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Stochastic modelling of DO and BOD components in a stream with random inputs

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Abstract

A stochastic model for the evolution of DO and BOD components along a river with independent BOD point inputs has been developed. The model examines the case in which the initial conditions and the concentrations of the inputs are affected by uncertainty. The uncertain quantities are modelled as random variables, for which any kind of probability distribution can be adopted. The possibility of separately analysing the different components of BOD (e.g., CBOD and NBOD) is included. A semi-analytical expression for the joint probability density function (pdf) of the concentrations is derived. The application of this relationship greatly reduces the computation efforts compared to Monte-Carlo methods. A procedure for the analytical determination of the concentration moments is also described.
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1. Introduction

One of the most important anthropogenic impacts on the environment is the disposal of wastes that originate from human activities. Among liquid wastes, wastewaters contaminated by biodegradable pollutants constitute a common by-product of both civil settlements and industrial facilities. This class of substances is known as biochemical oxygen demand (BOD), as it is made up of carbonaceous and nitrogenous matter that is oxidized by aerobic microorganisms, resulting in a deficit in the concentration of dissolved oxygen (DO) in the water body. Since small quantities of such contaminants are often present even in pristine environments, the discharge of BOD contaminated wastewaters

into natural rivers has become a consolidated habit. However, excessive BOD loads are detrimental for the quality of river water, as the resulting low DO concentration makes the river unsuitable for the life of flora and fauna. Consequently, a number of models for the prediction of water quality modifications due to BOD discharges have been formulated.

The first models, starting from the basic work by Streeter and Phelps [1], adopted a deterministic approach. The main feature of deterministic models is that all the characteristics of the system are considered to be known, that is, boundary and initial conditions and model parameters are assigned a unique value, which is considered to be exact. The value of contaminant concentration C along the river at any time can then be computed. However, it is commonly recognized that there are many sources of uncertainty that affect contaminant dynamics. This uncertainty is mainly due to three aspects: firstly, the natural heterogeneity of real

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rivers is often difficult to synthesize in a single value of a parameter, and uncertainty on the values of initial and boundary conditions (e.g., source terms) is often present. Secondly, calibration measurements that are used for the estimation of the values of parameters are always affected by experimental errors. Finally, simple models can be inadequate to describe the complexity of the actual physical phenomena that occur in rivers.

In order to consider these approximations, probabilistic methods have been developed over the last two decades, that describe the uncertain initial and boundary conditions and parameters as random variables or stochastic processes. These kinds of models can be grouped into three main typologies: first-order error analysis, Monte-Carlo methods, and stochastic differential equations. First-order error analysis is a simple approach that gives an estimate of the variance of the concentration as a function of the moments of the uncertain parameters (e.g., [2–4]). The limit of this approach is that its results are not valid for non-linear models and that only the concentration variance is provided. The Monte-Carlo method is a popular numerical technique that is often used to evaluate the probability density function (pdf) of the concentration C (e.g., [2,5–7]); however, it often requires great computational efforts, and its results are generally valid only for the specific simulated case. Stochastic differential equations derive from deterministic models in which model parameters, initial and boundary conditions are described by random variables or stochastic processes [8,9]. Even though this approach implies greater analytical difficulties than the previous methods, it allows—at least for simple models—analytic expressions to be obtained for the pdf and moments of the concentrations (e.g., [10–19]). A review on the various applications of stochastic models to contaminant fate problems can be found in [20].

This paper describes a stochastic model for the study of the evolution of DO and BOD components in a river with BOD point inputs. Such inputs can represent discharges from wastewater treatment plants or industrial facilities, as well as small, polluted tributaries. The case in which the main sources of uncertainty are the BOD concentration of the inputs and the concentrations of both BOD and DO at the initial section of the modelled reach is addressed. The uncertainties due to oversimplifications of the actual physical processes are not addressed. This model represents the extension of a previous work [20] in which only the total BOD evolution was described, and it is based on a system of stochastic differential equations with random boundary conditions. The model allows (i) any kind of probabilistic distribution of the random inputs to be chosen, (ii) semi-analytical expressions of the pdf of the BOD and DO concentrations to be obtained, and (iii) different types of BOD components (e.g., carbonaceous and nitrogenous BOD) to be considered. The possibility of choosing any statistical distribution for the random concentrations is important because greater flexibility—with respect to the often adopted Gaussian distribution—is thus obtained. The semi-analytical solution consists of a multiple integral, which can be evaluated through numerical methods (when the analytical resolution is not attainable) in a very fast way. Finally, it can be important to separately analyse the different classes of substances (e.g., carbonaceous and nitrogenous) that BOD is composed of, since they play different roles as nutrients in the river ecosystem [21,22].

2. Description of the model

The river is approximated as a uniform, steady, turbulent open channel flow with constant discharge, Q, and mean velocity, U. A reference axis, x, that coincides with the stream direction, is defined. It is assumed that the effects of dispersion are negligible compared with those of advection and reactions, so that the river can be modelled as a plug-flow system [21]. If a Lagrangian point of view is adopted, it is possible to follow a generic slice Ω of infinitesimal width as it moves along the stream; let $t = x/U$ be the travel time of Ω, and $C(t)$ and $O(t)$ its section-averaged concentrations of BOD and DO, respectively. Position, x, is therefore replaced by travel time, t. It should be noted that, since dispersion is neglected, each flow element can be regarded as independent of the other elements.

Let us assume that n independent point inputs of BOD are located at x_i, $i = 1, \ldots, n$; for the sake of simplicity, let $x_1 = 0$. The BOD concentration of the generic ith input is assumed to be uncertain, and is therefore described as a random variable with known pdf $p_i(C_i)$. In fact, in several cases the concentration of an input varies in time in a non-deterministic way. This can be the case, for instance, of a sewer as well as an industrial discharge. The concentration pdf should be determined on the basis of the specific production cycle and technologies. It should be noticed that no restriction is set to the shape of the pdfs $p_i(C_i)$, and non-Gaussian distributions can thus be chosen to describe skewed and/or non-negative valued pdfs.

The initial river concentrations of BOD and DO at $x = 0$, namely C_0 and O_0, are also treated as random variables, with joint pdf $p(C, O, t = 0) = p_0(C_0, O_0)$. The inputs $p_i(C_i)$ are considered to be independent, i.e., no correlation exists among the random variables C_i, $i = 1, \ldots, n$. On the contrary, some degree of correlation generally exists between the initial concentrations C_0 and O_0. The water discharge Q_i of each input is assumed to be much smaller than the river discharge Q, so that the river discharge remains constant along the examined reach.

When the element Ω passes the ith input, at time $t_i = x_i/U$, it receives a random amount of BOD that
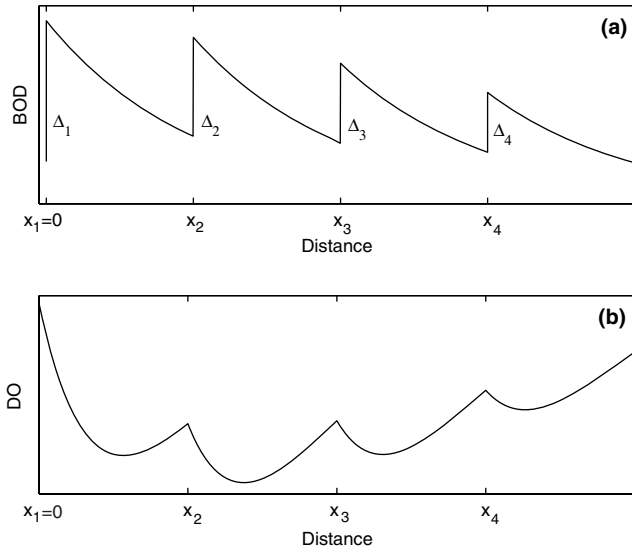
Fig. 1. Qualitative evolution of BOD (a) and DO (b) concentration along the stream.

causes an increment Δ_i^C in the river BOD concentration. This random increment can therefore be related to the BOD concentration of the input C_i

$$\Delta_i^C = \frac{Q_i}{Q} C_i \tag{1}$$

as long as $Q_i \ll Q$, and the corresponding pdf $p_i(\Delta_i^C)$ of the random increment can be defined. In this work, the concentrations C_i have therefore been replaced by the corresponding random jumps Δ_i^C.

The resulting situation is sketched in Fig. 1a: whenever the element Ω passes an input, it "samples" a value from the pdf $p_i(\Delta_i^C)$, and eventually undergoes a series of random jumps.

It is assumed that the river receives no DO from the inputs. This simplification is acceptable because the DO concentration is limited by the saturation concentration O_{sat} (which is a function of the water temperature, and is assumed to be constant); as shown by Eq. (1), the DO input concentration would be further reduced by the dilution factor $Q_i/Q \ll 1$. As a result, the river would receive a very small amount of DO, which can therefore be neglected. This assumption also leads to a prudential underestimation of the river DO concentration.

Let us now define the ith subreach as the river segment between two consecutive inputs located at x_i and x_{i+1}, that is, $x \in [x_i, x_{i+1}]$. As the element Ω moves along the ith subreach, BOD and DO undergo a series of biological reactions and reaeration phenomena that are described by the well-known model proposed by [1]

$$\frac{dC}{dt} = -k_i^C C, \tag{2}$$

$$\frac{dD}{dt} = k_i^C C - k_i^A D, \tag{3}$$

where the DO is replaced by the river DO deficit $D(t) = O_{sat} - O(t)$, $C(t)$ is the river BOD concentration, t is the travel time, k_i^C is the first-order decay constant for the ith subreach, and k_i^A is the reaeration constant for the ith subreach. Even though simple, the Streeter–Phelps model is recognized as being able to describe the main features of BOD and DO dynamics in rivers. More complex versions of the model have been proposed to consider other possible sources, sinks and chemical components. An extension of the model that is considered in this paper (see, e.g., [21,23–25]) is

$$\frac{dC}{dt} = -k_i^C C, \tag{4}$$

$$\frac{dN}{dt} = -k_i^N N, \tag{5}$$

$$\frac{dD}{dt} = k_i^C C + k_i^N N - k_i^A D, \tag{6}$$

where $C(t)$ and $N(t)$ are now the carbonaceous (CBOD) and nitrogenous (NBOD) components of BOD, respectively, and k_i^C and k_i^N the respective decay constants for the ith subreach. It should be understood that the total BOD concentration is now given by the sum of C and N, whereas in Eqs. (2) and (3), the total BOD concentration is simply given by C. This subdivision can be of interest because the two species are important as macronutrients in the stream ecology [21,22]. The extension of the model to subdivisions into more components—e.g., fast- and slow-decaying BOD—is straightforward, and is not shown here.

The qualitative behaviour of DO along a subreach is shown in Fig. 1b. While the BOD concentration undergoes a monotonic decay (compare Fig. 1b with a), after an initial phase of decay the concentration of DO reaches a minimum (provided that the subreach is long enough), after which the reaeration process leads to an asymptotic increase towards the saturation concentration O_{sat}.

The overall dynamics of BOD and DO (i.e., model (2)–(3)), with the addition of the random source term (1), can be described by the system of stochastic differential equations

$$\frac{d\overrightarrow{X}(t)}{dt} = \overrightarrow{K}\overrightarrow{X}(t) + \overrightarrow{P}(t), \quad t > 0 \tag{7}$$

in which

$$\overrightarrow{X}(t) = \begin{bmatrix} C(t) \\ D(t) \end{bmatrix}, \quad \overrightarrow{K} = \begin{bmatrix} -k_i^C & 0 \\ k_i^C & -k_i^A \end{bmatrix},$$

$$\overrightarrow{P}(t) = \begin{bmatrix} \sum_{i=1}^{n} \delta(t - t_i)\Delta_i^C \\ 0 \end{bmatrix},$$

where $\delta(\cdot)$ is the Dirac delta function, and $\overrightarrow{P}(t)$ represents the point source term corresponding to the inputs at $t = t_i$, $i = 1, \ldots, n$. In this paper, it is assumed that the

input pdfs $p_i(\Delta_i^C)$, $i = 1,\ldots,n$ and the joint pdf of the initial concentrations $p(C_0, D_0) \equiv p_0(C, D)$ at $t = 0$ are known. It should be noticed that the initial concentrations C_0 and D_0 can be correlated. The aim of the paper is to solve Eq. (7) for the joint probability density function $p(\overrightarrow{X}, t) = p(C, D, t)$ at a generic travel time t.

For the case of three chemical components (i.e., model (4)–(6)), Eq. (7) holds together with

$$
\overrightarrow{X}(t) = \begin{bmatrix} C(t) \\ N(t) \\ D(t) \end{bmatrix}, \quad \overline{K} = \begin{bmatrix} -k_i^C & 0 & 0 \\ 0 & -k_i^N & 0 \\ k_i^C & k_i^N & -k_i^A \end{bmatrix},
$$

$$
\overrightarrow{P}(t) = \begin{bmatrix} \sum_{i=1}^n \delta(t - t_i)\Delta_i^C \\ \sum_{i=1}^n \delta(t - t_i)\Delta_i^N \\ 0 \end{bmatrix},
$$

where Δ_i^C and Δ_i^N are, respectively, the random increments in CBOD and NBOD due to the ith input, $i = 1,\ldots,n$. In this case, the input pdfs $p_i(\Delta_i^C, \Delta_i^N)$ and the initial pdf $p(C_0, N_0, D_0) \equiv p_0(C, N, D)$ are assumed to be known. Since each input discharges both CBOD and NBOD, the random jumps Δ_i^C and Δ_i^N are expected to be correlated.

3. Solutions

The steps to determine the pdf $p(\overrightarrow{X}, t)$ and the moments of the concentration distribution are presented in this section. Since, from a mathematical point of view, model (4)–(6) is similar to the simpler model (2)–(3), with only the addition of the independent equation (5), the solutions are derived for the simpler case of two components. The results for three components are given more briefly.

3.1. Probability density functions

3.1.1. Two component model
Let us consider the generic point downstream to the nth input. The formal solution of the linear stochastic differential Eq. (7) can be written as

$$
C(t) = C_0 e^{-\gamma_{1,n+1}} + \sum_{j=1}^n \Delta_j^C e^{-\gamma_{j,n+1}}, \tag{8}
$$

$$
D(t) = D_0 e^{-\alpha_{1,n+1}} + C_0 \varphi_{1,n}^C + \sum_{j=1}^n \Delta_j^C \varphi_{j,n}^C, \tag{9}
$$

where $t > t_n$, and with

$$
\gamma_{j,i} = \sum_{\ell=j}^{i-2} k_\ell^C(t_{\ell+1} - t_\ell) + (1 - \delta_{i,n+1})k_{i-1}^C(t_i - t_{i-1})
$$
$$
+ \delta_{i,n+1}k_{i-1}^C(t - t_{i-1}), \tag{10}
$$

$$
\alpha_{j,i} = \sum_{\ell=j}^{i-2} k_\ell^A(t_{\ell+1} - t_\ell) + (1 - \delta_{i,n+1})k_{i-1}^A(t_i - t_{i-1})
$$
$$
+ \delta_{i,n+1}k_{i-1}^A(t - t_{i-1}), \tag{11}
$$

$$
\varphi_{j,i}^C = \sum_{\ell=j}^i q_\ell^C(e^{-\gamma_{j,\ell+1} - \alpha_{\ell+1,i+1}} - e^{-\gamma_{j,\ell} - \alpha_{\ell,i+1}}), \tag{12}
$$

$$
q_i^C = \frac{k_i^C}{k_i^A - k_i^C}, \tag{13}
$$

where $\delta_{i,j}$ is the Kronecker delta function. It should be noticed that $\gamma_{i,i} = \alpha_{i,i} = 0$.

In order to derive the concentration pdf at a generic travel time, it is more straightforward to split Eqs. (8) and (9) into two parts, that correspond to two distinct phases of the travelling of an element Ω along the river: (i) the movement in the subreaches between two consecutive inputs and (ii) the passages in correspondence to the inputs.

Let us first consider the generic ith subreach between the ith and the $(i + 1)$th inputs and define $p(C, D, t_i^-)$ and $p(C, D, t_i^+)$ as the joint pdf of the BOD and DO deficit immediately upstream and downstream to the ith input. In this subreach, the dynamics of $C(t)$ and $D(t)$ is deterministic and is governed by Eqs. (2) and (3), whose solution is

$$
\overrightarrow{X}(t) = \overrightarrow{A}(t) \cdot \overrightarrow{X}_0, \quad t \in [t_i^+, t_{i+1}^-], \tag{14}
$$

where

$$
\overrightarrow{X}(t) = \begin{bmatrix} C(t) \\ D(t) \end{bmatrix}, \quad \overrightarrow{X}_0 = \begin{bmatrix} C(t_i^+) \\ D(t_i^+) \end{bmatrix},
$$
$$
\overrightarrow{A}(t) = \begin{bmatrix} e^{-k_i^C(t-t_i)} & 0 \\ q_i^C(e^{-k_i^C(t-t_i)} - e^{-k_i^A(t-t_i)}) & e^{-k_i^A(t-t_i)} \end{bmatrix}. \tag{15}
$$

Eq. (14) establishes a deterministic link between the upstream concentration vector, $\overrightarrow{X}_0$, and the downstream one, $\overrightarrow{X}(t)$. It is then possible to write [8]

$$
p(\overrightarrow{X}, t) = |\overrightarrow{A}^{-1}| \cdot p(\overrightarrow{X}_0 = \overrightarrow{A}^{-1}\overrightarrow{X}). \tag{16}
$$

Eq. (16) can be applied to derive the concentration pdf at a generic $t \in [t_i^+, t_{i+1}^-]$, given the pdf at t_i^+. For $t = t_{i+1}^-$, in particular, it provides the relationship between $p(\overrightarrow{X}, t_i^+)$ and $p(\overrightarrow{X}, t_{i+1}^-)$, that is, the overall effect on the concentration pdf of the travelling of Ω through the ith subreach. The introduction of (15) into (16) leads to

$$
p(C, D, t_{i+1}^-) = e^{\gamma_{i,i+1} + \alpha_{i,i+1}}
$$
$$
\cdot p\big[Ce^{\gamma_{i,i+1}}, De^{\alpha_{i,i+1}} + Cq_i^C(e^{\gamma_{i,i+1}} - e^{\alpha_{i,i+1}}), t_i^+\big], \tag{17}
$$

where $\gamma_{j,i}$, $\alpha_{j,i}$, and q_i^C have been defined by (10), (11), and (13), respectively.

Eq. (17) provides the desired link between the concentration pdfs at the upstream and downstream ends of the

*i*th subreach. A relationship between the two concentration pdfs at t_i^- and t_i^+ is now sought for the second step. When the element Ω passes the *i*th input, its BOD concentration increases by a random quantity Δ_i^C which is extracted from the corresponding distribution $p_i(\Delta_i^C)$, while the DO concentration remains unchanged:

$$\vec{X}(t_i^+) = \vec{X}(t_i^-) + \vec{\Delta}_i, \tag{18}$$

in which

$$\vec{\Delta}_i = \begin{bmatrix} \Delta_i^C \\ 0 \end{bmatrix}.$$

The resulting downstream joint pdf is given by the convolution of all the possible upstream concentrations together with all the possible random jumps, that is,

$$p(C, D, t_i^+) = \int_0^C p(C - \Delta_i^C, D, t_i^-) p_i(\Delta_i^C) \, d\Delta_i^C. \tag{19}$$

It is now possible to recursively apply (for $i = 1, \ldots, n$) Eqs. (17) and (19), thus obtaining the analytical solution at a generic travel time. The solution at the generic $t > t_n$ is

$$p(C, D, t) = e^{\gamma_{1,n+1} + \alpha_{1,n+1}} \int_0^{f_n} \cdots \int_0^{f_1} p_0[f_1 - \Delta_1^C, h_1]$$
$$\cdot p_1(\Delta_1^C) \, d\Delta_1^C \cdots p_n(\Delta_n^C) \, d\Delta_n^C, \tag{20}$$

where

$$f_j = \begin{cases} Ce^{\gamma_{j,j+1}}, & j = n, \\ (f_{j+1} - \Delta_{j+1}^C)e^{\gamma_{j,j+1}}, & j = n-1, \ldots, 1 \end{cases} \tag{21}$$

$$h_j = \begin{cases} Cq_j^C(e^{\gamma_{j,j+1}} - e^{\alpha_{j,j+1}}) + De^{\alpha_{j,j+1}}, & j = n, \\ (f_{j+1} - \Delta_{j+1}^C)q_j^C(e^{\gamma_{j,j+1}} - e^{\alpha_{j,j+1}}) + e^{\alpha_{j,j+1}}h_{j+1}, \\ \quad j = n-1, \ldots, 1, \end{cases} \tag{22}$$

and $\gamma_{j,i}$, $\alpha_{j,i}$, and q_i^C are given by (10), (11), and (13), respectively.

The convolution integrals in Eq. (20) can only be analytically solved for certain distributions (see [20]). When analytical resolution is not possible, the numerical resolution of Eq. (20) is very fast, and is generally considerably quicker than the application of a Monte-Carlo method. This happens because the contribution of the *n* inputs is simply evaluated by *n* convolutions, while the number of required Monte-Carlo samples would be equal to c^n, where *c* is the number of samples for each input pdf. Moreover, FFT-based algorithms exist that are extremely efficient in solving convolution integrals [26].

3.1.2. Three component model

The case of three substances is analogous: the formal solution of Eq. (7) at the generic $t > t_n$ is

$$C(t) = C_0 e^{-\gamma_{1,n+1}} + \sum_{j=1}^n \Delta_j^C e^{-\gamma_{j,n+1}}, \tag{23}$$

$$N(t) = N_0 e^{-\nu_{1,n+1}} + \sum_{j=1}^n \Delta_j^N e^{-\nu_{j,n+1}}, \tag{24}$$

$$D(t) = D_0 e^{-\alpha_{1,n+1}} + C_0 \varphi_{1,n}^C + N_0 \varphi_{1,n}^N$$
$$+ \sum_{j=1}^n \Delta_j^C \varphi_{j,n}^C + \sum_{j=1}^n \Delta_j^N \varphi_{j,n}^N, \tag{25}$$

where $\gamma_{j,i}$, $\alpha_{j,i}$, $\varphi_{j,i}^C$, and q_i^C are still given by (10)–(13), and

$$\nu_{j,i} = \sum_{\ell=j}^{i-2} k_\ell^N (t_{\ell+1} - t_\ell) + (1 - \delta_{i,n+1}) k_{i-1}^N (t_i - t_{i-1})$$
$$+ \delta_{i,n+1} k_{i-1}^N (t - t_{i-1}), \tag{26}$$

$$\varphi_{j,i}^N = \sum_{\ell=j}^i q_\ell^N (e^{-\nu_{j,\ell+1} - \alpha_{\ell+1,i+1}} - e^{-\nu_{j,\ell} - \alpha_{\ell,i+1}}), \tag{27}$$

$$q_i^N = \frac{k_i^N}{k_i^A - k_i^N}, \tag{28}$$

where $\delta_{j,i}$ is the Kronecker delta function. It should be noticed that $\nu_{i,i} = 0$.

For the *i*th subreach, the solution of (4)–(6) is still given by Eq. (14) with

$$\vec{X}(t) = \begin{bmatrix} C(t) \\ N(t) \\ D(t) \end{bmatrix}, \quad \vec{X}_0 = \begin{bmatrix} C(t_i^+) \\ N(t_i^+) \\ D(t_i^+) \end{bmatrix},$$

$$\vec{A}(t) = \begin{bmatrix} e^{-\gamma_{i,i+1}} & 0 & 0 \\ 0 & e^{-\nu_{i,i+1}} & 0 \\ q_i^C(e^{-\gamma_{i,i+1}} - e^{-\alpha_{i,i+1}}) & q_i^N(e^{-\nu_{i,i+1}} - e^{-\alpha_{i,i+1}}) & e^{-\alpha_{i,i+1}} \end{bmatrix}, \tag{29}$$

where $t \in [t_i^+, t_{i+1}^-]$. The introduction of (29) into (16) gives

$$p(\vec{X}, t_{i+1}^-) = e^{\gamma_{i,i+1} + \nu_{i,i+1} + \alpha_{i,i+1}} \cdot p[Ce^{\gamma_{i,i+1}}, Ne^{\nu_{i,i+1}}, De^{\alpha_{i,i+1}}$$
$$+ Cq_i^C(e^{\gamma_{i,i+1}} - e^{\alpha_{i,i+1}}) + Nq_i^N(e^{\nu_{i,i+1}} - e^{\alpha_{i,i+1}}), t_i^+], \tag{30}$$

which is analogous to (17).

At the *i*th input, Eq. (18) still holds with

$$\vec{\Delta}_i = \begin{bmatrix} \Delta_i^C \\ \Delta_i^N \\ 0 \end{bmatrix}.$$

The pdf immediately downstream of the *i*th input is therefore given by

$$p(\vec{X}, t_i^+) = \int_0^C \int_0^N p(C - \Delta_i^C, N - \Delta_i^N, D, t_i^-)$$
$$\cdot p_i(\Delta_i^C, \Delta_i^N) \, d\Delta_i^C \, d\Delta_i^N. \tag{31}$$

Finally, from (30) and (31), the analytical solution for the joint pdf of the concentrations at $t > t_n$ can be found as

$$p(C,N,D,t) = e^{\gamma_{1,n+1}+\nu_{1,n+1}+\alpha_{1,n+1}}$$
$$\times \int_0^{f_n} \int_0^{g_n} \cdots \int_0^{f_1} \int_0^{g_1} p_0[f_1 - \Delta_1^C, g_1 - \Delta_1^N, h_1]$$
$$\cdot p_1(\Delta_1^C, \Delta_1^N)\,\mathrm{d}\Delta_1^C\,\mathrm{d}\Delta_1^N \cdots p_n(\Delta_n^C, \Delta_n^N)\,\mathrm{d}\Delta_n^C\,\mathrm{d}\Delta_n^N,$$
(32)

where f_j is still given by Eq. (21), and

$$g_j = \begin{cases} Ne^{\nu_{j,j+1}}, & j = n, \\ (g_{j+1} - \Delta_{j+1}^N)e^{\nu_{j,j+1}}, & j = n-1, \ldots, 1, \end{cases}$$
(33)

$$h_j = \begin{cases} Cq_j^C(e^{\gamma_{j,j+1}} - e^{\alpha_{j,j+1}}) + Nq_j^N(e^{\nu_{j,j+1}} - e^{\alpha_{j,j+1}}) \\ \quad + De^{\alpha_{j,j+1}}, \quad j = n, \\ (f_{j+1} - \Delta_{j+1}^C)q_j^C(e^{\gamma_{j,j+1}} - e^{\alpha_{j,j+1}}) \\ \quad + (g_{j+1} - \Delta_{j+1}^N)q_j^N(e^{\nu_{j,j+1}} - e^{\alpha_{j,j+1}}) \\ \quad + e^{\alpha_{j,j+1}}h_{j+1}, \quad j = n-1, \ldots, 1. \end{cases}$$
(34)

3.2. Moment analysis

3.2.1. Two component model

The linearity of Eq. (7) allows the moments of the concentration distribution to be obtained. The moments provide less information than the joint pdf $p(\overrightarrow{X},t)$, but they synthesize the main features of the concentration distributions and can thus be useful for practical purposes. The method herein described allows the moments to be analytically derived in a straightforward way.

Eqs. (8) and (9) show how each input Δ_i^C and the initial concentrations C_0 and D_0 give independent contributions to the final concentrations $C(t)$ and $D(t)$. In order to explicit these contributions, Eqs. (8) and (9) can be rewritten as

$$C(t) = Y_{C_0} + \sum_{j=1}^n Y_{\Delta_j^C},$$
(35)

$$D(t) = Z_{D_0} + Z_{C_0} + \sum_{j=1}^n Z_{\Delta_j^C},$$
(36)

where

$$Y_{C_0} = C_0 e^{-\gamma_{1,n+1}}, \quad Y_{\Delta_j^C} = \Delta_j^C e^{-\gamma_{j,n+1}}$$

and

$$Z_{D_0} = D_0 e^{-\alpha_{1,n+1}}, \quad Z_{C_0} = C_0 \varphi_{1,n}^C, \quad Z_{\Delta_j^C} = \Delta_j^C \varphi_{j,n}^C.$$

The terms in Eqs. (35) and (36) are independent random variables whose distributions can be evaluated as

$$p(Y_{C_0}) = e^{\gamma_{1,n+1}}p_0(C_0 e^{\gamma_{1,n+1}}),$$
(37)

$$p(Y_{\Delta_j^C}) = e^{\gamma_{j,n+1}}p_j(\Delta_j^C e^{\gamma_{j,n+1}}), \quad j = 1, \ldots, n,$$
(38)

$$p(Z_{D_0}) = e^{\alpha_{1,n+1}}p_0(D_0 e^{\alpha_{1,n+1}}),$$
(39)

$$p(Z_{C_0}) = \frac{1}{\varphi_{1,n}^C}p_0\left(\frac{C_0}{\varphi_{1,n}^C}\right),$$
(40)

$$p(Z_{\Delta_j^C}) = \frac{1}{\varphi_{j,n}^C}p_j\left(\frac{\Delta_j^C}{\varphi_{j,n}^C}\right), \quad j = 1, \ldots, n,$$
(41)

where $p_0(C) = \int_0^{+\infty} p_0(C,D)\,\mathrm{d}D$ and $p_0(D) = \int_0^{+\infty} p(C,D)\,\mathrm{d}C$ are the marginal distributions of C_0 and D_0, respectively, and $\gamma_{j,i}$, $\alpha_{j,i}$, and $\varphi_{j,i}^C$ are still defined by (10)–(12).

Since $C(t)$ and $D(t)$ are given by the sum of independent random variables, their distributions can be found as the convolution integral of the pdfs defined in (37)–(41). Let us now define the Laplace transform

$$\mathscr{L}[p(C)] = P_C(s) = \int_0^\infty p(C)e^{-sC}\,\mathrm{d}C,$$

and recall the well-known theorem [27]

$$\mathscr{L}[p(aC)] = \frac{1}{a}P_C\left(\frac{s}{a}\right),$$
(42)

where a is a real number. The application of the Laplace transform to Eqs. (35) and (36), together with (37)–(42), gives

$$P_C(s) = P_{C_0}(se^{-\gamma_{1,n+1}}) \cdot \prod_{j=1}^n P_{\Delta_j^C}(se^{-\gamma_{j,n+1}}),$$
(43)

$$P_D(s) = P_{D_0}(se^{-\alpha_{1,n+1}}) \cdot P_{C_0}(s\varphi_{1,n}^C) \cdot \prod_{j=1}^n P_{\Delta_j^C}(s\varphi_{j,n}^C),$$
(44)

where $\gamma_{j,i}$, $\alpha_{j,i}$, and $\varphi_{j,i}^C$ are still given by (10)–(12).

Even though the Laplace antitransform of Eqs. (43) and (44) can seldom be evaluated, the moments of the marginal pdfs of $C(t)$ and $D(t)$ can be derived, provided the involved distributions can be Laplace transformed. First, we recall that

$$\mu_j^C(t) \equiv \int_0^{+\infty} C^j(t)p(C,t)\,\mathrm{d}C = (-1)^j\frac{\mathrm{d}^j P_C}{\mathrm{d}s^j}\bigg|_{s=0},$$
(45)

$$\mu_j^D(t) \equiv \int_0^{+\infty} D^j(t)p(D,t)\,\mathrm{d}D = (-1)^j\frac{\mathrm{d}^j P_D}{\mathrm{d}s^j}\bigg|_{s=0},$$
(46)

where $\mu_j^C(t)$ and $\mu_j^D(t)$ are the jth order non-central moments of $C(t)$ and $D(t)$, respectively, at the generic travel time t.

It is also possible to derive the corresponding central moments, $m_j(t)$, as (e.g., [28])

$$m_2 = \sigma^2 = \mu_2 - \mu_1^2,$$
(47)

$$m_3 = \mu_3 - 3\mu_1\mu_2 + 2\mu_1^3,$$
(48)

$$m_4 = \mu_4 - 4\mu_1\mu_3 + 6\mu_1^2\mu_2 - 3\mu_1^4,$$
(49)

and so on.

3.2.2. Three component model

The same passages can be repeated for the case of three components, thus obtaining the Laplace transforms of the three concentration pdfs. The equation for $P_C(s)$ is formally identical to (43), while the other expressions are

$$P_N(s) = P_{N_0}(se^{-v_{1,n+1}}) \cdot \prod_{j=1}^{n} P_{\Delta_j^N}(se^{-v_{j,n+1}}), \qquad (50)$$

$$P_D(s) = P_{D_0}(se^{-\alpha_{1,n+1}}) \cdot P_{C_0}(s\varphi_{1,n}^C) \cdot P_{N_0}(s\varphi_{1,n}^N)$$
$$\cdot \prod_{j=1}^{n} [P_{\Delta_j^C}(s\varphi_{j,n}^C)P_{\Delta_j^N}(s\varphi_{j,n}^N)], \qquad (51)$$

where $\alpha_{j,i}$, $\varphi_{j,i}^C$, $v_{j,i}$, and $\varphi_{j,i}^N$ are still defined as in (11), (12), (26), and (27), respectively.

The non-central moments of the concentrations can be derived according to (45), (46), and

$$\mu_j^N(t) = (-1)^j \frac{d^j P_N}{ds^j}\bigg|_{s=0}, \qquad (52)$$

and the central moments can be evaluated with (47)–(49).

4. Examples

In this section, the proposed solution has been applied to a hypothetical stream with a cross-sectionally averaged velocity $U = 0.2$ m/s. The three-component model was used, and the total BOD was split into its carbonaceous and nitrogenous components C and N, respectively. Two different situations were considered: first, the case of three independent BOD inputs was analyzed. The inputs were separated by a constant distance of 30 km, with the first input located at $x_1 = 0$ km. Secondly, a fourth input was added at 40 km. Each input was assumed to have a bivariate lognormal distribution $p_i(\Delta_i^C, \Delta_i^N)$, $i = 1, \ldots, n$, for the random increments [29]. A correlation coefficient $\rho = 0.9$ was chosen to consider the simultaneous discharge of CBOD and NBOD. For both cases, a trivariate lognormal distribution $p_0(C, N, D)$ has been adopted for the in-stream concentrations at $x = 0$. Again, a correlation coefficient $\rho = 0.9$ between CBOD and NBOD was assumed. The mean values for each distribution have been summarized in Table 1, while the same coefficient of variation $CV = 0.2$ was adopted for all the components of each distribution. The value $O_{sat} = 11$ mg/L for the DO saturation concentration was used; it approximately corresponds to a water temperature of 10 °C. Finally, the decay rates $k_i^C = 5 \times 10^{-6}$ s^{-1} and $k_i^N = 2 \times 10^{-6}$ s^{-1} were chosen for the CBOD and the NBOD, respectively, while the reaeration rate $k_i^A = 10^{-5}$ s^{-1} was adopted. For the sake of simplicity, k_i^C, k_i^N and k_i^A were considered to be constant along the whole examined length of the

Table 1
Locations and mean values of the initial concentrations (p_0) and of the random jumps (p_1, p_2, p_3, p_4)

	x (km)	μ_C (mg/L)	μ_N (mg/L)	μ_D (mg/L)
p_0	0	2	1	2
p_1	0	4	2	–
p_2	30	3	2.5	–
p_3	40	2	3	–
p_4	60	2	3	–

stream. It should be worth noting that the described problem could also be solved using a Monte-Carlo approach, but not without great computational efforts; for instance, if each component is sampled 10^2 times (which is the minimum for a significant statistical analysis), then a total of 10^{18} simulations would be required.

Eqs. (30) and (31) were recursively applied to find the pdf of the concentrations of the three chemical components along the stream. The joint pdf $p(C, N, D)$ was evaluated every 1.5 km, and it was used to derive the marginal distributions and the values of the moments. The marginal pdfs of the three concentrations at $x = 50$ km have been reported in Fig. 2a and b, for the three and four inputs cases, respectively. These pdfs can be useful to evaluate the uncertainty in the in-stream concentration due to the ensemble of all the possible inputs. The effects of the introduction of the fourth input at $x = 40$ km can be observed from a comparison of the two figures: at the considered location, both the CBOD and, to a greater extent, the NBOD pdfs shifted towards higher mean concentrations and have increased their variances, while the DO pdf has shifted towards lower concentrations without any appreciable modification of its variance.

The CBOD evolution along the river is shown in Fig. 3a and b; the series of jumps and decays described in the previous sections can be appreciated. The overall uncertainty in the CBOD concentration is represented by the 80% confidence interval, that is given by the 0.1 and 0.9 quantiles. It should be noticed that the inputs act as sources of uncertainty for the CBOD concentration, since the width of the confidence interval suddenly increases in correspondence to them. On the other hand, the uncertainty gradually decreases along each subreach, since the concentration asymptotically tends to the (certain) zero value. A comparison of the two figures shows that the CBOD concentration increased in the central part of the examined reach, while only small differences can be observed between the two cases at the end of the reach, where most of the CBOD had already been oxidized by the microorganisms. It should also be noticed that the uncertainty was not substantially modified by the presence of the new input at 40 km.

Fig. 4a and b shows the evolution of NBOD concentration along the stream. The qualitative behaviour is
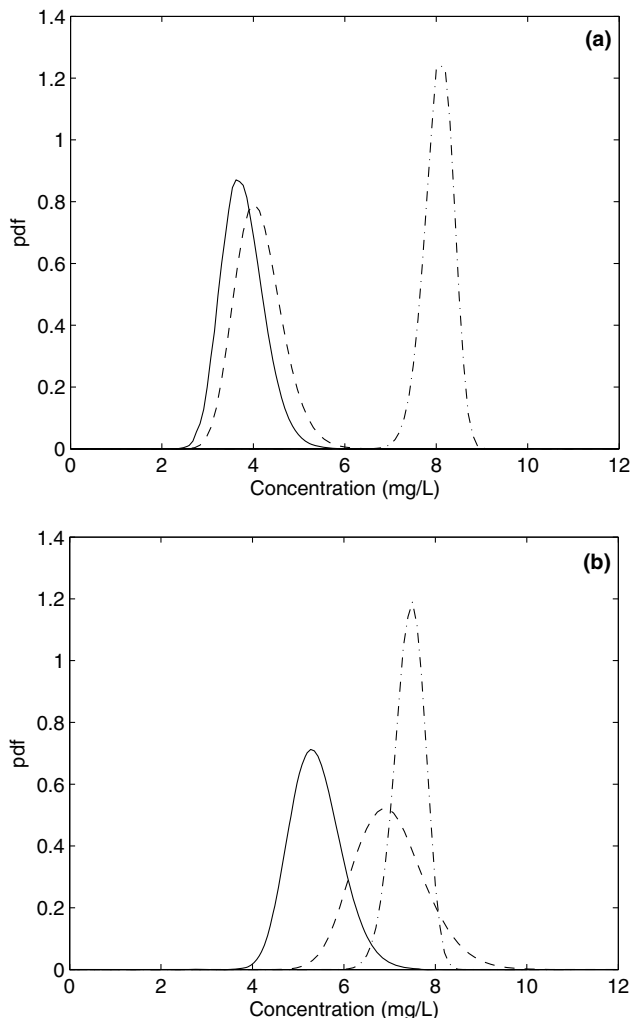
Fig. 2. Marginal probability density functions of CBOD (continuous line), NBOD (dashed line), and DO (dash-dotted line) concentrations at $x = 50$ km. Case of three (a) and four (b) point inputs.
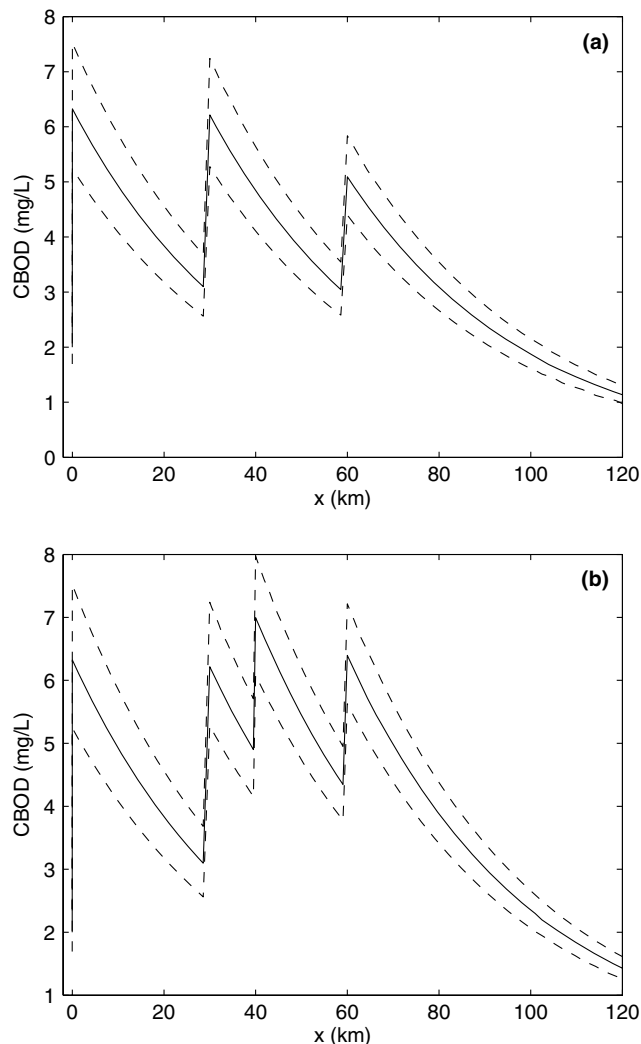

Fig. 3. CBOD mean value (continuous line), 0.1 and 0.9 quantiles (dashed lines) along the stream. Case of three (a) and four (b) point inputs.

similar to that of the CBOD, but the impact of the added input on the water quality is greater than in the CBOD case, due to the combined effect of the higher discharged mass and of the slower decay reactions.

The mean DO concentration along the river, with its confidence interval, has been represented in Fig. 5a and b. The sequence of DO microbial consumption and reaeration is evident; both the mean concentration and the width of the confidence interval are continuous, but their spatial derivatives are discontinuous in correspondence to the inputs. It should be noticed how the addition of the fourth input at $x = 40$ km affects the DO concentration to a great extent, increasing the overall mass of nutrients and thus the rate of oxygen consumption by the microorganisms. It should also be observed that the non-monotonic behaviour of the width of the confidence interval leads to high uncertainty levels in correspondence to the local minima, which represent the most critical points for the water quality.

Since the availability of dissolved oxygen is of crucial importance for an ecosystem, a useful tool for the analysis of river water quality is the probability P_{th} that the DO goes below a critical threshold O_{th} or, equivalently, the probability that the DO deficit exceeds the threshold value $D_{th} = (O_{sat} - O_{th})$

$$P_{th}(t) = \int_{D_{th}}^{+\infty} p(D, t)\, dD. \tag{53}$$

This probability can easily be evaluated from the marginal DO pdf, and it has been represented in Fig. 6 for the investigated cases. The threshold value $O_{th} = 8$ mg/L was chosen. The particular, non-trivial shape of these functions is due to the combined effect of the oxygen consumption and of the reaeration process. Fig. 6 shows that the introduction of the fourth input would lead a long segment of the river to have lower DO concentra-
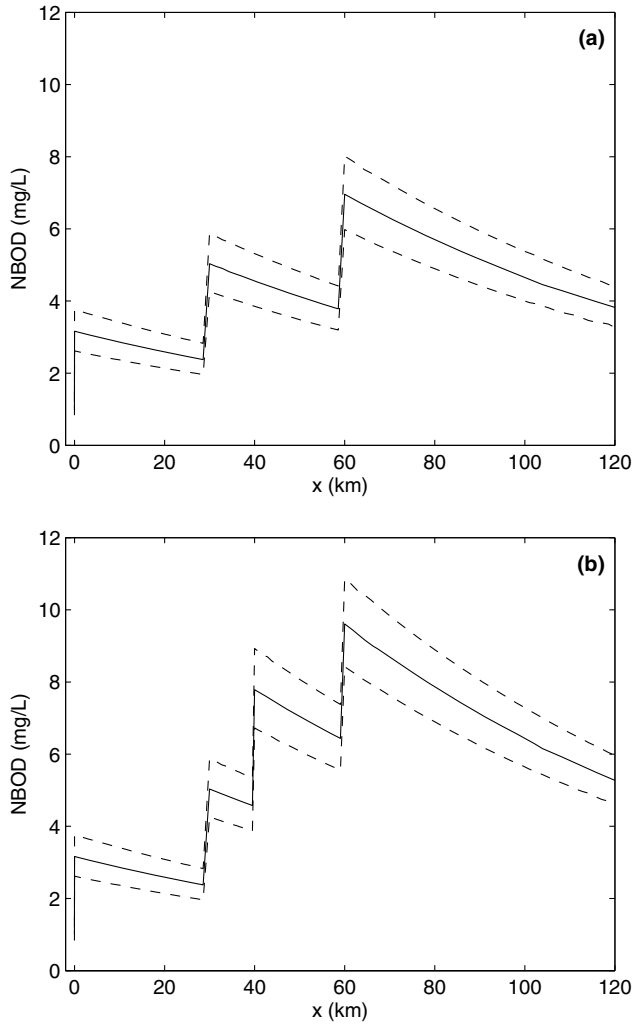
Fig. 4. NBOD mean value (continuous line), 0.1 and 0.9 quantiles (dashed lines) along the stream. Case of three (a) and four (b) point inputs.

Fig. 5. DO mean value (continuous line), 0.1 and 0.9 quantiles (dashed lines) along the stream. Case of three (a) and four (b) point inputs.

tions than 8 mg/L with $P_{th} \simeq 1$. The probability P_{th} can thus be a useful instrument to support decisions on water management.

5. Conclusions

A stochastic model for the analysis of the evolution of the concentrations of DO and BOD components along a stream has been presented in this paper. Of the many possible sources of uncertainty that can be encountered in river water quality problems, the presence of multiple independent BOD point inputs with uncertain concentrations has been considered. While some previous works only considered the Gaussian distribution for the uncertain parameters, in this work no restriction about the probability density functions of the input concentrations was made. This can be useful when the input concentration pdfs are best described
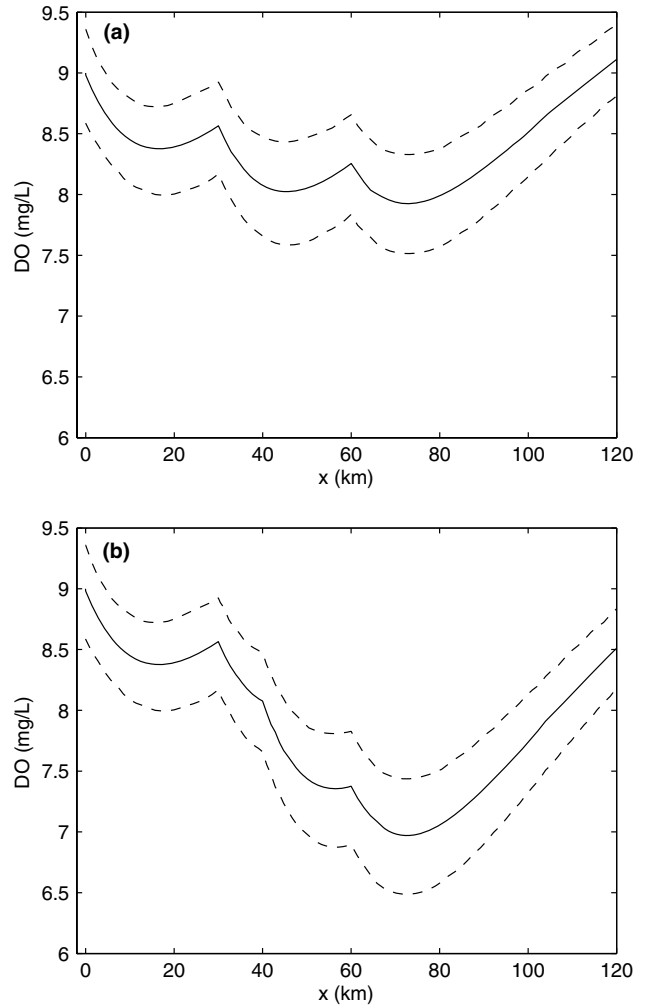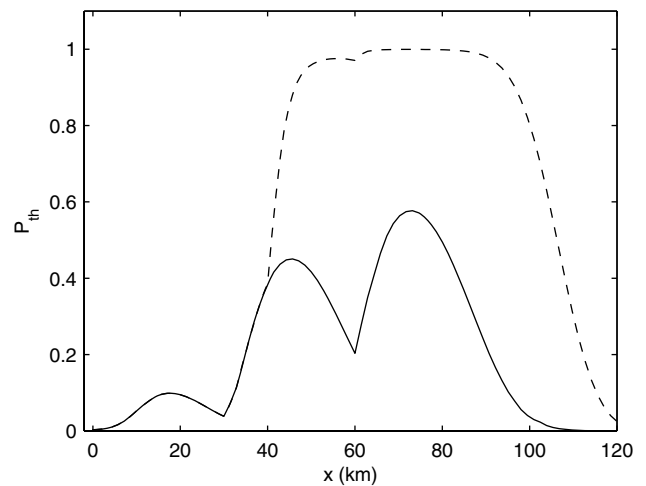

Fig. 6. Probability for the DO concentration to go below the threshold concentration $O_{th} = 8$ mg/L. Case of three (continuous line) and four (dashed line) point inputs.

by skewed distributions. Moreover, non-negative valued pdfs can be chosen, thus avoiding the problem of the negative tails of Gaussian distributions with high coefficients of variation. Correlations among the different BOD components that are released by each input were also included.

The joint DO and BOD concentration pdf can be derived from the proposed semi-analytical expressions. This joint pdf provides complete knowledge about the evolution of the concentrations. For instance, the probability of having a DO concentration below a threshold level can be inferred, thus determining the actual risk of critical conditions for the river ecosystem. When the semi-analytic relationships cannot be analytically evaluated and a numerical resolution is needed, our model allows to take advantage of the properties of convolution, which can be quickly solved using FFT-based algorithms. Since each input requires a convolution integral, the computation time grows linearly with the number of inputs. When the number of inputs is great, the present method may be preferred to a Monte-Carlo approach, for which the computation time exponentially increases with the number of inputs to be sampled.

A procedure for the evaluation of the moments of any order has also been presented. This procedure permits analytical expressions to be obtained for the moments of the concentration pdf, provided the latter can be Laplace transformed. Even though the moments provide less information than the joint pdf, the use of these analytical relationships provides an adequate description of the problem in a straightforward way.

The proposed examples have shown a possible application of the model as a support tool for the analysis of the overall effect of several point inputs on water quality. The evaluation of both the concentrations and the corresponding uncertainty of the DO and BOD components was attained. The adoption of a stochastic approach thus provides a practical method to derive information on the overall uncertainty, which is particularly useful to foresee possible events with low DO concentrations.

Acknowledgements

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