

Estimating water quality in river basins using linked models and databases

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Received 11 December 2007, in revised form 22 April 2008

Abstract. This paper describes the usage of linked models for assessment of water quality in a river basin. River water quality model QUAL2K and the Wennerblom (Älvborg) diffused pollution model were simultaneously applied for water quality and land-based pollution estimations. A software tool was developed to control the data flow between these models and databases. This tool provides automatic formation of a river model calculation scheme and assessment of river flow rates in every segment. The Pärnu River basin was chosen for testing the tool. Comparison with the measured data demonstrated an adequate behaviour of the linked models. Model simulations indicated that the diffused load forms an essential part in the total sea load and plays a significant role in the formation of river water quality.

Key words: modelling, water quality, nutrients, river basin management, databases.

INTRODUCTION

According to the Water Framework Directive (WFD), the water bodies should be managed on the basis of river basin districts and it is necessary to draw up a water management plan for each one of them. These plans have to demonstrate how to achieve the aim of the WFD of gaining a ‘good status’ for all waters by December 2015.

A large amount of information about a catchment in question is needed for generating water management plans. The national monitoring network does not cover all the rivers in Estonia. In the case of larger rivers, there may be more than one monitoring station in the river basin, but still their number is insufficient for estimating the water quality within the whole river basin. Therefore models have been used to simulate and predict the influence of different water management measures. The water quality in a river depends on the wastewater effluents and diffused sources from the catchment. Both types of pollution sources need to be taken into consideration in modelling river water quality.

The first considerable large-scale estimation of river water hydrochemical quality for the entire Estonian territory was started at the beginning of the 1960s at Tallinn University of Technology. The calculation methodology assumed that organic pollutants are decomposed as a result of dilution and biochemical oxidation in the recipient (Aitsam et al., 1965).

Pioneering developments of analytical methods for river water quality calculations were made by Paal (1976). The calculations of water quality were made according to the organic pollution parameter BOD along the river, using modelling based on the pollution load of point sources, river minimum runoff, and self-purifying capacity. Such calculations for different basins (Velner et al., 1967) and the entire Estonian territory (Türk et al., 1985) were carried out until the 1990s. Remarkable work in the application of the models for Estonia was done by V. Krysanova, A. Vassiljev, and A. Meiner, who developed modules for the SWIM model. The SWIM model is based on two previously developed models: SWAT (Arnold et al., 1993) and MATSALU (Krysanova et al., 1989; Krysanova et al., 1999). SWIM (Soil and Water Integrated Model) is a continuous-time spatially distributed river basin model, which simulates hydrology, vegetation, erosion, and nutrients (Krysanova et al., 1998; Krysanova & Becker, 1999). Currently Tallinn University of Technology in cooperation with other institutes investigates both the nutrients transport (Nõges et al., 2003; Iital et al., 2005; Leisk, 2006) and applications of models (Vassiljev & Stålnacke, 2005; Mourad et al., 2006; Vassiljev, 2006; Piirimäe, 2007). A promising series of investigations is underway at the University of Tartu to control nutrients loss from catchments. It focuses on the scale dependence of landscape metrics and the relationship between land use parameters (Uuemaa et al., 2005, 2007).

Land-based pollution estimation in Estonia needs additional research, in particular the role of different diffuse pollution sources in the formation of nutrient runoff from catchments should be further examined (Iital et al., 2003; Vassiljev et al., 2008). Numerous models exist for river basin calculations. Some of these models pay comprehensive attention to catchment processes, e.g. INCA (Wade et al., 2005) and IceCream (Posch & Rekolainen, 1993; Tattari et al., 2001). Some models are focused on river processes, e.g. QUAL2K (Chapra & Pelletier, 2003). The question is how to choose the relevant one? Some land-based pollution models attempt to describe this very complex system in a thoroughly detailed way. They include numerous processes and take into account dynamic conditions. In such models (e.g. INCA) the system is described by a large number of equations with many required parameters. As a rule, the results of these models depend crucially on the calibration of model parameters.

There are interlinked multi-model systems, where besides water quality estimation, economic aspects of management are taken into consideration as well. The MARE project serves as an example of such a decision support system (Wulff et al., 2003). The MARE project demonstrates what could be a cost-effective distribution of measures to achieve a desired environmental quality in the Baltic Sea. Although the MARE project is focused on marine systems manage-

ment, it requires river basin calculations to define external load conditions for the sea model.

Besides complex models, very simple calculation methods can be found as well. In the case of insufficient data simple models may be quite reasonable for environmental assessment. An example of such an uncomplicated method is the Wennerblom model (Lindström et al., 2000), in which land-based pollution is quite easy to calculate using an Excel spreadsheet.

There are certain aspects that need to be taken into account when selecting suitable aquatic models. Estonian rivers are short, their catchment areas and runoff are small. There are ca 500 rivers with a length of more than 10 km, two large lakes (Peipsi and Võrtsjärv), and ca 1200 small lakes in Estonia. The shoreline is ca 3800 km. For implementing WFD, Estonia is divided into three river basin districts consisting of nine sub-basins. According to the Estonian National Environment Monitoring Programme, hydrochemical analyses are carried out in 62 river stations. Monitoring frequency in these stations is up to 12 times a year. Hydrological parameters are observed daily in 39 locations. Point source data are measured 4 times a year. It is obvious that neither the frequency nor the spatial resolution of monitoring data is sufficient to describe the state of the environment in a region in detail. In addition, these are insufficient for initializing and calibrating sophisticated models. Therefore models are needed that would work with the limited available data. One such model is QUAL2K, which simulates stream water quality under steady-state conditions. In order to assess the conditions in the whole river basin, it is necessary to couple the QUAL2K model with a catchment model. This kind of separation into domains gives us the liberty of experimenting with different combinations of models.

The purpose of this work is to create a tool that is capable of linking stream and catchment models. The first attempt was a combination of the QUAL2K and Wennerblom models. Such tool mainly deals with the dataflow between the models. To automate the whole process it was decided to use a database for both initializing the models and storing simulation results. The Pärnu River basin was chosen for testing the tool.

DATA AND METHODS

Models

Two models were selected, one for estimating land-based pollution and the other for calculating the quality of river water. The first model is the Wennerblom model (Lindström et al., 2000) developed by Tord Wennerblom from the county of Älvborg in Sweden (also known as the Älvborg model). The second model chosen is QUAL2K.

The Wennerblom model allows calculation of nutrient fluxes to surface waters and separation of natural and human-caused loads. Such separation makes sense because measures can be primarily applied to reduce human-caused pollution.

One of the objectives of this work was to quantify the gross load of nitrogen and phosphorus from different sources. Currently the model coefficients are based on the measurements made in Sweden.

The model allows us to roughly estimate the most important sources of pollution. The Wennerblom model was preferred, as there is insufficiency of data for the calibration of a more sophisticated model for entire Estonia.

The main idea of the Wennerblom model is to divide the sources of nutrients into different groups and use group-specific coefficients in calculations. Separate calculation formulas are used for diffused and point sources. The diffused runoff of nutrients from different land-use types depends on water discharge:

$$M_{di} = a \times Q \times A_i + b, \quad (1)$$

where M_{di} is annual diffused runoff of nutrients from certain land-use type i , kg; Q stands for annual water runoff from the calculation area, mm; A_i is the area of land-use type i , km²; and a and b are model coefficients.

The influence of animal farms:

$$M_a = n_i \times p_i, \quad (2)$$

where M_a is annual diffused runoff of nutrients caused by animals, kg; n_i is number of livestock of group i ; and p_i is annual amount of nutrients from one livestock group i .

Point sources:

$$M_p = P_i \times r_i, \quad (3)$$

where M_p is annual amount of nutrients from point sources, kg; P_i stands for annual load of nutrients from point source i , kg; and r_i is reduction of nutrients due to treatment of point source i .

For lakes the standard annual values of 8 kg P/km² and 120 kg N/km² were used based on measurements of precipitation data.

The other model, QUAL2K, is a river and stream water quality model. It is a modernized version of the QUAL2E model (Brown & Barnwell, 1987). The following features characterize QUAL2K:

- one dimensional (the channel is well-mixed vertically and laterally)
- steady-state hydraulics (non-uniform, steady flow is simulated)
- diurnal heat budget (the heat budget and temperature are simulated as a function of meteorology on a diurnal time scale)
- diurnal water-quality kinetics (all water-quality variables are simulated on a diurnal time scale)
- heat and mass inputs (point and nonpoint loads and abstractions are simulated).

In the QUAL2 models the river is divided into reaches. A steady-state flow balance is implemented for each model reach:

$$Q_i = Q_{i-1} + Q_{in,i} - Q_{ab,i}, \quad (4)$$

where Q_i is outflow from reach i into reach $i+1$, m^3/d ; Q_{i-1} is inflow from the upstream reach $i-1$, m^3/d ; $Q_{in,i}$ is the total inflow into the reach from point and nonpoint sources, m^3/d ; and $Q_{ab,i}$ is the total outflow from the reach due to point and nonpoint abstractions, m^3/d .

The QUAL2K model includes 16 state variables: conductivity, inorganic suspended solids, dissolved oxygen, slowly reacting organic matter, fast reacting organic matter, dissolved organic nitrogen, ammonia nitrogen, nitrate nitrogen, dissolved organic phosphorus, inorganic phosphorus, phytoplankton, detritus, pathogen, alkalinity, total inorganic carbon, and bottom algae.

For all model state variables except the bottom algae a general mass balance for a constituent in a reach is written as:

$$\frac{dC_i}{dt} = \frac{Q_{i-1}}{V_i} C_{i-1} - \frac{Q_i}{V_i} C_i - \frac{Q_{ab,i}}{V_i} C_i + \frac{E_{i-1}}{V_i} (C_{i-1} - C_i) + \frac{E_i}{V_i} (C_{i+1} - C_i) + \frac{W_i}{V_i} + S_i, \quad (5)$$

where C_i is variable concentration for reach i , g/m^3 ; t is time, d ; Q_i is outflow from reach i into reach $i+1$, m^3/s or m^3/d ; V_i is volume of i th reach; E_i is bulk dispersion coefficient between reaches i and $i+1$, m^3/d ; W_i is external loading of the constituent to reach i , g/d or mg/d ; and S_i is sources and sinks of the constituent due to reactions and mass transfer mechanisms, $\text{g}/\text{m}^3/\text{d}$ or $\text{mg}/\text{m}^3/\text{d}$.

For bottom algae the transport and loading terms are omitted.

The QUAL2 models have been widely tested, calibrated, and used in many parts of the world. The QUAL2K model does not calculate land-based pollution; it requires diffuse pollution as an input. Therefore the Wennerblom model needs to be run first so that the QUAL2K model can use the results.

Interface for linking the models with databases

The Estonian Environment Information Centre (EEIC) maintains numerous Estonian environmental databases and information systems (Environmental Indicators, Environment Monitoring Programme, Information System of Environmental Permits, Waste Data Management System, Information System of Air Pollution Sources, Estonian Nature Information System EELIS, Fisheries Information System, Greenhouse Gas Emissions Trading Registry, Water Cadastre).

The Environmental Register is an interface meant to unite these separate databases. It is currently under development but once completed, it will become an essential data source for this tool.

For calculating land-based pollution, *Corine Land Cover 2000* and data from the Estonian Ministry of Agriculture were used. In fact, the database organized for the coupled Wennerblom and QUAL2K models is a link to different EEIC databases. It contains information about rivers and tributaries (names, lengths, slopes, locations where tributaries flow into the parent river, river sub-basin areas, hydrological measurements, etc.), point sources (amounts and locations), diffuse sources (land cover types, animal farms, etc.).

A software has been designed linking the models with these databases. It generates the calculation structures of models, initializes the models with input data, and stores calculation results in a database. It is also possible to visualize the results. Schematic presentation of this system is shown in Fig. 1.

This tool simplifies the whole process of modelling – a user needs only to select a river and it automatically generates the structure of the calculation and assimilates the model's input data.

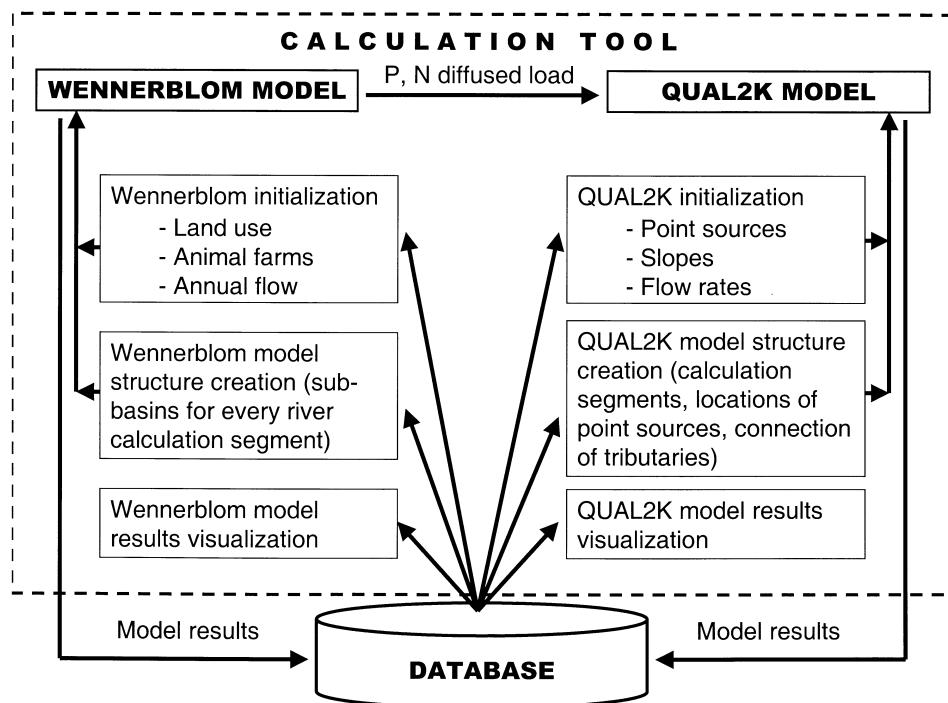


Fig. 1. Calculation tool.

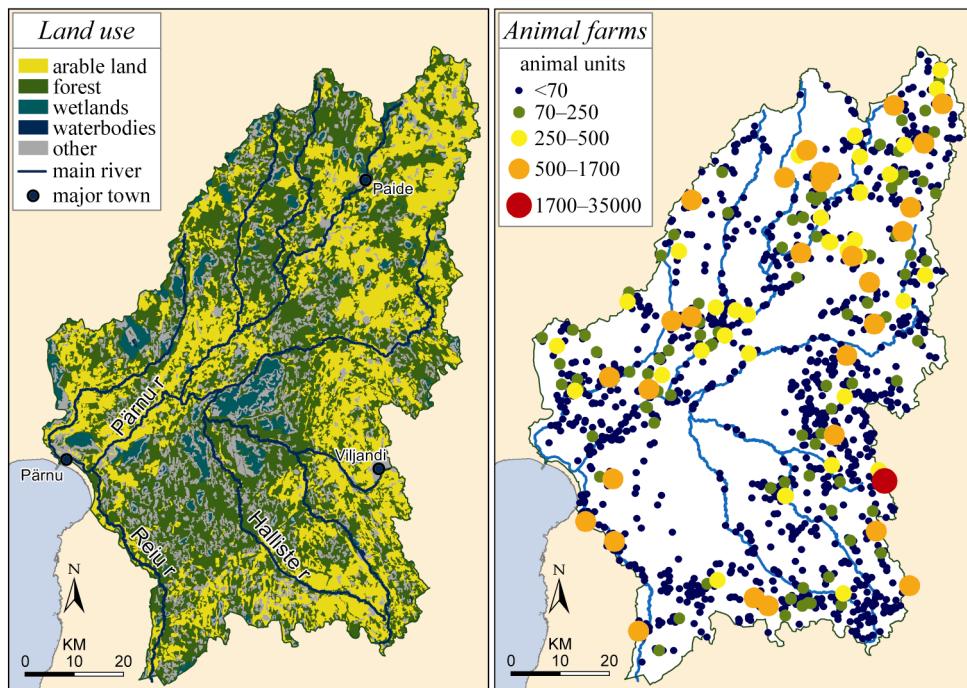


Fig. 2. Land use and animal farms in the basin of the Pärnu River.

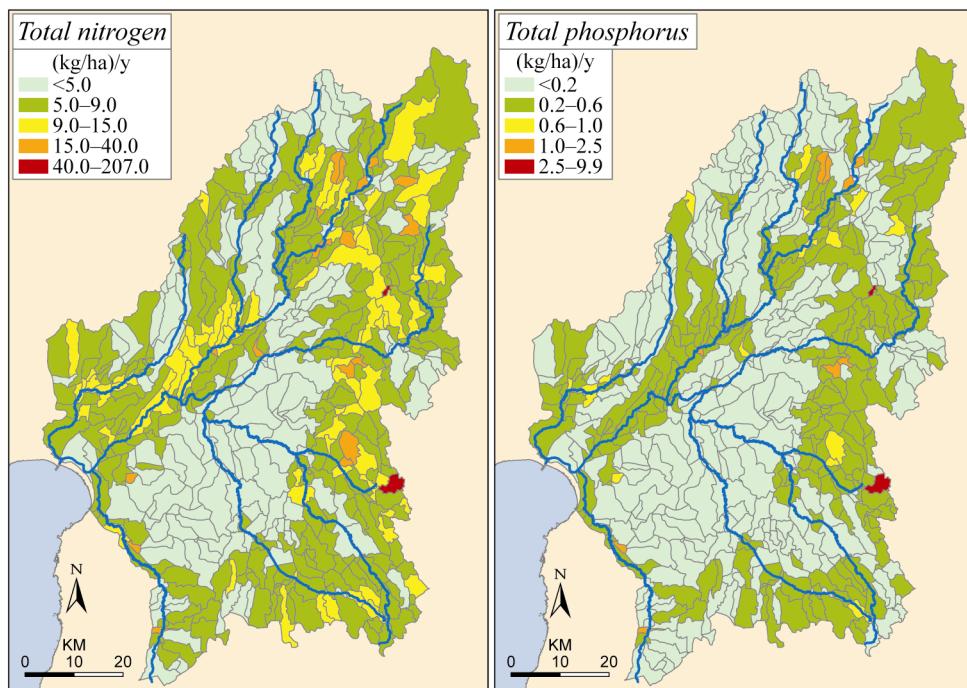


Fig. 3. Modelled runoff of nutrients in the basin of the Pärnu River.

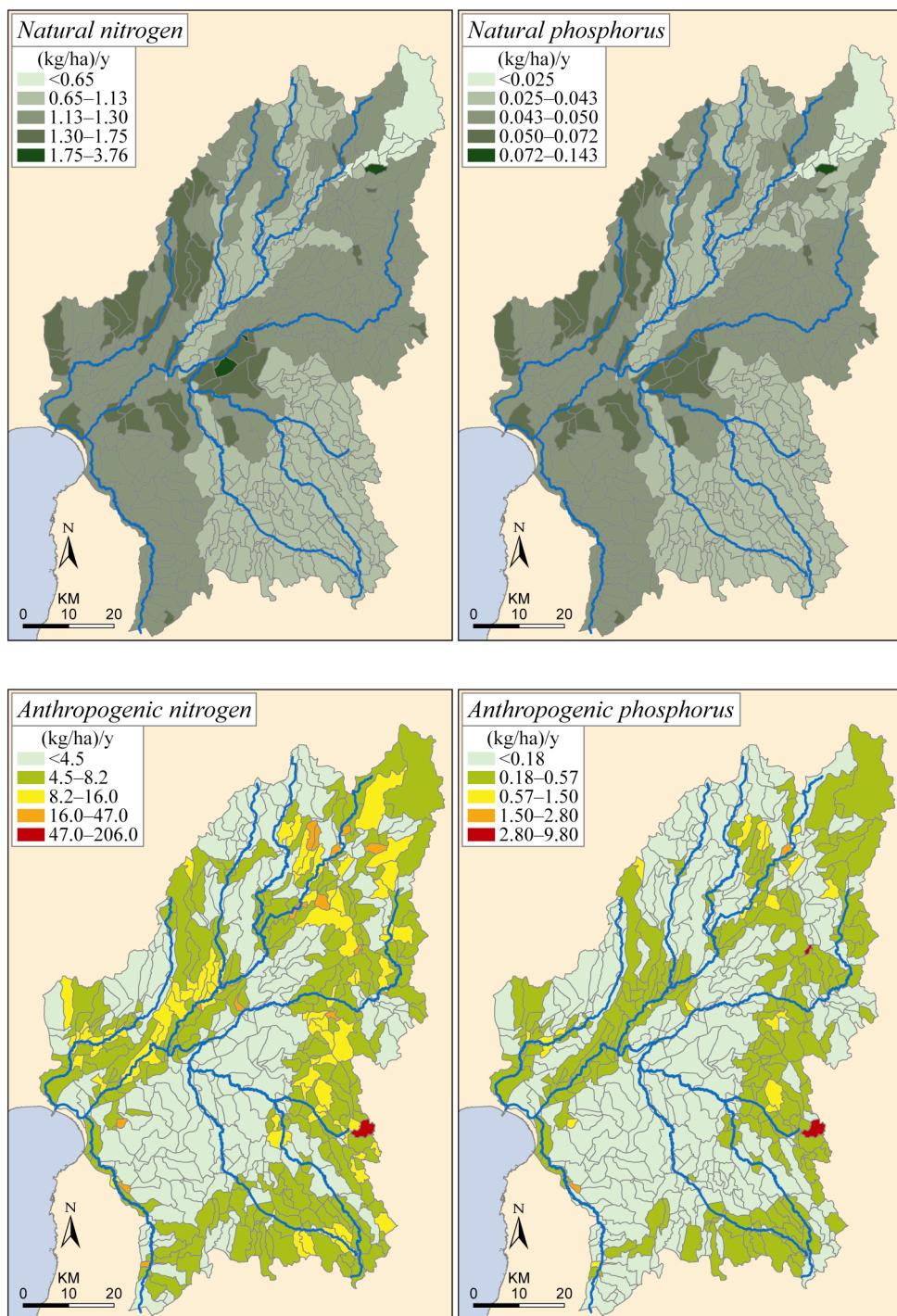


Fig. 4. Modelled natural and anthropogenic portions in nutrients runoff.

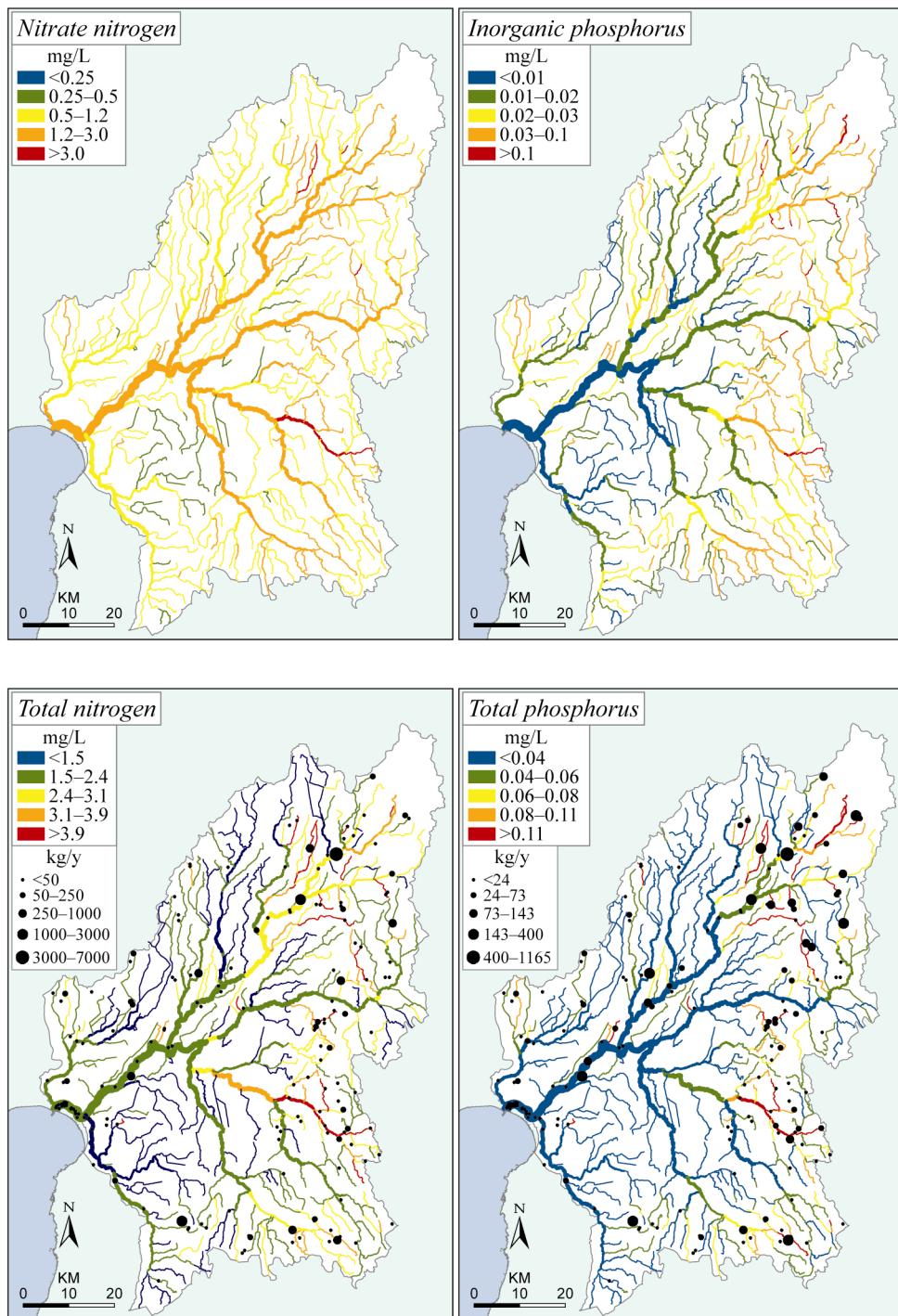


Fig. 5. Modelled nutrients in the Pärnu River.

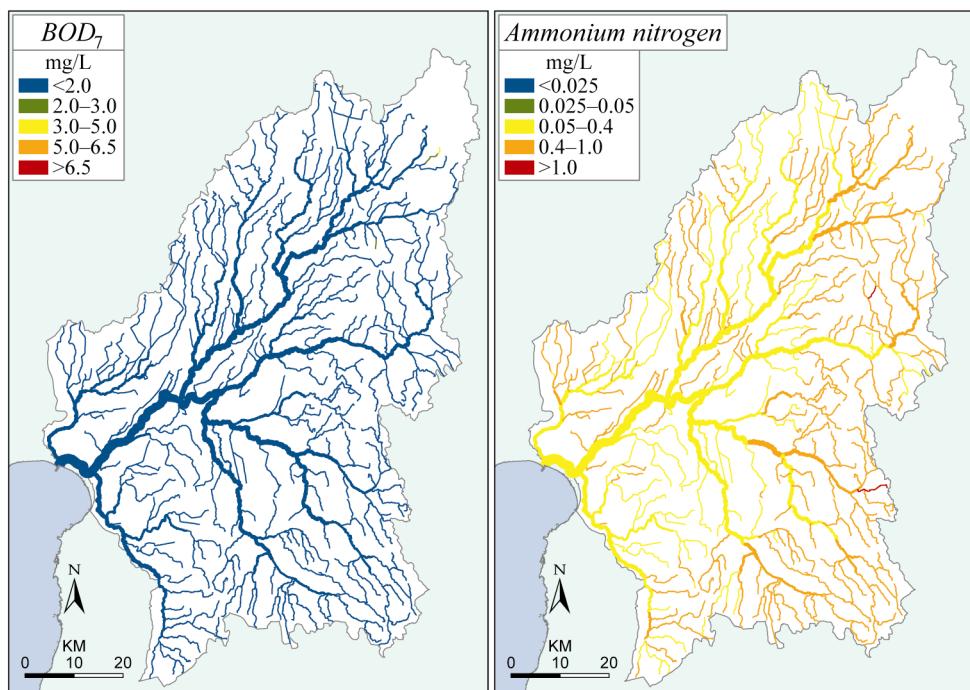


Fig. 6. Modelled BOD₇ and NH₄-N in the Pärnu River.

Application area

The model system was applied for the Pärnu River. The Pärnu River is the second longest river in Estonia with a length of 143 km. Its basin (6911 km^2) consists of the most prevalent landscapes in Estonia. The upper reaches of the Pärnu River and its tributaries flow through the best agricultural lands in Estonia. Near the town of Paide the landscape changes radically. There are large mire systems and extensive forests in the river basin downstream from Paide. The total population in the basin of the Pärnu River is 189 100, of whom ca 56% (105 500) live in towns. There are 637 villages and 11 towns in this river basin. The majority of the villages are small. The largest town is Pärnu (51 400). Others with more than 5000 inhabitants include Viljandi and Paide. The river's daily runoff is measured at nine hydrological stations and the water quality parameters are monitored at nine hydrochemical stations in the basin of the Pärnu River. All these data are stored in the EEIC database. Figure 2 shows the land use and location of animal farms, major towns, and main rivers in the basin.

RESULTS AND DISCUSSION

For calculations the Pärnu river system was divided into 1.7-km segments. The total number of segments reached 1948, which enabled to receive comprehensive information about the water quality status in the entire river basin. Several problems emerged in automatic generation of the model structure. For instance, the current elevation map is available only with a 10-m vertical resolution. This is insufficient for the generation of accurate river slopes for every calculation segment. A more precise elevation map is needed for the automatic creation of the calculation scheme for the river system. In some cases rivers pass through small lakes or reservoirs. This was another problem as the QUAL2K is not customized for lake calculations. The problem was solved by adjusting retention times for the corresponding calculation segments.

The calculations were carried out based on the data from the year 2005. Some common features of the modelled area are presented in Table 1.

The models run ca 10 min using a PC to calculate the whole basin of the Pärnu River.

The output of the Wennerblom model is the total amount of nitrogen and phosphorus generated by any given sub-basin in a year. The calculated land-based nitrogen and phosphorus runoff from the sub-basins of the Pärnu River is presented in Figs 3 and 4. The anthropogenic fraction is prevailing in the total nutrients runoff. The enormously high anthropogenic nitrogen and phosphorus values in one of the south-eastern sub-basins are caused by a giant farm in the vicinity of Viljandi with approximately 100 000 pigs. It is obvious that such a pollution source needs more accurate calculations, which would also take into account additional information about how the manure is handled. In general the

Table 1. The basin of the Pärnu River: common descriptive features of the modelled area

Descriptive feature	Value
Total number of modelled rivers, streams, and ditches	273
Total length of all streams	3257 km
Total area of arable land	2346 km ²
Total area of forests	3318 km ²
Total area of wetlands	353 km ²
Max height in modelled area	118.5 m (Pandivere)
Min height in modelled area	0 m (Pärnu bay)
Flow rate in rivers	Average of year 2005
Number of hydrological stations (bases for flow rates)	9 active stations
Number of modelled sub-basins	542
Number of point sources	169
Number of modelled river segments	1948
Max segment length	1.7 km

results of the Wennerblom model showed quite large variation in nutrient concentrations from different sub-basins, emphasizing the need to keep a rather detailed structure of land-based pollution models.

Land-based pollution sources are unevenly distributed in river basins. Since nutrients from diffuse sources take part in chemical and biological processes, their exact input locations need to be determined. The model results depend on whether the inflow from diffused sources along the river is uniform or variational.

The Wennerblom model output was used as the input data for the QUAL2K model. The QUAL2K model results are presented in Figs 5 and 6, where the modelled nutrients, BOD₇, and NH₄-N are shown.

The Pärnu, Halliste, and Reiu rivers were selected for the comparison of model results with measured data (Figs 7–9). The calculations were made with annual mean runoff conditions, therefore the measured data were selected from the period when flow rates in the monitoring stations were close to the calculated flow rates. The comparison demonstrates acceptable agreement between model results and observed data.

For illustrating the difference between the model output and the measured data in all monitoring stations, four graphs were created (Fig. 10). The x-axis represents the model output of nutrient concentrations sorted in ascending order. The y-axis represents measured concentrations. The diagonal solid line represents exact agreement between modelled values and measured data. In the case of total phosphorus and PO₄ there is a weak agreement between the model results and measured data. This can be attributed to the poor correlation between the phosphorus concentration and river flow rate. The correlation between the nitrogen concentration and river flow rate is better. Therefore the model results are compatible to measured data in the case of total nitrogen and NO₃. Neither is a perfect match, but since steady-state model results were compared to momentary measurements such difference is to be expected.

Estimating water quality

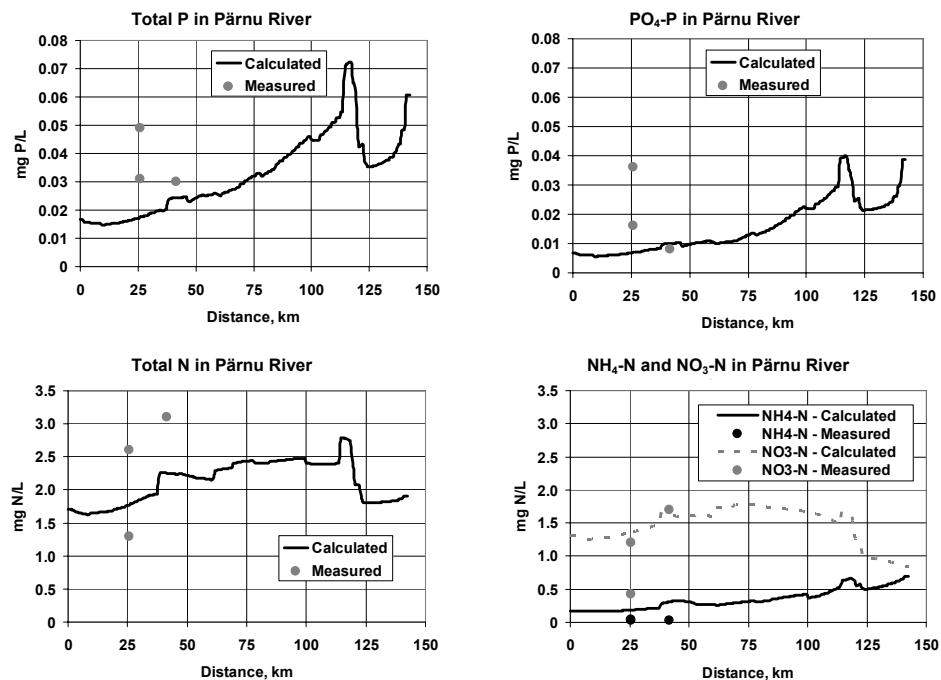


Fig. 7. Comparison of model results and monitoring data in the Pärnu River.

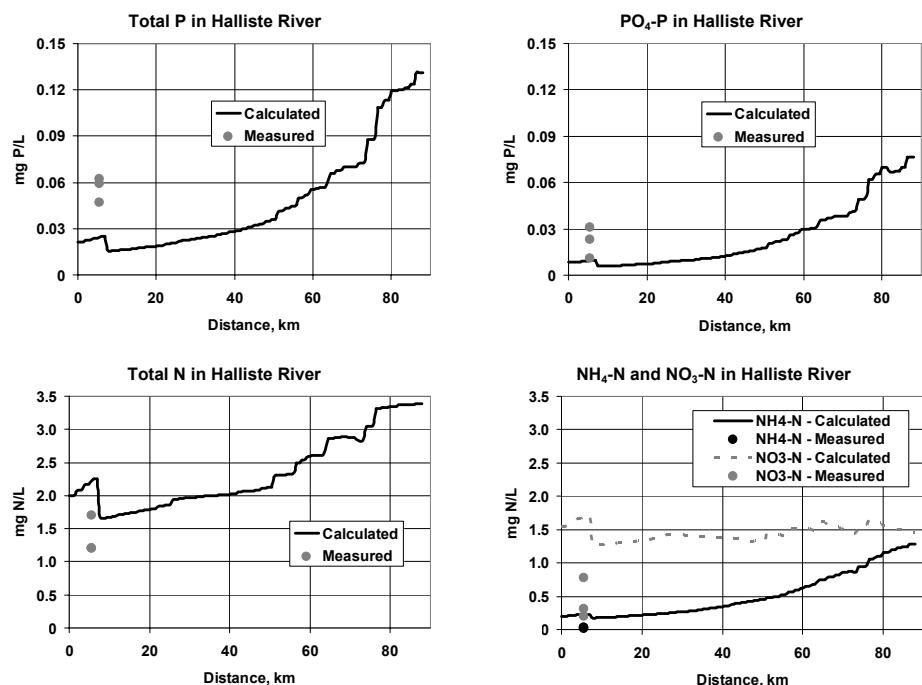


Fig. 8. Comparison of model results and monitoring data in the Halliste River.

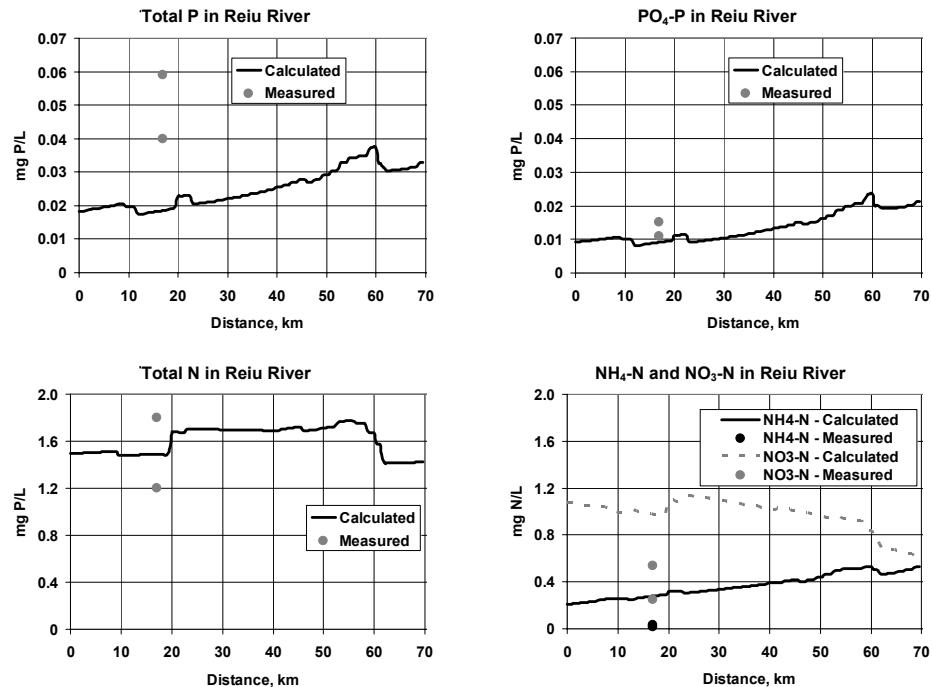


Fig. 9. Comparison of model results and monitoring data in the Reiu River.

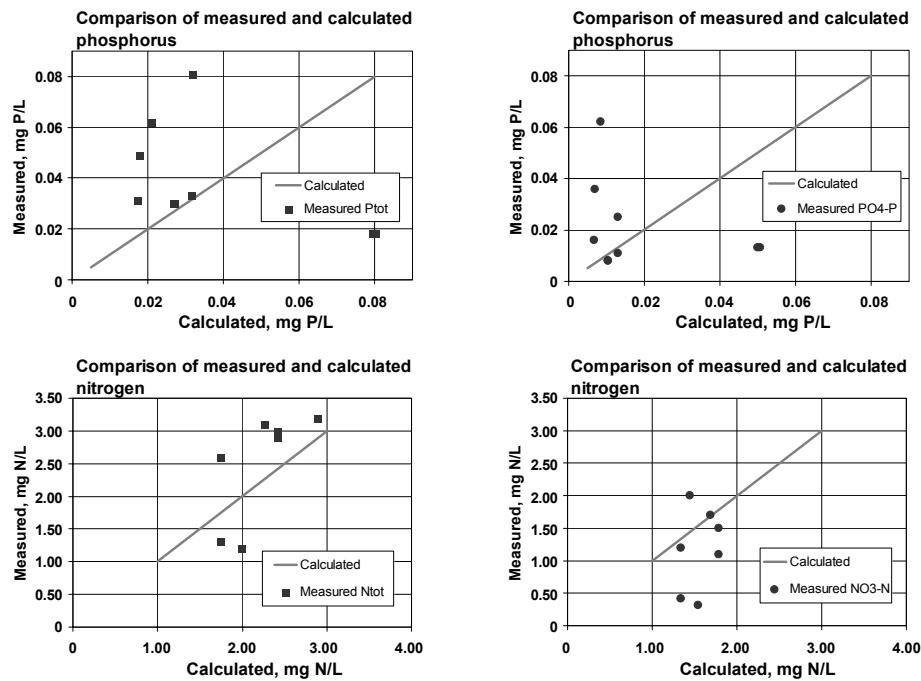


Fig. 10. Comparison of model results in all monitoring stations.

CONCLUSIONS

In this work an attempt was made to help decision-makers to evaluate the chemical state of a river basin. The major outcome is a tool that uses a database for initializing the models. The selected models were QUAL2K for river water quality simulation and Ålvborg–Wennerblom for diffused pollution estimation. The case study of the basin of the Pärnu River shows that the strength of this tool lies in its ability to offer comprehensive information about a large region. It presents the estimated diffused pollution from every sub-basin and demonstrates the influence of point sources describing the distribution of pollution along the river. For further development of the tool it is necessary to specify the nutrient runoff coefficients for Estonian conditions.

The tool enables the combination of different models and allows:

- automatic formation of a model calculation scheme (QUAL2K);
- automatic estimation of river flow rates in every segment (QUAL2K);
- linking of the models with databases (automatic assimilation of up-to-date data for the models input and storing the calculation results).

The majority of Estonian rivers are small and low in water. The results of test application show that land-based pollution can be very unevenly distributed and it is often the main supply of nutrients to these rivers. The division into many small sub-basins is recommended for the modelling of river water quality in Estonia.

Because of the shortage of data it is essential to use models that do not need detailed input data for the assessment of the water quality in large river basins. A high synergy can be achieved by combining the advantages of different models.

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Andmebaasidega rajanev veekvaliteedi modelleerimine

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On käsitletud valgala veekvaliteedi hindamiseks loodud tarkvaralist vahendit ja selle rakendamisvõimalusi. Valgalas toimuvate protsesside modelleerimiseks on kasutatud kaht mudelit. Hajureostust arvutatakse Wennerblomi mudeliga, mis võimaldab eristada looduslikke ja inimtekkelisi koormusallikaid. Veekvaliteeti piki jõge arvutatakse ühedimensioonilise QUAL2K mudeli abil. Mudelite koostöö on lahendatud selliselt, et Wennerblomi väljundit kasutatakse QUAL2K sisendina. Loodud tarkvara ühendab mudelid andmebaasidega, võimaldades nii mudelite otsest alglähtestamist, tulemuste salvestamist kui ka visualiseerimist. Süsteemi rakendati Pärnu jõgikonnas, kus saavutati rahuldag mudeli tulemuste ja mõõtmisandmete kokkulangevus. Kokkuvõtlikult võib tödeda, et loodud vahend võimaldab tulemuslikult kasutada riikliku seire andmeid ja nende abil hinnata valgala keskkonnaseisundit.