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Model based on dimensional analysis for prediction of nitrogen and phosphorus concentration in the River Laborec

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Abstract

The main aim of this paper is to develop a model for pollutant concentration prediction in a stream. The developed model that determines nitrogen and phosphorus concentrations in a river is based on a dimensional analysis. Applications of dimensional analysis to water quality modelling are presented, pointing out possibilities of applying this methodology in water quality research. We investigate how dimensional analysis can be applied to water quality modelling and which benefits it can bring to researchers in this area. The models were developed, calibrated and evaluated using measured data from the River Laborec in eastern Slovakia.

1 Introduction

In recognition of the adverse impacts of pollutants and the need for integrated water management, the EU has introduced a series of Directives aimed at reducing nutrients in aquatic systems (Wade et al., 2002b). The Water Framework Directive (2000/60) demands new approaches for managing and improving surface and groundwater quality across the European Union, with emphasis shifting from chemical towards ecological water quality standards. There are also older Directives aimed at reducing the impact of nitrogen and phosphorus pollution, which include the Nitrate, Habitat and Waste-water Treatment Directives. Since many EU policies aim to control nutrients in river systems, there is a need to understand the combined result of their implementation. The recent emphasis on integrated catchment planning and unifying EU directives has led to considerable research interest in the study of river systems. In particular, the pursuit of models and modelling frameworks capable of predicting water quality across ranges of spatial and temporal scales has provided key motivation. Recent European initiatives include the Land Ocean Interaction Study (LOIS) (Jarvie et al., 1998; Wade et al., 2002b); the Large Scale Processes in Ecology and Hydrology (LSP) project (Neal et al., 1997; Langan et al., 1997) and Integrated Nitrogen in European Catchments (INCA)

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project (Wade et al., 2002a). INCA is a model that links hydrological behaviour, the microbiological processes controlling nitrogen transformation and multiple sources of nitrogen inputs to catchments in eight European countries (Jarvie et al., 2002b; Kaste and Skjelkvale, 2002; Langusch and Matzner, 2002a,b; Rankinen et al., 2002, 2006; Whitehead et al., 1998a,b, 2002). Enhanced availability of phosphorus and nitrogen is a cause for eutrophication of water bodies. There are many studies focusing on nutrient loads in rivers (Beaujouan et al., 2001; Butturini and Sabater, 2002; Cosby et al., 1997; Goolsby et al., 2000; Jarvie et al., 2002a; Johnes, 1996; Neal et al., 1997, 2006; Pieterse et al., 2003; Le et al., 2010; Wade et al., 2001; Wang and Lewis, 2009; Ruiz et al., 2002a,b). Several investigations have examined trends in nitrogen and phosphorus concentrations. Certain decreases in nutrient concentrations have been found in recent years in Swedish agricultural rivers (Ulén and Fölstrer, 2007), Latvian rivers (Stålnacke et al., 2003) and Slovakian rivers (Bendíková, 2004). This is most evident in areas where agricultural activities and use of fertilisers has decreased. Mainly human activities have increased the loads of total nitrogen and total phosphorus in running waters, and this may have a serious impact on their ecological quality.

European management strategies have tended to address single issues (e.g. diffuse or point sources) or particular regions (e.g. upland or lowland areas). However, it is recognised that the nutrient status of river systems reflects the combined contribution of sources: fertiliser inputs, atmospheric deposition and sewage discharges (Wade et al., 2002a). Superimposed on these anthropogenic inputs, an integrated management approach is required (Langan et al., 1997). In particular, such an approach is needed to assess the likely impacts of land management and climatic change on EU river nutrient concentrations and loads (Wade et al., 2002a). The importance of this is acknowledged in the United States of America, where an integrated approach is being implemented through permit trading between diffuse and point source polluters (EPA, 1999). There is no clear-cut distinction between point sources or diffuse sources (non-point sources) (Chapman, 1996). The major point sources of pollution to fresh waters originate from the collection and discharge of domestic waste waters, industrial wastes or certain agricultural activities, such as animal husbandry. Most other agricultural activities, such as pesticide spraying or fertiliser application, are considered as diffuse sources. In general, with increasing discharge point sources of contaminants are diluted, whereas diffuse sources show increased concentrations. In order to predict the pollutant concentrations in rivers it is necessary to model water quality. There are various mathematical models for water resource systems, as mentioned for example in Straškraba (1994), Rauch et al. (1998), Somlyódy et al. (1998); or Borah et al. (2003).

During the past decades several models which predict the concentration profiles after a discharge of pollutants in a river have been developed. Application of these models to a river leads to discrepancies between predicted and measured concentration profiles.

Dimensional Analysis is a well-known methodology in physics, chemistry and other traditional engineering areas. In its simplest form, dimensional analysis is used to check the meaningfulness of a set of equations (dimensional homogeneity). In the last century dimensional theory has been profoundly investigated: its highest achievement is the Buckingham theorem (or pi-theorem), which states that any equation modelling a physical problem can be rearranged in terms of non-dimension ratios, thus limiting the variables to be handled, and especially enriching the inner physical knowledge of the studied phenomenon (Miragliotta, 2010).

A model that predicts nitrogen and phosphorus concentrations in a river has been developed and is presented here. The developed model that determines concentrations of pollutants in a water stream is based on dimensional analysis. The fundamentals of modelling pollutant prediction in a water stream consist in derivation of function dependency from expressed non-dimension arguments. Non-dimension arguments are stated from variables which influence the occurrence of pollutants. From this function dependency it is possible to obtain concentration values of a pollutant in a water stream. In general this dependency has exponential status. Its transformation to a logarithmical coordinate system renders it equivalent to linear status, which makes working with the model easier and makes it simpler to determine the parameters of linear status. A model for prediction of nitrogen and phosphorus concentrations in a water

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stream has been developed for the River Laborec in eastern Slovakia. The differences between the model described in this paper and measured concentrations are also discussed. The use of dimensional analysis for water quality modelling is a new approach here.

2 Material and methods

The model describing pollutant concentration in a water stream is based on the formation of non-dimension arguments π_i from the stated variables influencing the pollutant concentration. Their valuable feature is that in all existing systems of units they have the same numerical size and they have no dimension. Formation of the model consists in derivation of functional dependence from the expressed non-dimension variables, which in general always has exponential character. Transformation of this function into logarithmic coordinates gives it linear character, which makes working with the model easier and enables the parameters of the linear function to be determined (Čarnogurská 1998, 2000; Mäsiar and Kamenský, 2001; Vilčeková and Šenitková, 2009).

The most important part for the model development is selection of appropriate variables. For determination of pollutant concentration in a water stream using dimensional analysis it is essential to state the parameters which characterize the water stream, and which may be measured (Zeleňáková and Švecová, 2006):

- Flow Q [$m^3\,s^{-1}$], or mass flow Q_m [$kg\,s^{-1}$],
- Catchment area F [m^2],
- Velocity of water in the stream υ [$m\,s^{-1}$],
- Temperature of water T_w [K],
- Temperature of air T_a [K],

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– Pollutant concentration C_i [kg m^3].

All the given variables are presented in basic dimensions, which is the condition for dimensional analysis application.

The general relation among the selected variables, which can affect the pollutant concentration, can be put down in the next form in order that each parameter is considered with the same dimension

$$\phi(Q_\mathrm{m}, F, \upsilon, T_\mathrm{w}, C_i, T_\mathrm{a}) = 0. \tag{1}$$

The created dimensional matrix-relation (Eq. 3) has the rank of matrix $m = 4$ and its lines are dimensionally independent from each other. From $n = 5$ independent variables at matrix rank m, it is possible to set up $i = n - m$ of non-dimension arguments.

$$\begin{array}{c|ccccc|}
 & Q_\mathrm{m} & F & \upsilon & T_\mathrm{w} & C \\
\mathrm{m} & 0 & 2 & 1 & 0 & -3 \\
\mathrm{s} & -1 & 0 & -1 & 0 & 0 \\
\mathrm{kg} & 1 & 0 & 0 & 0 & 1 \\
\mathrm{K} & 0 & 0 & 0 & 1 & 0
\end{array}. \tag{2}$$

The following equation is valid

$$\pi_i = Q_\mathrm{m}^{x_1} \cdot F^{x_2} \cdot \upsilon^{x_3} \cdot T_\mathrm{w}^{x_4} \cdot C_i^{x_5} \cdot T_\mathrm{a}^{x_6}. \tag{3}$$

Selection of the unknown parameter is done twice $x_1 = 1$; $x_1 = 0$. For the system of two vectors, for non-dimension arguments, the following is finally valid

$$\begin{array}{ccccccc}
 & x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \\
\pi_1 & 1 & -1 & -1 & 0 & -1 & 0 \\
\pi_2 & 0 & 0 & 0 & -1 & 0 & 1
\end{array}. \tag{4}$$

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The sought dimensional homogeneous function in non-dimension form is

$$\phi(\pi_1, \pi_2) = 0. \tag{5}$$

After adjustment is valid

$$\phi\left(\frac{Q_\mathrm{m}}{F \cdot \upsilon \cdot C_i}, \frac{T_\mathrm{a}}{T_\mathrm{w}}\right) = 0. \tag{6}$$

Non-dimension argument π_1 contains the unknown parameter C_i, so this argument can be expressed as a function of argument π_2 in the form

$$\pi_1 = \phi(\pi_2). \tag{7}$$

The real course of the dependence (Eq. 7) of non-dimension arguments π_1 to π_2 in logarithmic coordinates is depicted in Fig. 2. The relation (Eq. 7) between independent argument π_2 and dependent argument π_1 can be defined by the exponential equation

$$\pi_1 = A \cdot \pi_2^B. \tag{8}$$

The regression regression coefficients can be calculated by the method of the least squares. After completing the relation TSI (Eq. 8) the relation characterizing the pollutant concentration in a river is obtained in the form

$$\frac{Q_\mathrm{m}}{F \cdot \upsilon \cdot C_i} = A \cdot \left(\frac{T_\mathrm{a}}{T_\mathrm{w}}\right)^B. \tag{9}$$

After modification the following equation is valid

$$C_i = A^{-1} \cdot T_\mathrm{a}^{-B} \cdot \upsilon^{-1} \cdot F^{-1} \cdot Q_\mathrm{m} \cdot T_\mathrm{w}^B. \tag{10}$$

Relation (Eq. 10) represents the model of the pollutant concentration in water stream. The model is valid for each pollutant, but it is necessary to calculate new regression coefficients A and B.

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2.1 Study area

Prediction of pollutant concentration in a water stream was performed in the River Laborec in Eastern Slovakia – Fig. 1. Water quality in this river has been monitored in river stations over a long period.

Required data were obtained from the Slovakian Water Management Company in Košice and the Slovak Hydrometeorological Institute in Košice.

Data sources

For modelling water quality in a water stream, as mentioned above, it is essential to know the parameters that influence water quality. Modelling based on dimensional analysis was applied. The relevant parameters are flow of water in the river (discharge), its catchment area, velocity of water in the stream, temperature of the water, temperature of the air and measured concentrations of the pollutant – nitrogen and phosphorus.

Data measured during the course of eight years, from 1995 to 2002 (12 values in a year) were used. Statistically processed data are presented in table 1 (one average value for each month over nine years). It is possible to develop a model for prediction of the pollutant in each river station where the input parameters are known. This paper presents the development of the model for the prediction of nitrogen and phosphorus concentrations at the river station Laborec-Ižkovce, at river kilometre 10.30.

3 Results and knowledge achieved

According to the known relevant parameters (from Table 1) the non-dimension arguments were stated. Figure 2 depicts the dependency of non-dimension arguments for nitrogen concentrations and Fig. 3 depicts the dependency of non-dimension arguments for phosphorus concentrations.

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The regression equation for nitrogen concentrations takes the form

$$y = 0.0039 \cdot x^{13.805} \tag{11}$$

and for phosphorus concentrations

$$y = 0.1868 \cdot x^{9.7892} \tag{12}$$

where y is independent argument π_1, x is dependent argument π_2.

The regression coefficients are then

A = 0.0039 (for nitrogen) and 0.1868 (for phosphorus),

B = 13.805 (for nitrogen) and 9.7892 (for phosphorus).

Pollutant concentrations were calculated according to Eq. (10), the developed model for prediction of pollutant concentration in a water stream; on the basis of measured input parameters and determined regression coefficients.

3.1 Model calibration

In Tables 2 and 3 the values of measured and predicted nitrogen and phosphorus concentrations are compared.

Uncertainty was calculated from the equation

$$\sigma = \frac{1}{n} \cdot \sum_{i=1}^{n} \frac{\left| c_{\text{measured}} - c_{\text{predicted}} \right|}{c_{\text{measured}}} \cdot 100. \tag{13}$$

3.2 Model verification

The developed models were verified for the next eight years – 2003–2010.

Comparison of measured and predicted nitrogen concentration in river is shown in the Fig. 4. Figure 5 depicts measured and predicted phosphorus concentration in Laborec River-Ižkovce river station.

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There were 96 measured and predicted values of nitrogen and phosphorus concentrations, as shown in Figs. 4 and 5. The average uncertainty was calculated according to Eq. (13) and the result was 31.33 % for the verified nitrogen model and 32.30 % for the verified phosphorus model. This is appropriate for modelling such phenomena as concentration of pollutants in a water stream. Negligible differences between measured and predicted concentrations are allowable. Differences occur for a variety of reasons, e.g. rainfall, influence of source of pollution, outflow of waste water. The big differences, as can be seen in Fig. 4 (measurement 42) could occur because of an error in taking a sample or in determining concentration. The proper variables for dimensional analysis also have to be used.

4 Discussion

The Buckingham π theorem is the core to dimensional analysis. This theorem describes how every equation involving n variables can be rewritten as an equation of $n-m$ dimension parameters, where m is the number of fundamental dimensions used. Furthermore it provides a method for computing these non-dimension arguments from the given variables. This provides a method for computing sets of these parameters from the given variables, even if the form of the equation is still unknown. The choice of non-dimension arguments is not unique: Buckingham's theorem provides a way of generating sets of non-dimension arguments (Zeleňáková and Čarnogurská, 2008).

It is clear that input data and selection of relevant parameters are the most important factors in predicting pollutant concentration in a water stream.

The choice of variables is influenced by the ability of an organisation to provide the facilities, and trained operators, to enable the selected measurements to be made accurately. Full selection of variables must be made in relation to assessment objectives and specific knowledge of each individual situation (Chapman, 1996).

The flow and velocity of a stream can significantly affect its ability to transport pollutants. Thus measurement of velocity is extremely important in any modelling. It enables

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the prediction of movement of pollutants within water streams. Water bodies undergo temperature variations along with normal climatic variations which occur seasonally. The temperature of surface waters is influenced by latitude, altitude, time of day, time of year, the flow and depth of the water body. Temperature affects also the physical, chemical and biological processes in rivers and, therefore, the values of many variables. The size of the catchment area controls the fluctuations in water level, velocity and discharge. The final selection of variables is made in relation to the assessment objectives.

Calculated uncertainty can be considered as an acceptable factor. The differences between measured and predicted nitrogen and phosphorus concentrations can occur because the selection of relevant parameters did not involve all the effects which pollutant concentration depends on. The next reason may be that the measured values are not exactly stated.

5 Conclusions

Agriculture and urban activities as has been mentioned above are major sources of nitrogen and phosphorus in aquatic ecosystems. These non-point inputs of nutrients are difficult to measure and regulate because they derive from activities dispersed over wide areas of land and are variable in time due to effects of the weather. Nutrient enrichment seriously degrades aquatic ecosystems and impairs the use of water particularly for drinking, industry, agriculture and recreation (Carpenter et al., 1998).

Water quality modelling can be a valuable tool for water management since it can simulate the potential response of the aquatic system to such changes as the increase in nutrient levels. The use of generally available models should be verified with data obtained from the river for which its use is being considered.

River quality models seek to describe the spatial and temporal changes in constituents which are of concern. This paper presents the possibility of pollutant concentration prediction in a water stream. The developed model is based on dimensional

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analysis, which is applied in engineering and water management to understand physical situations (Čarnogurská, 2000).

The main objectives of the present research are to investigate options for estimating the parameters of the models and to develop a usable model for concentration prediction in a stream.

The variation of pollutant concentrations in surface waters stimulates broad interest among scientists and researchers in the field of water pollution control. Models are useful in defining the nature of water systems and the relations among their components. Some models have been developed and verified for the River Laborec in eastern Slovakia. Based on the study results, it can be concluded that the water quality prediction model is highly applicable to this regulated large river for water quality management.

This approach could be used to calculate the parameters for other similar streams, if the coefficients in the equations were similar. Alternatively, further work would be needed to explore how these coefficients vary between streams.

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Table 1. Values of relevant arguments and measured nitrogen and phosphorus concentrations.

	Q_m kg s^{-1}	F m^2	υ m s^{-1}	T_a K	T_w K	C_N kg m^{-3}	C_P kg m^{-3}
1	37 343.80	4.468×10^9	1.340	272.60	277.60	0.002419	4.00×10^{-5}
2	30 409.00	4.468×10^9	1.258	270.34	277.58	0.002162	3.88×10^{-5}
3	85 402.00	4.468×10^9	1.788	278.04	279.58	0.002345	3.94×10^{-5}
4	66 219.60	4.468×10^9	1.650	281.20	281.10	0.002230	3.88×10^{-5}
5	80 227.20	4.468×10^9	1.792	290.56	289.16	0.001894	3.62×10^{-5}
6	33 690.60	4.468×10^9	1.316	295.90	291.54	0.001727	3.52×10^{-5}
7	42 386.00	4.468×10^9	1.356	295.06	294.78	0.003409	3.92×10^{-5}
8	35 370.60	4.468×10^9	1.334	297.58	296.80	0.001372	3.52×10^{-5}
9	30 224.80	4.468×10^9	1.264	293.78	292.72	0.001351	3.60×10^{-5}
10	54 306.20	4.468×10^9	1.434	287.96	287.66	0.001279	3.88×10^{-5}
11	57 952.25	4.468×10^9	1.510	285.03	283.98	0.001820	4.52×10^{-5}
12	30 954.40	4.468×10^9	1.266	276.00	280.18	0.001761	4.78×10^{-5}

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Table 2. Values of non-dimension arguments, predicted concentrations, uncertainty for nitrogen.

	$C_{measured}$ $kg\,m^{-3}$	π_2 –	π_1 –	$C_{predicted}$ $kg\,m^{-3}$	σ %
1	0.002419	0.981988	0.002052	0.002055	15.03
2	0.002162	0.973917	0.001670	0.001998	7.59
3	0.002345	0.994492	0.003341	0.002958	26.13
4	0.002230	1.000356	0.002705	0.002292	2.75
5	0.001894	1.004842	0.003431	0.002403	26.92
6	0.001727	1.014955	0.001885	0.001197	30.68
7	0.003409	1.000950	0.002610	0.001770	48.06
8	0.001372	1.002628	0.002061	0.001467	6.92
9	0.001351	1.003621	0.001939	0.001305	3.36
10	0.001279	1.001043	0.002903	0.002142	67.44
11	0.001820	1.003698	0.003123	0.002093	15.03
12	0.001761	0.985081	0.001754	0.001727	1.96

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Table 3. Values of non-dimension arguments, predicted concentrations, uncertainty for phosphorus.

	$C_{measured}$ kg m^{-3}	π_2 –	π_1 –	$C_{predicted}$ kg m^{-3}	σ %
1	4.000×10^{-5}	0.981988	0.155932	3.989×10^{-5}	0.27
2	3.880×10^{-5}	0.973917	0.139434	3.751×10^{-5}	3.32
3	3.940×10^{-5}	0.994492	0.271322	6.041×10^{-5}	53.32
4	3.880×10^{-5}	1.000356	0.231500	4.792×10^{-5}	23.50
5	3.620×10^{-5}	1.004842	0.276793	5.116×10^{-5}	41.33
6	3.520×10^{-5}	1.014955	0.162776	2.652×10^{-5}	24.65
7	3.920×10^{-5}	1.000950	0.178467	3.710×10^{-5}	5.34
8	3.520×10^{-5}	1.002628	0.168587	3.096×10^{-5}	12.04
9	3.600×10^{-5}	1.003621	0.148660	2.765×10^{-5}	23.18
10	3.880×10^{-5}	1.001043	0.218448	4.491×10^{-5}	15.76
11	4.520×10^{-5}	1.003698	0.189409	4.420×10^{-5}	2.20
12	4.780×10^{-5}	0.985081	0.114483	3.394×10^{-5}	29.00

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Nitrogen and phosphorus concentration in the River Laborec

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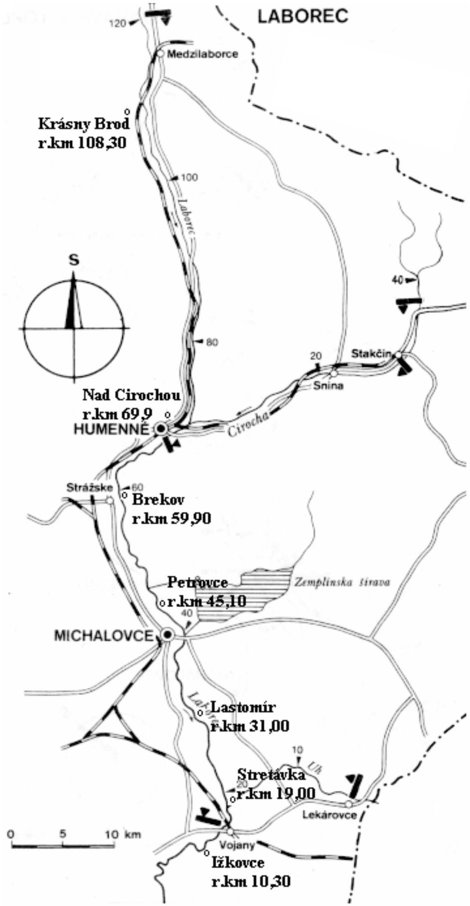

Fig. 1. River Laborec – Eastern Slovakia.

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Nitrogen and phosphorus concentration in the River Laborec

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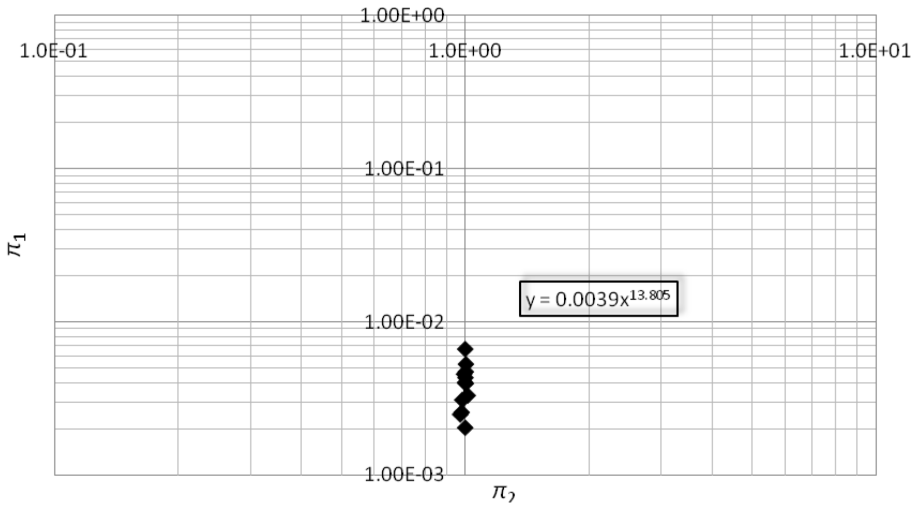

Fig. 2. Non-dimension arguments and regression line in logarithmic coordinates for nitrogen concentrations.

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Nitrogen and phosphorus concentration in the River Laborec

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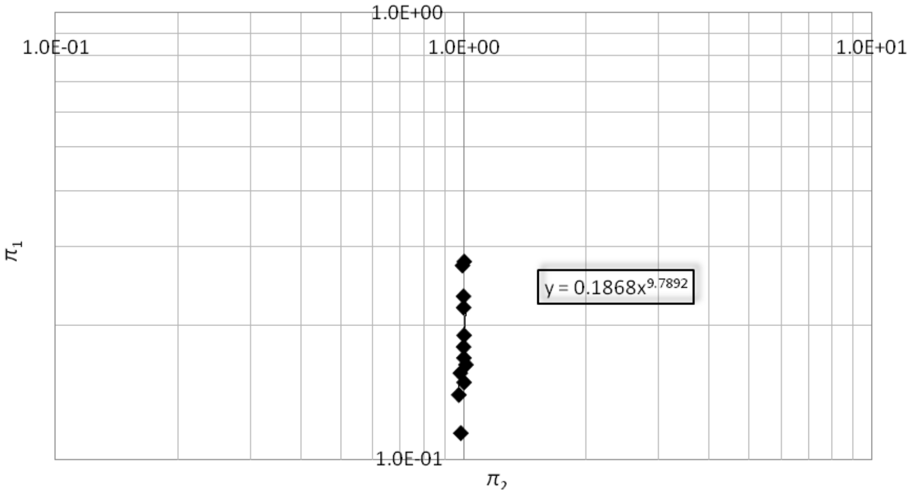

Fig. 3. Non-dimension arguments and regression line in logarithmic coordinates for phosphorus concentrations.

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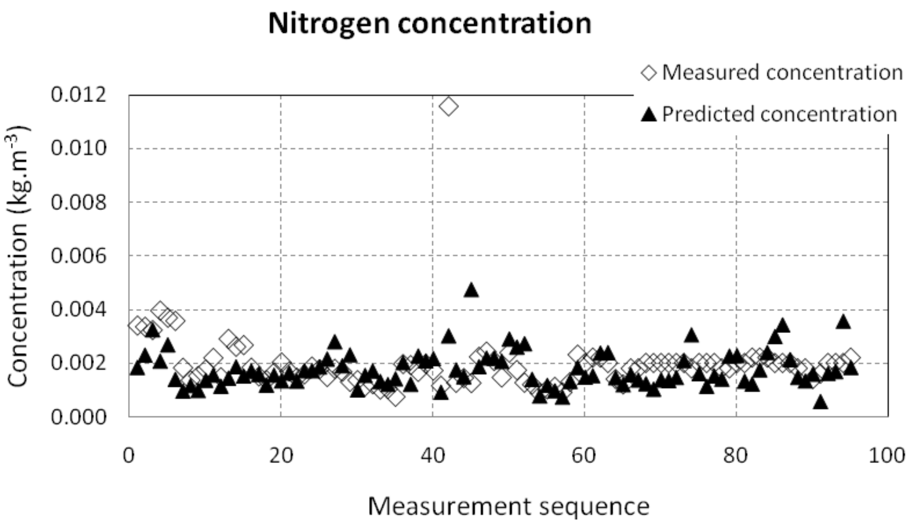

Fig. 4. Comparison of measured and predicted nitrogen concentrations in river.

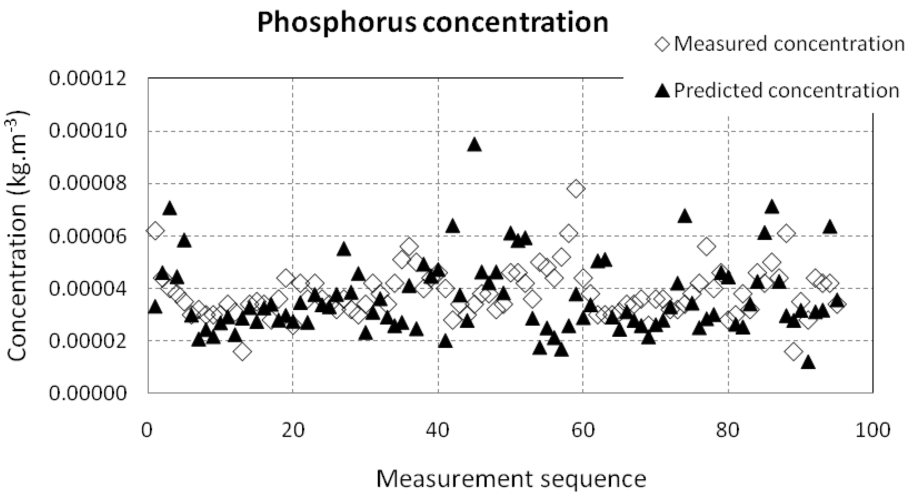

Fig. 5. Comparison of measured and predicted phosphorus concentrations in river.