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Abstract

This paper is devoted to the identification of a pollution source in a river. A simple mathematical model of such a problem is given by a one-dimensional linear advection-dispersion-reaction equation with a right hand side spatially supported in a point (the source) and a time varying intensity, both unknown. There exist some identifiability results about this distributed system. But the numerical estimation of the unknown quantities require the introduction of an approximated model, whose identifiability properties are not analyzed usually. This paper has a double purpose: - to do a complete identifiability analysis of the differential system considered for estimating the unknown parameters, - to propose a new numerical global search of these parameters, based on the previous analysis. Another consequence of this approach is that it gives the unknown pollution intensity directly as the solution of a differential equation. Lastly, the numerical algorithm is described in detail, completed with some applications.

1 Introduction

The quality of the water is of a crucial interest in our society. It can be estimated by measuring, for example, the quantity of organic matters contained in the water. This paper is concerned with the determination of the location and the intensity of a pollution source from the measurements of a pollutant concentration linked to organic matters. The model, given here, corresponds to a river portion of length L surrounded by factories or other possible pollution sources. A first simple model is given by a linear advection-dispersion-reaction equation (see [10] and [12] for details):

$$\begin{cases} \dfrac{\partial u}{\partial t}(x,t) - D\dfrac{\partial^2 u}{\partial x^2}(x,t) + V\dfrac{\partial u}{\partial x}(x,t) + Ru(x,t) = \lambda(t)\delta(x-a)\,, \quad (x,t) \in]0,L[\times]0,T[\\ u(x,0) = g(x),\ x \in]0,L[\,, \\ u(0,t) = 0,\ t \in]0,T[\,,\ \dfrac{\partial u}{\partial x}(L,t) = 0,\ t \in]0,T[\,, \end{cases} \tag{1}$$

where u, D, V, and R denote the substrate concentration, the dispersion coefficient, the transport velocity and the reaction coefficient respectively. The right hand side member depends on two unknown parameters: $\lambda \in \mathcal{L}$ (the set of functions $\mathcal{L}$ will be specified in the remainder), the flow rate of the pollutant, and $a \in]0,L[$, the location of the source. The function g is assumed to be smooth, at least in $C^2(0,L)$, and $\delta(x-a)$ is the Dirac mass at the point a.

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The pollution is assumed to be known at the initial time and the boundary conditions translate the unidirectional nature of the transport. Indeed there is no significant transport upstream, therefore the concentration is assumed to be zero at some point situated upstream ($x = 0$). On the other hand the downstream point $x = L$ is far enough from the source so that a zero gradient can be considered.

It is well-known that the problem (1) has a unique solution that is smooth enough in a neighborhood of L since $a \in]0, L[$. So, it makes sense to define $u(L, t)$ as the observation function:

$$y(t) = u(L, t)\,,\ t \in (0, T). \tag{2}$$

In order to test a new approach, a first study was done when λ is constant [17]. It was proved that, when the initial conditions are considered known, the observation function y is sufficient to obtain the identifiability of the pollution source in the model (1) whereas when they are unknown, a second point of observation has to be added. In order to estimate the parameters λ and a, an approximated system was used and its global identifiability was proved by using an elimination approach [11]. From the identifiability analysis, a new numerical procedure of parameter estimation was elaborated and tested.

It is the same idea which is developped in this paper but the variation in time of the pollution intensity increases the complexity of the solution. For the model (1), results of identifiability, obtained by using a decomposition on a basis of eigenfunctions, and parameter identification were given in [6] with two points of observation, one upstream, the other downstream from the source provided the flow rate is zero on an interval $[T, T + \delta T]$ $(T > 0)$. And the proposed numerical method is local and based on a least-squares regularized method.

In this paper, an approximate system is obtained from an approximation of the Dirac mass by a smooth function and a semi-discretization in space. It consists of a system of differential equations, the size of which corresponds to the number of discretization points of the interval $[0, L]$. First, the paper is focused on the proof of the identifiability of the so-obtained model, based on an elimination approach. Then it is shown how the previous identifiability analysis leads to a numerical global search of the localization of the pollution source and the pollution intensity. Indeed the unknown function $\lambda(t)$ is computed from the solution of a differential equation directly, without truncating its decomposition on a basis function as it is done usually. This method is close to the one proposed by B. Laroche and al. [9] or F. Olliver and al. [14].

The paper is presented as follows: section 2 introduces the approximation differential system, section 3 gives identifiability results, section 4 explains in detail the numerical algorithm and presents some numerical results.

2 The semi-discretized model

Let us begin by recalling an identifiability result about the model (1). Let us denote the dependence of u on (λ, a) by $u|(\lambda, a, g); x, t|$. The following result of the identifiability of the model (1) has been shown in [6]. Let λ and $\tilde{\lambda}$ be two functions in $L^2(0, T)$, such that $\lambda(t) = \tilde{\lambda}(t) = 0$ for $T^* < t < T$, and let a and $\tilde{a}$ be two points in $]\xi_1, \xi_2[$ where ξ_1 or ξ_2 is a "strategic" point. Then the model (1), completed with the observations:

$$y_1|(\lambda, a, g); t| = u|(\lambda, a, g); \xi_1, t|\,,\ y_2|(\lambda, a, g); t| = u|(\lambda, a, g); \xi_2, t|$$

is identifiable, i.e.: $\exists t_1$ $(0 < t_1 < T)$ such that if $y_1|(\lambda, a, g); t| = y_1|(\tilde{\lambda}, \tilde{a}, g); t|$ and $y_2|(\lambda, a, g); t| = y_2[(\tilde{\lambda}, \tilde{a}, g); t]$, $\forall t \in]0, t_1[$, then $(\tilde{\lambda}, \tilde{a}) = (\lambda, a)$. The assumption considered here $(\lambda(t) = 0$ for $T^* < t < T)$ corresponds to the case of an accidental pollution stopped at time T^*, while recording of the concentration u is continued until a later time T.

Now, the model used for the numerical estimation of the parameters is introduced. Firstly, since regular functions are needed to use differential algebra, the Dirac mass $\delta(x - a)$ is approximated by a

Gaussian function:

$$w(x) = \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{(x-a)^2}{\sigma^2}}, \tag{3}$$

where the coefficient σ will be chosen so that the error between the solution of (1) and the solution of the continuous model with $\delta(x-a)$ replaced by $w(x)$ be smaller than the error of the semi-discretized scheme. Indeed, if $\check{u}$ is the solution of (1) with the Dirac mass substituted by (3), the following estimation can be easily shown:

$$\forall \epsilon > 0,\ \exists \sigma^* > 0, \text{ such as if } 0 < \sigma < \sigma^* : \parallel u(t) - \check{u}(t) \parallel_2 \leq \frac{\lambda_{max}\epsilon}{\kappa}\sqrt{1-e^{-\kappa T}}e^{-\nu L},$$

with $\nu = -\frac{V}{2D}$ and κ is an ellipticity constant.

Then the system (1) is discretized in space by a centered difference scheme. If $(N+1)$ discretization points $(x_i)_{0<i<N}$ in space are considered, it leads to:

$$\begin{cases} \dot{u}(x_1,t) + \left(\frac{V}{h} + 2\frac{D}{h^2} + R\right) u(x_1,t) - \frac{D}{h^2}u(x_2,t) = \lambda(t)w(x_1) + h\epsilon_1(t), \\ \\ \dot{u}(x_i,t) - \left(\frac{V}{h} + \frac{D}{h^2}\right) u(x_{i-1},t) + \left(\frac{V}{h} + 2\frac{D}{h^2} + R\right) u(x_i,t) - \frac{D}{h^2}u(x_{i+1},t) = \lambda(t)w(x_i) + h\epsilon_i(t), \\ i = 2, ..., N-1, \\ \\ \dot{u}(x_N,t) - \left(\frac{V}{h} + 2\frac{D}{h^2}\right) u(x_{N-1},t) + \left(\frac{V}{h} + 2\frac{D}{h^2} + R\right) u(x_N,t) = \lambda(t)w(x_N) + h\epsilon_N(t), \end{cases} \tag{4}$$

where $h = \frac{L}{N}$, $x_i = ih$ for $i = 0, ..., N$ and

$$\epsilon_i(t) = -\frac{1}{2}V\frac{\partial^2 u}{\partial x^2}(x_i,t) + \frac{h}{6}\left(\varphi_{1,i}D\frac{\partial^4 u}{\partial x^4}(x_i + \varphi_{2,i}h, t) - V\frac{\partial^3 u}{\partial x^3}(x_i + \varphi_{1,i}h, t)\right)$$

with $|\varphi_{k,i}| < 1$, $k = 1,\ 2$.

Consequently, the flow rate λ is assumed to be $C^{N-1}([0,T])$, whatever is the value of N.

The value $w(x_i)$, defined by (3), is explicited as:

$$w(x_i) = \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{a^2}{\sigma^2}} e^{-\frac{(ih)^2}{\sigma^2}} \left(e^{h\frac{2a}{\sigma^2}}\right)^i \tag{5}$$

Let us introduce:

$$\begin{gathered} \alpha = \frac{V}{h} + \frac{D}{h^2},\ \beta = -\left(\frac{V}{h} + 2\frac{D}{h^2} + R\right),\ \gamma = \frac{D}{h^2} \\ \ell(t) = \frac{\lambda(t)}{\sigma\sqrt{\pi}} e^{-\frac{a^2}{\sigma^2}},\ k_i = e^{-\frac{(ih)^2}{\sigma^2}},\ Q = e^{h\frac{2a}{\sigma^2}}, \end{gathered} \tag{6}$$

$$u_h(t) = \begin{pmatrix} u(x_1,t) \\ \vdots \\ u(x_N,t) \end{pmatrix},\ b_h(t) = \begin{pmatrix} k_1 l(t) Q \\ \vdots \\ k_N l(t) Q^N \end{pmatrix},\ A_h = \begin{pmatrix} \beta & \gamma & 0 & \dots & 0 \\ \alpha & \beta & \gamma & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \alpha & \beta & \gamma \\ 0 & \dots & 0 & \alpha+\gamma & \beta \end{pmatrix}. \tag{7}$$

Thus, the system (4) completed with the initial condition gives

$$\begin{cases} u_h'(t) = A_h u_h(t) + b_h(t) + h\epsilon_h(t), \\ u_h(0) = g_h, \end{cases} \tag{8}$$

where $g_h = \begin{pmatrix} g(x_1) \\ \vdots \\ g(x_N) \end{pmatrix}$.

Neglecting the derivatives of order greater than two, the following system is obtained:

$$\begin{cases} v_h'(t) = A_h v_h(t) + b_h(t), \\ v_h(0) = g_h, \end{cases} \tag{9}$$

where v_h is an approximated solution of (8). Indeed, since $A_h = (a_{i,j})$ is a real tridiagonal matrix whose coefficients verify $a_{k,k+1} \times a_{k+1,k} > 0$ for $k = 1, \ldots, n$, it is similar to a Hermitian matrix and its eigenvalues are real. Besides, according to the Gerschgorin theorem, these eigenvalues are negative. Hence, according to the expressions of u_h and v_h and the Gerschgorin theorem, one gets:

$$\exists C > 0, \ \| u_h(t) - v_h(t) \|_\infty \leq \frac{|h| C K_h}{R}$$

where K_h is the condition number of A_h. In the simulations, N has been chosen so that K_h is the smallest possible, that is $N + 1 = 150$.

3 Identifiability of the semi-discretized model

The numerical estimation of the parameters is based on (9), consequently its identifiability analysis has to be performed. First results about the identifiability concept can be found in Walter [18]. In the 90's Diop and Fliess [5], Fliess and Glad [7], and Ollivier [13] proposed a new approach of identifiability based on differential algebra, and which does not require the existence of a control. Boulier et al [1] have introduced the concept of charasteristic presentation (or decomposition), leading to an algorithm of differential elimination called "'Rosenfeld-Groebner algorithm"' and implemented in the package Diffalg in Maple [2]. This identifiability approach ignores the initial conditions of the system. But the initial conditions can play a crucial role [3], [16] and a software based on "Rosenfeld-Groebner algorithm" and which takes them into account has been written [3], [4].

A very important repercussion of the identifiability analysis is the elaboration of differential polynomials linking outputs, parameters and inputs if any, in the most cases allowing the obtention of parameter estimates without any a priori knowledge. In the context of the considered semi-discretized differential model, the unknown parameters are not only constants but also functions and there is no input. Then, the classical approaches based on differential algebra for identifiability analysis [3], [16] cannot be used. Let us begin by recalling some basic definitions and giving some useful notations.

3.1 Basic concepts of differential algebra

In the following, a differential polynomial $p(x)$ is a polynomial in some variables, functions of time, $x_1, \ldots, x_n, y_1, \ldots, y_m$ and a finite number of its derivatives with coefficients in the field K, K is the field of rational numbers $\mathbb{Q}$ or a field extension $\mathbb{Q}(\alpha_1, \ldots, \alpha_r)$ where $\alpha_i, i = 1, \ldots, r$ are some constants.

The differential polynomials generate a ring in the indeterminates $x_1, \ldots, x_n, y_1, \ldots, y_m$ with their derivatives up to any order. It is called a *differential ring* $K\{x_1, \ldots, x_n, y_1, \ldots, y_m\}$. A *differential ideal* of a differential ring R is an ideal of R stable under derivations. If $p_1, \ldots, p_s$ are elements of R, the differential ideal denoted $I = [p_1, \ldots, p_s]$ generated by the $p_i, i = 1, \ldots, s$ is the set of all elements of R that are linear combinations (with elements of R for coefficients) of $p_i, i = 1, \ldots, s$ and their derivatives up to any order.

The *radical differential ideal* $J = \{p_1, \ldots, p_s\}$ generated by the $p_i, i = 1, \ldots, s$ is the set of all element of R a power of which belongs to $I = [p_1, \ldots, p_s]$. Considering a set S of differential polynomials, a differential polynomial p vanishes on all the zeros of s if and only if p belongs to the radical differential ideal generated by S [1], [2].

Any radical differential ideal can be decomposed into an intersection of some differential ideals (said *characterizable)* and the obtained representation is called a *characteristic decomposition.* These ideals

are defined by sets of differential polynomials, differential *characteristic sets* which are kinds of canonical forms, [15], [16].

The notion of *ranking* is fundamental in elimination methods. It is a well-ordering over the indeterminates and their derivatives. An elimination ranking denoted "$\prec$" has been used, which is such that

$$\begin{cases} u_i^{(k)} \prec u_i^{(k+p)} \\ u_i^{(k)} \prec u_j^{(l)} \Longrightarrow u_i^{(k+p)} \prec u_j^{(l+m)} \end{cases}$$

for any indeterminates u_i and u_j and arbitrary integers k, l, m and p. On the other hand, an orderly ranking has been also used, which satisfies, with the same notations ($p > 0$) $u_i^{(k)} \prec u_j^{(k+p)}$. The notation used in Diffalg to set an orderly ranking is $[u_1, .., u_n]$ (leftmost elements are greater than rightmost ones and the derivatives are ordered by an orderly ranking). The highest ranking variable or derivative of a variable in a differential polynomial is called the *leader* of the polynomial.

3.2 Identifiability approach by elimination

The system (9) can be rewritten as a differential polynomial system that is completed with the observation $y = v_N$ and with $\dot{Q} = 0$ and $\dot{k}_i = 0$ ($i = 1, \ldots, N$) since Q and k_i are constant. The resulting system can be described by the following differential polynomials:

$$(Sd_N) \begin{cases} \dot{v}_1 - (\beta v_1 + \gamma v_2 + k_1 \ell Q) = 0, \\ \dot{v}_2 - (\alpha v_1 + \beta v_2 + \gamma v_3 + k_2 \ell Q^2) = 0, \\ \ldots \\ \dot{v}_{N-1} - (\alpha v_{N-2} + \beta v_{N-1} + \gamma v_N + k_{N-1} \ell Q^{N-1}) = 0, \\ \dot{v}_N - ((\alpha + \gamma) v_{N-1} + \beta v_N + k_N \ell Q^N) = 0, \\ y - v_N = 0, \ \dot{Q} = 0, \\ \dot{k}_i = 0, k_i \neq 0 \text{ for } i = 1, \ldots, N. \end{cases} \tag{10}$$

It is assumed that the constants α, β, γ are not solutions of algebraic equations.
Then, the differential ideal generated by the equations of (Sd_N) can be considered in the differential ring $K\{v_1, ..., v_N, y, \ell, Q, k_1, \ldots, k_N\}$ generated by the field of constants $K = \mathbb{Q}(\alpha, \beta, \gamma)$, the states $(v_i)_{1 \leq i \leq N}$, the output y, the unknown function ℓ, the unknown parameter Q and the constants k_i for $i = 1, \ldots, N$. And, this section is devoted to the identifiability of the function ℓ and the parameter Q that is considered. The following identifiability definition, where $\mathcal{U} = \mathcal{L} \times]0, T[$ represents the admissible set of the parameters, is used:

Definition 3.1 *The model (Sd_N) is globally identifiable at $(\ell, Q) \in \mathcal{U}$ if there exists a finite time $t_1 > 0$ such that if $y[(\tilde{\ell}(t), \tilde{Q}); t] = y[(\ell(t), Q); t]$ for all $t \in [0, t_1]$, with $(\tilde{\ell}, \tilde{Q}) \in \mathcal{U}$, then $(\tilde{\ell}, \tilde{Q}) = (\ell, Q)$.*
The model (Sd_N) is locally identifiable at $(\ell, Q) \in \mathcal{U}$ if there exists an open neighbourhood W of (ℓ, Q) such that (Sd_N) is globally identifiable at (ℓ, Q) with $\mathcal{U}$ restricted to W.

It is well in line with the classical identifiability definitions in the case of models whose the structure depends only on constant parameters.

The main result is given in the following theorem.

Theorem 3.1 *The radical of the ideal generated by (Sd_N) endowed with the ranking*

$$[Q, \ell, y, k_1, \ldots, k_N] \prec [v_1, \ldots, v_N] \tag{11}$$

admits a characteristic decomposition which is defined by the following characteristic set $\mathcal{C}$:

$$\begin{array}{c} \{\dot{Q}, \dot{k}_1, \ldots, \dot{k}_N, P(y, \ell, Q, k_1, \ldots, k_N), R_1(y, \ell, Q, v_1, k_1, \ldots, k_N), R_2(y, \ell, Q, v_2, , k_1, \ldots, k_N), \\ \ldots, R_{N-1}(y, \ell, Q, v_{N-1}, k_1, \ldots, k_N), R_N(y, \ell, Q, v_N, k_1, \ldots, k_N)\}. \end{array} \tag{12}$$

with

$$P(y,\ell,Q,k_1,\ldots,k_N) = f_N(y) + \sum_{i=0}^{N-1} c_{N,i}(Q)\ell^{(i)}. \tag{13}$$

The leader of the polynomial P is y, and the leader of the polynomial R_j is v_j for $j = 1,\ldots,N$.
The function $f_N(y)$ is a linear function depending on y and its derivatives and whose the highest derivative whith respect to y is y^{N-1}. Besides, the each term of the sequence $(c_{N,i})_{i=1,\ldots,N}$ is a constant depending on Q and the parameters of the initial system α, β and γ. This sequence is defined by:

- ⋆ *for $r = 1$:*

$$c_{1,0} = -k_N Q^N, \tag{14}$$

- ⋆ *for $r = 2$:*

$$\begin{cases} c_{2,0} = \beta k_N Q^N - (\frac{V}{h} + 2\frac{D}{h^2})k_{N-1}Q^{N-1}, \\ c_{2,1} = -k_N Q^N. \end{cases} \tag{15}$$

- ⋆ *for $r \in [3,N]$:*

$$c_{r,r-1} = -k_N Q^N, \tag{16}$$

$$c_{r,0} = -\gamma\alpha c_{r-2,0} - \beta c_{r-1,0} - (\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-2}k_{N-r+1}Q^{N-r+1}, \tag{17}$$

$$c_{r,i} = c_{r-1,i-1} - \beta c_{r-1,i} - \alpha\gamma c_{r-2,i}, \text{ for } i = 1,\ldots,r-3, \tag{18}$$

$$c_{r,r-2} = c_{r-1,r-3} - \beta c_{r-1,r-2}, \tag{19}$$

$$c_{r,r-2} = c_{2,0} - (r-2)\beta c_{2,1}. \tag{20}$$

Proof - The proof will be decomposed in two steps. The first one consists in proving the following lemma; the second one in proving that the $c_{r,i}$ are constants depending on Q and the parameters of the initial system.

Lemma 3.1

For all integer $r \in [1,N]$, the following equalitie holds:

$$(\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1}v_{N-r} = g_{r,N}(t) + \sum_{i=0}^{r-1} c_{r,i}l^{(i)}(t), \tag{21}$$

with $g_{r,N}(t)$ a linear function in v_N and its derivatives defined by

$$\begin{cases} g_{1,N} = \dot{v}_N - \beta v_N, \\ g_{2,N} = \ddot{v}_N - 2\beta\dot{v}_N + (\beta^2 - (\frac{V}{h} + 2\frac{D}{h^2})\gamma)v_N, \\ g_{r+1,N} = \dot{g}_{r,N}(t) - \beta g_{r,N}(t) - \alpha\gamma g_{r-1,N}(t), \text{ pour } r \in [3,N-1]. \end{cases} \tag{22}$$

and where the $c_{r,i}$ are defined by (14), (15), (16), (17), (18) and (19).

Proof of the lemma 3.1 - (21) is proved by an induction argument on r. The expression of the $c_{r,i}$ given by (15), (16), (17), (18) and (19) will be deduced from it.

- r=1: the following relations must be proved

$$\begin{cases} (\frac{V}{h}+2\frac{D}{h^2})v_{N-1}(t) = g_{1,N}(t) + c_{1,0}l(t), \\ c_{1,0} = -k_N Q^N. \end{cases} \tag{23}$$

The last equation of the system can be rewritten:

$$(\frac{V}{h}+2\frac{D}{h^2})v_{N-1} = \dot{v}_N - \beta v_N - lk_N Q^N. \tag{24}$$

Thus, for $g_{1,N} := \dot{v}_N - \beta v_N$ and $c_{1,0} := -k_N Q^N$, (21) for $r = 1$ and (14) are verified.

- r=2: it must be proved:

$$\begin{cases} (\frac{V}{h}+2\frac{D}{h^2})\alpha v_{N-2}(t) = g_{2,N}(t) + c_{2,0}l(t) + c_{2,1}l^{'}(t), \\ c_{2,0} = \beta k_N Q^N - (\frac{V}{h}+2\frac{D}{h^2})k_{N-1}Q^{N-1}, \\ c_{2,1} = -k_N Q^N. \end{cases} \tag{25}$$

From the (N-1)th equation of the system, an expression of v_{N-2} in function of v_{N-1} and v_N can be obtained, that is:

$$\alpha v_{N-2} = \dot{v}_{N-1} - \beta v_{N-1} - \gamma v_N - lk_{N-1}Q^{N-1}.$$

In multiplying this last equation by $(\frac{V}{h}+2\frac{D}{h^2})$ and in substituting $(\frac{V}{h}+2\frac{D}{h^2})v_{N-1}$ and $(\frac{V}{h}+2\frac{D}{h^2})\dot{v}_{N-1}$ by their expression deduced from (24), one gets:

$$(\frac{V}{h}+2\frac{D}{h^2})\alpha v_{N-2} = g_{2,N} + \left(\beta k_N Q^N - (\frac{V}{h}+2\frac{D}{h^2})k_{N-1}Q^{N-1}\right) l - k_N Q^N l^{'}, \tag{26}$$

with $g_{2,N} := \ddot{v}_N - 2\beta\dot{v}_N + (\beta^2 - (\frac{V}{h}+2\frac{D}{h^2})\gamma)v_N$. Thus, if $c_{2,0} := \beta k_N Q^N - (\frac{V}{h}+2\frac{D}{h^2})k_{N-1}Q^{N-1} = -\beta c_{1,0} - (\frac{V}{h}+2\frac{D}{h^2})k_{N-1}Q^{N-1}$ and $c_{2,1} := -k_N Q^N$, the relations (21) for $r = 2$ and (15) are proved.

- In order to prove the relation for $r = 3$, the following equalities must be established:

$$\begin{cases} (\frac{V}{h}+2\frac{D}{h^2})\alpha^2 v_{N-3}(t) = g_{3,N}(t) + \sum_{i=0}^{2} c_{3,i}l^{(i)}(t), \\ c_{3,0} = -\beta c_{2,0} - \alpha\gamma c_{1,0} - (\frac{V}{h}+2\frac{D}{h^2})\alpha k_{N-2}Q^{N-2}, \\ c_{3,1} = c_{2,0} - \beta c_{2,1}, \\ c_{3,2} = -k_N Q^N. \end{cases} \tag{27}$$

In multiplying the (N-2)th equation by $(\frac{V}{h}+2\frac{D}{h^2})\alpha$, one gets:

$$(\frac{V}{h}+2\frac{D}{h^2})\alpha^2 v_{N-3} = (\frac{V}{h}+2\frac{D}{h^2})\alpha\dot{v}_{N-2} - (\frac{V}{h}+2\frac{D}{h^2})\alpha\beta v_{N-2} - (\frac{V}{h}+2\frac{D}{h^2})\alpha\gamma v_{N-1} - (\frac{V}{h}+2\frac{D}{h^2})\alpha l k_{N-2}Q^{N-2}.$$

In substituting $(\frac{V}{h}+2\frac{D}{h^2})v_{N-1}$, $(\frac{V}{h}+2\frac{D}{h^2})v_{N-2}$ and $(\frac{V}{h}+2\frac{D}{h^2})\alpha\dot{v}_{N-2}$ deduced from the relations (23) and (26), the following equality is obtained:

$$(\frac{V}{h}+2\frac{D}{h^2})\alpha^2 v_{N-3} = g_{3,N} + \sum_{i=0}^{2} c_{3,i}l^{(i)}, \tag{28}$$

with $g_{3,N} := \dot{g}_{2,N} - \beta g_{2,N} - \alpha\gamma g_{1,N}$, $c_{3,0} := -\beta c_{2,0} - \alpha\gamma c_{1,0} - (\frac{V}{h}+2\frac{D}{h^2})\alpha k_{N-2}Q^{N-2}$, $c_{3,1} := c_{2,0} - \beta c_{2,1}$, $c_{3,2} := c_{2,1} = -k_N Q^N$. Thus, (21), (16), (17), (18) and (19) for $r = 3$ are proved.

- Suppose now that (21), (16)-(19) are verified until $r \in [1, N-1]$. Then, the $(N-r)$th equation after multiplying it by $(\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1}$ can be rewritten:

$$\begin{aligned}(\frac{V}{h} + 2\frac{D}{h^2})\alpha^r v_{N-r-1} = (\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1}\dot{v}_{N-r} - (\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1}\beta v_{N-r} \\ -(\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1}\gamma v_{N-r+1} - (\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1} l k_{N-r} Q^{N-r}.\end{aligned} \tag{29}$$

Or, according to the induction hypothesis at the ranks $r-1$ and r, one gets:

$$\left\{\begin{array}{l}(\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-2} v_{N-r+1} = g_{r-1,N} + \sum_{i=0}^{r-2} c_{r-1,i} l^{(i)}, \\ (\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1} v_{N-r} = g_{r,N} + \sum_{i=0}^{r-1} c_{r,i} l^{(i)}.\end{array}\right. \tag{30}$$

Thus, in taking again (29) and in substituting $(\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-2} v_{N-r+1}$, $(\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1} v_{N-r}$ and $(\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1}\dot{v}_{N-r}$ by the expressions given by (30), the following equality is obtained:

$$\begin{aligned}(\frac{V}{h} + 2\frac{D}{h^2})\alpha^r v_{N-r-1} &= (\dot{g}_{r,N} - \beta g_{r,N} - \alpha\gamma g_{r-1,N}) + (-\beta c_{r,0} - \alpha\gamma c_{r-1,0} - (\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1} k_{N-r} Q^{N-r}) l \\ &+ \sum_{i=1}^{r-2} (c_{r,i-1} - \beta c_{r,i} - \alpha\gamma c_{r-1,i}) l^{(i)} + (c_{r,r-2} - \beta c_{r,r-1}) l^{(r-1)} + c_{r,r-1} l^{(r)}.\end{aligned} \tag{31}$$

If $g_{r+1,N}(t) := \dot{g}_{r,N}(t) - \beta g_{r,N}(t) - \alpha\gamma g_{r-1,N}(t)$, $c_{r+1,0} := -\beta c_{r,0} - \alpha\gamma c_{r-1,0} - (\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-1} k_{N-r} Q^{N-r}$, $c_{r+1,i} := c_{r,i-1} - \beta c_{r,i} - \alpha\gamma c_{r-1,i}$, for $i = 1, \ldots, r-2$, $c_{r+1,r-1} := c_{r,r-2} - \beta c_{r,r-1}$ and $c_{r+1,r} := c_{r,r-1} = -k_N Q^N$, the relations (21), (16), (17), (18) and (19) are proved at the rank $r+1$.
Thus, the lemma is valid for all $r \in \lfloor 1, N-1 \rfloor$ and gives some recurrence relations defining the $c_{r,i}$.

In order to finish the proof of the theorem, it remains to establish that the each term of the sequence $(c_{N,i})_{i=1,\ldots,N}$ is a constant depending on Q and the parameters of the initial system. It will be first proved for the sequence $(c_{r,0})_{r\in[1,N]}$, then for $(c_{r,r-2})(r \in [3, N])$ and finally for $(c_{r,i})_{i\in[1,r-3]}$ $(r \in [3, N])$.

The sequence $(c_{r,0})_{r\in[1,N]}$.
$c_{1,0}$ and $c_{2,0}$ are given by (14) and (15) respectively and depend on the constants of the system and on Q.
The equation (17), that is $c_{r,0} = -\gamma\alpha c_{r-2,0} - \beta c_{r-1,0} - (\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-2} k_{N-r+1} Q^{N-r+1}$ can be rewritten under the following matrix form $u_r^0 = S u_{r-1}^0 - w_r^0$ where
$u_r^0 = \begin{pmatrix} c_{r-1,0} \\ c_{r,0} \end{pmatrix}$, $S = \begin{pmatrix} 0 & 1 \\ -\alpha\gamma & -\beta \end{pmatrix}$, $w_r^0 = \begin{pmatrix} 0 \\ (\frac{V}{h} + 2\frac{D}{h^2})\alpha^{r-2} k_{N-r+1} Q^{N-r+1} \end{pmatrix}$.

It is a linear sequence of order 1 whose the initial condition is
$u_2^0 = \begin{pmatrix} c_{1,0} \\ c_{2,0} \end{pmatrix} = \begin{pmatrix} -k_N Q^N \\ \beta k_N Q^N - (\frac{V}{h} + 2\frac{D}{h^2}) k_{N-1} Q^{N-1} \end{pmatrix}$.
It also can be rewritten:

$$u_r^0 = S^{r-2} u_2^0 - \sum_{j=0}^{r-3} S^j w_{r-j}^0. \tag{32}$$

Thus, $(c_{r,0})_{r\in[3,N]}$ depends only on the constants of the initial system and on Q.

The sequence $(c_{r,r-2})$ for $r \in [3, N]$
Let's prove that $c_{r,r-2} = c_{2,0} - (r-2)\beta c_{2,1}$ for $r \in [3, N]$ by an induction argument on r.

- r=3: The term $c_{3,1}$ has been found in the poof of the previous lemma and is equal to $c_{2,0} - \beta c_{2,1}$.

- Suppose that the relation is true until the rank $r \in [3, N-1]$, that is $c_{r,r-2} = c_{2,0} - (r-2)\beta c_{2,1}$. From (19), one gets:

$$c_{r+1,r-1} = c_{r,r-2} - \beta c_{r,r-1}. \tag{33}$$

Or, by hypothesis, $c_{r,r-2} = c_{2,0} - (r-2)c_{2,1}$ and according to (16) and the second relation of (15), $c_{r,r-1} = -k_N Q^N = c_{2,1}$:

$$\begin{aligned} c_{r+1,r-1} &= c_{2,0} - (r-2)\beta c_{2,1} - \beta c_{2,1} \\ &= c_{2,0} - (r-1)\beta c_{2,1}. \end{aligned} \tag{34}$$

Thus, (20) is proved for all $r \in [3, N]$ and since $c_{2,0} = \beta k_N Q^N - (\frac{V}{h} - 2\frac{D}{h^2})k_{N-1}Q^{N-1}$ and $c_{2,1} = -k_N Q^N$, $c_{r,r-2}$ for $r \in [3, N]$ depends only on the constants of the system and on Q.

The sequence $(c_{r,i})_{i\in[1,r-3]}$ for $r \in [3, N]$ fixed

In the theorem, the sequence $(c_{r,i})_{i\in[1,r-3]}$ was defined in fixing r and by varying i. The idea of the proof consists in fixing i and varying r. Since $r \in [3, N]$ and $i \in [1, r-3]$, if i is fixed in $[1, N-3]$, then $r \in [i+3, N]$.

Let's prove by an induction argument on i that the sequence $(c_{r,i})_{i+3<r<N}$ depends only on the constants of the system and on Q.

- If $i = 1$ ($r \in [4, N-3]$), according to the second relation of (15) with $r = 2$ and (19) with $r = 3$, one gets $c_{2,1} = -k_N Q^N$ and $c_{3,1} = c_{2,0} - \beta c_{2,1} = 2\beta k_N Q^N - (\frac{V}{h} + 2\frac{D}{h^2})k_{N-1}Q^{N-1}$. The equation (18) can be rewritten under the following matrix form:

$$u_r^1 = S u_1^1 + w_r^1$$

where
$u_r^1 = \begin{pmatrix} c_{r-1,1} \\ c_{r,1} \end{pmatrix}$, $S = \begin{pmatrix} 0 & 1 \\ -\alpha\gamma & -\beta \end{pmatrix}$, $w_r^1 = \begin{pmatrix} 0 \\ c_{r-1,0} \end{pmatrix}$

with the initial condition

$$u_3^1 = \begin{pmatrix} c_{2,1} \\ c_{3,1} \end{pmatrix} = \begin{pmatrix} -k_N Q^N \\ 2\beta k_N Q^N - (\frac{V}{h} + 2\frac{D}{h^2})k_{N-1}Q^{N-1} \end{pmatrix}.$$

The sequence $(u_r^1)_{r\in[4,N-4]}$ is a linear sequence of order 1 which can be rewritten

$$u_r^1 = S^{r-3}u_3^1 - \sum_{i=0}^{r-4} S^j w_{r-j}^1 \tag{35}$$

and where the w_{r-j}^1 are deduced from (32). Thus, $(c_{r,1})_{r\in[4,N]}$ depends only on the constants of the initial system and on Q.

- Suppose that the proposition is true until $i \in [1, N-4]$ and let's prove that it is true for $i+1 \in [1, N-3]$. According to (16) with $r = i+2$ and (20) with $r = i+3$, one gets $c_{i+2,i+1} = -k_N Q^N$ and $c_{i+3,i+1} = c_{2,0} - (i+1)\beta c_{2,1} = (i+2)\beta k_N Q^N - (\frac{V}{h} + 2\frac{D}{h^2})k_{N-1}Q^{N-1}$. The equation (18) can be rewritten:

$$u_r^{i+1} = S u_{r-1}^{i+1} + w_r^{i+1}$$

where
$u_r^{i+1} = \begin{pmatrix} c_{r-1,i+1} \\ c_{r,i+1} \end{pmatrix}$, $S = \begin{pmatrix} 0 & 1 \\ -\alpha\gamma & -\beta \end{pmatrix}$, $w_r^{i+1} = \begin{pmatrix} 0 \\ c_{r-1,i} \end{pmatrix}$

with the initial condition

$u_{i+3}^{i+1} = \begin{pmatrix} c_{i+2,i+1} \\ c_{i+3,i+1} \end{pmatrix} = \begin{pmatrix} -k_N Q^N \\ (i+2)\beta k_N Q^N - (\frac{V}{h} + 2\frac{D}{h^2}) k_{N-1} Q^{N-1} \end{pmatrix}$.
Thus, the sequence $(u_r^{i+1})_{r\in[i+4,N]}$ is a linear sequence of order 1 which can be rewritten

$$u_r^{i+1} = S^{r-i-3} u_{i+3}^{i+1} + \sum_{j=0}^{r-i-4} S^j w_{r-j}^{i+1} \tag{36}$$

and whose the w_{r-j}^{i+1}, $j \in [0, r-i-4]$ are deduced from the recurrence hypothesis and depend only on the constants of the initial system and on Q. Thus, the property is true at the rank $i+1$.

Remark 3.1 *In this context, the systems (Sd_N) and $(\mathcal{C})$ defined by*

$$\begin{cases} P(y, \ell, Q, k_1, \ldots, k_N) = 0, \\ R_1(y, \ell, Q, v_1, k_1, \ldots, k_N) = 0, \\ R_2(y, \ell, Q, v_2, k_1, \ldots, k_N) = 0, \\ \ldots \\ R_{N-1}(y, \ell, Q, v_{N-1}, k_1, \ldots, k_N) = 0, \\ R_N(y, \ell, Q, v_N, k_1, \ldots, k_N) = 0, \\ \dot{Q} = 0, \\ \dot{k}_i = 0, k_i \neq 0 \text{ for } i = 1, \ldots, N. \end{cases} \tag{37}$$

and deduced from $\mathcal{C}$ (cf. (12)) are equivalent systems. The radical of the ideal generated by $(\mathcal{C})$ endowed with the ranking

$$[Q, \ell, y, v_1, \ldots, v_N, k_1, \ldots, k_N] \tag{38}$$

admits a characteristic decomposition which is defined by the polynomials given by (Sd_N).

Remark 3.2 *Thereafter, we will suppose that the speed of the substrat concentration at the initial time do not vary near the observation point, that is $\dot{v}_{N-1}(0)$ will be supposed equal to $\dot{v}_N(0)$ and consequently it is assumed to be known. Indeed, the numerical estimation of parameters has been done with this assumption, which numerically is translated into $\dot{v}_{N-1}(0) = \dot{v}_N(0)$.*

Now let us prove the main identifiability result:

Theorem 3.2 *Suppose that $v_i(0) \geq 0$ for $i = 1, \ldots, N$ and $\dot{v}_{N-1}(0)$ are known. Then, the model (Sd_N) is globally identifiable at $(\ell, Q) \in \mathcal{U}$.*

Proof - The theorem 3.1 gives the parameter-output polynomial which verifies:

$$f_N(y) + \sum_{i=0}^{N-1} c_{N,i}(Q) \ell^{(i)} = 0. \tag{39}$$

This equation is a linear differential equation of order $N-1$ ($c_{N,N-1} \neq 0$). In order to show the model identifiability, it would be enough to show the identifiability of the parameter Q which implies the identifiability of the parameters $c_{N,i}$. Then, the identifiability of ℓ will be deduced from the resolution of the differential equation (39).

- *Identifiability of Q and $\ell(0)$ by using (Sd_N)*

System (Sd_N) gives:

$$\begin{array}{l} k_N \ell Q^N = \dot{y} - (\alpha + \gamma) v_{N-1} - \beta y \\ k_{N-1} \ell Q^{N-1} = \dot{v}_{N-1} - (\alpha v_{N-2} + \beta v_{N-1} + \gamma y) \end{array} \tag{40}$$

These equations taken in 0 give $k_N \ell(0) Q^N$ and $k_{N-1}\ell(0)Q^{N-1}$, this leads to the identifiability of Q and then of $\ell(0)$.

Some expressions of Q and $\ell(0)$ can be given:

$$Q = \frac{k_{N-1}}{k_N} \frac{\dot{y}(0) - (\alpha+\gamma)v_{N-1}(0) - \beta y(0)}{\dot{v}_{N-1}(0) - (\alpha v_{N-2}(0) + \beta v_{N-1}(0) + \gamma y(0))} \tag{41}$$

$$\ell(0) = \frac{k_N^{N-1}}{k_{N-1}^N} \frac{(\dot{v}_{N-1}(0) - \alpha v_{N-2}(0) - \beta v_{N-1}(0) - \gamma v_N(0))^N}{(\dot{v}_N(0) - (\alpha+\gamma)v_{N-1}(0) - \beta v_N(0))^{N-1}}. \tag{42}$$

From this study, it can be deduced that the position of the pollution source depends only on the observation and the flow rate at the initial time. Therefore, since the coefficients $(c_{N,i})_{i=1,\dots,N}$ are function of Q and the constants of the system, they are identifiable.

- *Identifiability of ℓ by using ($\mathcal{C}$)*

Now, it remains to establish that $(\dot{\ell}(0), \dots, \ell^{(N-1)}(0))$ can be uniquely determined from the observation. The following property is proved, for $i = 2, ..., N$, by using polynomials $R_1, \dots, R_N$ and an induction argument:
"$\ell^{(i-1)}(0)$ and $(v_{N-j-1}^{(i-j-1)}(0))_{j=-1,0,\dots,i-2}$ are uniquely determined from y and $(v_i(0))_{i=1,\dots,N}$."
The proof is based on an elimination method and gives the way to obtain an explicit expression which can be obtained by Maple as it will be explained in the section 4.1.

Consequently the function $\ell(t)$ is the unique solution of the differential equation (39) completed with the initial conditions $(\ell(0), \dot{\ell}(0), \dots, \ell^{(N-1)}(0))$, which are uniquely determined from the observation and the initial conditions. This gives the identifiability of the function ℓ.

Remark 3.3 *Since $Q = e^{\frac{2ah}{\sigma^2}}$, the unknown parameter a is identifiable and, from (41), is given by:*

$$a = \frac{N\sigma^2}{2L} log[\frac{k_{N-1}}{k_N} \frac{\dot{y}(0) - (\alpha+\beta)v_{N-1}(0) - \beta y(0)}{\dot{v}_{N-1}(0) - (\alpha v_{N-2}(0) + \beta v_{N-1}(0) + \gamma y(0))}]. \tag{43}$$

Besides, $\ell(0) = c\lambda(0)e^{-\frac{a^2}{\sigma^2}}$, with $c = \frac{1}{\sigma\sqrt{\pi}}$, gives the identifiability of $\lambda(0)$.

4 Numerical parameter identification

For estimating the numerical values of the unknown parameters (λ, a), the measurement is done at discrete times $(t_i)_{1<i<M}$, which induces a numerical evaluation of observation derivatives involved in the parameter-output polynomial, and, consequently, a numerical error. The choice of the derivatives evaluation will be also crucial. The method proposed by M. Fliess and H. Sira-Ramirez in [8] will be used in the numerical applications. This method does not necessitate any knowledge *a priori* of statistical properties of the signals. Furthermore, the estimators lay on explicit formulas.
The previous identifiability's study will give a numerical procedure for getting explicit formulas of the unknown parameters which allow a first approximation of them, without *a priori* knowledge, as it is explained below.

4.1 Presentation of the method

- *Expression of ℓ and its derivatives in zero*
  The estimation of a comes from (43). The flow rate will be calculated from the solution of the following differential system of first order:

$$\begin{cases} \dot{L}(t) &= AL(t) + F(t), \\ L(0) &= L_0 \end{cases} \tag{44}$$

where $L(t) = (\ell(t), \ell^{'}(t), \ldots, \ell^{(N-2)}(t))$,

$$A = -\frac{1}{c_{N,N-1}} \begin{pmatrix} 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ldots & \vdots \\ c_{N,0} & c_{N,1} & c_{N,2} & \ldots & c_{N,N-2} \end{pmatrix}$$

$$F(t) = -\frac{1}{c_{N,N-1}} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ f_N(y) \end{pmatrix}.$$

L_0 will be computed more precisely later.
The matrix A is diagonalizable. Indeed, it can be proved that if the characteristic polynomial of A has a multiple root then α, β and γ are solutions of an algebraic equation which has been excluded. Therefore, the linear differential system is solved by a direct solution using the diagonalization of the matrix A: $D = P^{-1}AP$, $L = PZ$. It gives:

$$\dot{L}(t) = AL(t) + F(t) \iff \dot{Z}(t) = DZ(t) + P^{-1}F(t). \tag{45}$$

Let us denote by $(d_{i,j})_{1\leq i\leq N-1, 1\leq j\leq N-1}$ the coefficients of the matrix D, $(\tilde{f}_1(t), \ldots, \tilde{f}_{N-1}(t))$ (resp. $(z_i)_{i=1,\ldots,N-1}$) the coefficients of the vector $\tilde{F}(t) = P^{-1}F(t)$ (resp. Z). The solution of the system (45) is reduced to the solution of:

$$\begin{cases} \dot{z}_1(t) & = d_{1,1}z_1 + \tilde{f}_1(t), \\ & \vdots \\ \dot{z}_{N-1}(t) & = d_{N-1,N-1}z_{N-1} + \tilde{f}_{N-1}(t). \end{cases} \tag{46}$$

Since $f_N(y)$ is a linear function of the observation and its derivatives, it can be rewriten:

$$\sum_{j=0}^{N-1} u_j y^{(j)}$$

where the coefficients u_j are obtained by using Maple, and depend only of the constants of the initial system α, β, γ.
The wellknown solution of (46) is given by:

$$z_i(t) = z_i(0)e^{d_{i,i}t} + \sum_{j=0}^{N-1} \left[d_{i,i}^j I_i(t) + \tilde{u}_{i,j} \sum_{l=0}^{j-1} \left(d_{i,i}^{j-1-l} (y^{(l)}(t) - y^{(l)}(0)e^{d_{i,i}t}) \right) \right] \tag{47}$$

where

$$I_i(t) = \int_0^t y(t)e^{-d_{i,i}(t-s)}ds\,,\ \tilde{u}_{i,j} = P^{-1}(i, N-1)u_j.$$

Consequently, the flow rate is given by

$$\lambda(t) = \ell(t)e^{\frac{a^2}{\sigma^2}}\sigma\sqrt{\pi}, \tag{48}$$

where

$$\ell(t) = P(1,1)z_1(t) + \ldots + P(1, N-1)z_{N-1}(t). \tag{49}$$

In order to determinate $z_i(0)$, that is $L(0)$, the package Diffalg is used. For example, with $N+1 = 11$ points, the ranking $[v_1, \ldots, v_{10}, k_1, \ldots, k_{10}, y, q, \ell]$ is applied to the equations (10). It leads to

polynomials which contain ℓ and its derivatives of order n ($n = 1, ..., 9$), y and its derivatives and $v_1, ..., v_{10}$. For example, it leads to the following expression of $\dot{\ell}$:

$$\dot{\ell} = (\ddot{v}_{10} - (\alpha+\gamma)\alpha v_8 - (\alpha+\gamma)\beta v_9 - (\alpha+\gamma)\gamma v_{10} - (\alpha+\gamma)k_9 Q^9 \ell - \beta v'_{10})/k_{10}/Q^{10}, \tag{50}$$

hence

$$\ell'(0) = (\ddot{y}(0) - (\alpha+\gamma)(\alpha v_8(0) + \beta v_9(0) + \gamma v_{10}(0) + k_9 Q^9 \ell(0) + \beta \dot{y}(0))/k_{10}/Q^{10}. \tag{51}$$

The other derivatives are deduced by the same way.

- *Evaluation of the observation derivatives*
  As it can be noticed, some observation derivatives of important order have to be estimated. For evaluating them, the method proposed in [8] will be used in the numerical applications. It is based on Mikusinski fields and the estimators depend on explicit formulas given below.
  First, the derivatives in 0 will be given. Let x a real function, analytic around 0. The Taylor expansion of $x(t)$ is $x(t) = \sum_{n\geq 0} x^{(n)}(0)\frac{t^n}{n!}$ and it can be approximated on an interval $(0, \epsilon)$ by $x_p(t) = \sum_{n=0}^{p} x^{(n)}(0)\frac{t^n}{n!}$ ($x_p^{(n)}(0) = x^{(n)}(0)$) which verifies:

$$\frac{d^{p+1}}{dt^{p+1}} x_p = 0. \tag{52}$$

  In the operational domain, (52) gives:

$$s^{p+1}x_p - s^p x_p(0) - s^{p-1}\dot{x}_p(0) \ldots - x_p^{(p)}(0) = 0. \tag{53}$$

  The derivatives in zero, $x_p^{(i)}(0) = \frac{d^i}{dt^i} x_p(t) \mid_{t=0}$ are also obtained from the solution of the system of linear equations ($m = 0, \ldots, p$, $\nu \geq p+1$):

$$s^{-\nu}\frac{d^m}{ds^m}\left\{x_p^{(p)}(0) + x_p^{(p-1)}(0)s + \ldots + x_p(0)s^p\right\} = s^{-\nu}\frac{d^m}{ds^m}\left\{s^{p+1}x_p\right\}. \tag{54}$$

  By the wellknown rules of th operational calculus, and by replacing x_p by x, the following formula, in the time domain, are deduced:

  - $m = p$,

$$x_p(0) = \frac{1}{a(0,p,\nu)t^{\nu-1}} \sum_{i=0}^{p} b(i,p,\nu) \int^{(\nu-i-1)} (-t)^i x(t),$$

  - $m = p-1, ..., 0$:

$$x_p^{(p-m)}(0) = \frac{1}{a(p-m,m,\nu)t^{\nu-1}} \left[\sum_{i=0}^{m} b(i,m,\nu) \int^{(m+\nu-i-p-1)} (-t)^i x(t) - \sum_{j=0}^{p-m-1} x^{(j)}(0) a(j,m,\nu) t^{j+m+\nu-p-1}\right] \tag{55}$$

    where, for $m \in [0,p]$, $\nu \geq p+1$,

$$a(j,m,\nu) = \frac{(p-j)!}{(p-j-m)!(j+m+\nu-p-1)!},\ b(i,m,\nu) = C_m^i \frac{(p+1)!}{(p+1-m+i)!}.$$

    and for $i < j$:

$$\begin{aligned}\int^{(j-i)} (-t)^i x(t) &= \int_0^t \int_0^{\tau_1} \ldots \int_0^{\tau_{j-i-1}} (-\tau_{j-i})^i x(\tau_{j-i}) d\tau_{j-i} \ldots d\tau_2 d\tau_1 \\ &= \frac{(-1)^i}{(j-i-1)!} \int_0^t (t-\tau)^{j-i-1} \tau^i x(\tau) d\tau.\end{aligned} \tag{56}$$

In order to estimate the derivatives in t, the Taylor expansion of $x(t) = \sum_{n\geq 0} a_n \frac{t^n}{n!}$ is considered. It can be approximated by $x_p(t) = \sum_{n=0}^{p} a_n \frac{t^n}{n!}$, where $a_n = x_p^{(n)}(0)$. Thus a polynomial approximation of $x(t)$ in a neighborhood of t also. For evaluating the derivatives, it is sufficient to derivate the so-obtained polynomial approximation.

4.2 Numerical results

For checking the validity of our approach, an accidental pollution has been simulated in a river during 4 hours with: $L = 1000m$, $V = 0.66m/s$, $R = 10^{-5}/s$, $D = 5m^2/s$. λ is built from the function

$$\lambda(t) = \sum_{i=1}^{3} 3\alpha_i e^{-\beta_i (t-\tau_i)^2}, \tag{57}$$

with $\alpha_1 = 1.2$, $\alpha_2 = 0.4$, $\alpha_3 = 0.6$, $\beta_1 = 10^{-6}s^{-2}$, $\beta_2 = 5.10^{-6}s^{-2}$, $\beta_3 = 10^{-6}s^{-2}$, $\tau_1 = 4500s$, $\tau_2 = 6500s$, $\tau_3 = 9000s$. The observation corresponds to $y(t) = u(L,t)$. The measured observation y (Fig. 1) was simulated from the true signal $\bar{y}$ obtained by solving (1) with a classical finite element scheme, the pollution location being a mesh point. Therefore, the Dirac mass is approximated by putting the whole mass in this point. The output y is supposed to follow a random law with $\bar{y}$ mean and $(s\bar{y})^2$ variance. The coefficient s is computed so that the relative error has a maximum value of 0.05 with an error probability less than 0.003. Thus, if $y = \bar{y} + \sigma\bar{y}\eta_0$ with η_0 following the reduced normal law, σ is chosen so that $P\left(\left|\frac{y-\bar{y}}{\bar{y}}\right| \leq 0.05\right) = 0.997$ or $P\left(|\eta_0| \leq \frac{0.05}{\sigma}\right) = 0.997$. According to the table of the reduced normal law, $\sigma \approx 0.017$.

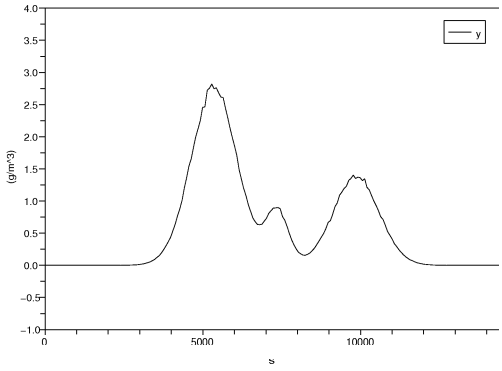

Figure 1: Observation when the pollution source is located at a=442m.

Algorithm - The numerical estimation of the unknown parameters is based on the following semi-discretized scheme:

$$\begin{cases} \dot{v}_1(t) + \left(\frac{V}{h} + 2\frac{D}{h^2} + R\right) v_1(t) - \frac{D}{h^2} v_2(t) = \lambda(t) \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{(h-a)^2}{\sigma^2}}, \\ \dot{v}_i(t) - \left(\frac{V}{h} + \frac{D}{h^2}\right) v_{i-1}(t) + \left(\frac{V}{h} + 2\frac{D}{h^2} + R\right) v_i(t) \\ \qquad\qquad - \frac{D}{h^2} v_{i+1}(t) = \lambda(t) \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{(ih-a)^2}{\sigma^2}}, \ i = 2, ..., N-1, \\ \dot{v}_N(t) - \left(\frac{V}{h} + 2\frac{D}{h^2}\right) v_{N-1}(t) + \left(\frac{V}{h} + 2\frac{D}{h^2} + R\right) v_N(t) = \lambda(t) \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{(Nh-a)^2}{\sigma^2}}, \\ v_i(0) = g(x_i), \ i = 1, \ldots, N, \\ y_\sigma(t) = v_N(t). \end{cases} \tag{58}$$

The factories, i.e. the pollution sources, are assumed to be located between $400m$ and $900m$. The computation has been done with $N+1=11$ points, which is a very small number for such a distributed system but which allows the symbolic computation of (13). Besides, let us recall that the aim of this work is to make a first evaluation of the parameters.

Before giving numerical results, notice that (43), and (48) depend on the parameter σ which has to be chosen as good as possible. Indeed, σ is crucial for approximating the Dirac mass, and, in theory, it has to be taken very small, but it is not the case owing to the numerical errors introduced by estimating the derivatives for example. After some numerical tests, it has been decided to take σ in the interval $[0.01; 0.5]$. Now, for a given value $\tilde{\sigma}$ of σ in this interval, the numerical estimations of the unknown parameters, $(a_{\tilde{\sigma}}, \lambda_{\tilde{\sigma}})$, are given by (43), and (48). Afterwards, the corresponding $y_{\tilde{\sigma}}$ is obtained by solving (58) and the following relative error is computed:

$$e_{\tilde{\sigma}} = 0.5\frac{\text{norm}(y - y_{\tilde{\sigma}})}{\text{norm}(y)}.$$

Consequently, the value of σ is chosen such that it gives the smallest relative error, and an estimate of the parameters corresponds to this choice. It is summarized in the following algorithm:
Step 1: **for** $\tilde{\sigma}$ **from** 0.01 **to** 0.5

- estimation of $a_{\tilde{\sigma}}$ and $\lambda_{\tilde{\sigma}}$ by using (43), and (48).
- estimation of $y_{\tilde{\sigma}}$ by solving (58) and by using the function ode of scilab.
- estimation of the relative error $e_{\tilde{\sigma}} = 0.5\frac{\text{norm}(y - y_{\tilde{\sigma}})}{\text{norm}(y)}$

Step 2: Find the smallest relative error, which leads to the estimate of $\tilde{a}$, $\tilde{\lambda}$.

Remark 4.1

Since the data are noisy, the error on the estimation of $\ell(0)$ and a with respect to the error on the initial conditions has to be evaluated. Denote by v_i the non noisy concentrations of substrate, v_{i,ϵ_i} the noisy concentration which is supposed to follow a random law with v_i mean and $(sv_i)^2$ variance. It also can be written $v_{i,\epsilon_i} = v_i + \epsilon_i$ ($\epsilon_i = sv_in_i$ where n_i follows the normal law $N(0,1)$).

Let us denote $z = \dot{v}_{N-1}(0) - \alpha v_{N-2}(0) - \beta v_{N-1}(0) - \gamma v_N(0)$, $\tilde{z} = \dot{v}_N(0) - (\alpha+\gamma)v_{N-1}(0) - \beta v_N(0)$, then (42) can be rewritten:

$$\ell(0) = \frac{k_N^{N-1}}{k_{N-1}^N}\frac{z^N}{\tilde{z}^{N-1}}$$

and with straightforward notations,

$$\ell_\epsilon(0) = \frac{k_N^{N-1}}{k_{N-1}^N}\frac{z_\epsilon^N}{\tilde{z}_\epsilon^{N-1}}.$$

Therefore, the following equality is obtained:

$$\mid \ell_\epsilon(0) - \ell(0) \mid = \frac{k_N^{N-1}}{k_{N-1}^N} \mid z_\epsilon \left(\frac{z_\epsilon}{\tilde{z}_\epsilon}\right)^{N-1} - z\left(\frac{z}{\tilde{z}}\right)^{N-1} \mid .$$

Or, from the Neuman conditions ($v_{N-2} \simeq v_N$, $v_{N-1} \simeq v_N$), the expressions $\frac{z}{\tilde{z}} \simeq 1$ and $\frac{z_\epsilon}{\tilde{z}_\epsilon} \simeq 1$ are obtained, hence:

$$\begin{aligned} \mid \ell_\epsilon(0) - \ell(0) \mid &\simeq \frac{k_N^{N-1}}{k_{N-1}^N} \mid z_\epsilon - z \mid \\ &\simeq e^{-\frac{(N-1)L^2}{N\sigma^2}} \mid \dot{\epsilon}_N(0) + R\epsilon_N(0) \mid . \end{aligned} \tag{59}$$

Since σ is taken small in the numerical work, the exponential is negligible. Thus, $\ell(0)$ is few sensitive to the initial conditions. Now, look at the sensitivity of the position of the pollution source with respect to the initial conditions. Notice a_ϵ obtained from (43) in substituting $\ell(0)$ by $\ell_\epsilon(0)$ and $v_i(0)$ by v_{i,ϵ_i}. Thus,

$$\begin{aligned} \mid a_{\tilde{\epsilon}} - a \mid &= \frac{N\sigma^2}{2L} \mid \log\left(\frac{\tilde{z}_\epsilon}{\tilde{z}}\right) - \log\left(\frac{z_\epsilon}{z}\right) \mid \\ &= \frac{N\sigma^2}{2L} \mid \log\left(\frac{z}{\tilde{z}}\frac{\tilde{z}_\epsilon}{z_\epsilon}\right) \mid \end{aligned} \tag{60}$$

Thus, in taken σ sufficiently "small", the error on the position will be negligible. Consequently, if σ is chosen small enough, the location may be estimated with a good accuracy, as it will be confirmed by the numerical simulations.

The simulations have been performed on the time interval $[2000, 14400]$, and the initial time corresponds to 2000. Furthermore, the derivatives of the observation at the initial time have been computed by applying the method introduced in the previous section, with $p = 1$ and $\nu = 2$ for the first derivative and $p = 9$ and $\nu = 12$ for higher derivatives.

The results obtained by the algorithm can be summed up as follows:

- ⋆ For $a = 442m$, the results are $\tilde{a} = 441.6m$ and the curve of the flow rate is represented in Fig. 2. The relative error is equal to 0.25.
- ⋆ For $a = 547m$, the results are $\tilde{a} = 546.5m$ and the curve of the flow rate is represented in Fig. 3. The relative error is equal to 0.04.
- ⋆ For $a = 621m$, the results are $\tilde{a} = 623.6m$ and the curve of the flow rate is represented in Fig. 4. The relative error is equal to 0.099.
- ⋆ For $a = 853m$, the results are $\tilde{a} = 849.2m$ and the curve of the flow rate is represented in Fig. 5. The relative error is equal to 0.12.

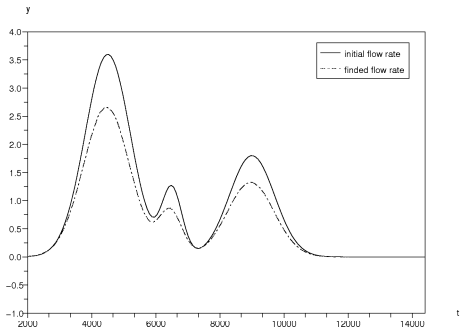

Figure 2: Flow rate obtained when $a = 442m$

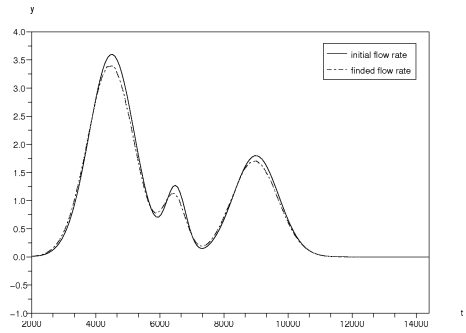

Figure 3: Flow rate obtained when $a = 547m$

The results are quite satisfactory, due to the search of the parameter σ in the approximated system. However, the flow rate found in the first case is not as good as in the others. Indeed, since a is located far from the observation point, a degradation of the substrate, which is traduced by the coefficient R, has happened.

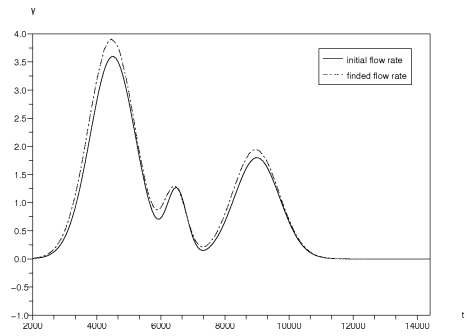

Figure 4: Flow rate obtained when $a = 621m$

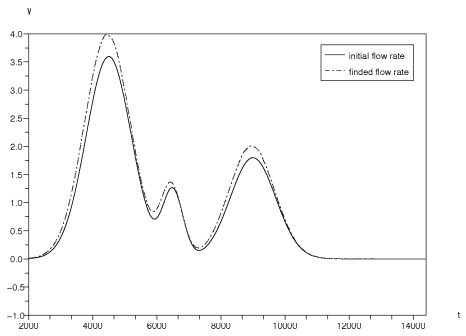

Figure 5: Flow rate obtained when $a = 853m$

5 Conclusion

In this paper an original method for estimating time-varying parameters in a distributed system without using a basis of special functions has been tested. It consists in elaborating an approximated system whose identifiability has been proved by an elimination procedure whatever the mesh refinement. The identifiability analysis leads to the development of numerical algorithms of global optimization. Of course, since it is an elimination approach, some derivatives of important order appeared. However, the method developed by M. Fliess and H.Sira-Ramirez proposed an effective way to estimate them without any knowledge *a priori* of statistical properties of the signals. Finally, some numerical simulations are confirming the interest ot the proposed approach.

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