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Modelling of nitrogen concentrations in water from drained peat soils

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ABSTRACT

In addition to traditional sources, drained peat soils have been found to be a significant source of nitrogen in Estonia. As a result, supplementary measures are required to improve water quality in rivers. Modelling is a widespread method to select means for improving water quality. At present, modelling of nitrogen in rivers has been concentrated on the influence of agricultural activity. However, drained peat can increase nitrogen concentrations even without fertilization and farming activities. This investigation describes the attempt to model water quality in the watershed with a large share of drained peat soils. The results showed a good alignment between measured and modelled nitrate concentrations using the MACRO and the SOILN for MACRO models. Some measures to improve water quality were tested using these models.

Key words | drained peat soils, MACRO, modelling, nutrient loads, river water pollution, SOILN

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INTRODUCTION

One of the main environmental pressures on the marine ecosystem in the Baltic Sea region and thus also in Estonia is the eutrophication caused by the oversupply of nutrients. Although HELCOM (Baltic Marine Environment Protection Commission – Helsinki Commission) countries have agreed on joint efforts to reduce the nutrient load on the marine ecosystem (HELCOM 2018), recent data analyses show that riverine nutrient loads in Estonia have increased in some rivers (Iital *et al.* 2010; Kaur *et al.* 2017). An increase in nitrogen (N) concentrations has been detected in watersheds with very low human activity (Iital *et al.* 2010) and despite the overall decrease of fertilizer usage. This has initiated a discussion as to whether there are additional nutrient sources that contribute to the overall load, which have been underestimated. Hoffmann *et al.* (2000) assumed that increases in pollution by nutrients may be caused by wide-scale melioration. For example, the drainage of peat soils leads to the decomposition of peat and increases fluxes of nutrients to watercourses (Heikkinen 1994; Kløve 2001; Kløve *et al.* 2010). The drainage of peatlands results in peat oxidation and changes their physical and chemical properties significantly (Litaor *et al.* 2008; Verhoeven & Setter 2010), which can result in high nitrate-nitrogen (NO_3-N) concentrations in the pore water of drained peatlands. This is caused by the aeration of peat and subsequent mineralization and nitrification of organic N (Tiemeyer *et al.* 2007). In Europe, mineralization of nitrogen from peat soils is regarded as another possible source of nutrients (EC Eurostat 2011). An increase of nitrogen concentrations in some Estonian river basins with a high percentage of drained peat soils has also been observed by Vassiljev *et al.* (2016).

To analyse the influence of the nitrogen emissions coming from drained peat soils in Estonia, a statistical study was conducted (Vassiljev *et al.* 2016; Kaur *et al.* 2017). The diffuse unit-area source emission coefficients of nitrogen in Estonian rivers were estimated for the whole of Estonia and for a smaller study area near the capital Tallinn. The results from both the cases showed that drained peat soils were the highest diffuse source contributor in the unit-area loads. The loads from drained peat soils were up to 2.3 times higher than those from arable land (Vassiljev *et al.*

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2016; Kaur *et al.* 2017), which is considered as the main nitrogen contributor in Estonia (Estonian Ministry of Environment 2016). In order to plan appropriate measures for reducing the nitrogen leaching, sophisticated hydrological and water quality models are required to analyse nitrogen concentrations in watersheds with a large share of drained peat soils. The main objective of this article is to assess the suitability of MACRO and SOILN for MACRO for modelling the water quality in watersheds with a high percentage of drained peat soils. A 5.5-year period was selected for model calibration and a 5.5-year period for validation. The article uses the results from Vassiljev *et al.* (2018); but this analysis is more comprehensive, based on the larger data volume and time period.

MODELS AND STUDY AREA

Modelling of nitrogen leaching is a two-step procedure. In the first step, the water fluxes are modelled because water is the carrier of nitrogen. In the second step, the chemical behaviour and the leaching of nitrogen in soils are modelled. Most of the conceptual hydrological models cannot provide the data needed to calculate the nitrogen transformations in soil (e.g. take into account the changes in soil temperature), which makes it difficult to couple them with nitrogen-leaching models. Therefore, the MACRO model was used in this study to simulate water quantity. It was developed to simulate the data needed for calculations of nitrogen transformation in soils. The only drawback is that the model is one-dimensional and developed for analysing small homogeneous areas at a field or plot scale. Major carbon (C) and nitrogen (N) flows and corresponding processes in soils and plants were modelled using the SOILN model.

In the MACRO model, the soil profile is divided into micro- and macropores. Soil macropores (e.g. root and worm holes, and structural shrinkage cracks) allow rapid non-equilibrium fluxes of water in soil (Beven & Germann 1982), and consequently, influence the leaching of nitrogen quite significantly (Larsson & Jarvis 1999). The exchange of water and nutrients between micro- and macropores is usually ignored by hydrological models developed for watersheds. Studies in peat soils have indicated the presence of macropores (Litaor *et al.* 2008), which makes the MACRO model suitable for modelling water quantity in areas with drained peat soils. Input variables for the MACRO model include air temperature and humidity, precipitation, wind speed and solar radiation for each day. In addition, it needs information about soil profiles. Output variables include besides water flow into the river system also all information needed for the calculation of nitrogen transformation in soil.

The SOILN model (Larsson & Jarvis 1999) simulates major carbon (C) and nitrogen (N) flows and corresponding processes in soils and plants. Flow and state variables are simulated at a field level with a daily time step. Input variables such as daily data on the air temperature, solar radiation, evaporation, soil heat and water conditions are gained from the MACRO model. The soil vertical profile is divided into layers. In each layer, mineral N is represented by one pool for ammonium N and one for nitrate N. Ammonium N is usually regarded as immobile, whereas the nitrate form is transported with the water fluxes (a special option can also make ammonium mobile). The ammonium pool might be increased by the nitrogen supplied from manure application, mineralization of organic material and by atmospheric deposition, and it is decreased by immobilization to an organic material, nitrification to the nitrate pool and plant uptake. The nitrate store is increased through the nitrification of the ammonium pool, fertilization and atmospheric deposition. The leaching, denitrification and plant uptake reduce the amount of nitrate N in the soils. Water flows that transport nitrate N between the layers is responsible for nitrogen leaching. The rate of the decomposition of organic matter depends on soil moisture and temperature conditions. Nitrogen dynamics of the organic matter is governed by C flows, and mineralization or immobilization depends on the C/N ratio of the decomposed material and the availability of mineral N (Johnsson *et al.* 1987). SOILN for MACRO takes into account the nitrate exchange between the macro- and micropores (Jarvis 1994; Larsson & Jarvis 1999). The SOILN model obtains data about water fluxes and the temperature from the MACRO model. Additional data on fertilization and other sources of nitrogen were obtained from national databases. Output variables besides water flow (obtained from MACRO) include information about the concentrations of nitrates in water coming into the river system. In modelling on the watershed scale, it is required to divide a watershed into homogeneous one-dimensional areas that have the same soils, the same depth of ground water, vegetation, etc. The modelling scheme has to include the simulation of water fluxes and nitrogen movement in the river system. The models were adapted according to the scheme described in Vassiljev *et al.* (2004).

In this study, water quantity and quality were modelled at a watershed with a large percentage of peat soils (Leivajõgi River). The whole area of the watershed covers 79 km^2, and the river length is 17 km with an average discharge of 0.77 m^3/s at the point of water quality measurements. Annual average precipitation is 704 mm and the temperature 5.9 °C. The map of the watershed is given in Figure 1(a). Soil types in the watershed were estimated on the basis of a digital soil map obtained from the Estonian Land Board. A digital CORINE land cover map was used to derive land use statistics. The two maps were intersected to generate an overall map with soil types and land use in the watershed (Figure 1(b)). The analysis of soil and land use maps revealed that there are four dominant areas in the watershed – forest on peat soils, forest on loam soils, pastures on peat soils and arable land on loam soils. The distribution of the four dominant areas in the watershed is shown in Figure 1(b).

The four dominant land use soil type areas are all situated at different parts of the watershed and can contain profiles with different ground water depths. This was taken into account in the selection of a suitable methodology. The most precise measurements of the ground water levels and ground elevations are manual measurements, which

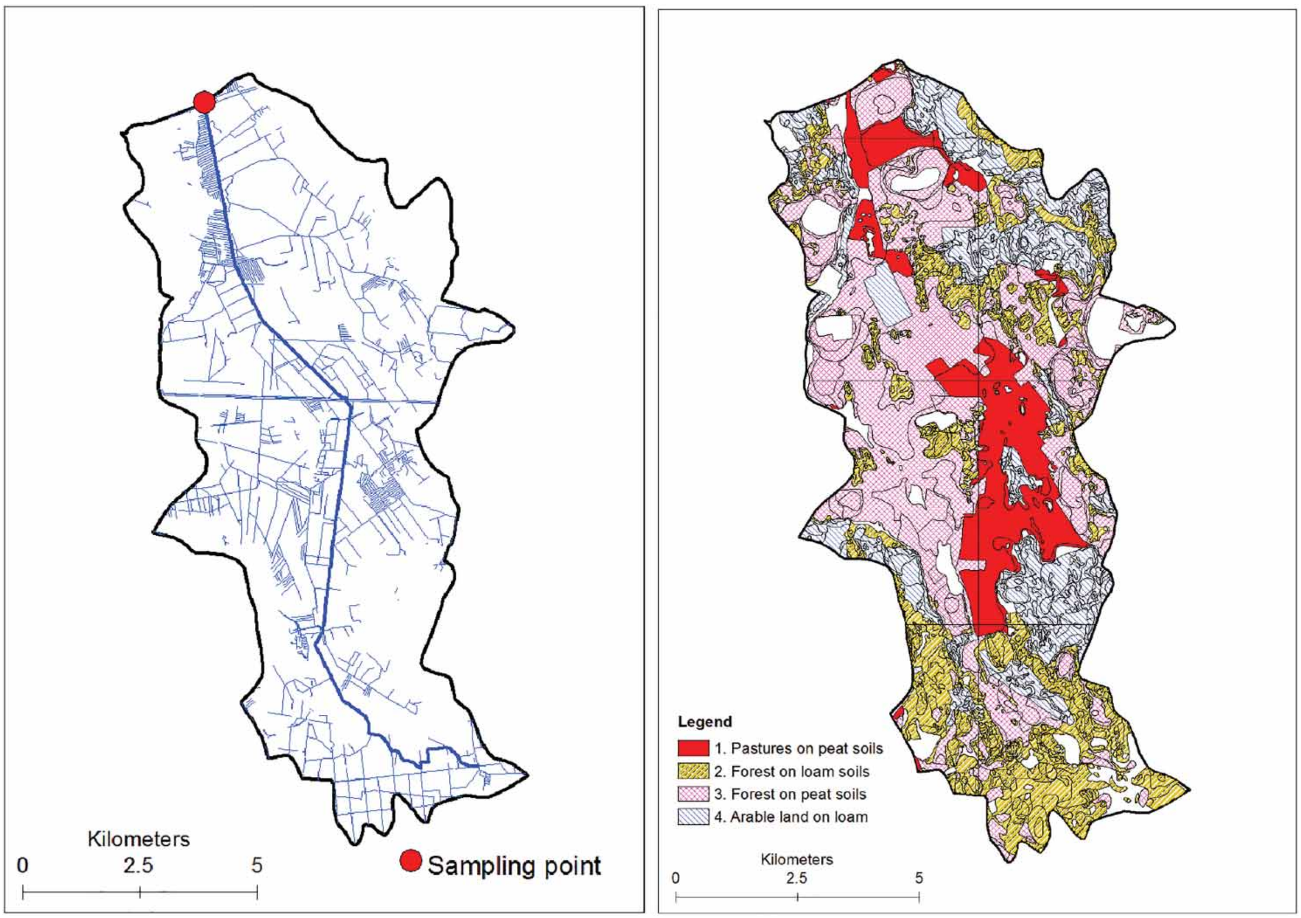

Figure 1 | Map of the River Leivajõgi watershed.

however are labour-consuming. Therefore, in our study, five profiles with different depths of ground water were selected. For these profiles, a series of calculations were performed and an optimization procedure was used to find the areas that occupy each soil profile.

The characteristics of the watershed are given in Table 1. The watershed contains quite large areas of peat soils; arable and farming activity is low. The main soil types in the watershed are peat (45.6%) and clay loam (35.2%). All the areas covered with water (rivers, lakes, bogs, etc.) are drawn together to wetlands.

The data presented in this study were gathered from the Estonian national monitoring programme database. Water flow was measured daily, and grab samples of water were collected during the national monitoring programme according to national legislation. The sampling rate changed from the year 2010 from 12 to six times per year. The sampling point was at the outlet of the watershed under investigation (Figure 1(a)). The measurement points of the discharge and the water quality do not overlap exactly but are close to each other. Water samples were analysed in an accredited laboratory.

RESULTS

The content of organic matter in peat soils is usually very high (>90%). The experience of the authors shows that most of the hydrological models fail to perform with soils containing a high rate of organic matter. For this reason, only the MACRO and the SOILN for MACRO models were used in this study.

Table 1 | Soil areas (%) of different land use types for the Leivajõgi watershed (numbers in bold indicate areas used in modelling)

Land use/soil	Sandy loam	Clay	Sand	Clay loam	Peat	Sum
Arable	0.9	0.0	0.3	**16.4**	2.3	19.9
Pasture	0.4	0.0	0.2	1.7	**13.4**	15.8
Forest	1.5	0.0	3.7	**16.5**	**29.7**	51.4
Natural grass	0.0	0.0	0.0	0.6	0.2	0.8
Wetland						**9.9**
Others						2.2
Total						100

Four types of dominant areas described earlier (Figure 1(b)) were used for modelling. For each area, modelling was accomplished for five different profiles with a total depth of 30, 60, 90, 120 and 170 cm. Selected profiles cover the typical range of depths of the zone of aeration in the studied watershed. All profiles were divided into 10 layers of different thickness. Parallel calculations using the farming algorithm (Topping *et al.* 1998) were used in order to decrease the computing time. Results of calculations for each profile (20 altogether) were exported into an Excel workbook in order to use the optimization procedure. The total water inflow into the river system is the sum of runoffs from the areas described by these soil profiles. It is necessary to take into account a part of precipitation that falls onto areas covered by water (e.g. river and wetlands). Water flow from such areas in a warm season was found as the difference between the precipitation and evaporation. For a cold period when the water flow depends on the temperature, a more complex approach was used. For instance, water coming onto the wetland areas during snow melting was assumed to be equal to water coming onto the surface of the watershed. Coefficients for each profile were found through the optimization procedure. Solver in Microsoft Excel contains two different approaches applicable for optimization in the present cases – Nonlinear and Evolutionary Generalized Reduced Gradient. Calculations showed that the first of these was unable to provide reasonable results obviously because of too many parameters. The evolutionary approach took much more time but resulted in better solutions. The scheme described in Vassiljev *et al.* (2004) was used to simulate the moving of the water flow and nitrate N along the river system until the measurement point.

Daily water flow and concentrations of nitrate nitrogen were modelled for 11 years. Half of this period was used for calibration and the other half for validation. The efficiency of modelling was estimated by the Nash–Sutcliffe efficiency (NSE) (Nash & Sutcliffe 1970) for the validation period. The NSE is a normalized statistic that determines the relative magnitude of the residual variance ('noise') compared to the measured data variance ('information') (Moriasi *et al.* 2007). It indicates how well the plot of the observed versus the simulated data fits the 1:1 line. The NSE was computed using the following equation:

$$\mathrm{NSE} = 1 - \left[\frac{\sum_{i=1}^{n} (Y_i^{\mathrm{obs}} - Y_i^{\mathrm{sim}})^2}{\sum_{i=1}^{n} (Y_i^{\mathrm{obs}} - Y^{\mathrm{mean}})^2}\right] \tag{1}$$

where Y_i^{obs} is the ith observation for the constituent being evaluated, Y_i^{sim} is the ith simulated value for the constituent being evaluated, Y^{mean} is the mean of the observed data for the constituent being evaluated and n is the total number of observations. In general, model simulation can be judged as satisfactory if NSE > 0.50 (Moriasi *et al.* 2007). Values smaller than 0.0 indicate that the mean observed value is a better predictor than the simulated value, which implies unacceptable performance. The calibration of the model was accomplished within the years 2006–2011 (first half of the year 2011). NSE coefficients were 0.63 for water flow and 0.61 for nitrate nitrogen. Years for validation were 2011 (second half of the year 2016). NSE coefficients were lower – 0.51 and 0.5, respectively. Results can still be considered good, taking into account that precipitations were measured quite far (about 20 km) from the watershed.

It should be noted that calibration was accomplished simultaneously for the water flow and the concentrations to achieve a maximal sum of the NSE for the water flow and the NSE for the concentrations.

Figures 2 and 3 show the results of modelling water discharge for the calibration and validation periods. As can be seen, at some points, the maximal flow is over- or underestimated most likely due to precipitations measured outside the watershed. At the same time, the shape of the hydrographs is described well. Figures 4 and 5 present the modelled and the measured concentrations of NO_3-N. The figures show that the concurrence of the modelled and the measured concentrations is good and the trends are similar in the calibration and validation period (NSE 0.61 and 0.5, respectively). Clearly, differences in the maximal flow lead to differences in the modelled and the measured concentrations; resulting from the analysis of the input data, the reason is that the measured NO_3-N concentrations increase with the increase in the measured water flow (Figure 6).

The analysis showed also that similar to the measured data, the modelled concentrations increase with the increase in the water flow (Figure 6). Both dependencies (for measured and modelled variants) are non-linear (increase rate is lower at higher discharge). Such behaviour is common for diffuse pollution of nitrogen (e.g. Hanslík *et al.* 2016) in rivers with a low level of point pollution. This shows that the models selected for use in this study are appropriate for modelling nitrogen

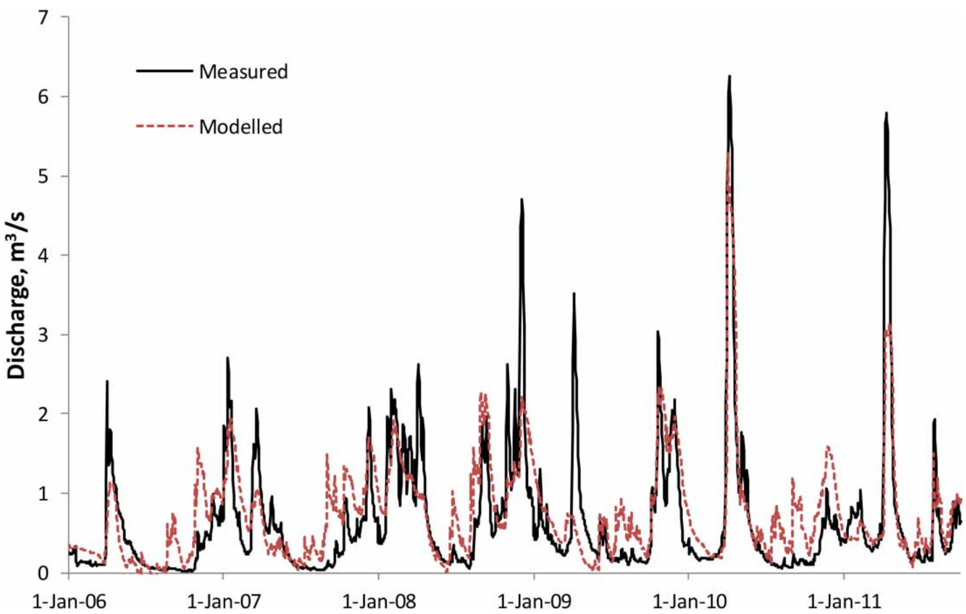

Figure 2 | Measured and modelled water discharge (calibration period).

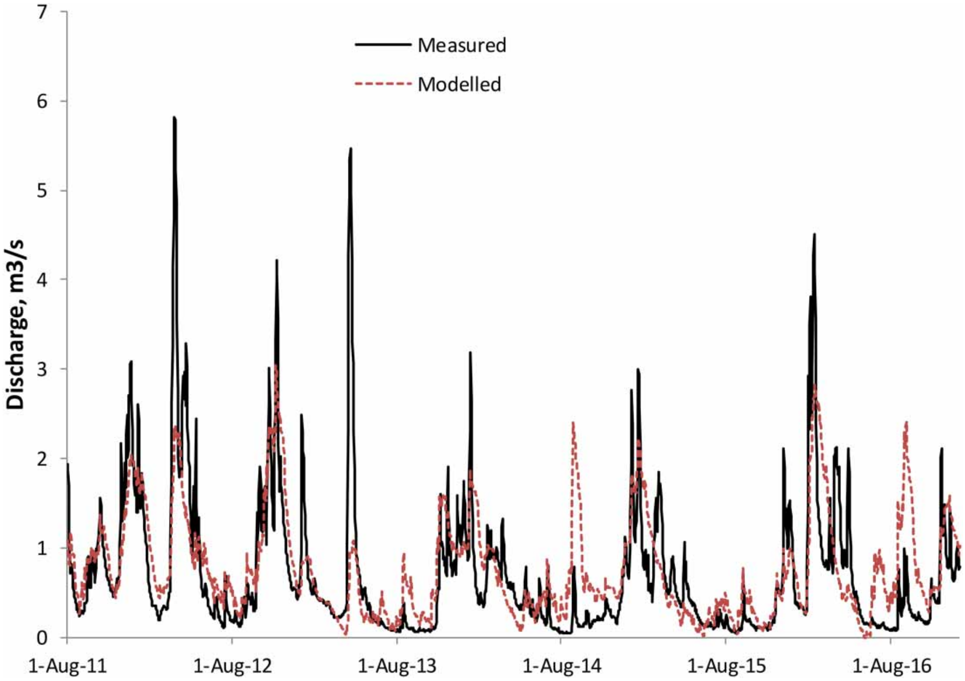

Figure 3 | Measured and modelled water discharge (validation period).

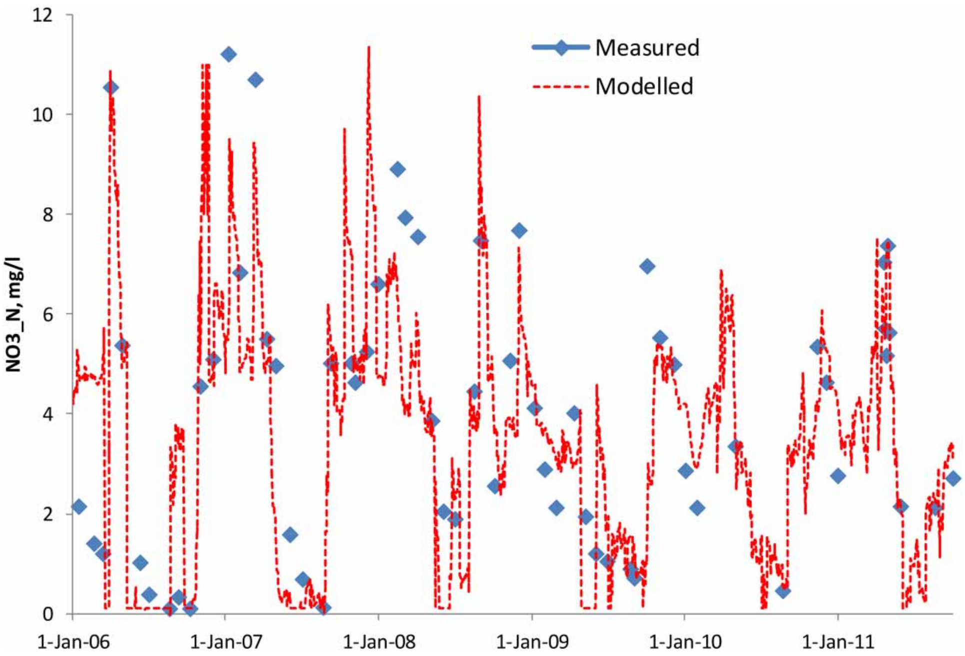

Figure 4 | Measured and modelled nitrate nitrogen (calibration period).

leaching from drained peat areas as other models mostly show a decrease in concentrations with an increased discharge.

Figure 7 shows that both modelled and measured averaged annual concentrations fluctuate over the study period. The rate of fertilization usage in arable lands

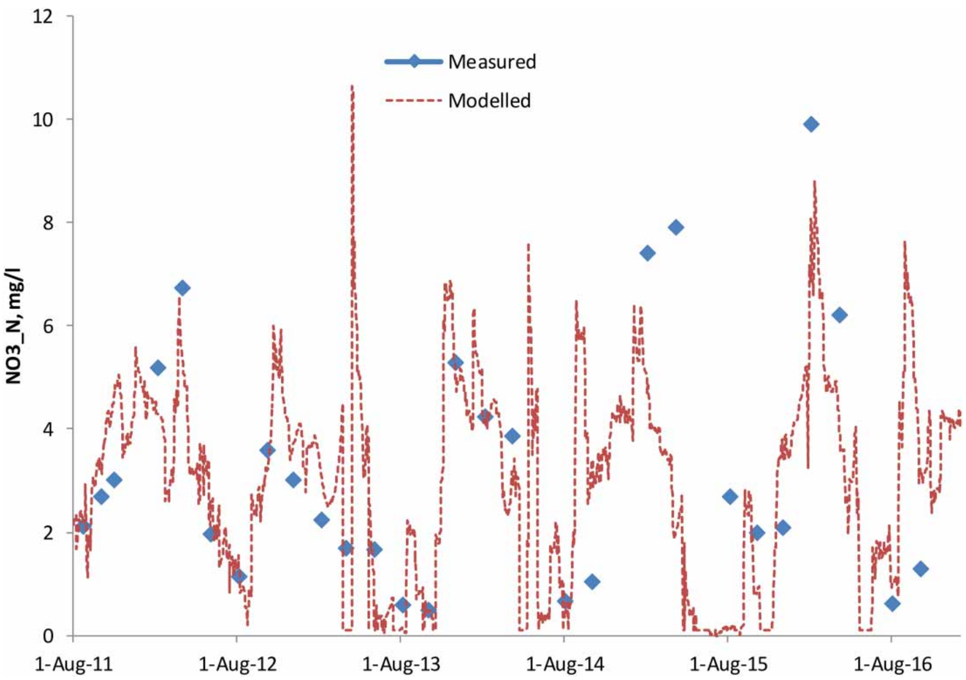

Figure 5 | Measured and modelled nitrate nitrogen (validation period).

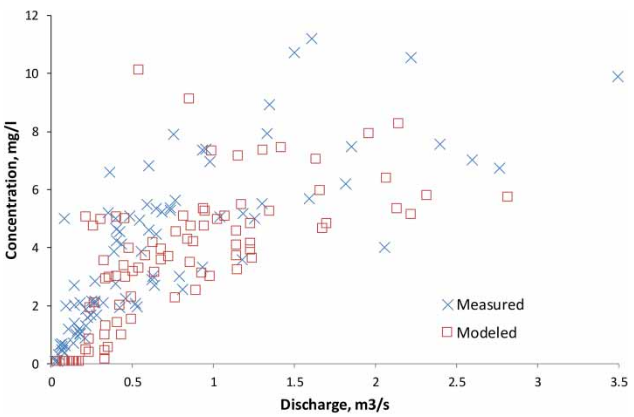

Figure 6 | Dependence of nitrate-nitrogen concentrations on water discharge.

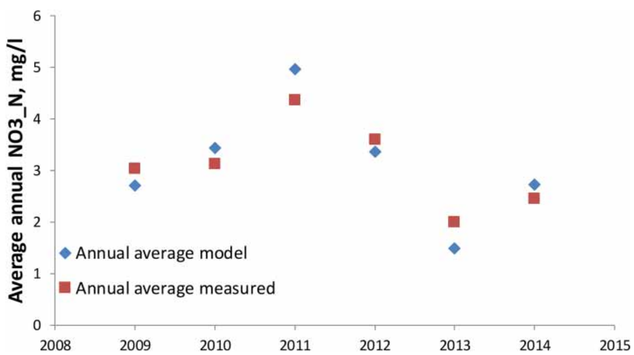

Figure 7 | Annual average concentrations.

was kept the same over the study period (Statistics Estonia 2015). Therefore, fluctuations of NO_3-N concentrations are connected with weather changes. The amplitude of the changes is almost the same in the modelled and the measured values. Therefore, meteorological conditions have to be taken into account while analysing the trends in nitrate concentrations in the watershed.

DISCUSSION

This section discusses some applications of the models to find measures and actions for improving the water quality from the watersheds with a high ratio of drained peat soils. The MACRO model suitable for modelling of water runoff from soils with a high content of organic matter (almost 100% of organic) was tested in the watershed with a high percentage of drained peat soils. As compared with other hydrological models, this model provides all necessary information to the respective SOILN model to calculate the concentration of NO_3-N in a river. In addition, the MACRO model enables an analysis of the exchange of water and nitrogen between the micro- and macropores. Moreover, this study showed that the field-scale model is applicable also at the watershed scale. Thus, these models demonstrate high reliability in the analysis of soils of that type. As a result, the models enable an analysis of the influence of different water protection measures to improve water quality. Importantly, in addition to the traditional sources of nutrients (e.g. arable lands), the influence of peat soils as an additional source can be addressed.

Successful attempts at modelling for a watershed with a high percentage of drained peat areas can be used to find solutions for the reduction of nitrate concentrations. Such actions targeted to a large amount of similar watersheds are of high importance in Estonia. Two different measures to reduce the nitrogen flow were modelled with MACRO and SOILN to exemplify the reliability of the models: (1) increasing the distance between the drains and (2) decreasing the depth of the drains. Table 2 presents the results of the analysis of the first measure, providing cumulative export of nitrates (for 11 years) from one square metre of peat profile with a depth of drain of 170 cm.

Table 2 shows that a significant (>50%) decrease of nitrate export into a river can be achieved by extending the distance between the drains up to 10 km. Agricultural drainage pipes are typically designed at a depth of 0.6–1.2 m from the ground and at a spacing of 10–30 m (Blann *et al.* 2009). Therefore, extending the distance between the concurrent lines beyond the limit brings the systems to the contradiction with the initial aim of the drains to form a dense network of conduits for removing the excessive water (Gurovich & Oyarce 2015). Table 2 shows that extending the distance between the drains decreases the nitrate export. The decrease is so slow that this measure is considered as inefficient and is not recommended for implementation in watershed management.

Decreasing the depth of the drains has a profound influence on the reduction of the nitrogen flow. As shown in Figure 8, decreasing the depth ca. three times, from 155 to 55 cm, will result merely in five times lower nitrogen concentrations. As noted above, these numbers are in line with typical drain installation depths. Decreasing the depth of the drains decreases the peat profile that is in contact with oxygen and as a result decreases the peat amount under oxidation. Also, many other studies have found a similar trend between the depth and the nitrogen flow (Kladivko *et al.* 2004; Nangia *et al.* 2010). With the decrease in the depth of the drains, it is essential to reduce the distance between the drains to sustain the same effect on excess water removal. Although this might bring along higher construction costs, a positive effect on the nitrogen outflow is evident, and thus this measure could be applied for watershed management. Changes of vegetated conditions may also be used as an additional measure to reduce the nitrogen flow (Giannini *et al.* 2015).

Table 2 | Nitrate export (for 11 years) at different distances between drains

Distance between drains, m	Nitrate export, g/m^2
20	106.81
40	104.97
160	101.87
1,000	91.46
10,000	50.37

CONCLUSIONS

In this study, water quantity and quality of the watershed with a high percentage of peat soils were modelled using models initially developed for field-scale use. The analysis

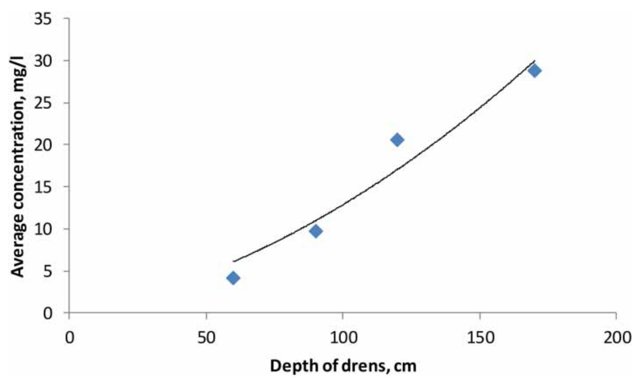

Figure 8 | Dependence of nitrate concentrations on different drain depths.

of CORINE and soil maps showed that four dominant areas prevail on the watershed: forest on peat, forest on clay loam, arable on clay loam and pastures on peat. Calculations were accomplished for five different soil profiles. Areas occupied by each profile were estimated by optimization to obtain a maximal value of sum NSE coefficients for the water flow and NO_3-N concentrations. Daily water flow and concentrations of nitrate nitrogen were modelled for 11 years. The reliability of modelling was estimated by the NSE. The investigation showed that the field-scale MACRO and SOILN for MACRO models may be successfully applied at the watershed scale. A good fit between measured and modelled nitrate-nitrogen concentrations using MACRO and SOILN for MACRO models was found. In addition, it was concluded that nitrate concentrations depend on weather conditions that may lead to a positive trend of nitrates in rivers with very low human activity.

This result is significant for Estonia where the main sources of diffuse nutrient loads are expected to come from agriculture and forestry. However, studies have shown that nitrogen loads from drained peat soils can be larger than those from arable lands (Vassiljev *et al.* 2016; Kaur *et al.* 2017). Models used in this study allow modelling of the water quantity and quality at the watersheds with a high content of peat soils and therefore are applicable to the planning activities of River Basin Management. According to the opinion of official authorities, the increase in nitrogen concentrations in rivers is linked with agricultural activities; however, the results of modelling showed that in this case, changes in the NO_3-N level may depend on the meteorological conditions rather than on human activity. Therefore, River Basin Management, with a focus on drained peat soils, needs additional solutions to improve the quality of water in rivers. Initial results showed that nitrate concentrations may be decreased by decreasing the depth of drains.

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