Modeling of river pollution: a 2D systems approach

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ABSTRACT The paper presents some applications of 2D system theory to the problem of modeling river pollution phenomena. The dynamical evolution of the biological oxygen demand (BOD) and dissolved oxygen (DO) in an one-dimensional river is represented under various physical assumptions.

1 Introduction

The unquestioned success of the state space methods in 1D theory mainly relies on the solution of control problems based on explicit synthetic algorithms for (static or dynamic) compensators. Along the same lines, one of the main achievements of 2D theory is the formulation of feedback regulation procedures based on the introduction of state space models that depend on two independent variables.

The aim of this paper is to point out how 2D state space models can be used in representing the river pollution process. The results we present have a preliminary character. Further research will, it is to be hoped, do much to clarify advantages and drawbacks of different 2D models, but we may feel confident that the outlines at least are broadly valid. Actually, once a 2D state model has been suitably validated, many results already available in 2D literature offer promising applications in monitoring and control of river pollution.

To keep the paper within an acceptable size, we found it impossible to give a detailed account of unidimensional continuous time Streeter-Phelps models. Thus we only select from the current mine of literature some references [1,2], that seem well suited for our modelling purposes. 2D systems are outlined in section 2, but the development of 2D theory has been carried out only to the extent necessary for the subsequent sections. Thus most important topics had to be omitted and the reader inclined to pursue the subject further is referred to [3-5], which contain a large bibliography up to 1989. Section 3 is devoted to a fairly detailed analysis of the problem of representing pollution dynamics via 2D state space models, when longitudinal dispersion can be neglected. Finally, a number of 2D models that incorporate the diffusion process are discussed in section 4.

2 2D state space models

The first contributions [6-8] that discussed the problem of defining dynamical systems with input, output, and state functions depending on two independent variables appeared nearly 15 years ago.

In principle, they were motivated by the necessity of investigating recursive structures for processing two-dimensional data. The processing has been performed for a long time using discrete filters, given by ratios of polynomials in two indeterminates or by algorithms assigned via difference equations. The idea that originated research on 2D systems consisted in considering these algorithms (i.e., transfer functions and difference equations in two indeterminates) as external representations of dynamical systems and hence in introducing for such systems the concepts of state and its updating equations. It turns out that the models obtained in this way are suitable for providing state-space descriptions for a large class of processes which depend on two independent variables. Typically, they apply to two-dimensional data processing in various fields, as sonarology, X-ray image enhancement, image deblurring, digital picture processing, etc. Also, 2D systems constitute a natural framework for modelling multivariable networks, large-scale systems obtained by interconnecting many subsystems, and, in general, physical processes where both space and time have to be taken into account.

From the very beginning, deep and substantial differences from the theory of dynamical systems in one variable have been evidenced. These are due to the mathematical tools to be used and, above all, to the concept of space itself and to the structure of state updating equations. In this case, there is no "canonical" algebraic construction that provides an intrinsic meaning to a finite dimensional state. Thus several state models have been introduced, with different recursive structures, although they are generated by the same underlying idea that a recursive computation is made possible by a finite dimensional local state and that the complete information on the past is kept by an infinite sequence of local states of global state.

The support of a 2D dynamics is constituted by the discrete plane \( \mathbb{Z} \times \mathbb{Z} \). Usually, a partial order is introduced in it, by taking the product of the orderings of the coordinate axes. Sometimes, however, it is convenient to refer to different coordinates in a finite subset of \( \mathbb{Z} \times \mathbb{Z} \), using a transformation as

\[
\begin{bmatrix}
0 & 1 \\
1 & 0
\end{bmatrix} \cdot \begin{bmatrix}
\mathbf{h} \\
\mathbf{k}
\end{bmatrix}
\]

(2.1)

where \( M \) is a unimodular matrix in \( \mathbb{Z}^{2 \times 2} \). In these cases the partial order in \( \mathbb{Z} \times \mathbb{Z} \) may consist of the product of the orderings of the new coordinate axes (see fig. 2.1).

![fig.2.1](image)

We associate with each point \((h,k) \in \mathbb{Z} \times \mathbb{Z}\) a local state \(x(h,k) \in \mathbb{R}^n\), that determines the output value \(y(h,k)\). The updating of the local states is given by a linear recursive equation, that involves local states and input values at some points that precede \((h,k)\), according to the partial order.

Depending on the delay structure of the updating equations, there are essentially two different kinds of 2D state space models. First order models (that include also Roemer's models) are characterized by the following state space equations:

\[
x(h+1,k+1) = A_1 x(h,k+1) + A_2 x(h+1,k) + B_1 u(h,k+1)
\]

\[
y(h,k) = C x(h,k)
\]

(2.2)

and second order models (that include Attali's models) by equations:

\[
x(h+1,k+1) = A_1 x(h,k+1) + A_2 x(h+1,k) + A_3 x(h,k) + B_1 u(h,k+1)
\]

\[
y(h,k) = C x(h,k)
\]

(2.3)

Slight modifications are sometimes useful; a couple of models in next sections is based on a first order state updating structure, while the input-state map is second order:

\[
x(h+1,k+1) = A_1 x(h,k+1) + A_2 x(h+1,k) + B_1 u(h,k+1)
\]

\[
y(h,k) = C x(h,k)
\]

(2.4)

However (2.4) can be also viewed as a particular case of (2.3), with \(A_3 = 0\).
Local states that appear in the above equations do not exhibit the separation property, in the sense that, giving a single local state at \( \{h, k\} \) is not enough for computing the local states that follow \( z(\cdot, k) \) according to the partial ordering.

Actually, obtaining the whole evolution of a 2D system requires to know all local states that belong to a suitable infinite subset \( (= \text{separation set}) \) of \( \mathbb{Z} \times \mathbb{Z} \). Some examples of separation sets for systems having equations (2.2) are shown in fig. 2.2.

\[ \text{fig. 2.2} \]

3 2D Streeter-Phelps model

In this section we aim to introduce and discuss 2D space-time models that describe the process of natural self-purification of a river. The underlying biochemical hypotheses are the same as in the classical Streeter-Phelps model: modifications only account for the discretization of both space and time variables.

We shall assume throughout that the variables of BOD and DO concentrations on the river cross sections are much less important than the longitudinal ones. So we may confine ourselves to "one-dimensional" river models. One further hypothesis, to be relaxed later on in this section, is that hydrological variables, in particular the stream velocity \( v \), are constant all over the river stretch.

The first stage in constructing a 2D model is to divide the river into elementary reaches of length \( \Delta t \). The time step \( \Delta t \) and the elementary reach \( \Delta x \) are connected by \( \Delta t = \Delta x/v \), so a water element centered in \( i \) at time \( t \) will be centered in \( i + \Delta x \) at time \( t + \Delta t \).

Let \( \beta_i(t) \) and \( d_i(t) \) denote BOD concentration and DO deficit (w.r.t. to the saturation level) that exist in an elementary river reach centered in \( i \) at time \( t \). Computing BOD and DO values at \( i + \Delta x, t + \Delta t \) is based on a discretized balance equation, accounting for

- the self-purification process, due to the degradation of the originally discharged pollutants by bacteria. We assume that it decreases BOD concentration of the same amount \( a \beta_i(t, i+\Delta x) \) it increases the DO deficit;
- the respiration process, taking place water/oxygen interface. The simplest hypothesis is that DO deficit is reduced by an amount given by \( a \beta_i(t, i+\Delta x) \);
- BOD sources (effluents, local runoff, etc.) \( l_i(t, \cdot) \) and possibly reoxidation plants \( m_i(x, \cdot) \).

3.1 Models structure

Since longitudinal diffusion and dispersion are not taken into account, the values of the variables at the point \( (h, i, k+\Delta t) \) of the discrete plane \( \{(h, i, k) | (h, i) \in \mathbb{Z} \times \mathbb{Z} \} \) only affect the values at \( \{(h+\Delta t, i, k) | (h, i) \in \mathbb{Z} \times \mathbb{Z} \} \), i.e. along the diagonal line passing through \( (h, i, k) \).

The resulting balance equations are easily obtained and have the following structure

\[
\beta((h+1) \Delta t, (k+1) \Delta x) = \left( [1 - a \Delta t] \beta(h+1, k, \Delta x) + M \psi(h, k) + l_i(h, k) \right) \Delta x \\
\Delta (h+1) \Delta t = a \beta(h, k) \Delta x \\
\Delta (k+1) \Delta t = -a \beta(h, k) \Delta x
\]

Letting

\[ \pi_i(h, k) := \frac{\beta(h, k)}{a \beta(h, k)} \quad \psi_i(h, k) := \frac{\psi(h, k)}{a \beta(h, k)} \quad l_{i,q}(h, k) := \frac{l_i(h, k)}{a \beta(h, k)} \]

Equations (3.2) are rewritten as a second order 2D model

\[
z(h+1, k+1) = \left[ \begin{array}{cc} 1 & a \Delta t \\ a \Delta t & 1 - a \Delta t \end{array} \right] z(h, k) \\
+ \left[ \begin{array}{cc} (1 - a \Delta t)M & 0 \\ 0 & -(1 - a \Delta t)N \end{array} \right] \psi(h, k) \\
= A z(h, k) + B \psi(h, k)
\]

Remarks The above 2D model can be thought of as the juxtaposition of infinitely many copies of the same 1D system, each copy being associated with a different diagonal of the discrete plane. The elementary volume of water that at time 0 in position \( h, k \) is characterized by a state \( \{0\} := z(0, k) \) at time \( t = \Delta t \)

There are other methods by which one can proceed to build up a 2D state space model. It would be tedious and unnecessary to discuss here all of them; we confine ourselves to illustrate the structure of a first order model, with local states of dimension 2, which illustrates the advantages one gets if the coordinates \( (h, k) \) of the points in the discrete plane are not directly identified with time and space values of the physical model. This approach will prove to be fruitful in the next section, where diffusion will be taken into account.

We assume that the pair \( (h, k) \) is associated with the point \( (a, b) \in \mathbb{Z} \times \mathbb{Z} \) that satisfies

\[ a = h - k, \quad b = k. \]

So, the points of the separation set \( \{(a, b) | a + b = k \} \) represent locations \( k \Delta x \) along the river stretch at the same time instant \( k \Delta t \) and the points of the set \( \{(a, b) | b - k = a \} \) represent time instants \( a \Delta t = (a - k) \Delta t \) at the same location \( k \Delta x \).

Letting

\[ \text{fig. 3.1} \]
3.2 Initial conditions

In the continuous Streeter-Phelps model initial conditions (i.e. the values of BOD concentration and DO deficit at time \( t = 0 \)) as well as the boundary conditions (i.e. the values of BOD concentration and DO deficit at \( t = 0 \)) can be independently assigned. A different possibility consists in assigning only the boundary conditions at \( t = 0 \) for all \( t \geq t_0 \) \( (t_0 \in \mathbb{R} \) or \( t_0 = -\infty \)) in this case the solution can be computed in the region \( (t, t_1) \mid t \geq 0, t_1 > t_0 \).

When the discrete 2D model (3.3) is considered, local states can be arbitrarily assigned on the boundary of the positive orthant. There are also other possibilities: actually we are allowed to assigning independently conditions on all the diagonal lines of the plane (except one local state on each diagonal). Any one of the above sets of conditions is "reachable", since it can be thought of as produced by the application of suitable space/time distributions of BOD and DO sources.

Some caveats are in order when assigning conditions for model (3.9). First of all, the compositional of the local state specify the values of BOD concentration and DO deficit at the same time instant in two consecutive spatial locations. Thus, when local states are assigned as initial conditions on some line \( \{(h, k) \mid h \in \mathbb{Z}\} \) or along the boundary of the positive orthant, restrictions should be placed on the values of the states, so that the second and the fourth component of \( x(h, k) \) are equal to the first and the third component of \( x(h, k+1) \) respectively. So, when initializing the 2D system (3.9), the physical meaning of local states allows to consider only reachable arrays of admissible conditions.

One more aspect of the dynamical structure of the system, however, must be considered if the assignment of the initial states is to be meaningful. Namely, the state updating operation must not modify the original values of the given states on the boundary. If some boundary points are in the future of some others, it is patently inconsistent to compute the free state evolution by superposing local state values, as determined by the rule \( x(h, k) = A_{k}x(h, k) + A_{h}x(h, k) \). In fact, this would possibly modify boundary values themselves. In this connection we shall discuss here the problem of computing the formal power series associated with the doubly indexed sequence of states in two cases, seemingly the most significant ones.

Suppose first that local states have been assigned on the boundary \( \{(h, 0) \mid h \in \mathbb{Z}_+\} \cup \{(0, k) \mid k \in \mathbb{Z}_+\} \) of the first orthant and input values on \( (h, 0) \) \( h \geq 0, k > 0 \) \( (0, k) \) \( h > 0, k \geq 0 \). Due to the recursive structure of (3.9), the computation of \( z(h, k) \), \( h > 0, k > 0 \) only involves the initial local states \( x(h, 0) \) \( 0 < h < k \) \( \cup \{(0, k) \mid 0 < h < k \) \) and the input values \( u(h, k) \), \( 0 \leq h < k, 0 < k \leq k \) \( h > 0, k > 0 \) as shown in fig. 3.3

Consider the formal power series

\[
X_{2}(z_{1}, z_{2}) = \sum_{h,k>0} x(h,k) z_{1}^{h} z_{2}^{k} 
\]

associated to the doubly indexed array of local states \( x(h,k) \mid h,k > 0 \) and let \( X_{2}(z_{1}, z_{2}) \) be the corresponding free evolution induced by the assignment of local states on the boundary of the positive orthant. \( X_{2}(z_{1}, z_{2}) \) can be computed according to

\[
X_{2}(z_{1}, z_{2}) = \sum_{h,k>0} x(h,k) z_{1}^{h} z_{2}^{k} 
= \sum_{h,k>0} \left[ A_{2}x(h-1,k) + A_{2}x(h,k-1) \right] z_{1}^{h} z_{2}^{k} 
\]

On the other hand, forced evolution is easily obtained as

\[
X_{2}(z_{1}, z_{2}) = (I - A_{1}z_{1} - A_{2}z_{2})^{-1} \left( z_{1}A_{1} \sum_{h>0} x(0,h) z_{1}^{h} z_{2}^{0} + z_{2}A_{2} \sum_{k>0} x(0,k) z_{1}^{k} z_{2}^{0} \right) 
\]

where \( U(z_{1}, z_{2}) = \sum_{h,k>0} u(h,k) z_{1}^{h} z_{2}^{k} \) is the formal power series associated with the input sequence.

The second case we investigate constitutes a discrete analogue of assigning BOD and DO values at some point of the river (e.g. \( t = 0 \)) for all \( h \). This corresponds to specifying in model (3.3) local states on the line \( \{(h,0) \mid h \in \mathbb{Z} \} \) and input values on the half plane \( \{(h,k) \mid h \geq 0 \} \). An obvious role of the dimensionality of \( A_{2} \) and \( A_{3} \) is to guarantee that a single local state \( x(h,k) \) does not influence local states on the diagonal lines that do not intersect the set \( \{(h,k) \mid h = 1, k = 1 \} \). The following equations reveal the importance of this property as determining the free state evolution of the system

\[
x(h,0) = A_{2}x(h-1,0) + A_{2}x(h,1) 
\]

\[
x(0,k) = A_{1}x(0,k-1) + A_{1}x(0,k) 
\]

\[
x(h,k) = A_{2}x(h-1,k) + A_{2}x(h,k) 
\]

\[
X_{2}(z_{1}, z_{2}) = \sum_{h,k>0} x(h,k) z_{1}^{h} z_{2}^{k} 
= \sum_{h,k>0} \left[ A_{2}x(h-1,k) + A_{2}x(h,k-1) \right] z_{1}^{h} z_{2}^{k} 
\]

The state vector in the \( k \)-th river stretch is the coefficient of any monomial \( z_{1}^{h} z_{2}^{k} \) in (3.17), i.e. \( x(h,k) = [A_{1}^{h} A_{2}^{k}] x_{0} \). The assignment of initial states and the formal power series description of local set of boundary conditions in model (3.11) are similar to those for the model (3.9), but simpler because no constraints are needed among initial states. We leave the details to the reader.

To conclude this section we remark that an alternative to introducing a reachable set of boundary conditions always exists, and consists in considering input sequences that force boundary conditions on a 2D system originally at rest (e.g. on a river that is perfectly clean and aerated). In these cases, substituting forced dynamics for boundary conditions is a matter of taste and/or computational convenience.

3.3 Space-dependent dynamics

Our original assumption in this section was that all river parameters do not depend on \( l \). It is often the case, however, that certain parameters of the one-dimensional model are strongly influenced by the geometrical and physical at-
tributes of the underlying three-dimensional real model. Relaxing that assumption can certainly enhance our capability of modelling river phenomena. So in the remaining part of this section we suppose that the river velocity \( v \) as well as the coefficients \( a_1 \) and \( a_2 \) are dependent on \( x \) and \( t \).

It is not difficult to figure out situations where a dependence on \( t \) may arise. Apart from the obvious ones, refer to velocity variations, the dependence of \( a_1 \) on \( t \) is also to be avoided for the inhomogeneous bacterial oxidation (e.g. due to thermal variations or to same bacterial species that locally prevail on some others), while the dependence of \( a_2 \) may be connected with turbulences, falls etc., that induce some variations on the reservoir process.

While the time interval \( \Delta t \) is kept constant, the length \( \Delta l \) of the elementary reaches will vary so as to satisfy in all cases the condition \( \Delta l = \Delta l(x) \). More precisely, the river stretch will be divided into elementary reaches \( \Delta l = [x, x + 1] \), with \( \Delta l = \Delta l(x) \) so that an elementary volume of water in position \( x \) at time \( t \) will be in position \( x + \Delta l \) at time \( t + \Delta t \). After introducing two families of \( \Delta t \)-dependent coefficients \( a_1(x, t) \) and \( a_2(x, t) \), we are in a position to rewrite model (3.3) as follows:

\[
x(x + 1, t + \Delta t) = \begin{bmatrix} -a_1(x)\Delta t & 0 \\ a_2(x)\Delta t & -a_2(x)\Delta t \end{bmatrix} x(x, t) + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \Delta t f(x, t)
\]

(3.18)

where the local state vector is defined by

\[
x(x, t) = \begin{bmatrix} h(x, t) \\ \rho(x, t) \end{bmatrix}
\]

(3.19)

The 1D model (3.4) associated with (3.1) and (3.2) becomes now

\[
\xi(t + 1) = \begin{bmatrix} -a_1(x)\Delta t & 0 \\ a_2(x)\Delta t & -a_2(x)\Delta t \end{bmatrix} \xi(t) + \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Delta t f(x, t)
\]

(3.20)

In particular, the free evolution of (3.1) satisfies

\[
\xi(t + 1) = A_0\xi(t - 1) + \ldots + A_0(1)\phi_0(0)(0) = \Phi(t)\phi(0)
\]

(3.21)

with

\[
\Phi(t) = \sum_{\epsilon = \pm 1} \prod_{k=1}^{t} \left\{ \prod_{\epsilon = -1} \left[ 1 - a_2(x)\Delta t \right] \right\} \left\{ 1 - a_1(x)\Delta t \right\}
\]

(3.22)

The asymptotic behaviour of (3.21) can be deduced from the absolute criterion for infinite products \([0, 0] \). Actually, because of the inequalities \( 0 \leq a_2(x)\Delta t < 1, 0 \leq a_1(x)\Delta t < 1 \), a necessary and sufficient condition for having \( \lim_{t \to +\infty} \prod_{k=1}^{t} \left[ 1 - a_2(x)\Delta t \right] = 0 \) and \( \lim_{t \to +\infty} \prod_{k=1}^{t} \left[ 1 - a_1(x)\Delta t \right] = 0 \) is that both the following series

\[
\sum_{s=0}^{\infty} a_1(x) \quad \text{and} \quad \sum_{s=0}^{\infty} a_2(x)
\]

(3.23)

diverge.

We shall prove now that, when the series in (3.22) diverge, the term in position (2,1) of the transition matrix \( \Phi(t) \) converges to zero as \( t \to +\infty \). This shows that the divergence series in (3.23) constitute a necessary and sufficient condition for the self-purification of the river.

First of all, note that \( A_0\phi \) can be viewed as a diagonal block of a 3 \times 3 stochastic matrix

\[
A^{(0)}(\phi) = \begin{bmatrix} -a_1(\phi)\Delta t & 0 & 0 \\ a_2(\phi)\Delta t & -a_2(\phi)\Delta t & 0 \\ 0 & 0 & 1 \end{bmatrix}
\]

(3.23)

Therefore

\[
\Phi^{(0)}(\phi) = \Phi^{(0)}(\phi) - \Phi^{(0)}(\phi) + \ldots + \Phi^{(0)}(\phi) = \begin{bmatrix} \Phi(0) \\ \Phi(0) \\ \Phi(0) \end{bmatrix}
\]

(3.24)

is a stochastic matrix for all \( \epsilon \in Z_2 \). Next, apply the recursive equation \( \Phi^{(0)}(\phi) = \Phi^{(0)}(\phi) + \Phi^{(0)}(\phi) \) to obtain the following identity

\[
\Phi^{(n)}(\phi) = \begin{bmatrix} \Phi(0) \\ \Phi(0) \\ \Phi(0) \end{bmatrix}
\]

(3.25)

The monotonous character of the sequence \( \Phi^{(n)}(\phi) \) and the inequality \( \Phi^{(n)}(\phi) \leq \Phi^{(n)}(\phi) \leq 1 \), \( \forall n \), imply that the above sequence converges : \( \lim_{n \to +\infty} \Phi^{(n)}(\phi) = \Phi^{(\infty)}(\phi) \). Now, taking the limit on the right side of \( \pi = \pi^{(0)} + \pi^{(1)} + \pi^{(2)} \), and recalling that \( (\pi^{(n)}(\phi)) \) converges to 0, we see that the sequence \( \pi^{(n)}(\phi) \) converges to \( \pi^{(\infty)}(\phi) = 1 - \pi^{(\infty)}(\phi) \).

It remains to prove that \( \phi_2 = 0 \). Assume, by contradiction, \( \phi_2 > 0 \). Then there exists an integer \( m \) such that \( \phi_2(\phi) > \phi_2(\phi), \forall n \geq m \) and therefore

\[
\phi_2(\phi) = \phi_2(\phi) > \phi_2(\phi) > \phi_2(\phi) > \ldots \geq 0
\]

(3.26)

Taking into account that \( \sum_{\epsilon = \pm 1} \phi_2(\phi) \) diverges too, which is a contradiction, since \( \phi_2(\phi) \) is finite. We therefore have \( \phi_2 = 0 \) and \( \phi(0) \to 0 \quad as \quad t \to +\infty \).

4 2D diffusion models

The 2D models considered so far do not incorporate (longitudinal) diffusion and/or dispersion phenomena. As well known, introducing diffusion in Streeter-Phelps equations gives rise to partial differential equations that include the second derivatives w.r.t. the space coordinate. Although 2D analogs of continuous diffusion models may be obtained using a suitable discretization procedure, we prefer to stay here directly from a discrete representation of the diffusion mechanism and to set up a "first principles" derivation of 2D diffusion models.

4.1 Building an elementary model

Perhaps the simplest representation of the diffusion mechanism can be obtained by introducing in model (3.1) additional terms that account for BOD and DO diffusion between contiguous elementary reaches. Diffusion is therefore modeled by assuming that the BOD concentration of the elementary reach centered in \( x \) at time \( t \) undergoes variations in \( x \) that are proportional to the differences \( \beta(t, t - \Delta t) \) and \( \gamma(t, t - \Delta t) \).

Correspondingly, equation (3.1) has to be modified as follows:

\[
\beta(t, t - \Delta t) = \beta(t, t - \Delta t) - \beta(t, t - \Delta t) - \beta(t, t - \Delta t)
\]

(3.27)

Similarly equation (3.2) becomes

\[
\delta(t, t - \Delta t) = \delta(t, t - \Delta t) + \delta(t, t - \Delta t) - \delta(t, t - \Delta t) - \delta(t, t - \Delta t)
\]

(4.1)

Letting

\[
\phi(x, t) = \begin{bmatrix} \phi_1(x, t) \\ \phi_2(x, t) \\ \phi_3(x, t) \end{bmatrix}
\]

one gets a 2D system in form (3.2):

\[
x(x + 1, t + 1) = \begin{bmatrix} D_{\beta}(\Delta t) & 0 & 0 \\ 0 & a_1(\phi)\Delta t & 0 \\ 0 & 0 & a_2(\phi)\Delta t \end{bmatrix} \begin{bmatrix} x(x, t) \\ \phi_2(x, t) \\ \phi_3(x, t) \end{bmatrix} + \begin{bmatrix} \beta(t, t - \Delta t) \\ 0 \\ 0 \end{bmatrix} \Delta t
\]

(4.2)

with \( a_1 = a_1 + 2D_{\beta}, a_2 = a_2 + 2D_{\beta} \).

4.2 BOD and DO distributions

Assume first that a unitary BOD pulse at \( (0, 0) \) constitutes the forcing input to a river that is perfectly clear and aerated. This gives rise to a spatially symmetric distribution of BOD, that extends at time \( \Delta t \) from the abscissa \( x \) up to the abscissa \( 2\Delta l \). Having \( \Delta l \) as a center of symmetry.

The general local state response can be described by a formal power series

\[
X^{(n)}(x, t, \phi) = (I - A^{(0)}\phi - a_2(\phi)\Delta t - a_1(\phi)\Delta t) x^{(0)}(x, t, \phi) - B^{(0)}\phi x^{(0)}(x, t, \phi)
\]

with

\[
A^{(0)} = \begin{bmatrix} 0 \\ D_{\beta}(\Delta t) & 1 - a_1(\phi)\Delta t \\ 0 \end{bmatrix}, \quad A^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}
\]

(4.3)
The second component of $X[\pi](\tau_1, \tau_2)$ provides the BOD impulse response:

\[ X[\pi](\tau_1, \tau_2) = \frac{1}{2}\left( D_0 \Delta t + \frac{1}{2} \Delta \sigma \right) \left( 1 - 2 \psi(\tau_1, \tau_2) \right) \]

and the values of the BOD concentration at time $\Delta t$ can be found just by considering the polynomial in $R[\tau]$ that constitutes the coefficient of $x_i^2$ in the series above, i.e.

\[ x_2 \left( D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2) \right) \]

The power series representing the DO deficit distribution can be obtained along the same lines. After introducing the following shorthand notations:

\[
\begin{align*}
    d(x) &= D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2) + D_\psi \Delta t \frac{\Delta}{2} \\
    L &= |1 - a_1| \Delta t \\
end{align*}
\]

the DO deficit distribution is given by the series expansion:

\[ X[\pi](\tau_1, \tau_2) = \frac{1}{L} \left( D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2) + D_\psi \Delta t \frac{\Delta}{2} \right) \sum_{i=0}^{\infty} \frac{d(x)^i}{i!} \]

Suppose next that a time constant unitary input of BOD is applied on the 0th reach of the river. Using the superposition principle, we represent the BOD distribution as given by a power series in $\tau_1$, with coefficients in the ring $R[\tau_1]$ of formal power series in $\tau_2$:

\[ X[\pi](\tau_1, \tau_2) = \frac{1}{L} \left( D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2) + D_\psi \Delta t \frac{\Delta}{2} \right) \sum_{i=0}^{\infty} \frac{d(x)^i}{i!} \]

Accordingly, it can be inferred that a steady state BOD distribution settles down along the river, as represented by the series:

\[ X[\pi](\tau_1, \tau_2) = \frac{1}{L} \left( D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2) + D_\psi \Delta t \frac{\Delta}{2} \right) \sum_{i=0}^{\infty} \frac{d(x)^i}{i!} \]

The same reasoning shows that the space-time representation of the DO deficit is given by the formal power series expansion of:

\[ X[\pi](\tau_1, \tau_2) = \frac{1}{L} \left( D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2) + D_\psi \Delta t \frac{\Delta}{2} \right) \sum_{i=0}^{\infty} \frac{d(x)^i}{i!} \]

Here we obtain the steady state BOD distribution by expanding the rational function:

\[ \frac{Lx}{1 - x} \sum_{i=0}^{\infty} \frac{d(x)^i}{i!} \]

into a power series in $R[\tau_1]$.

### 4.3 Steady state distributions

The long term behaviour of the steady state distributions above are determined by the root locations of the polynomials $1 - D_0 \Delta t$ and $1 - d(x)$. Stability issues, in particular, are connected with root locations w.r.t. to the unitary circle. Since $D_\psi \Delta t$, $D_0 \Delta t$, $\Delta$, and $\Delta t$ are negligible w.r.t. to 1, is easy to check that the roots of $1 - D_0 \Delta t$ and $1 - d(x)$ are external w.r.t. the unitary disk. We conclude that, according to our physical intuition, stationary distributions of BOD concentration and DO deficit converge to zero as $t$ goes to infinity.

In order to get a more detailed information, we aim here to make a comparison of BOD and DO steady state regimes with and without diffusion. Analysing the shapes of BOD and DO distributions along the river stretch, requires to introduce first a partial fraction expansion of (4.6) and (4.7), and then to expand each fraction into a geometric power series.

**BOD distribution** Rewrite (4.6) as follows:

\[ X[\pi](\tau_1, \tau_2) = \frac{G_\psi \Delta t}{1 - D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2)} \]

with:

\[ G_\psi = \sqrt{\frac{\Delta t}{D_0 \Delta t}}, \quad b_1 = \frac{1}{1 - D_0 \Delta t}, \quad b_2 = \frac{1}{1 - D_0 \Delta t} \]

Moreover, let:

\[ \mu_1 = -a_1 \Delta t, \quad \mu_2 = -a_2 \Delta t \]

Hence, if $b_3 = 0$, and therefore polluting materials do not undergo diffusion, the denominator of (4.8) reduces to the first order polynomial $1 - \mu_1 \Delta t$. Otherwise, it factorizes as $(1 - \mu_1 \Delta t)(1 - \mu_2 \Delta t)$, with $\mu_1 < \mu_2$ when $\Delta t$ is small enough [10].

The partial fraction and the geometric series expansions of (4.8) give:

\[ X[\pi](\tau_1, \tau_2) = \frac{G_\psi \Delta t}{1 - D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2)} \]

and reduces to $\beta \Delta t$ when BOD does not undergo diffusion phenomena.

Some interesting conclusion can be drawn from these simple calculations. First, since $G_\psi \gg G_\mu$, the BOD regime with diffusion can be approximated by a decreasing geometric sequence with ratio $\mu_1$, perturbed by an oscillatory term, whose amplitude, infinitesimal as $t \to \infty$, is everywhere negligibly small. Second, when the model does not incorporate diffusion, the geometric sequence converges to zero more rapidly (since $\mu_1 < \mu_2$) and the oscillatory perturbation disappears.

**DO distribution** The comparison of the DO regimes with and without diffusion require to introduce some more notations. Rewrite first (4.7) as:

\[ X[\pi](\tau_1, \tau_2) = \frac{G_\mu \Delta t}{1 - \mu_1 \Delta t + 1 - 2 \psi(\tau_1, \tau_2)} \]

with:

\[ G_\mu = \sqrt{\frac{\Delta t}{1 - D_\psi \Delta t}}, \quad d_1 = \frac{1}{1 - D_0 \Delta t} \quad d_2 = \frac{1}{1 - D_\psi \Delta t} \]

and let:

\[ \mu_1 = 1 - a_2 \Delta t, \quad \mu_2 = -a_1 \Delta t \]

When diffusion phenomena are neglected, the denominator of (4.11) is the second order polynomial $(1 - \mu_1 \Delta t)(1 - \mu_2 \Delta t)$ and in that case the partial fraction expansion of (4.11) becomes:

\[ X[\pi](\tau_1, \tau_2) = \frac{G_\psi \Delta t}{1 - D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2)} \]

The DO deficit at the abscissa $[i + 2] \Delta t$:

\[ \delta \left( i + 2 \Delta t \right) = \frac{G_\psi \Delta t}{1 - D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2)} \]

can be viewed as a function of the real variable $i$, whose maximum value is attained when $\mu_1^2 \Delta t \mu_2 = \mu_2^2 \Delta t \mu_1$. Denoting by $[x]$ the integer part of the real number $x$, the maximum value of the sequence (4.12) is attained either at $i_M \leq i_{M}$ or at $i_{M} + 1$. Note that $i_{M}$ is a nonnegative number, as we may except from the physical assumption that the river is perfectly aerated at the abscissas $l = 0$ and therefore polluted injections at $l = 0$ increase the DO deficit on the subsequent reaches, until the natural reaeration balances the bacterial oxidative processes.

This leads to the important qualitative conclusion that the sequence (4.12) is a discrete analogue of the surf profile of DO concentration in the continuous Streeter-Phelps model.

Suppose now that diffusion is not negligible, so that the denominator of (4.11) factorizes into $(1 - \mu_3 \Delta t)(1 - \mu_4 \Delta t)(1 - \mu_5 \Delta t)$, with $\mu_3 < \mu_4 < \mu_5$. Confining ourselves to the case when multiple roots are excluded, i.e. when:

\[ \frac{b_2}{b_1} \neq \frac{b_1}{b_2} \quad \frac{b_2}{b_1} \neq \frac{1 + i \Delta t}{1 - i \Delta t} \]

we have [10]:

\[ X[\pi](\tau_1, \tau_2) = \frac{G_\psi \Delta t}{1 - D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2)} \]

or at $i_M + 1$. Note that $i_{M}$ is a nonnegative number, as we may except from the physical assumption that the river is perfectly aerated at the abscissas $l = 0$ and therefore polluted injections at $l = 0$ increase the DO deficit on the subsequent reaches, until the natural reaeration balances the bacterial oxidative processes.

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\[ \frac{b_2}{b_1} \neq \frac{b_1}{b_2} \quad \frac{b_2}{b_1} \neq \frac{1 + i \Delta t}{1 - i \Delta t} \]

we have [10]:

\[ X[\pi](\tau_1, \tau_2) = \frac{G_\psi \Delta t}{1 - D_0 \Delta t + 1 - 2 \psi(\tau_1, \tau_2)} \]

and reduces to $\beta \Delta t$ when BOD does not undergo diffusion phenomena.
Since $\beta/\mu_0$ are negligible w.r.t to 1, we are allowed to introduce the following approximations

$$G_{\text{exp}} \approx G_{\text{emp}} \approx \frac{G_2^2}{\beta_1 - \beta_2}, \quad G_{\text{int}} \approx G_{\text{ev}} = \frac{G_2}{\beta_1 - \beta_2},$$

which give the partial fraction expansion (4.14) the simpler structure

$$X_2^{(1)}(\tau_2) = \frac{2Z}{\beta_1 - \beta_2} - \frac{G_2}{\beta_1 - \beta_2} \left( \frac{1}{\tau_1^2} \right) \left( \frac{1}{\tau_2^2} \right),$$

and allow to express the DO deficit at the abscissa $(i+2)\Delta t$ as

$$\ell_t(i, (i+2)\Delta t) = G_{\text{exp}} \left[ \beta_1^{i+1} - \beta_2^{i+2} \right] + \cdots,$$  

The second term of (4.16) constitutes an oscillatory perturbation, that goes to zero as $i \to \infty$, and is negligible everywhe where the term 1.

### 4.4 Modelling diffusion velocity

An implicit assumption in equations (4.1)-(4.2) as well as in the corresponding state model (4.3) is that the diffusion velocity is equal to the velocity of the river. This is also clear from support of the impulse response. A BOD injection at time $i = 0$ on the origin of the space coordinates gives rise, for all $\tau$, to spatially symmetric distributions, whose maximum points lie on the diagonal of the first quadrant (i.e., on the support of the impulse response when diffusion is neglected) and the initial point is steadily at the abscissa $\Delta t$. This implies that the backward propagation of the diffusion wavefront exactly balances the advection velocity of the river.

![Fig. 4.1](image)

There are several ways for introducing 3D models where the diffusion and the advection velocity do not coincide. Here we shall only present a sampling of these methods and outline two conceptually different approaches to the problem. The first approach is based on the intuitive assumption that more complex dynamics require higher order systems to be represented; the second one exploits a suitable reinterpretation of the integer grid $Z \times Z$, along the same lines we followed for the third state model in sec. 2.1.

For sake of simplicity, we deal only with BOD diffusion equation. Assume that the elementary volume of water, centered at the abscissa $i$ at time $t$, attains the abscissa $i + 2\Delta t$ at time $t + \Delta t$, so that the advection velocity is $v = 2\Delta t/\Delta t$. We still keep in force the BOD degradation scheme considered at the beginning of this section, assuming in particular that diffusion in $\Delta t$ only affects contiguous elementary reaches. Thus the BOD updating equation takes the explicit form

$$\beta(t + 1\Delta t, (k + 2)\Delta t) = [1 - a_1\Delta t][\beta(t + \Delta t, k\Delta t)] + [1 - a_1\Delta t][\min(t + \Delta t, k\Delta t)]$$

$$+ D_\beta \left[ \beta(t + \Delta t, (k + 1)\Delta t) - \beta(t + \Delta t, k\Delta t) \right]$$

Letting

$$x(\Delta t, k + 1) = \left[ \begin{array}{c} x_1(t + \Delta t, k + 1) \\ x_2(t + \Delta t, k + 1) \\ \vdots \end{array} \right],$$

one gets a 2D system of the following form

$$x(\Delta t, k + 1) = A(t, \Delta t) x(t, k),$$

(4.18)

with

$$A(t, \Delta t) = \left[ \begin{array}{cccc} 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & \cdots \\
-1 & -a_1\Delta t & D_\beta & \cdots \end{array} \right], \quad A_1(t, \Delta t) = \left[ \begin{array}{cccc} 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\
0 & 0 & 0 & \cdots \\
-1 & -a_1\Delta t & D_\beta & \cdots \end{array} \right].$$

Assuming BOD concentration $\beta(t + \Delta t, k\Delta t)$ as the system output the impulse response is given by the power series expansion of the following transfer function

$$\frac{1}{1 - \beta(\Delta t, k\Delta t)} = \frac{1}{1 - \beta(t, \Delta t)} + \beta(t, \Delta t)\Delta t,$$

(4.19)

where $\beta(t, \Delta t)$ denotes the polynomial of (4.7). The support of (4.19) is represented in fig. 4.2, showing that the diffusion wavefront progresses with a velocity which is different from (actually, smaller than) the river advection velocity.

The second approach is reminiscent of the philosophy that underlines model (3.11). The interpretation of the grid $Z \times Z$, given in fig. 3.2 with reference to model (3.11) is well suited also for representing the diffusion model (4.1). In fact, letting

$$\beta(h, t, \Delta t) = \varphi(h - k, \Delta t),$$

and equation (4.1) is transformed into

$$x(\Delta t, h, k) = \varphi(k, h, \Delta t),$$

and therefore admits a 2D representation with a scalar state variable, provided that a suitable reinterpretation of the grid $Z \times Z$ has been performed.

The above examples constitute a particular application of a more general theory, that is outlined in [10].

### 5 References

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