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Convolution integral vs. finite difference for the inverse problem of detection of a contamination source in rivers

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ABSTRACT

The identification of the source of a contamination in a river, either accidental or intentional, is of extreme interest for both the technical and scientific communities. To this aim, the recent development of innovative wireless sensors, coupled with computational tools capable of analyzing big data almost in real-time, offers novel opportunities to develop early warning systems for the protection of surface waters. In the present paper, a novel approach is discussed, in which the unknown location and magnitude of pollution are looked through the solution of an inverse problem, based on the experimental detection of a contamination pattern and on a suitable mathematical model of the governing system. Provided that the geometry, the hydraulic parameters and the boundary conditions are sufficiently simple, the equations describing the conservation of contaminant mass can be solved formally. On the other hand, for more general conditions there is no alternative to the numerical solution. Benefits and drawback of these two alternatives are analyzed in the present paper for a hypothetical case study concerning the Volturno river reach, close to the city of Caserta in Southern Italy, schematized as a one-dimensional (1-D) steady uniform flow. Namely, the response to the contamination pattern is computed by both the exact solution based on the convolution of the pulse response and the finite difference Crank–Nicolson discretization of the governing equations. The comparison between the two approaches, provides interesting results in terms of effectiveness, computational complexity (central processing unit time) and model limitations, which may be of valuable help in the implementation of an identification network based on smart sensors.

Keywords: Smart sensor network; Surface water; Sensors; Contamination; Water protection

1. Introduction

The serious problem of river contamination is more and more frequent and essentially due to industrialization, rapid population growth and increase in urbanization [1], but also to the use of chemical agents in agricultural practices [2]. These contamination events can also occur accidentally, for example, during the interruption of service of a treatment plant but, unfortunately, in some cases, they occur intentionally as a consequence of non-authorized discharges of wastewaters.

To minimize the contamination risks of surface water, some actions have been adopted to control the anthropic activities both in the industry and in the agriculture. Recently, the 2008/105/EC Directive established a list of 33 priority

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substances requiring special attention concerning water protection, one-third of which are pesticides [3]. Most of the current techniques used for the determination of pollutant concentration, based on sophisticated laboratory equipment, are offline, and thereby unable to provide a desirable quick response to the contamination. Moreover, this equipment can be very expensive. Offline sensors allow only an occasional monitoring of the water quality, but not the identification of the contamination source, which would require several spatially distributed sensors and continuous-in-time measurements. To this aim, online instrumentation that implements standard analytical methods is currently available, even though it is generally expensive, often cumbersome, and it still poses some threats concerning installation and maintenance. Indeed, distributed and continuous-in-time measurements require a widespread sensor network with real-time monitoring that can provide an early warning system able to recognize the contamination source and to alert rapidly the authorities. In other terms, a dense array of low-cost sensors could lead to more protection than just few expensive monitoring stations.

The recent development of biosensors [4–11], based on different technologies – such as on luminescent bacteria, combined with the quantitative measurement of chemical parameters applying standard spectrophotometric/fluorimetric methods, quartz crystal microbalances, fluorimetric methods using specific organic liquid reagents, nanofiber materials with electrochemical techniques, optofluidic jet waveguide, microwave resonator, electrochemical, bio-based electrodes, etc – seems highly promising and able to provide devices for real-time monitoring of critical situations also at low costs [2]. These technologies can be arranged in a sensor network for water early warning, overcoming most of the operational difficulties described above, in which the sensors are the "eyes" of the system.

The threat of accidental contamination of water systems is not new, but in the past few years considerable effort has been devoted to develop mathematical algorithms in support of contamination events in water distribution networks [12]. The detection of the pollution source as the solution of an inverse problem involving contaminant transport in a river is less investigated. Basic concepts can be found in the works by Kirsch [13] and Okubo [14], whereas the interested reader is referred to the paper by El Badia et al. [15] for a detailed statement of the problem. Apart from the inherent difficulties resulting from the ill-posedness of this non-linear inverse problem [16], most of the practical approaches to this problem require the repeated solution of the governing equations describing contaminant transport. From the computational point of view, this requirement may become extremely demanding if discrete methods like finite differences or finite volumes are used.

Starting from the preliminary results reported in [2], in this paper, a novel identification algorithm, based on a parametric method for the contamination inputs, a suitable mathematical model for the contaminant mass conservation and transport, a genetic algorithm for optimization problem and a statistical approach to define the best solution, is proposed.

Within this framework, the present paper explores in detail two alternative approaches to the solution of the contaminant transport equation: the formal solution based on the convolution of the pulse response and the finite difference Crank–Nicolson discretization of the governing equations.

The benefits of the former approach are well known in the literature and have been exploited in the analysis of both single channels [17] and network channel systems [18] under both uniform and gradually varied flow regimes: since no approximation of the time and space derivatives is required, this method does not suffer from the consequences of finite accuracy, like diffusive or dispersive errors [19], which may significantly alter the outcome of the inverse problem. On the other hand, the numerical discretization of the governing equations cannot be avoided if a more sophisticated flow model has to be accounted for: for instance, if flow is inherently two-dimensional (2-D) or three-dimensional (3-D) [18].

The performance in terms of the detection of position, magnitude, duration and time of the contamination for several typical contamination scenarios (CS) is evaluated, considering a hypothetical case study inspired to a river reach enclosed between two sensors.

The paper is structured as follows: in section 2 the methodology for the identification of the unknown contamination source is discussed in detail, starting from the typical configuration of a sensor network in a river. Section 3 discusses the application of the identification algorithm to a synthetic case study and compares the corresponding results of the two approaches. Finally, conclusions are drawn in section 4.

2. Methodology

As proposed in [2], a sensor network can be implemented by disposing an array of B_n sensors along the river, illustrated schematically with an indefinite line in Fig. 1. While the issue of a detailed design of the sensor network is beyond the scope of the paper, we can observe that the river can be split into several reaches, each of which is bounded by two sensors B_s and B_{s+1}. Given the number of sensors, it is possible to limit the space where the contamination may have occurred as the distance between two subsequent sensors. The following identification variables are introduced to

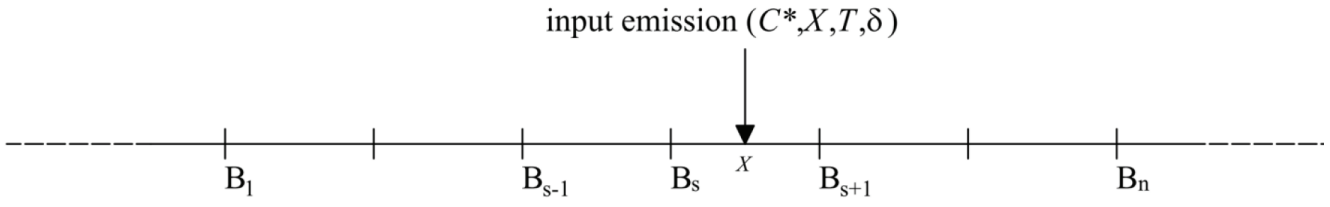

Fig. 1. Identification variables and network layout.

characterize the contamination event: the position along the reach X, the maximum concentration C^*, the lifespan δ and the injection time T.

The methodology proposed is based on the comparison between the measured (in B_s and B_{s+1}) and computed time history of a pollutant concentration in a given monitoring station, in order to identify the most likely position X, magnitude C^*, lifespan δ and injection time T of the contamination.

As far as the modeling of the process concerned, the transport of a conservative pollutant dissolved in the flowing water can be described as an advection–dispersion process and the 1-D equation for a non-prismatic open channel can be written as follows [20]:

$$\frac{\partial}{\partial t}\left(A\cdot C\right)=-\frac{\partial}{\partial x}\left(Q\cdot C\right)+\frac{\partial}{\partial x}\left(A\cdot D\frac{\partial C}{\partial x}\right) \tag{1}$$

where A is the river cross-section area, C the average solute concentration, D the dispersion coefficient, Q is the volumetric flow rate, t is the time and x is the streamwise coordinate. For steady uniform flow, when A, Q, D are constants and the mean velocity $U = Q/A$, Eq. (1) simplifies in:

$$\frac{\partial C}{\partial t}=-U\frac{\partial C}{\partial x}+D\frac{\partial^2 C}{\partial x^2} \tag{2}$$

Furthermore, to take into account the injection of the pollutant in the channel, it can be assumed that the mixing with ambient fluid is complete and instantaneous. Thus, the downstream concentration can be computed as follows:

$$C_D=\frac{C_U\cdot Q+C_p\cdot Q_p}{Q+Q_p} \tag{3}$$

where the C_D is the pollutant concentration just downstream the injection, C_U is the upstream pollutant concentration, Q_p and C_p are the flow rate and the concentration of pollutant, respectively.

The identification process is based on a real-time process driven by analysis of the measures of a couple of sensors in the network, B_s and B_{s+1}. For sake of simplicity, it is further assumed that shape of pollutograph is known: in the following, rectangular and triangular injection laws will be considered. Specifically, neglecting spills as well as phase transformations during the flow, the total mass of contaminant injected in the reach is conserved and it is measured by the downstream sensors B_{s+1}. Based on this information, it is possible to estimate the parameter C^* for a rectangular injection, discharging upstream at distance X with the same total mass measured by the downstream sensor B_{s+1} with a lifespan δ and a time delay T:

$$C^*=\frac{a}{\delta}\int_0^{\delta_m} C_m\cdot dt \tag{4}$$

where δ_m and C_m are the measured lifespan and concentration of pollutant in B_{s+1} and the shape parameter a is 1 for rectangular and 2 for triangular pollutograph, respectively. The identification process is carried out minimizing the following objective function (OF):

$$\mathrm{FO}=\sum_{t=0}^{t_{\max}}\sqrt{\left(C_m(t)-C_i(t)\right)^2} \tag{5}$$

where $t_{\max}$ is the total time of simulation, $C_i(t)$ is the pollutant concentration at time t computed in the downstream section by solving Eq. (2) with a proper method and $C_m(t)$ is the measured concentration at time t. For the minimization of FO (Eq. (5)) a genetic algorithm [21] was used. The identification process is schematically illustrated in the flowchart reported in Fig. 2.

The CS, used as inputs in the comparison, are assumed as a rectangular pollutograph (Fig. 3) and a triangular pollutograph (Fig. 4), whose parameters are the peak concentration magnitude C^*, lifespan δ and time delay T. In detail, four CS have been investigated:

- CS1 – a rectangular pollutograph in a clean reach (i.e., null concentration upstream);
- CS2 – a rectangular pollutograph over a constant upstream concentration C_{in} (measured by sensor B_s);
- CS3 – a triangular pollutograph in a clean reach;
- CS4 – a triangular pollutograph over a constant upstream concentration C_{in} (measured by sensor B_s).

For all of the four CS, the following boundary conditions applied:

$$\begin{cases} C=\text{const} & x=0 \\ \dfrac{\partial C}{\partial x}=0 & x=L \end{cases} \tag{6}$$

in which L denotes the distance between the two sensors.

As far as the solution of the partial differential equation (PDE; Eq. (2)) with boundary conditions (Eq. (6)) is concerned, the exact solution is available for the scenarios CS1 and CS2 [22]. On the other hand, the solution for CS3 and

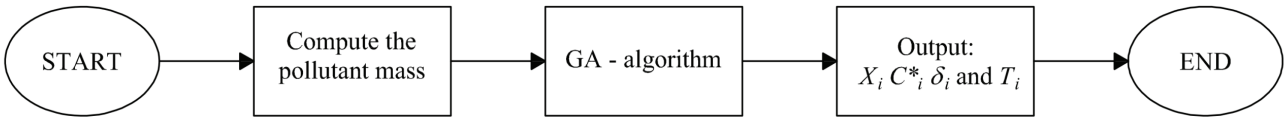

Fig. 2. Flowchart of pollution source identification algorithm.

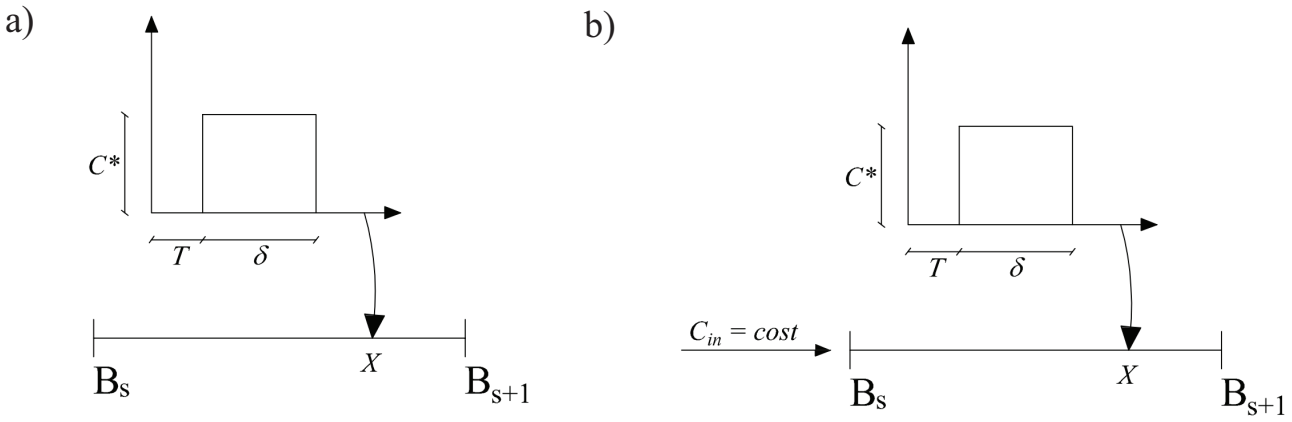

Fig. 3. Two input rectangular emission scenarios CS1 and CS2.

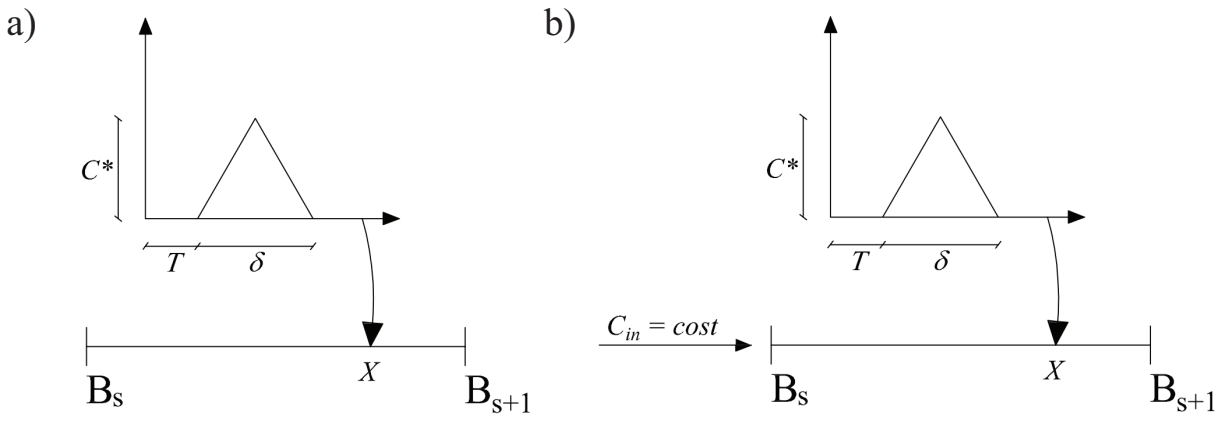

Fig. 4. Two input triangular emission scenarios CS3 and CS4.

CS4 can be formally deduced in terms of an integral expression with the procedure outlined in [22]. Indeed, the instantaneous value of the concentration in a generic cross-section can be computed with the following convolution integral:

$$C(x,t)=\int_0^t Ug(t-\tau)\left[\frac{1}{\sqrt{\pi D\tau}}e^{-\frac{(x-U\tau)^2}{4D\tau}}-\frac{U}{2D}e^{\frac{Ux}{D}}\operatorname{erfc}\left(\frac{x+U\tau}{\sqrt{\pi D\tau}}\right)\right]d\tau \quad (7)$$

in which the convolution kernel (the term in square brackets) represents the concentration in (x, t) in response to a Dirac-delta impulse at (x = 0, t = 0) [15]. Moreover, in Eq. (7) the arbitrary input function, $g(t)$ results from the combination of Eq. (3) with the scenario-specific pollutograph. The convolution integral is easily and efficiently evaluated with a straightforward numerical quadrature.

Alternatively, the PDE (2) with the same boundary conditions described above may be also solved numerically with the Crank and Nicolson finite-difference method [23,24] with spatial and temporal discretization steps denoted as Δt and Δx. It is worth to remark that in this case, Eq. (3) is discretized considering the spatial step Δx containing the injection point.

3. Sample application and results

The comparison between the two approaches, analytical and numerical, has been tested on a synthetic example, already proposed in [2], in which the considered river reach has a length of 10 km, a flow rate Q = 20 m^3/s, mean velocity U = 0.7 m/s and dispersion coefficient D = 10 m^2/s in compliance with hydraulic properties of a typical Italian alluvial river.

The analysis is conducted starting from the parameters of the assigned pollutographs (C_{in}, $C_{pollutant}$, δ, X, T) which are used to generate the synthetic "measured concentration" (MC) in the four scenarios. Their values are reported in Table 1. For sake of simplicity, in the following analysis, the injection time T has been set equal to zero.

Furthermore, the contaminant volume injected in all the four scenarios has been assumed equal to W = 10 m^3. Figs. 5 and 6 illustrate with continuous line the time evolution of the MC for CS 1–4.

In Tables 2 and 3, the identification results are reported, showing the effectiveness of the proposed approach based on the convolution integral (5): in both scenarios, very low values of FO, along with practically the correct value of the

maximum concentration C^*, the position X (with a maximum error of 50 m), lifespan δ and injection time T, have been identified.

As far as the numerical solution of Eq. (2) is concerned, the analysis has been repeated for three values of the space step Δx, assuming at first the value Δx = 28 m, a larger ($2\Delta x$) and a smaller one ($\Delta x/2$). The computational time needed to solve the identification problem is also reported in Tables 2 and 3.

In order to provide a more detailed assessment of the performance of the two approaches, Tables 4–7 report the values of four statistics of the temporal distribution of the MC at the downstream sensor, namely the mean concentration, the standard deviation (S.D.), the skewness and the curtosis.

Table 1
Contamination parameters

	CS1	CS2	CS3	CS4
C_U (mg/L)	0.00	0.30	0.00	0.30
C_p (mg/L)	5×10^3	5×10^3	5×10^3	5×10^3
C^* (mg/L)	2.626	3.218	2.494	3.230
δ (s)	900	900	1,800	1,800
X (m)	3,500	6,000	3,500	6,000
T (s)	0	0	0	0
W (m^3)	10	10	10	10

The previous tables show that the values of the parameters identified through the numerical solution of the governing equations are in worse agreement with the true ones compared with those obtained with the aid of the exact analytical solution. Correspondingly, the FO values are generally larger than those corresponding to the analytical solution.

Moreover, a slight but appreciable dependence of the identification results on the mesh spacing adopted is found. Finally, as far as the computational cost is concerned, the execution time is comparable only for the coarser mesh. The finest resolution considered caused an increase of more than one order of magnitude of the execution time, without any significant increase in the accuracy of pollutograph parameter estimation.

As far as the statistics of time history of the reconstructed downstream concentration are concerned, the analytical ones are found to coincide with the true ones, whereas those based on numerical solution are affected by a mesh-dependent inaccuracy, which in the present example is about 10% for the higher-order statistics.

Finally, the accuracy in the estimation of the maximum injected concentration $C_{p,max}$, based on the results of the

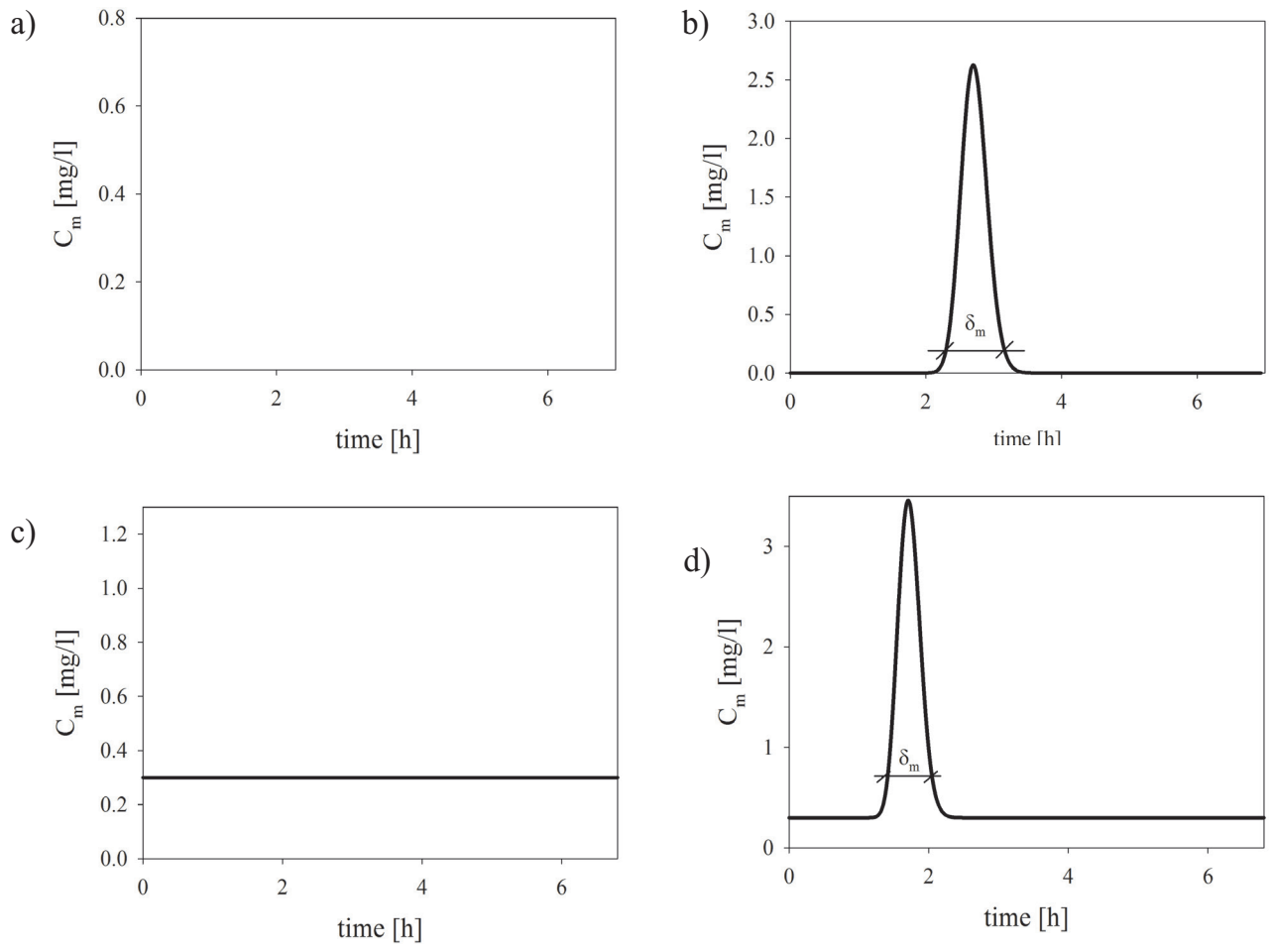

Fig. 5. Measured concentration in B_s and B_{s+1}, respectively, for CS1 (a) and (b); and CS2 (c) and (d).

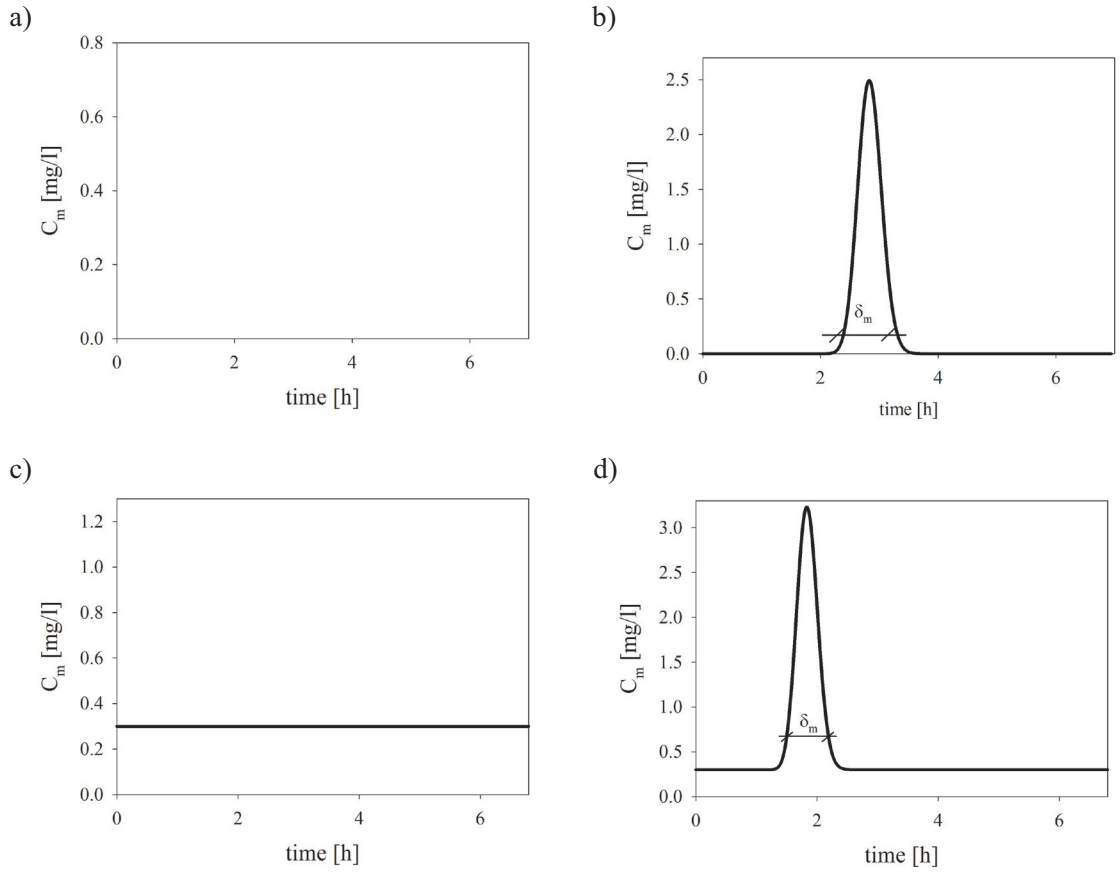

Fig. 6. Measured concentration in B_s and B_{s+1}, respectively, for CS3 (a) and (b); and CS4 (c) and (d).

Table 2
Identification results for CS1 and CS2

		C^* (mg/L)	δ (s)	X (m)	T (s)	Run time (s)	FO
CS1	Analytical	2.627	900	3,500	0	3×10^2	7.13×10^{-12}
	Finite difference [Δx]	2.665	910	3,503	0	6×10^3	190.48
	Finite difference [$\Delta x/2$]	2.667	920	3,498	0	1×10^5	229.10
	Finite difference [$2\Delta x$]	2.652	820	3,495	0	2×10^3	638.92
CS2	Analytical	3.449	914	6,004	0	2×10^3	99.26
	Finite difference [Δx]	3.544	909	5,986	0	3×10^3	76.98
	Finite difference [$\Delta x/2$]	3.532	933	5,987	0	4×10^4	293.36
	Finite difference [$2\Delta x$]	3.547	748	5,983	0	2×10^3	707.92

Table 3
Identification results for CS3 and CS4

		C* (mg/L)	δ (s)	X (m)	T (s)	Run time (s)	FO
CS3	Analytical	2.493	1,800	3,500	0	6×10^2	1.52×10^{-09}
	Finite difference [Δx]	2.494	1,801	3,504	0	8×10^3	9.45
	Finite difference [$\Delta x/2$]	2.494	1,802	3,489	0	5×10^4	126.63
	Finite difference [$2\Delta x$]	2.488	1,718	3,496	0	5×10^3	465.53
CS4	Analytical	3.234	1,800	6,000	0	6×10^2	0.19
	Finite difference [Δx]	2.927	1,873	6,022	0	3×10^3	280.61
	Finite difference [$\Delta x/2$]	2.955	1,459	5,880	0	5×10^4	12,384.00
	Finite difference [$2\Delta x$]	2.921	1,509	5,890	0	3×10^3	12,376.00

Table 4
Identification results for CS1

		Mean	S.D.	Skewness	Curtosis
CS1	True	0.1800	0.5500	3.3056	9.9224
	Analytical	0.1802	0.3027	3.3014	9.9050
	Finite difference [Δx]	0.1790	0.3059	3.3448	10.2090
	Finite difference [$\Delta x/2$]	0.1789	0.3053	3.3330	10.1166
	Finite difference [$2\Delta x$]	0.1790	0.3061	3.3468	10.2250

Table 5
Identification results for CS2

		Mean	S.D.	Skewness	Curtosis
CS2	True	0.4561	0.5535	3.8150	13.6894
	Analytical	0.4802	0.3703	3.6907	12.7691
	Finite difference [Δx]	0.4794	0.3813	3.7658	13.3606
	Finite difference [$\Delta x/2$]	0.4794	0.3798	3.7575	13.2949
	Finite difference [$2\Delta x$]	0.4778	0.3797	3.7845	13.5033

Table 6
Identification results for CS3

		Mean	S.D.	Skewness	Curtosis
CS3	True	0.1800	0.5347	3.1986	9.1826
	Convolution	0.1800	0.5347	3.1986	9.1826
	Finite difference [Δx]	0.1799	0.5344	3.1981	9.1773
	Finite difference [$\Delta x/2$]	0.1799	0.5349	3.2026	9.2090
	Finite difference [$2\Delta x$]	0.1799	0.5342	3.1887	9.1069

Table 7
Identification results for CS4

		Mean	S.D.	Skewness	Curtosis
CS4	True	0.4800	0.5853	3.5339	11.5664
	Convolution	0.4800	0.5853	3.5339	11.5664
	Finite difference [Δx]	0.4514	0.5154	3.6437	12.3343
	Finite difference [$\Delta x/2$]	0.5462	0.7721	3.3467	10.1303
	Finite difference [$2\Delta x$]	0.4524	0.5100	3.6544	12.4903

Table 8
Identification of the peak concentration for all scenarios

	$C_{p,\max}$ (mg/L)			
	CS1	CS2	CS3	CS4
True	5.0000	5.0000	5.0000	5.0000
Analytical/convolution	5.0000	4.2688	5.0000	5.0000
Finite difference [Δx]	4.9451	4.9505	4.9451	6.6354
Finite difference [$\Delta x/2$]	4.8913	4.8232	4.8913	8.5182
Finite difference [$2\Delta x$]	4.2688	6.0160	5.4878	8.2359

identification procedure, has been assessed. The estimated values of the peak concentration for the four investigated CS are reported in Table 8.

Table 8 shows that the procedure based on the solution of Eq. (2) by the convolution integral performs also from this point of view generally better than the one involving the finite difference approach. Remarkably, the former approach estimates the true peak concentration within 15% accuracy, independently on the presence of an upstream pollutant concentration. On the other hand, the finite difference approach exhibits a systematic decay of the performance for scenarios CS2 and CS4 (without an upstream pollutant concentration) compared with CS1 and CS3 (with upstream pollutant concentration).

Based on the above results, in the considered scenarios the approach based on the convolution integral (or on the exact solution for the CS1 and CS2 scenarios) therefore allows more accurate and efficient solution to the pollution source identification problem. However, this advantage is counterbalanced by the restriction to simple geometries and constant parameters, which limits the validity of the formal solution (Eq. (7)). On the other hand, the procedure based on the numerical solution of the transport equation can be in principle extended to the case of non-uniform distribution of the flow velocity and/or of the diffusion coefficient, to 1-D time-dependent flows as well as to contamination problem involving even 2-D or 3-D flow fields, provided that a suitable computational power is available.

Further research will be devoted to investigate the effect on the identification of potential source of disturbance such as measuring errors, uncertainties in the flow parameters, unknown shape of the pollutograph. The results of the above analysis may represent a valuable help in the design of a sensor network in a river, especially if early warning and rapid reaction to the contamination event have to be guaranteed.

4. Conclusions

The identification of the pollution source in a river may be regarded as an inverse problem driven by the MCs upstream and downstream the injection point. Common approaches to this problem require the repeated solution of the governing equations expressing the convective/diffusive contaminant transport, which is usually performed by means of discrete numerical methods. In the present paper, an alternative strategy based on the solution of the contaminant transport equation built by means of the convolution integral of the impulse response, has been explored. These two approaches have been embedded in a heuristic optimization algorithm and

compared with reference to a sample synthetic application. In the considered examples, the approach based on the convolution integral provided at the same time more accurate results and a considerable reduction of the computational cost. However, the procedure based on the finite-difference solution of the transport equation can be easily extended to more complex flow fields of certain practical applications, for which the formal solution is not available.

Symbols

A	—	River cross-section area, m^2
B_s	—	Sensors
C	—	Average solute concentration, mg/L
C^*	—	Maximum concentration, mg/L
C_D	—	Pollutant concentration just downstream the injection, mg/L
$C_{i(t)}$	—	Pollutant concentration at time t, mg/L
C_m	—	Concentration of pollutant, mg/L
$C_{m(t)}$	—	Measured concentration at time t, mg/L
C_p	—	Concentration of pollutant, mg/L
$C_{p,\max}$	—	Maximum injected concentration of pollutant, mg/L
C_U	—	Upstream pollutant concentration, mg/L
D	—	Dispersion coefficient, m^2/s
L	—	Distance between the two sensors, m
Q	—	Volumetric flow rate, m^3/s
Q_p	—	Flow rate of pollutant, m^3/s
T	—	Injection time, s
t	—	Time, s
$t_{\max}$	—	Total time of simulation, s
U	—	Mean velocity, m/s
X	—	Position along the reach, m
x	—	Streamwise coordinate, m
δ	—	Lifespan, s
δ_m	—	Measured lifespan, s
Δx	—	Space step, m

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