Pollution source localisation in a simple river branch

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Abstract. Modern water quality monitoring system enables detailed observation of water quality parameters. Measured data of the pollution concentration time course can be consequently used for determination of the pollution source position. Paper deals with the solution of inverse problem, where the pollution source and its position is determined from the pollution concentration time courses obtained in the monitored watercourse profile located downstream. The main objective of this paper is to introduce the simple method for solution of pollution spreading inverse task and to analyse the accuracy of this method application. For this aim, a software tool was developed. Two different analytical solutions equation for this tool were used. For the method verification, data from a field tracer experiment were used. The experiment was performed on a lowland channel with extensive vegetation coverage. The test results show, that the proposed procedure is feasible, the numeric solution is reliable, stable and fast. Results of tests have also indicated the impact of used analytical solution equation and also the software tool ability to fit the specific conditions in the real streams.

1. Introduction

Water resources are considered as one of the most valuables resources on the Earth, so the protection of water resources is currently one of the priority roles declared by human society [1]. Water and its accessibility currently represent one of the basic limits of society development [2] [3].

Almost all water management activities are more or less focused on water resources protection, both the water quality and quantity. Recently, a lot of different types of pollution are occurring in surface water. In addition to classical pollution (such as organic, inorganic substances, metals, etc.), research is currently focusing on micropollutants (substances often occurring in small amounts, but still capable of highly negatively influence the biocoenosis in hydrosphere). These are different species and groups of substances such as organic or inorganic various specific substances with toxic, persistent or bio-cumulative properties, eventually various residues or metabolites of these substances [4].

Pollution gets into surface waters by different ways, but a very dangerous case is the uncontrolled leakage of pollutant substances into surface waters (industrial or ecological accidents). In some cases, such leakages may be classified as an environmental crime, where the pollution originator is very often unknown. The identification of the source of pollution is then often a complicated and hard-to-implement task, given the efforts of the originator of the accident to conceal the event and avoid legal sanctions.

From hydrodynamic point of view, the determination of the pollution source is very problematic due to the high degree of uncertainty. In the case of a watercourse network, the situation is much more complicated and it is very difficult to determine the point of discharge by conventional procedures. The task can be easier in the case of a simple reach of a watercourse.
A significant help in detecting the accidental pollution sources can be the water quality monitoring systems, which can monitor not only the occurrence and total amount of monitored substances, but also the concentrations time course of these substances in the monitored watercourse profile. Such water quality monitoring system enables the use of the obtained data of the pollution time course to determine the position of the pollution source. Accuracy of such detection procedure depends on various factors. The main objective of this paper is to analyse the accuracy of the localisation task solution depending on method, used in forward modelling in the localisation procedure.

2. Theoretical background

2.1. Dispersion

One-dimensional advection–dispersion equation (ADE), describing these processes in flowing fluid, can be written in form [5]:

\[
\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} = D_x \left( \frac{\partial^2 C}{\partial x^2} \right) + M_s
\]

where \( C \) is the substance concentration (kg.m\(^{-3}\)), \( v_x \) is the fluid velocity in longitudinal direction (m.s\(^{-1}\)), \( D_x \) is the coefficient of dispersion in the longitudinal direction (m\(^2\) s\(^{-1}\)), \( t \) is the time (s), \( M_s \) express the substance sources or sinks (kg m\(^{-3}\) s\(^{-1}\)), \( x \) is the distance in the longitudinal direction (m).

In our experiments, we use for so-called forward modelling a numerical simulation model based on two different 1D analytical solutions of the ADE (Eq. 1) valid for simplified conditions and instantaneous solute input. The first one was in form [6]:

\[
C(x, t) = \frac{M}{2A \sqrt{\pi D_x t}} \exp \left( \frac{-(x - \bar{v}t)^2}{4 D_x t} \right)
\]

where \( M \) is the substance mass (kg), \( A \) is the cross-sectional area of the watercourse (m\(^2\)) and \( \bar{v} \) is the average flow velocity in the watercourse.

The second analytical solution was in form [7]:

\[
C(x, t) = \frac{M}{A \sqrt{D_x G_{MB} t}} \exp \left[ \frac{x - \bar{v}t}{\sqrt{D_x G_{MB} t}} \right] - \exp \left( \frac{x - \bar{v}t}{\sqrt{D_x G_{MB} t}} \right)
\]

where \( D_x G_{MB} \) is the coefficient of dispersion in the x-axis direction (m\(^2\) s\(^{-1}\)) according the Gumbel model approach [7].

The simplified conditions include steady and uniform fluid flow and a conservative substance, lateral and vertical homogeneous concentration of transported substance (which is the necessary condition for 1D application of ADE) as well as streambed of prismatic shape.

Zero substance concentration in watercourse (initial and boundary conditions) and no lateral inflows are assumed. If conditions for the zero initial and boundary conditions cannot be met, it is necessary to divide the watercourse into parts (sections) [8].

2.2. Inverse task

The inverse task – pollution source detection based on the monitoring results is not a typical water quality modelling task. Classical modelling solves changes of water quality at known initial and boundary conditions in the direction of water flow. It means, that amount, release time and time course of discharged pollutant and hydraulic conditions are known. Then the model results are time courses of pollutant concentrations in individual watercourse profiles. In this way, majority of current simulation models are conceived - they can simulate the pollution spreading (and its concentration) forwards, i.e. in the flow direction.

Solution of the inverse problem, where the source of pollution is unknown and should be determined by the pollution concentration time courses in the monitored watercourse profile, is addressed by several authors [9], [10], [11].

This task is often understood as a mathematical and academic problem. Published theoretical solutions are relatively difficult to implement in practice. In doing so, the inverse task -representing
determination of the pollution source position in a simple reach of the watercourse is often simplified. As it was mentioned above, in the case of a watercourse network, the situation is much more complicated ([12], [13]).

Determining the position of the pollution source based on the substance concentration time course has no direct and deterministic solution. It is necessary to mention, that besides the unknown location of the pollution source, the flow rate of the pollution as well as the time course of the pollution concentration at the source place are also unknown.

Each solution gives only probable or approximate results, and therefore solutions based on probabilistic models and simple analytical solutions of advection-dispersion equation (ADE) are often published [14]. These solutions, however, do not consider the specific hydromorphological and hydraulic conditions of river, canal or sewer networks (network topology, time-varying hydraulic states in the network).

Because of that, the paper also analyses the influence of two analytical solutions used for the governing equations of so-called forward modelling in the inverse task solution procedure on accuracy of pollution source localisation prediction. For this reason, we used a simple model, based on a simulation-optimisation approach, as defined by [15].

In our approach, we use a simulation model for the concentration prediction from the possible sources locations. This simulation model is coupled with an optimization procedure.

The optimization algorithm is designed to determine the source location as guiding variable, searching the minimal sum of square differences between measured and modelled data. The optimisation function (procedure) is based on the minimal sum of square error (SSE) between the measured and modelled values, i.e.

\[
SSE = \sum_{t=t_1}^{t=t_2} (c_{m,t} - c_{s,t})^2
\]

where SSE is the sum of square error, \(t_1\) is the time when the measurement starts (s) and \(t_2\) is the time when the measurement ends (s), \(c_{m,t}\) is the measured value (concentration) at the time \(t\) \((kg.m^{-3})\), \(c_{s,t}\) is the simulated value in the time \(t\) \((kg.m^{-3})\).

The optimisation procedure for the distance of the pollution source is based on the searching of the minimum value of the objective function (SSE). All the parameters of this search procedure (minimum and maximum distance, distance step \(\Delta x\)) have to be defined by the user. To ensure to find a global optimum solution (global minimum of the SSE function), the whole range of possible source distances is scanned with defined distance step and the SSE function values are computed in corresponding distances. This will avoid the convergence of the search procedure to some local minimum of the SSE function, which differs from the global minimum of the SSE function. The found minimal value of the SSE function and the corresponding distance \(x_{min}\) is then used as a central point of the next iteration cycle of the localisation procedure. In this next step, the previously described scan procedure is repeated with redefined parameters - the minimal distance is redefined as the point left from the \(x_{min}\) value \((x_{min} - \Delta x)\) and the maximal distance is the point right from the \(x_{min}\) value \((x_{min} + \Delta x)\). This procedure is repeated until a defined precision is achieved.

3. Methods

3.1. Field experiment

Field tracer experiments were performed at the Malina stream in August 2018. The Malina stream is a modified watercourse, typical for the lowland areas in south – west Slovakia. The originally constructed cross-sectional profile of this watercourse was changed by vegetation occurrence (Figure 1).
Figure 1. Picture of the Malina channel close to the village Zohor (GPS 48.3348, 16.9674).

Measured discharge during the experiments in the examined watercourse reach was $0.18 - 0.19 \text{ m}^3 \text{s}^{-1}$. The measured water level slope was $0.19\%$, the total length of the experimental stream reach was $3510 \text{ m}$, the measured average velocity was very low due the vegetation – $0.045 \text{ m.s}^{-1}$. The shape of the watercourse in the examined reach can be considered prismatic. The average depth was $0.54 \text{ m}$ with a maximum value of about $0.66 \text{ m}$, the watercourse width was about $7.5 \text{ m}$ [16]. The coefficient of dispersion ($D_x$), evaluated by use of Eq. 1 was $1.163 \text{ m}^2 \text{s}^{-1}$, using the Eq. 2 it was $2.57 \text{ m}^2 \text{s}^{-1}$ [17]. These values are consistent with measurements performed on similar channels [18]. The experiments were performed in the middle of growing season, so there was a high degree of aquatic vegetation occurrence in the channel. There was submerged vegetation in the central part of the channel, as well as approximately up to one meter of emerged vegetation on both banks. Both kinds of vegetation (submerged in the stream bed and emerged along the stream banks) formed so-called dead zones. The time course of the tracer concentrations (pollutogram) during the tracer experiment is shown on Figure 2.
3.2. Inverse task experiments
For the evaluation of the inverse task procedure, own software tool was developed using the MS Visual Basic software as an integrated environment for the software coding. The developed software tool followed the principles described in the theory part of this paper.

For the inverse task procedure parameters summarized in Table 1 were used.

| Parameter                        | Unit      | Value   |
|----------------------------------|-----------|---------|
| Min. distance                    | [m]       | 0       |
| Max. distance                    | [m]       | 10000   |
| Nr. of division intervals        | [+]       | 10      |
| Required precision               | [m]       | 0.1     |
| Dispersion coefficient in Eq. 1  | [m².s⁻¹]  | 1.163   |
| Dispersion coefficient in Eq. 2  | [m².s⁻¹]  | 2.576   |
| Average velocity                 | [m.s⁻¹]   | 0.045   |

4. Results and discussion
Progress of the inverse task solution procedure for described two analytical solutions (Eq. 2, Eq. 3) is shown on the Figure 3.

As it can be seen on this figure, the effective solution was achieved approximately after 10 iterations; further iterations were performed to achieve the required numerical accuracy (less than 0.1 m in subsequent iteration steps). The whole iteration process (20 iterations) takes approximately 14 seconds on a PC.

The resulting pollution source distance using Eq. 2 was 3710.033 m (relative error 5.7%), using Eq. 3 was 3570.354 m (relative error 1.72%). The concentration time courses for the optimal solutions (computed pollution source distance) and its comparison with the measured values is demonstrated on the Figure 4. The relatively big difference in the results achieved according the Eq.2 and Eq.3 is caused by the better fit of the Eq. 3 in case of specific conditions in the examined stream (vegetation, extensive presence of dead zones), as demonstrated on Figure 4. This better fit also allows more precise
determination of the dispersion coefficient from tracer experiments (Figure 2) and consequently better fit in the pollution source localisation procedure (Figure 4).

It is necessary to mention, that the usability of the Eq. 2 and Eq. 3 is limited to the conditions, described in the part 2.1. The main assumptions comprise instantaneous pollution entry, prismatic streambed, steady uniform flow and conservative pollutant. In real conditions, the most problematic assumption is the instantaneous pollution entry and occurrence of aquatic vegetation.

Figure 4. Optimal solution (best fit with measured data) of the computed and modelled concentration time courses in the pollution source localisation procedure (according corresponding equation).

5. Conclusions
Analysis of accuracy of used inverse task solution method results was examined and described in this paper. In this scope, a simple iterative procedure for the numerical inverse task solution (pollution source localisation) was developed. The accuracy of the inverse task procedure was tested with two different approaches – analytical solutions of the ADE equation, defined as Eq. 2 and Eq. 3. The applicability and feasibility of the proposed procedure was tested and verified by the experimental tests based on real field experiments. Values of hydraulic parameters used in numerical tests were taken from measured values from these field experiments.

Results of analysis show, that the proposed procedure is feasible, the numerical solution is reliable, stable and fast. The relative error of the computed distance of pollution source was 5.7% (by Eq. 2 application) and 1.72% (by Eq. 3 application), respectively. The difference in the results- the distance error (method precision) shows, that it is also very important to use in the inverse tasks suitable and appropriate models. It does not automatically mean a mathematically and computationally complicated model, but a model adapted to local conditions. Therefore, we will focus our research on the conditions of use of the models with regard to their abilities and the boundary conditions in which they will be applied.

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