Monitoring based localisation of pollution sources

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Abstract. Water quality modelling is currently very effective and important tool in context of the task to ensure the required quality of water resources, respectively, to achieve (maintain) good water status according the Water Framework Directive (2000/60/EC). This paper analyses the current status in numerical modelling of pollution dispersion in streams and use of some modelling approaches for the inverse task. Inverse task means a modelling technique, which is focused on the localisation of unknown pollution source (typical common models or equations are rather focused on the pollution spreading simulation, whereas the pollution source location is known). Paper offers an idea of such inverse task solution. It is based on the known pollution concentration time courses or it can be based on the results of the on-line monitoring of the specific water quality parameters as well. For the application of inverse tasks in conditions of real streams and rivers a large number of various requirements and conditions in specific river should be considered, i.e. the non-prismatic river bed, occurrence of dead zones, dispersion rate etc. Paper also describes the first version of the software for solving inverse tasks and preliminary experiences of using this software.

1. Introduction

Currently, in water quality modelling practice are prevailing tasks, for which initial and boundary conditions are known and the model is solving pollution concentration in downstream direction. It is typical for the tasks of this type, that the quantity, the time course of discharge and concentration of emitted pollutant, as well as the hydraulic conditions in the stream are known parameters. The result of such modelling tasks is a time course of pollutant concentration in the particular stream locations. The overwhelming majority of existing simulation models is conceived exactly for that purpose - their focus is on pollution modelling, i.e. such models are able to simulate the pollution spreading (concentration) only downstream and these models require to enter strictly all the initial and boundary conditions (discharges, concentrations of the pollutant).

However, in practice converse problems may occur: pollution concentration time courses in specific locations are known (e.g. based on the on-line monitoring), but pollution discharge location, as well as the pollution time course are unknown. The objective of this task is to determine the location of pollution outlet (localization task) as well as the overall mass and time course of pollution concentration. This type of task can occur in case of accidental pollution, if the origin of the pollution is not known, or even with intentional act that can be defined as an offense or crime (illegal business - production of various substances, illegal wastewater outlets etc.).
2. The theoretical part - inverse tasks

As mentioned above, most of the current models are focused on modelling the pollution spreading in downstream direction. The inverse task – pollution outlet localization on the basis of known monitoring data is referred as a “inverse problem”. It should be noted, that such inverse task has not always an unequivocal solution, but the result is usually few plausible solutions. Inverse problem is currently far more understood as a math problem, verified practical applications or commercial software that would deal with the inverse problem are not currently known. In the scientific literature a number of works dealing with these issues can be found, e.g. [1,2,3], but in general it can be stated, that the presented methods and solutions are relatively complex and complicated, and in the practice there is a large number of limitations and restrictions.

Based on such definition, we believe that the general and exact analytical solution of inverse problem is not possible: every solution, using any method will generate only the approximate solution or estimate, or will generate a particular - most probable solution among number of plausible solutions (simulations), the results of which are in best coincidence with monitored data.

Overall, we can divide the solving methods of inverse problems into the following groups:

- **Empirical methods**, e.g. [4,5].
- **Simple methods** based on simplified analytical solutions of the advection – dispersion equation. These methods focus on the simulation of the individual (potential) pollution incidents, using for simulation simple analytical solutions and consequently comparing of simulation results with measured (monitored) data. The advantage of these methods is their simplicity, the possibility of governing equations modifications for the specific conditions (e.g. occurrence of dead zones, etc.). Their disadvantage is the necessity of large amounts of numerical simulations, thereby long computation time.
- **More complex procedures** focused on the inverse numerical simulation in upstream direction. From a mathematical point of view these methods are more accurate, but also more complicated and more difficult to code [1,2].

For practical solution of an inverse problem following assumptions are often taken:

- The pollution is conservative.
- There is a simple pollution source, which means, the stream is defined as a simple river section without tributaries and lateral inflows.

Pollution conservatism means that examined pollution is not subject to any physical, chemical or biological (biochemical) processes that take place in the stream. It is obvious that absolutely conservative substance in reality does not exist, so it is realistic to require that ongoing changes are not random and fast, but rather slow and steady (slow changes - assume that the concentration changes are reflected in the order of days or in a longer time period).

In case of a not conservative pollutant (polluting substance is a subject of physical, chemical or biological processes), inverse problem could be solved by similar processes, but decomposition (concentration decrease) of the substance should be considered in the simulation.

Assuming single pollution source means, that in the investigated river section is only one, spatially invariant source of pollution, which emits pollution directly into the river (not into tributary). Another assumption is a single river section, i.e. the deployment of monitoring sections will clearly determine the river section, where the pollution enters into the river. This simplifies the inverse task to localise the source of pollution in a particular river section without tributaries. The monitoring results in downstream end of the examined river section are the basis for the source localisation.

For proper operation of such localization tool the key task will be the determination of the exact hydraulic parameters (discharges, cross sectional area, velocity) in the stream. The task will be even more complicated by the fact, that the hydraulic parameters may vary depending on the hydrological situation (discharge) in the river.

3. Proposed method of pollution sources localization
The project VEGA Nr. 1/0805/16 focuses on methods for practical solutions of inverse problems, i.e. localisation of pollution sources. The following section describes proposed method, which will be further developed and improved.

The general solution method is based on the computation of simulations for (all possible) boundary conditions:
- Different distances between the source and the monitoring profile.
- For the various alternatives of pollution concentrations time courses.

Simulation results of each of these alternatives will be compared with data monitoring - simulation that will best match the monitored data can be considered as probable solution. The simulation itself is based on simplified analytical solution, which (as discussed further in this paper) should be further modified and developed.

In principle, it as a “brute force” method. The risk of such method is in the computer time, necessary to carry out a huge number of numeric simulations. This computational time will depend on the length and time steps, which implies the total number of simulations needed. Under the term ‘adjustable length interval’ can be a distance between points understood, where the pollution outlet is assumed (discretisation of stream section length), but also number of river sub-sections, where individual definition of constant hydraulic parameters is assumed. Simulation time step is used for time discretization of the pollution inflow. Decreasing the time step \( dt \) increases the number of possible pollution inflow (time courses) variations and thus the simulations count. A key factor in the choice of the time step \( dt \) is variability of pollution inflow. The choice of time step will be one of the key tasks and we assume to perform huge amount of numerical tests to obtain the optimal value of the time step \( dt \).

Another assumption is the time invariability, proportionality principle and the superposition principle. Time invariability means that the pollution input causes always the same time course of the pollution concentration (pollutogram) independently of pollution entry in other time steps. In other words, if the pollution entry will shift the timeline with time step \( dt \), then the resulting pollutogram will also move the time \( dt \), and does not change its shape or size.

The proportionality principle means that the system (river) response is linearly proportional to the input, i.e. if the concentration will increase twice, then the output (concentration pollutogram) will be also two times bigger.

The last assumption is that the output concentrations, obtained by transformation of unit inputs, can be added together (superposition principle). This assumption is generally valid, if the concentrations are low, whereas in high concentrations, close to the saturation concentration, this assumption is not valid. However, if we assume that the monitored concentrations are sufficiently low, it is possible to apply the superposition principle of full concentration range. A summation of transformed particular pollution time courses then determines the final resulting concentration time course (pollutogram).

The definition of the parameters needed for the pollution transport simulation in a river has to reflect the fact, that the basic hydraulic parameters, characterizing the flow in a stream, are variable in time, depending on the current hydrological situation. It is therefore necessary to define the flow area, the average flow speed, eventually the discharge characterized as a function of the water depth. This principle is common in hydrological measurement profiles and hydrology service is generally able to provide such data. Inverse task should be then solved with such specific hydrological parameters, which were monitored during event (accident).

Another problem is the spatial variation of hydraulic parameters. In solving inverse problems, we assume spatial discretization - the distribution of the investigated river branch into several sections in which we can assume constant hydraulic conditions (flow velocity, depth, cross-sectional area...). The resulting pollution pollutogram will be then simply the result of the partial transformation of the input pollutogram in particular sub-sections of the investigated river branch.

Risk of the proposed inverse problem solution procedure is the sensitivity of the method to various influences, such as hydraulic stream parameters and the precision of the numerical description of the dispersion process in real streams, especially the presence of dead zones, singularities, etc. This results
from the fact that the solution of the given inverse task is determined simply by the similarity of measured and modelled pollutograms. This clearly demonstrates the need for further research and improvement of modelling procedures focused on dispersion processes in conditions of real streams.

4. Results

For project implementation a SW tool was developed (working title Locator Of Pollution Source - LOPS), according to the principles described in the previous section. The basic input parameters of the SW are the longitudinal length step dx, the time step dt, sensitivity of the pollution entry (number of intervals), the searching procedure starting length (ending length is the river branch length). Besides this it is necessary to enter the monitored pollutogram, as well as the basic hydraulic parameters of the river section (currently only one section is implemented) – average flow velocity, cross sectional area and dispersion coefficient.

The first version of the LOPS successfully passed the tests with virtual (modelled) data and was preliminary tested also on real data. The test with real data and various input pollutograms were performed on a small mountain creek. Beside this was the LOPS also tested on real data from earlier tracer experiments on lowland stream, but only with instantaneous pollution injection, thus the tests should be extended with different pollution input conditions on different streams types.

The test results show, that for each field experiment can be achieved at least one good pollution input localisation, with the minimal best fit length error up to 10 percent. The problem is, that this best result was achieved with various and heterogeneous combination of SW tool computation parameters and it is not possible to determine, which parameter combination is the best one. Decrease of time or length steps, as well as increase of the SW tool input sensitivity generally does not guarantee better localisation results. A very big results heterogeneity was achieved for the pollutions source localisation length. Average localisation error (about 30%) is typically 10-30 times bigger, compared to the minimal error (less than 10%), the maximal localisation error is as well very high, typically higher the 50%.

Tests of sensitivity confirmed two important factors, that significantly improves the results of the LOPS computational procedure – pollution input sensitivity parameter and the average flow velocity. The first parameter is in fact the number of intervals, in which is pollution input unit divided to. Higher numbers of intervals lead to better results, but on the other hand significantly extend the computational time. For the second parameter – the average flow velocity - almost linear dependency of the LOPS results was confirmed and this parameter seems to be the crucial one.

During the LOPS SW test was another issue found: the localization results are based on the search for the best fit between the monitored and modelled data, but the current (first) version of the LOPS routine is not able to represent some special particular problems, e.g. occurrence of dead zones in the investigated stream, so there is significant difference between the pollutograms. Therefore, one of the main tasks in the future should be to use (or to develop) simple computational routines, based on analytical solutions, which incorporate modelling of particular dispersion problems and irregularities.

5. Conclusions

Systems for water quality on-line monitoring in rivers have a great potential for the control, eventually management of water quality in rivers. They enable operational monitoring and control of discharges of specific substances. In case of water quality accidents (acute and extraordinary deterioration of water quality) such systems can provide the information necessary for operational measures, as well as to provide data for models to simulate a prediction of water quality in real time. Specific problem related to the on-line monitoring is the polluters identification. This type of task can occur in case of accidental pollution, where the polluter is not known, as well as cases of operational or explorative monitoring of water bodies. As noted above, general and accurate analytical solutions of inverse problems are currently not known, using any method always gives us only the approximate solution or an estimate, eventually the choice of a particular solution – the most probable case from a number of
possible simulations, the results of which fits best with monitored data. In this paper we also describe the pollution source localization SW – LOPS. It represents one of possible approaches how to solve the inverse problem, which is universal and simple. The preliminary tests of the LOPS show various SW tool accuracy and overall results heterogeneity. Sensitivity analysis of the SW tool has shown high correlation between the SW tool results and the velocity input value, so it means that the river flow velocity is the crucial parameter for the SW localisation tool accuracy.

Another crucial issue will be to use (or to develop) simple computational routines, based on analytical solutions, which are able to simulate particular dispersion problems and irregularities to achieve better coincidence of measured and modelled pollutograms and thus better localisation results.

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