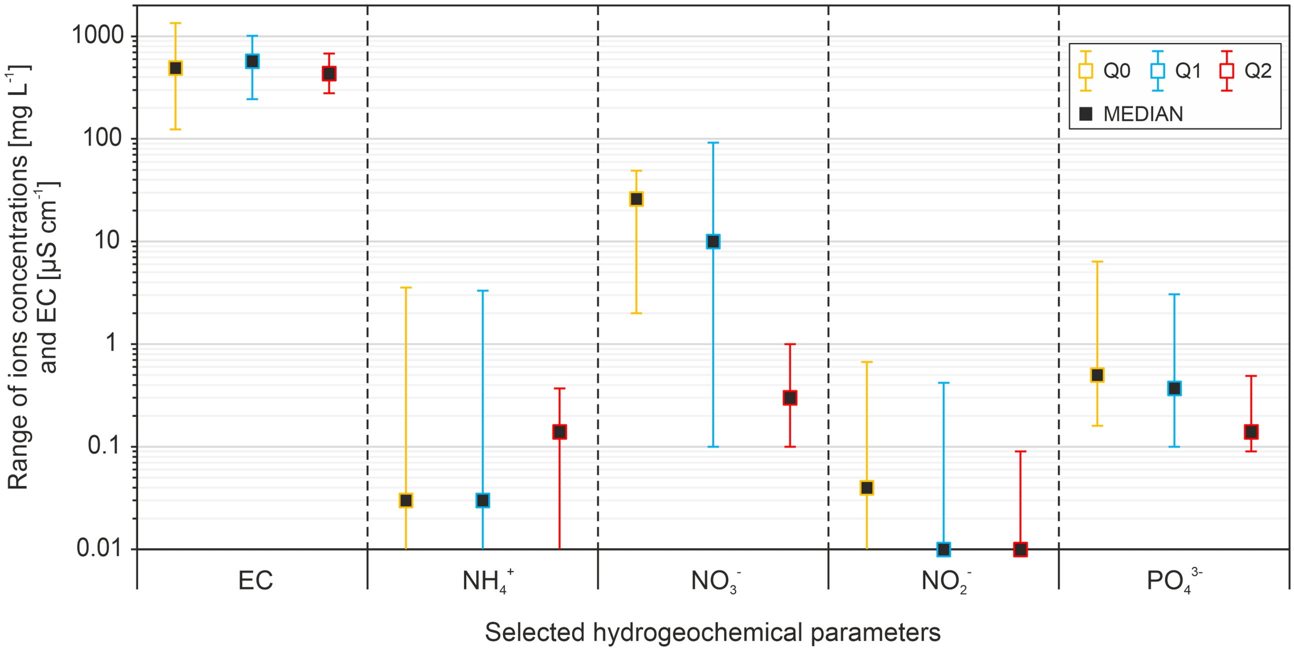

Figure 10: **Dependence of selected hydrogeochemical parameters concentration range to the type of aquifer occurrence.**
Explanation of abbreviations: EC – electrical conductivity, NH_4^+ – ammonium, NO_2^- – nitrites, NO_3^- – nitrates, PO_4^{3-} – phosphate, Q0 – shallow perched aquifer, Q1 – upper/shallow Quaternary aquifer, Q2 – lower Quaternary aquifer.

The concentrations of detected pesticides in soil samples (chlorpyrifos-ethyl, anthraquinone, glyphosate and AMPA) ranged from 0.05 to 0.35 mg kg^{-1}. The highest concentrations were obtained in August in water from drainage ditches for metazachlor (2.0 mg L^{-1}), glyphosate (4.7 mg L^{-1}) and AMPA (2.0 mg L^{-1}). In the surface water samples and sediment samples taken from the Bay of Puck, none of the 309 substances from the pesticides group were found (Pazikowska-Sapota et al., 2020). On the base of obtained results, it can be concluded that the overall level of impact of farms from the Puck Commune on the environment, including the quality of the waters of the Bay of Puck, is relatively low. It should be noted, however, that among the studied farms, there were some whose environmental pressure determined by the surveys and specified pressure indicators had an unusually large dimension.

3.2 Calibration and validation results

3.2.1 SWAT

SWAT calibration allowed to meet all 3 calibration criteria described earlier. The annual groundwater recharge fluxes obtained from the model were 36 to 146 mm yr^{-1}, vs the reference range of 19 to 186 mm yr^{-1}. Average annual evapotranspiration in the model was 459 mm yr^{-1} vs the reference range 450 to 495 mm yr^{-1}. Finally, the average annual biomass (dry mass) production in the forest HRU's was 6.1 to 8.5 t ha^{-1} yr^{-1} vs. the reference range of 6.5 to 7.5 t ha^{-1} yr^{-1}.

Validation was performed by comparing the daily simulated and observed flow rates for the period of operation of the monitoring network, i.e., 01.06.2018–30.07.2019, the parameter ME equals to -0.012, MSE 0.032, and RMSE 0.18. In the case of biomass, crop yields obtained in the modelled basin are, depending on HRU parameters, for example for winter wheat from 5.9 to 7.3 t ha^{-1} yr^{-1} (average according to surveys 6.4 t ha^{-1} yr^{-1}), for canola from 2.6 to 3.4 t ha^{-1} yr^{-1} (surveys 3.8 t ha^{-1} yr^{-1}) (Dzierzbicka-Glowacka et al., 2019). Overall, the model performance was considered satisfactory and no further attempt was undertaken to improve biomass and yield predictions. Pesticide calibration was not included because in the watercourses modelled, the presence of Diflufenican was detected in only 1 sample (Pazikowska-Sapota et al., 2020).

3.2.2 GroundPuck

Figure 10 and Figure 11 shows that in most control points a satisfactory agreement between the measured and calculated groundwater heads was obtained. The indicators of fit quality were as follows:

- mean error 0.29 m,

- mean absolute error 1.10 m,
- root-mean-square error 1.79 m.

The lowest convergence is observed in the upper aquifer (Q1), mainly in the southwestern part of the model area. It is a result of difficulties in the spatial projection of the aquifer layer, variation of hydraulic conductivity values and probability of perched aquifer (Q0) occurrence, which can be responsible for the increase of groundwater recharge.

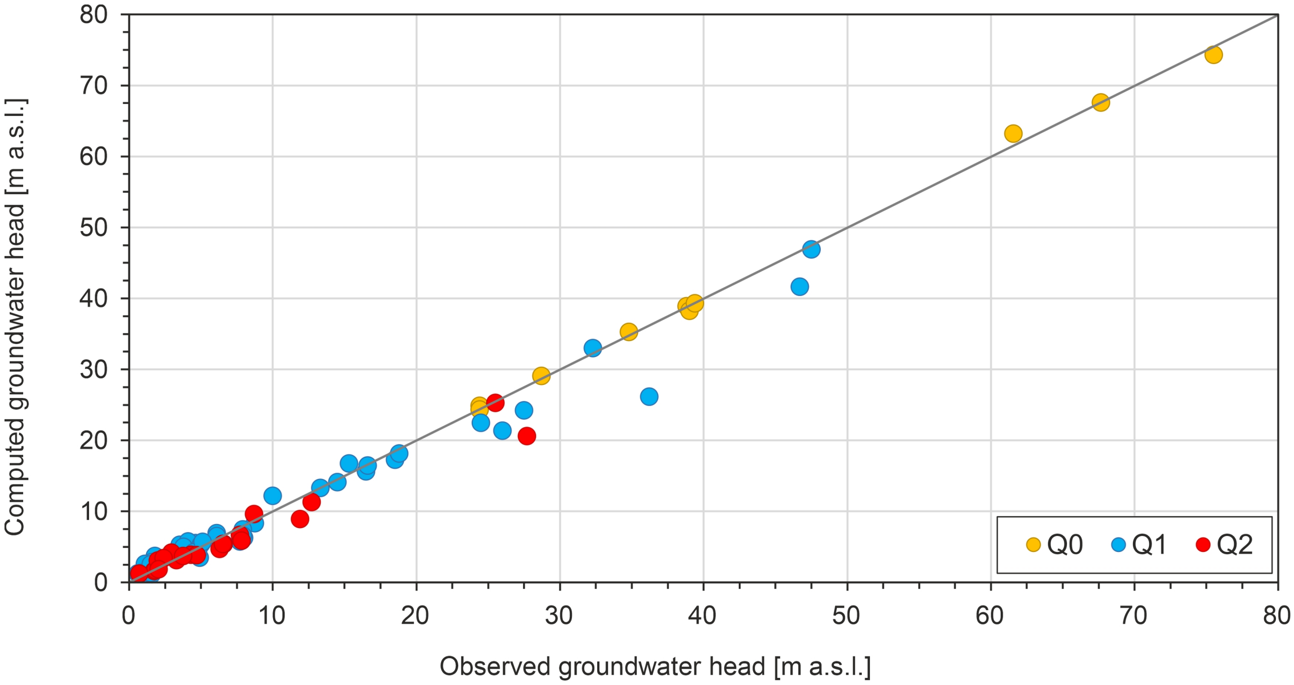

Figure 11: **Plot of observed versus computed groundwater heads in steady-state model.** Explanation of abbreviations: Q0 – shallow perched aquifer, Q1 – upper/shallow Quaternary aquifer, Q2 – lower Quaternary aquifer, m a.s.l. – meters above sea level.

Taking into account the number of chemical analysis, the distribution of sampling points and the mosaic variability of the nitrates concentrations in groundwater (that may indicate the local influence of pollution source), it would be difficult and less reliable to compare the results of simulations with use of reference points method. Therefore, we approached the validation holistically and operated with the observed and simulated range values of N-NO_3^- concentrations for the whole area of groundwater study. Table 1 shows a reasonable agreement between measurements and model in each aquifer.

Table 1: Calculated and measured N-NO_3^- groundwater concentration.

Layer	calculated N-NO_3^- [mg L^{-1}]	measured N-NO_3^- [mg L^{-1}]
Perched aquifer (Q0)	8.0×10^{-8} – 17.72	0.45 – 11.06
Upper aquifer (Q1)	3.8×10^{-6} – 62.88	<0.02 – 20.78
Lower aquifer (Q2)	0.0012 – 1.00	<0.02 – 0.23

In addition, the calculated amount of water discharged from the upper (Q1) and lower (Q2) aquifers are in a good agreement with the results of previous studies related to groundwater outflow to the Bay of Puck (Piekarek-Jankowska, 1994; Kryza and Kryza, 2006; Jaworska-Szulc, 2009; Lidzbarski, 2015). In our model, the total groundwater discharge to the sea from Q1 and Q2 is 1286 m^3 h^{-1}, which corresponds to 92 m^3 h^{-1} per kilometer of the coastline. The flow rate varies from 58 m^3 h^{-1} km^{-1} in the upland areas to 152 m^3 h^{-1} km^{-1} in the river valleys. Piekarek-Jankowska (1994) reported the rate of groundwater discharge to the Bay of Puck in the same area ranging from 21 to 165 m^3 h^{-1} km^{-1}, with an average of 98 m^3 h^{-1} km^{-1}, while Jaworska-Szulc (2009) estimated the rate of groundwater discharge to the Bay of Puck in the Reda river valley as 165 m^3 h^{-1} km^{-1}.

3.2.3 EcoPuckBay

We validated the EcoPuckBay model for two hydrodynamic parameters (temperature and salinity) and four biochemical parameters (oxygen, nitrates, phosphates, chlorophyll-a). Detailed results for the hydrodynamic part of the EPB model validation have been described in Dybowski et al. (2019), while biochemical part validation of the EPB model has been extensively presented in Dybowski et al. (2020b). In both cited studies, we used modified Taylor diagrams, because in our opinion their use (together with mean error) is the best way to present the quality of model data in relation to environmental measurements. The EPB model simulation run has been performed for the time period from January 2011 to December 2018. The Voivodship Inspectorate of Environmental Protection (VIEP) in Gdańsk provided monitoring data from January 2014 to Decemver 2017, the NEMO-Nordic model data covered 2014-2016 years, and NEMO-SCOBI model data covered 2014-2017. Measurement data from s/y Oceania was taken during the 2018 summer cruise. Table 2 summarizes the statistical comparison between the EPB modelled results and reference data.

Table 2: Statistical comparison between modelled by EPB and reference data

parameter (reference set)	RMSE	STD	ME	Pearson's r
Temperature [°C] (VIEP)	1.45	5.67	-0.83	0.97
Temperature [°C] (NEMO-Nordic)	1.33	6.01	-0.31	0.98
Temperature [°C] (s/y Oceania)	2.85	5.29	-1.16	0.92
Salinity (VIEP)	0.67	0.60	0.16	0.58
Salinity (NEMO-Nordic)	0.97	0.70	-0.24	0.17
Salinity (s/y Oceania)	0.40	0.84	-0.03	0.90
O_2 [mmol m^{-3}] (VIEP)	31.03	35.97	22.20	0.71
O_2 [mmol m^{-3}] (NEMO-SCOBI)	29.02	35.95	-1.73	0.75
N-NO_3^- [mmol m^{-3}] (VIEP)	2.19	2.87	0.74	0.66
N-NO_3^- [mmol m^{-3}] (NEMO-SCOBI)	4.20	3.82	1.02	0.60
P-PO_4^{3-} [mmol m^{-3}] (VIEP)	0.21	0.21	-0.03	0.56
P-PO_4^{3-} [mmol m^{-3}] (NEMO-SCOBI)	0.29	0.15	-0.47	0.59
Chlorophyll-a [mg m^{-3}] (VIEP)	2.89	3.59	-0.04	0.64
Chlorophyll-a [mg m^{-3}] (NEMO-SCOBI)	4.74	2.40	-2.86	0.63

The correlation coefficients ranges: from 0.92 to 0.98 for temperature, from 0.17 to 0.90 for salinity (where 0.17 is for comparison with the numerical model (NEMO-SCOBI) which horizontal resolution is about 40 times lower than EPB), and from 0.56 to 0.75 for biochemical variables (O_2, NO_3^-, PO_4^{3-}, Chlorophyll-a).

Correct stratification of temperature and salinity (especially in vertical profiles using data from s/y Oceania) indirectly also gives information about the correctness of vertical mixing in the model. While the spatio-temporal agreement with VIEP monitoring data allows us to state that the currents are also correctly represented in the model. In the case of sea surface height (SSH), the resolution of the model data (also the fact that the model produced mean values from the 6-hour time window) and the lack of access to measurement data forced us to abandon direct validation of SSH. It should be emphasized that the SSH is not of main interest in the presented tool, but is only an additional variable that we have decided to show.

For ammonia and silicates, we have compared, for the purpose of this article, our results from EPB model to the International Council for the Exploration of the Sea (ICES) data (https://www.ices.dk/data) and summarized in Table 3. Comparing the mean values and their standard deviations, we conclude that the range of variability of the concentration of ammonia and silicates is correct.

Table 3: Comparison between modelled by EPB and reference ICES data

parameter (data source)	min	mean	STD	max
NH_4^+ [mmol m^{-3}] (ICES)	0.10	12.62	9.00	75.50
NH_4^+ [mmol m^{-3}] (EPB)	3.33	15.57	3.11	27.60
SiO_3^{2-} [mmol m^{-3}] (ICES)	0.10	0.87	0.99	10.40
SiO_3^{2-} [mmol m^{-3}] (EPB)	0.01	0.82	1.04	10.98

In the case of pesticides, as a result of extensive monitoring in the waters of the Bay of Puck, no pesticides were detected (only 1 sample with Diflufenican detected). The EPB model, based on the inflow of pesticides from the SWAT model, distributes the biochemical load (including pesticides) inside the Bay of Puck, and these values are below the limit of quantification.

The last parameter group of EPB labelled as 'nutrient spread' (nitrate, phosphate, ammonia,max spread) is described in the article by Dybowski et al. (2020b). The nutrient spread module describes the diffusion and advection of nutrients under the influence of sea currents. Data on the flow and concentration of nutrients are provided once a day at the land–water border from the SWAT model.

There are no references in the literature to studies using numerical models with such high resolution as the EPB for the studied area. However, the concentration of nutrients in the Gulf of Gdańsk (of which the Bay of Puck is a part) is monitored and thoroughly investigated (Lysiak-Pastuszak, 2000; Kot-Wasik et al., 2003; Kruk-Dowgiałło and Szaniawska, 2008), and the use of the EPB model should make it easier to assess the environmental state of the Bay of Puck.

3.3 WaterPUCK toolkit's capabilities

The real potential of the WaterPUCK toolkit lies in its practical implementation in the form of an online service that is easy to access and simple to use. The whole set of developed tools is available through the website https://waterpuck.pl/en/ ("PRODUCTS" tab). In the following subsections, we are presenting the capabilities offered by key modules of the created toolkit.

3.3.1 Database

The WaterPUCK database is a tool that connects and enables the communication between the individual elements of the solution. It is operated from the map view level and allows the user to find the necessary data and meta-information in a short time. All measurement points collected in the database are visualised in the form of markers placed on the map. The data can be downloaded directly to the local device and can also be presented in the form of a graph in a web browser. Table 4 shows the ranges of nitrate nitrogen and phosphate phosphorus measured concentrations for different environments in the studied area.

Table 4: The ranges of nitrate and phosphate measured concentration in different locations in the studied area.

sampling site [unit]	N-NO_3^-	P-PO_4^{3-}
soils [mg kg^{-1}]	2.60-392.0	2.20-79.50
drainage ditches [mg L^{-1}]	0.02-15.50	0.01-7.65
surface water [mg L^{-1}]	0.13-12.90	0.02-0.45
groundwater [mg L^{-1}]	0.06-8.35	0.03-1.63
SGD [mg L^{-1}]	0.00-7.10	0.00-1.60
seawater [mg L^{-1}]	0.00-0.80	0.00-0.09

The maximum observed nitrate nitrogen and phosphate phosphorus concentrations decrease with the subsequent environments in which they are propagated. An exception to this rule is the transition from surface water to groundwater. Here we observe higher concentrations in groundwater than in surface water for phosphates phosphorus. Data on nitrate and phosphate concentrations in surface run-off for Puck Commune's watershed were published (Matej-Lukowicz et al., 2020; Wojciechowska et al., 2019a,b) and the range of variation of N-NO_3^- and P-PO_4^{3-} presented in the Table 4 is consistent with previous studies. The concentration of orthophosphates for SGD is consistent with the Szymczycha et al. (2012) study, while the maximum concentration of nitrates for SGD is significantly higher than in the quoted study.

Measurements of nutrients' concentrations with the highest possible spatial and temporal resolution, while maintaining an accurate and high-quality database allows for the highest quality studies in the field of water contamination from agricultural activity.

3.3.2 Surface water model

The user can perform (using a web interface) a simulation of agricultural pollution entering the Bay of Puck with surface run-off. The quality and quantity of water inflow are calculated in the SWAT model. Two modes for visualising the results are available:

1. General data — where one can simulate and produce forecast for the concentrations of selected nutrients and pesticides in surface run-off and rivers within the Puck Commune (WaterPUCK SWAT (General data mode), 2021);

2. Calculator — allows the user to perform simulations after making changes regarding crops, doses, and types of fertilisers and plant protection products (WaterPUCK SWAT (Calculator mode), 2021).

In the General data view, it is possible to select two parameters for presentation: soil and channel assessment. Soil assessment shows the spatial variability of nutrients (nitrogen and phosphorus compounds) present in surface run-off. Channel assessment shows the time variability of flow rate and the amount of nutrients present in watercourses [kg] as well as pesticides (as mg of active substance). Meteorological conditions have a significant impact on the amount of nutrients leached out by surface run-off. The optimal dose of the fertiliser should depend on the forecasted rainfall, therefore through the online interface, the user has to choose one of the following rainfall scenarios: real rainfall, dry year simulation (70% real rainfall) and wet year (120% real rainfall).

General data mode allows presenting results in two ways: graphical presentation of the entire analysed area, with the option of choosing a displayed period; the exact value for the selected place or section of the river. In addition, for watercourse results, it is possible to present a time series of nutrient and/or pesticide concentrations in the watercourses over a selected period of time.

In the Calculator mode, one should mark the field location for which the simulation will be carried out. In the place indicated on the map, a house symbol appears and at the same time, a list of required inputs shows up. The user should enter the size of the analysed field and the planned doses of fertiliser and pesticide. From the drop-down lists, plant type, fertiliser type, and pesticide type can be chosen. After selecting the plant, based on the tested agricultural calendars, input files for the SWAT model will be generated, regarding the agricultural practices used, e.g., date of sowing, ploughing, fertilising, harvesting, etc. Files are created for each agricultural HRU. After performing a full simulation for the changed land development and dosing of fertilisers and pesticides, a preview known from the general view will be displayed, enabling a thorough analysis of the results obtained. In addition, under the map, a comment on the amount of nutrients leaching will appear.

3.3.3 GroundPuck

The associated web interface service allows the user to visualise the results of simulations: groundwater heads and concentrations of nitrogen in nitrate form (N-NO_3^-) for a selected day from the simulation period. Visualisation is possible for one of the three layers of the model representing aquifers (water-bearing layer) — Q_0 — layer 1 of the model, Q_1 — layer 3 of the model and Q_2 — layer 5 of the model, as shown in Figure 4.

The user has to choose the date using the calendar shown on the webpage. From the dropdown lists below the calendar, one can choose the type of data (groundwater head or N-NO_3^- concentration) and the considered aquifer (Q_0, Q_1, Q_2). Next, one has to click the “Generate map” button, to display the data of interest on the map.

The groundwater head values are given in m a.s.l. (the values can be higher than the ground surface elevation, due to artesian pressures in some regions of the model). The concentrations of N-NO_3^- are given in mg L^{-1}.

The results of groundwater simulations are passed to the hydrodynamic and ecological models of the Bay of Puck (the rate of groundwater discharge from Q_1 and Q_2 aquifers to the sea and the corresponding loads of N-NO_3^-).

3.3.4 EcoPuckBay

Another tool that is directly fed with data from both the SWAT and GroundPUCK models is the EPB model. For the convenience of presentation, we have created separate entries for individual components of the model, i.e., the hydrodynamic part of EPB, the biochemical part of EPB, and the Nutrient Spread Model.

The presentation of data from the EPB model is handled in a very intuitive way in each of the three presentation modes. In the first step, a day is selected from the calendar. Then for the hydrodynamic part, one of the four physical parameters (i.e., temperature, salinity, sea level, or currents), for the biochemical part, one of the seven parameters (i.e., nitrate, phosphate, ammonia, silicate, chlorophyll-a, oxygen or pesticide), and for the Nutrient Spread Model, one of the four options (i.e., nitrate, phosphate, ammonia, or maximum spread range). Finally, for the hydrodynamic and biochemical part, one of the three available data presentation methods (i.e., area maps, time series, or vertical section) is selected.

Using the Nutrient Spread Model, it is possible to model the expected distribution of agricultural substances in the waters of the bay in a short period of time (10 days), which can be helpful when extreme events occur and in making decisions to mitigate the negative effects associated with them. For example, when the forecast predicts very intense rainfall, regulations may be issued encouraging farmers to postpone fertilisation, which will also be beneficial for them.

3.3.5 Use of the WaterPUCK toolkit by farmers

According to the Nitrates Directive, farmers have to calculate the doses of nitrogen fertiliser. This ensures that fertilisation is appropriate to the plants’ nutritional requirements and is economical and sustainable. The WaterPUCK product makes it possible to calculate the environmental impact of a selected fertilisation scheme. It focuses on the nutrients that have the most destructive effect on the ecosystem — nitrogen and phosphorus.

The farmer can estimate the fertiliser losses during the production cycle by selecting different available fertilizers and applying them at a chosen location.

The farmer using the WaterPUCK toolkit can also calculate nitrogen losses for different fertilisation plans. For example, on a field of 100 hectares of winter wheat (with expected yield of 5 tonnes ha^{-1}), a pre-sowing application of 75 kg ha^{-1} of urea, then 218 kg ha^{-1} of Nitrochalk (calcium ammonium nitrate) in the first dose, and finally 130 kg ha^{-1} of urea in the second dose resulted in 2578 kg of nitrogen and 312 kg of phosphorus (including mineral:77 kg N, 9 kg P) for entire year. However, when we increase the expected value of the yield to 7 tonnes ha^{-1}, using 75 kg ha^{-1} of urea in pre-sowing, 316 kg ha^{-1} of Nitrochalk in the first dose and 186 kg ha^{-1} in the second dose, then we get 2647 kg of nitrogen and 314 kg of phosphorus (including mineral:118 kg N, 9 kg P) for entire year.

The above example was presented for a field located close to the coastline (not further than 2 km), however, if we apply the same data for a field located approximately three times further from the coastline, the following results will be obtained: 1128 kg of nitrogen and 130 kg of phosphorus (including mineral:42 kg N, 2 kg P) for entire year (expected yield of 5 tonnes ha^{-1}), and 1140 kg of nitrogen and 136 kg of phosphorus (including mineral:65 kg N, 2 kg P) for entire year (expected yield of 7 tonnes ha^{-1}).

From the previous examples, we know what nitrogen losses occur when using urea for pre-sowing, so let's replace it with Polifoska 17/17/18 (with a dose of 200 kg ha^{-1} in order to keep the amount of nitrogen similar to the amount used in the example using urea), then we will get: 2564 kg of nitrogen and 315 kg of phosphorus (including mineral:64 kg N, 12 kg P) for entire year (expected yield of 5 tonnes ha^{-1} from filed located near the coastline).

In the last example, we will check what the result of nitrogen loss will be when replacing urea used in the second dose with ammonium sulfate (with a dose of 176 kg / ha, which does not change the amount of nitrogen compared to the example with urea), and then we will get: 2568 kg of nitrogen and 312 kg of phosphorus (including mineral:72 kg N, 9 kg P) for entire year (expected yield of 5 tonnes ha^{-1} from filed located near the coastline).

4 Discussion

The online WaterPUCK toolkit, which is the result of both environmental research (aimed at verifying the mathematical models and their correct parameterisation) and numerical research, gives a real advantage to several target groups.

The first group of recipients of the created toolkit are farmers. Using the tools available from WaterPUCK online interface, they can calculate the nutrient balance, nutrient efficiency and the amount of nitrogen that is leached out of the field when planning the fertilisation. These tools allow farmers to make more efficient use of the means of production available on their farms while respecting the environment and, as a result, reduce the amount of substances that could potentially endanger them.

Important information for the farmer is the amount of nutrient loss depending on the form of nitrogen in the fertiliser. The user can compare possible fertilisation variants and thus evaluate their efficiency and reduce losses. Calculate what losses will occur when using different forms of nitrogen (e.g., amides and nitrates). The product takes into account the spatial variation of soil parameters, so that each farmer has an individual view of fertiliser losses. The diversity of soils and a large database of fertilisers makes it possible to analyse many variants of cultivation and fertilisation. This makes the tool flexible and gives it potential in local agricultural advisory services. The calculator makes it possible to visualise the spatial variation of nutrient losses over the whole municipality.

The SWAT model is a tool that also contributes to increasing knowledge on the optimal production means dosage. The use of SWAT is very intuitive as the farmer indicates on the map the location of his farm and enters data on the planned crop, fertilisation and protection plans for the next production period. As a result, receives feedback on the environmental impact of the changes for different assessments and rainfall scenarios.

Another group are scientists for whom quick access to detailed data on the state of environmental pollution from the place of application, through propagation, to various places of its accumulation is essential. It also creates the possibility of conducting research in a comprehensive manner without omitting the complexity of the issue. In addition, the knowledge gathered in such a comprehensive way makes it possible to develop predictions of possible long-term environmental effects, which is necessary to implement effective strategies to protect the environment.

Quick access to very detailed phenomena taking place in the environment may be also extremely important for testing hypotheses about the dynamic of those processes. For example, using the data presentation interface for the EPB model, we can observe a very interesting phenomenon of anti-cyclonal eddy and its impact on all monitored variables inside the bay. This kind of knowledge is highly important for a short-term assessment of the impact of various types of extreme pollution that may arise from water treatment system failures.

The interest group for which the use of our solution may be beneficial is the policymakers. With the help of solutions developed and described in this study, it is expected to benefit from provided expert knowledge and make responsible long-term decisions respecting the assumptions of sustainable development of rural areas with particular attention to environmental protection.

It should be mentioned that there are currently solutions in use that partially overlap with the toolkit we proposed and were collected and briefly described in the Table 5.

Table 5: Solutions similar to WaterPUCK toolkit.

similar solution	short description
Farm Carbon Calculator	A calculator for farms to determine greenhouse gas emissions (Farm Carbon Calculator, 2021).
COMET-Farm	In addition to greenhouse gas emissions, the calculator estimates the reduction of nitrous oxide emissions based on location (state and county), plot size, surface soil texture, approximate historical land use changes, cultivation and fertilisation practices, future land management and carbon storage practices and the current consumption of electricity from fossil fuels. (COMET-Farm tool, 2021; Eve et al., 2014)
Cool Farm Tool	Internet platform estimating greenhouse gas emissions by farms, monitoring biodiversity on the farm, impact on surface waters,including water consumption (The Cool Farm Tool, 2021; Hillier et al., 2011).
Agrecalc	Calculates greenhouse gas emissions emitted by farms or enterprises (Agrecalc, 2021).
Afolu Carbon Calculator	Calculator of carbon dioxide emissions as a result of the implementation of projects (including regular farming), agricultural and forestry (Afolu Carbon Calculator, 2021; Winrock International, 2014).
Greenhouse in Agriculture	Multifunctional calculators (set of calculators) measuring greenhouse gas emissions by farms and livestock breeders, depending on the breed of animals and the species kept (Greenhouse in Agriculture, 2021).
Farm Water Calculator	It coexists with the dry matter calculator, but the two are not integrated with each other. They allow for the estimation of yields with given initial parameters (similar to the WaterPUCK toolkit). The water consumption calculator allows one to estimate consumption, calculate possible savings, diversify water supply sources (Farm Water Calculator, 2021).
CSF Water Deficit Calculator	Tool for calculating the water deficit in the area of crops. Only available for parts of the US East Coast. Calculates deficits for plants that are selected as part of the calculator completion (CSF Water Deficit Calculator, 2021).
The Healthy Farm Index (HFI) Biodiversity Calculator	Measuring the level of ecosystem services to agriculture and the farm's effectiveness in terms of maintaining biodiversity in the area of crops. The calculator has many functionalities, but it does not calculate indicators related to water and soil quality (The Healthy Farm Index (HFI) Biodiversity Calculator, 2021; Noll et al., 2020).
Water Quality Index	A calculator that allows one to determine the indicators of surface water quality for a given latitude and longitude. Universal, directed to all interested parties (Water Quality Index, 2021).

Although there are many common features among the solutions presented in the Table 5, our solution is the only one that comprehensively addresses the environmental impact of agriculture from the production planning stage to the final propagation of pollution in the aquatic environment (both land and marine). For example, A Cool Farm Tool and COMET-Farm (Vetter et al., 2018; Ziegler et al., 2016) focuses mainly on the carbon cycle or, for aquatic environment, on water footprint caused by irrigation. There is also an interesting study on so-called Healthy Farm Index by Quinn et al. (2013), but it is mainly focused on biodiversity.

5 Conclusions

Solutions that comprehensively connect the marine and land environment are essential for resource monitoring and management, especially in the coastal zone which plays a beneficial role for humans. Moreover, considering the individual elements of the solution as separate and unconnected may lead to an underestimation/overestimation of the potential effects of planned regulation.

Improved understanding of sea-land interactions, in the context of hazardous substances, will contribute to achieving the goals set by European legislation, which aims to improve the state of marine waters, that is also the ultimate result of WaterPUCK project implementation. The systematic use of the WaterPUCK toolkit by farmers (particularly the farm balance calculator, nitrogen leaching calculator and SWAT's Calculator mode) allows for more efficient management of production means while respecting the environment.

Creation of environmental database and its availability for decision-makers, environmental NGOs and other interested stakeholders is an additional indirect benefit for the society achieved from WaterPUCK toolkit implementation. The environmental database gathers data from the literature, monitoring and adds new data obtained within the project with the aim to inform management authorities of the Bay of Puck, including public consultations. This is especially important as publicly available data are still scarce and access to them is often restricted.

The WaterPUCK toolkit is designed so that it can be applied to other regions around the world. A necessary condition for the success of its application is to carry out the calibration process described in this study. The key was to set up the database in such a way that each of the system's component tools could easily use the necessary information for its correct operation, which was ensured in our solution.

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A Statistical measures used for model system evaluation

To estimate numerical models accuracy we made calculation using standard measures such as mean error (ME), mean absolute error (MAE), mean squared error (MSE), root mean squared error (RMSE), standard deviation (STD), and Pearson correlation coefficient (Pearson's r):

$$ME = \frac{1}{n}\sum_{i=1}^{n}(X_i - Y_i) \tag{1}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|X_i - Y_i| \tag{2}$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(X_i - Y_i)^2 \tag{3}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(X_i - Y_i)^2} \tag{4}$$

$$STD = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(X_i - \overline{X}\right)^2} \tag{5}$$

$$\text{Pearson's } r = \frac{\sum_{i=1}^{n}\left(X_i - \overline{X}\right)\left(Y_i - \overline{Y}\right)}{\sqrt{\sum_{i=1}^{n}\left(X_i - \overline{X}\right)^2}\sqrt{\sum_{i=1}^{n}\left(Y_i - \overline{Y}\right)^2}} \tag{6}$$

where X_i – i-th measured value from sample; Y_i – i-th simulated value corresponding to measured point; n – the total number of observations, and $\overline{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$.

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