SECOND ORDER TOPOLOGICAL DERIVATIVE FOR THE INVERSE PROBLEM IN DIFFUSION WITH RETENTION

Jairo R. de Faria

Ana P. P. Wyse

Antonio J. B. dos Santos

jairo@ci.ufpb.br

anawyse@ci.ufpb.br

boness@ci.ufpb.br

Departamento de Computação Científica, Universidade Federal da Paraíba

Av. dos Escoteiros, s/n, Mangabeira VII, 58055-000, João Pessoa–PB, Brasil

Luiz Bevilacqua

bevilacqua@coc.ufrj.br

Instituto Alberto Coimbra, COPPE, Universidade Federal do Rio de Janeiro

Av. Horácio Macedo 2030, Centro de Tecnologia, Cidade Universitária, 21941-914, Rio de Janeiro–RJ, Brasil

Flavio P. Costa

pietrobon_costa@yahoo.com.br

Departamento de Ciências Exatas e Tecnológicas, Universidade Estadual de Santa Cruz

Campus Soane Nazaré de Andrade, Km 16, BR-415, 45662-900, Ilhéus–BA, Brasil

Abstract. *Several relevant phenomena studied in scientific computing, like population spreading with partial hold up of the population to guarantee territorial domain, chemical reactions inducing adsorption processes and multiphase flow thorough porous media, Brownian motion in the speckle light field, for instance, are modeled by diffusion with retention. A new and general formulation of this problem was presented recently by Bevilacqua et. al., where the resulting governing equation is a fourth order differential partial equation. The new parameters associated to this higher order term need to be estimated, which leads to an inverse problem.*

In this work we shall consider the retention phenomena as a singular perturbation of the classical diffusion and rewrite the inverse problem as an optimization problem, taking into account the usual shape functional given by squared residues between experimental data and predicted values. Then, we derive the first and second order topological asymptotic expansion of this functional. Numerical results obtained using first and second topological derivative are presented and discussed.

Keywords: *Topological Derivative, Inverse Problem, Diffusion–Retention*

1 INTRODUCTION

The applicability of classical approach to the diffusional flux by Fick's law can be sufficient for many practical modelling purposes; however, these forms imply diffusion as a local or short range effect, with systems describing the variation of relatively small concentrations. Due to complexity of some processes, it is not enough simply manipulate diffusivity parameters, it is necessary to complement the Fick's law by including, for example, terms of higher order into the classical modeling. This applies to some anomalous diffusion processes, which can be due to adsorption processes, anisotropy, partial and temporal retention of particles and many others physicochemical phenomena that need improvement of the analytical formulation due to side effects not included in the classical diffusion modeling.

In Bevilacqua et al. (2011a) the authors present a modelling where a fourth order term arise naturally when the flux distribution for the diffusional process is fractionated due to introduction of control parameter β. This parameter can not be absorbed either by diffusion coefficient or by fourth order coefficient describing the retention, so that it characterizes a fraction of concentration which is able to diffuse. Many practical problems can be modeled by this equation, nevertheless a formulation involving new terms also includes complementary coefficients to be estimated. So, experimental specific techniques, together with an inverse analysis, can be useful to determine them.

Inverse Problems belong to a very important multidisciplinary area of research with applications in industry, medicine, engineering and science. Although the definition of direct and inverse problems may seem somewhat subjective, inverse problem are, in general, ill-posed while direct ones are well posed in the sense of Hadamard (1902). In this work, we examine the inverse problem given by the identification of the diffusion and retention parameters introduced in the formulation proposed by Bevilacqua et al. (2011a). This matter has been studied by Silva et al. (2013, 2014b,a).

As usual in inverse problem literature, we shall consider the associated minimization problem of a functional that measures the quadratic distance between measured data (from the model) and simulated ones taking into account parameters artificially introduced in the model. Different algorithms are generated according to the procedure chosen to generate the comparison parameters and the computational cost criteria must be taken into account. Considering the retention term as an infinitesimal singular perturbation of pure diffusion, we shall propose a new algorithm taking into account the topological asymptotic expansion of the shape functional to be minimized.

Topological derivative was introduced by Sokołowski and Zochowski (1999) and defined as the first-order correction of the asymptotic expansion of a shape functional with respect to an infinitesimal singular perturbation. This concept gives a theoretical justification for the bubble method, formally considered by Eschenauer et al. (1994) and it has been successfully applied to a large variety of problems, like topological optimization, inverse problems and image processing, for instance. An account of which may be found in the recent monograph by Novotny and Sokołowski (2013).

In the next section, it is straightly presented the formulation proposed by Bevilacqua et al. (2011a) and formulated an inverse problem approaching topological derivative by an asymptotic expansion of functional. Section 3 consider a singularly perturbed problem by a small parameter, showing that the topological derivative depends only of the solution of its partner unperturbed; moreover we derive the second order topological derivative for the functional in two cases, one of them has known analytical solution and confirms the hypothesis of the previous section. In section 4 it is formulated a finite element approximation to solve numerically the model. Scenarios obtained by numerical simulations are shown in section 5, comparing exact and numerical solution of model, followed by a brief discussion of the results and suggestions for further investigation.

2 PROBLEM FORMULATION

Anomalous diffusion process, where the mean squares variance grows slower (subdiffusion) or faster (superdiffusion) than a Gaussian process, has been modeled by fractional differential equations. In this paper, however, we shall adopt the recent analytical formulation for the simulation of the phenomena of diffusion with retention, introduced by Bevilacqua et al. (2011a). In that paper, the authors started from a discrete mathematical formulation, introducing a parameter $0 < \beta \leq 1$ to represent a fraction able to diffuse from total concentration, thus $(1 - \beta)$ is the temporaly retained fraction, making the diffusion slower than for the classical diffusion problem.

Considering symmetric distribution, each neighboring cells $(n - 1)$ and $(n + 1)$ is loaded with a fraction $\beta/2$ of the concentration p in the cell n at each time step. Thus, the redistribution of contents of each cells is governed by the algebraic expressions

$$p_n^t = (1-\beta)p_n^{t-1} + \frac{1}{2}\beta p_{n-1}^{t-1} + \frac{1}{2}\beta p_{n+1}^{t-1}, \tag{1}$$

$$p_n^{t+1} = (1-\beta)p_n^{t} + \frac{1}{2}\beta p_{n-1}^{t} + \frac{1}{2}\beta p_{n+1}^{t}. \tag{2}$$

After a carefully manipulation of these equations, the difference terms are:

$$\frac{\Delta p_n^{t+\Delta t}}{\Delta t} = \beta\left(\frac{1}{2}\frac{L_0^2}{T_0}\frac{\Delta^2 p_n}{\Delta x^2} + \frac{O(\Delta x^2)}{\Delta x^2} - (1-\beta)\frac{1}{4}\frac{L_1^4}{T_0}\frac{\Delta^4 p_n}{\Delta x^4}\right)^{t-\Delta t}, \tag{3}$$

where T_0, L_0 and L_1 are scale factors. Calling the constants $K_2 = \frac{L_0^2}{2T_0}$ and $K_4 = \frac{L_1^4}{4T_0}$ and assuming the $p(x,t)$ sufficiently smooth, we can take the limit as $\Delta t \mapsto 0$ and $\Delta x \mapsto 0$, getting:

$$\frac{\partial p}{\partial t} = \beta K_2 \frac{\partial^2 p}{\partial x^2} - \beta(1-\beta)K_4\frac{\partial^4 p}{\partial x^4}, \qquad 0 < x < L, \quad t > 0. \tag{4}$$

Note that if $\beta = 1$, the problem is reduced to the classical Gaussian distribution; it is because the structure contained in the standard diffusion equation is totally preserved. The negative term corresponds to non-Fickian part that characterizes the retention effect. In general, the Eq.(4) involves parameters of different orders of magnitude $K_4 = O(10^{-2}K_2) = O(10^{-4}\beta)$, as we can see inBevilacqua et al. (2011a,b), for example, and the retention term is significantly lower than the diffusive coefficient.

In this work, due to the parameters magnitude differences, we consider the retention term as a small perturbation of the pure diffusion, and we rewrite the problem (4) in a context of singularly perturbed problems. The perturbed problem (**Problem** (P_ε)) consists of finding $p_\varepsilon(x,t)$, defined on $x \in (0, L)$ and $t > 0$, which satisfy the following problem:

$$\frac{\partial p_\varepsilon}{\partial t} = D\frac{\partial^2 p_\varepsilon}{\partial x^2} - \varepsilon\frac{\partial^4 p_\varepsilon}{\partial x^4}, \tag{5}$$

with initial-boundary conditions given by

$$\begin{aligned} p_\varepsilon(0,t) &= a_0, \quad p_\varepsilon(L,t) = a_L, \\ \left.\frac{\partial^2 p_\varepsilon}{\partial x^2}\right|_{x=0} &= \left.\frac{\partial^2 p_\varepsilon}{\partial x^2}\right|_{x=L} = 0, \\ p_\varepsilon(x,0) &= f(x), \end{aligned} \tag{6}$$

where $D = \beta K_2$ and $\varepsilon = \beta(1-\beta)K_4$ are constant parameters associated to diffusion and retention, respectively, $f(x)$ a given initial function, a_0 and a_L are constants that satisfies the compatibility conditions, i.e. $a_0 = f(0)$ and $a_L = f(L)$. For the unperturbed problem (**Problem** (P)) we discarded the retention term and obtain a simple diffusion problem, consists of finding $p_0(x,t)$ which satisfy the problem:

$$\frac{\partial p_0}{\partial t} = D\frac{\partial^2 p_0}{\partial x^2}, \tag{7}$$

with the same initial-boundary conditions like those defined in (6).

2.1 Inverse problem

The characterization of the complete inverse problem consists in determining both D and ε simultaneously. However, for a sake of simplicity, let us assume in this paper that the diffusion parameter D is previously known.

Thus, the aim of this work is to reconstruct the retention parameter ε taking into account a set of N measurements $\mathbf{p}_{exp} = \{p^1_{exp}, ..., p^N_{exp}\}$ and a set of N noisy predicted values $\mathbf{p}_\varepsilon = \{p^1_\varepsilon, ..., p^N_\varepsilon\}$, from Problem (5 - 6). As usually adopted in topological derivative approach for inverse problems, we shall consider the minimization of an associated shape functional. A very natural suitable choice is the quadratic distance between $\mathbf{p}_{exp}$ and $\mathbf{p}_\varepsilon$:

$$\text{Min } \Psi(\varepsilon) = \sum_{i=1}^{N} (p^i_{exp} - p^i_\varepsilon)^2. \tag{8}$$

Here, we shall consider the asymptotic expansion of functional (8). This approach has several advantages, mainly in the computational cost point of view. In fact, as will be demonstrated in the next section, topological derivative depends only on the solution of the unperturbed problem, i.e., given the solution of the Eq. (7), it is possible get an estimate for ε.

In more general cases, topological derivative depends on the solutions original and adjunct unperturbed problems (Novotny and Sokołowski, 2013). On the other hand, second order topological derivative has non local terms (Rocha de Faria and Novotny, 2009) resulting in higher computational cost. However, in this particular case, where we are considering the fourth order PDE model given by Bevilacqua et al. (2011a), the second order topological derivative depends only the unperturbed problems, i.e., problems associated to pure diffusion models, as will become clear in next sections.

3 TOPOLOGICAL DERIVATIVE

Singularly perturbed problems occur when the model is disturbed by a infinitesimal parameter ε, which degenerates not smoothly to original problem as $\varepsilon \to 0$. Nucleation of holes, creation of inclusions in the domain, insertion of source terms or perturbation in the main term of the PDE are examples of singularly perturbed problems, which have important applications as topology optimization, image processing and inverse problems, for instance.

In the last fifteen years topological derivative (Sokołowski and Zochowski, 1999) has been proven an effective tool for dealing with these kind of problems (Novotny and Sokołowski, 2013). In fact, topological derivative gives the topological asymptotic expansion of a shape functional with respect to a singularly infinitesimal perturbation. The most remarkable fact about first order topological derivative is that this term depends only on the unperturbed problem and, consequently, its computational cost is very low. In fact, it is necessary to solve just one problem (or two problems, in the case of the adjunct methodology) to estimate the minimum of the functional about a singular infinitesimal perturbation.

Let us consider a singularly perturbed problem by a small parameter ε, whose solution is denoted by p_ε. We are denoting by $\Psi_\varepsilon(p_\varepsilon)$ a shape function associated to the perturbed problem. Analogously, consider the unperturbed problem ($\varepsilon = 0$), where the solution is denoted by p_0 and the corresponding shape functional is $\Psi(p_0)$. Suppose $\Psi_\varepsilon(p_\varepsilon)$ admits the following topological asymptotic expansion

$$\Psi_\varepsilon(p_\varepsilon) = \Psi(p_0) + \gamma_1(\varepsilon)\mathcal{T} + \gamma_2(\varepsilon)\mathcal{T}^2 + o(\gamma_2), \tag{9}$$

where $\gamma_1(\varepsilon)$, $\gamma_2(\varepsilon)$ (called first and second correction functions of Ψ_ε, respectively) are positive. Further, $\gamma_2/\gamma_1 \to 0$ and $o(\gamma_2)/\gamma_2 \to 0$ as $\varepsilon \to 0$. In this case, the functions $\mathcal{T}$ and $\mathcal{T}^2$ are called the first and second order topological derivative (Rocha de Faria and Novotny, 2009), respectively.

Next, let us consider the model given by Eq. (5) as a singularly perturbed problem and compute the second order topological asymptotic analysis of the shape functional (8) to obtain the reconstruction of retention parameter ε.

In order to introduce the main ideas of the proposed methodology, we present the calculation of the topological derivative for functional (8) considering two basic cases. In the first one (Case A), we choose a problem whose analytical solution is known to introduce systematic analysis of the entire process behind the calculations. Thus, we obtain the explicit form of asymptotic expansion of functional and consequently, we can identify each one of its terms and assign it the order of the topological derivative. In the second case (Case B), we introduce a generalized methodology to be used in the numerical calculation of first and second order topological derivative of shape functional (8).

Case A: an example with analytical solution

In this particular example, consider the problems (P) and (P_ε), described by Eqs, (5-7) with $x \in (0,1)$, $t > 0$, the initial condition $f(x) = \sin \pi x$ and the boundary conditions $a_o = a_1 = 0$. The analytical solution of the unperturbed problem (P) is given by:

$$p_0(x,t) = e^{-D\pi^2 t} \sin \pi x. \tag{10}$$

On the other hand, the solution of problem (P_ε) is given by:

$$p_\varepsilon(x,t) = e^{-D\pi^2 t} e^{-\varepsilon \pi^4 t} \sin \pi x. \tag{11}$$

Note that if parameters D, ε, $\hat{D}$ and $\hat{\varepsilon}$ satisfy $D + \varepsilon\pi^2 = \hat{D} + \hat{\varepsilon}\pi^2$, from Eq. (11) we can infer that parameters D and ε are not simultaneously identifiable. Then, it is necessary to solve the inverse problem of identification of D and ε in two steps. As previously mentioned, we admit here that the diffusion coefficient D is already known.

As the goal is to investigate the asymptotic expansion of the solution $p_\varepsilon(x,t)$, let us consider the following approximation

$$e^{-\varepsilon\pi^4 t} = 1 - \varepsilon\pi^4 t + \frac{\varepsilon^2\pi^8 t^2}{2} + o(\varepsilon^2), \tag{12}$$

into Eq.(11). It follows that

$$\begin{aligned} p_\varepsilon(x,t) &= p_0(x,t) - \varepsilon\pi^4 t p_0(x,t) + \frac{\varepsilon^2\pi^8 t^2}{2} p_0(x,t) + o(\varepsilon^2) \\ &\approx p_0(x,t) - \varepsilon\pi^4 t p_0(x,t) + \frac{\varepsilon^2\pi^8 t^2}{2} p_0(x,t) = p_\varepsilon^{asymp}(x,t). \end{aligned} \tag{13}$$

Note that Eq. (13) indicates that if $p_0(x,t)$ is known, we have an approximation (as good as ε is small) for $p_\varepsilon(x,t)$, denoted by $p_\varepsilon^{asymp}(x,t)$. Furthermore, given an experimental set of data for p_ε we can have an estimative for the retention parameter ε. In fact, taking into account the asymptotic expansion of $p_\varepsilon(x,t)$ given by Eq. (13) into the shape functional (8), we have

$$\begin{aligned} \Psi_\varepsilon(\varepsilon) &= \sum_{i=1}^{N} (p^i_{exp} - p^i_\varepsilon)^2 = \sum_{i=1}^{N} (p^i_{exp} - p^i_0)^2 + 2\varepsilon\pi^4 \sum_{i=1}^{N} t(p^i_{exp} - p^i_0)p^i_0 \\ &+ \varepsilon^2\pi^8 \sum_{i=1}^{N} t^2(2p^i_0 - p^i_{exp})p^i_0 + o(\varepsilon^2). \end{aligned} \tag{14}$$

Considering Eq.(9), we can identify $\gamma_1(\varepsilon) = 2\varepsilon\pi^4$, $\mathcal{T} = \sum_{i=1}^{N} t(p^i_{exp} - p^i_0)p^i_0$, $\gamma_2(\varepsilon) = \varepsilon^2\pi^8$ and $\mathcal{T}^2 = \sum_{i=1}^{N} t^2(2p^i_0 - p^i_{exp})p^i_0$.

In this simple example we can observe the most important property of the topological derivative: this term depends only the unperturbed problem and, therefore, it is very cheap from a computational point of view. Although, in this particular example it is also true for the second order topological derivative, it is not true in general cases (Rocha de Faria and Novotny, 2009).

In order to identify the retention parameter ε we consider the first and second order topological asymptotic expansion. Putting $\Psi_\varepsilon(\varepsilon) = 0$ and disregarding the terms $o(\varepsilon)$ in Eq. (14), we obtain, taking into account first order topological asymptotic expansion,

$$\varepsilon_1 = -\frac{\sum_{i=1}^{N} (p^i_{exp} - p^i_0)^2}{2\pi^4 \sum_{i=1}^{N} t(p^i_{exp} - p^i_0)p^i_0}, \tag{15}$$

as the 'first-order' estimate for ε.

On the other hand, considering second order topological asymptotic expansion, the minimum of the expression (14), where we had disregarding the terms $o(\varepsilon^2)$, is given by

$$\varepsilon_2 = -\frac{\sum_{i=1}^{N} t(p^i_{exp} - p^i_0)p^i_0}{\pi^4 \sum_{i=1}^{N} t^2(2p^i_0 - p^i_{exp})p^i_0}, \tag{16}$$

where ε_2 is a 'second-order' estimate for ε.

Case B: the general case

Let us consider again the problems (P) and (P_ε), described by Eqs, (5-7) and build an efficient numerical methodology to obtain the topological derivative. For this, consider the asymptotic expansion of $p_\varepsilon(x,t)$ given by:

$$p_\varepsilon(x,t) = p_0(x,t) + \varepsilon w_1(x,t) + \varepsilon^2 w_2(x,t) + w_\varepsilon(x,t), \tag{17}$$

where $w_1(x,t)$ and $w_2(x,t)$ are independent of the parameter ε. In fact, taking into account Eq. (17) and the problems (P) and (P_ε), we got that $w_1(x,t)$ is the solution of the following auxiliary problem:
Problem (W_1): Given p_0, find $w_1(x,t)$ such that

$$\frac{\partial w_1}{\partial t} \quad - \quad D\frac{\partial^2 w_1}{\partial x^2} = -\frac{\partial^4 p_0}{\partial x^4}, \tag{18}$$

whith initial-boundary conditions given by

$$w_1(0,t) = w_1(L,t) = 0; \quad \left.\frac{\partial^2 w_1}{\partial x^2}\right|_{x=0} = \left.\frac{\partial^2 w_1}{\partial x^2}\right|_{x=L} = 0; \quad w_1(x,0) = 0, \tag{19}$$

where $x \in (0,L)$ and $t > 0$.

Further $w_2(x,t)$ is associated to a pure diffusion problem and w_ε compensates the discrepancy produced by the previous terms. More specifically, these terms are solutions of the following problems:
Problem (W_2): Given $w_1(x,t)$, find v_0 such that

$$\frac{\partial w_2}{\partial t} - D\frac{\partial^2 w_2}{\partial x^2} = -\frac{\partial^4 w_1}{\partial x^4}, \tag{20}$$

with initial-boundary conditions given by

$$w_2(0,t) = w_2(L,t) = 0; \quad \left.\frac{\partial^2 w_2}{\partial x^2}\right|_{x=0} = \left.\frac{\partial^2 w_2}{\partial x^2}\right|_{x=L} = 0; \quad w_2(x,0) = 0, \tag{21}$$

Finally, w_ε satisfies:
Problem (W_ε): Given w_2 and ε, find $w_\varepsilon(x,t)$ such that

$$\frac{\partial w_\varepsilon}{\partial t} \quad - \quad D\frac{\partial^2 w_\varepsilon}{\partial x^2} + \varepsilon\frac{\partial^4 w_\varepsilon}{\partial x^4} = -\varepsilon^3\frac{\partial^4 w_2}{\partial x^4}, \tag{22}$$

whith initial-boundary conditions given by

$$w_\varepsilon(0,t) = w_\varepsilon(L,t) = 0; \quad \left.\frac{\partial^2 w_\varepsilon}{\partial x^2}\right|_{x=0} = \left.\frac{\partial^2 w_\varepsilon}{\partial x^2}\right|_{x=L} = 0; \quad w_\varepsilon(x,0) = 0. \tag{23}$$

It is easy to observe that $w_\varepsilon = o(\varepsilon^2)$. Therefore, this term may be disregarded.

In summary, first of all, we need to solve the unperturbed problem given by Eq. (7). Then, the solution $p_0(x,t)$ is post-processed and the term $-\partial^4 p_0/\partial x^4$ is the source term in the Problem (W_1). Finally, after solve Problem (W_1) and a post-processing of the solution (w_1), we can solve the Problem (W_2).

Then, putting the ansätz (17) into the shape functional (8), we get

$$\begin{aligned}\Psi_\varepsilon &= \sum_{i=1}^{N}\left(p^i_{exp} - p_0 - \varepsilon w_1 - \varepsilon^2 w_2 + o(\varepsilon^2)\right)^2 \\ &= \Psi_0 - 2\varepsilon\sum_{i=1}^{N}(p^i_{exp} - p_0)w_1 - \varepsilon^2\left(2\sum_{i=1}^{N}(p^i_{exp} - p_0)w_2 - \sum_{i=1}^{N} w_1^2\right) + o(\varepsilon^2). \quad (24)\end{aligned}$$

In Section 5.1 we show that first order topological derivative not proved to be a good estimator for the retention parameter. Therefore, in this general case we will consider only the "second order" estimator ε_2 given by:

$$\varepsilon_2 = -\frac{\sum_{i=1}^{N}(p^i_{exp} - p_0)w_1}{2\sum_{i=1}^{N}(p^i_{exp} - p_0)w_2 - \sum_{i=1}^{N} w_1^2}. \quad (25)$$

4 FINITE ELEMENT APPROXIMATION

In order to solve the time-dependent problems $(P), (W_1)$ and (W_2) numerically, let $\Omega \equiv (0, L)$ denote the spatial domain and $I \equiv (0, T)$ the time interval of interest, $W = H^2_a(\Omega) = \{w(x,t) \in H^2(\Omega) \mid w(0,t) = a_0; w(L,t) = a_L\}$ and $V = H^2_0(\Omega)$, be the set of trial functions and the space of weighting functions, respectively. Let $[0,T] = \bigcup_{n=1}^{N}[t_n, t_{n+1}]$ be a uniform temporal discretization and $\Delta t = t_n - t_{n-1}$ the time step. The spatial domain is discretized using an uniform finite element partition consisting of n_e elements Ω_e such that $\overline{\Omega} = \bigcup_{n=1}^{n_e}\Omega_e$ and $\bigcap_{n=1}^{n_e}\Omega_e = \emptyset$. Our choice is to construct $W_h = \{w_h(x,t) \in C^1(\Omega) \mid w_h(0) = w_h(L) = 0, \forall w_h(\Omega_e) \in \hat{P}_3(\Omega_e)\} \subset W$ and $V_h \subset V$, where $\hat{P}_3(\Omega_e)$ are the Hermite's polynomials of third degree. Then, the approximations to problems are given by

Problem (P_h): Find $p^h_0(x,t) \in W_h$, $\forall t \in I$, such that

$$\int_0^L \frac{\partial p^h_0}{\partial t} v_h d\Omega + D\int_0^L \frac{\partial p^h_0}{\partial x}\frac{\partial v_h}{\partial x} d\Omega = 0, \quad \forall v_h \in V_h, \quad (26)$$

with initial-boundary conditions given by

$$p^h_0(0,t) = a_0; \quad p^h_0(1,t) = a_1; \qquad w(x,0) = f(x). \quad (27)$$

Problem (W_{1h}): Given p^h_0, find $w^h_1(x,t) \in W_h$, $\forall t \in I$, such that

$$\int_0^L \frac{\partial w^h_1}{\partial t} v_h d\Omega + D\int_0^L \frac{\partial w^h_1}{\partial x}\frac{\partial v_h}{\partial x} d\Omega = -\int_0^L \frac{\partial^2 p_{oh}}{\partial x^2}\frac{\partial^2 v_h}{\partial x^2} d\Omega, \quad \forall v_h \in V_h, \quad (28)$$

with initial-boundary conditions given by

$$w^h_1(0,t) = w^h_1(L,t) = 0; \quad w^h_1(x,0) = 0. \quad (29)$$

For the **Problem (W_{2h})**, we take **Problem (W_{1h})** replacing $p^h_0 = w^h_1$ and $w^h_1(x,t) = w^h_2(x,t)$.

In the last procedures, it is necessary a transient algorithm to obtain the required numerical solutions of the semi-discrete problems. For this, we take the approximation at time t to be of the form $w^h_1(x,t) = \sum_{j=1}^{n_p} w_j(t)\varphi_j(x)$ and $v_h(x,t) = \sum_{j=1}^{n_p}\varphi_j(x)$ to construct the finite element interpolation and weighting functions, respectively, where n_p is the total number of degrees of freedom and $\varphi_j(x)$ the global shape function. Thus, each of the spatial discrete problems (P_h) and (W_{1h}), not excluding the Dirichlet boundary condition nodes, leads to an ordinary differential system

$$\begin{aligned} \sum_{j=1}^{n_p}\left[M_{ij}\frac{dw_j}{dt}+K_{ij}w\right] &= F_i, \qquad t\in I;\quad 1\leqslant i\leqslant n_p, \\ w_i(0) &= f_i(x), \end{aligned} \tag{30}$$

where $F_i = 0$ to problem (P_h), $f_i(x) = 0$ to problem (W_{1h}) and

$$M_{ij} = \int_{\Omega_e}\varphi_i(x)\varphi_j(x)d\Omega_e, \tag{31}$$

$$K_{ij} = \int_{\Omega_e}D\varphi_i'(x)\varphi_j'(x)d\Omega_e, \tag{32}$$

$$F_i = \int_{\Omega_e}p_o^h(x_i)\varphi_j'(x)d\Omega_e, \tag{33}$$

which may be rewritten in the following matrix form:

$$\begin{aligned} \mathbf{M}\dot{\mathbf{w}}+\mathbf{K}\mathbf{w} &= \mathbf{F}, \\ \mathbf{w}(\mathbf{0}) &= \mathbf{f}(\mathbf{x}), \end{aligned} \tag{34}$$

The transient algorithm to be used here to solve the above system is based on generalized trapezoidal family of methods, presented in Hughes (1987), which consists of the following equations:

$$\begin{aligned} \mathbf{M}\boldsymbol{\nu}_{n+1}+\mathbf{K}\mathbf{w}_{n+1} &= \mathbf{F}_{n+1}, \\ \mathbf{w}_{n+1} &= \mathbf{w}_n+\Delta t\boldsymbol{\nu}_{n+\alpha}, \\ \boldsymbol{\nu}_{n+1} &= (1-\alpha)\boldsymbol{\nu}_n+\alpha\boldsymbol{\nu}_{n+1}, \end{aligned} \tag{35}$$

where $\boldsymbol{\nu}_n$ and $\mathbf{w}_n$ are the approximations to $\dot{\mathbf{w}}(t_n)$ and $\mathbf{w}(t_n)$, respectively; $\mathbf{F}_{n+1} = \mathbf{F}(t_n)$, Δt is the constant time step and $\alpha \in [0, 1]$ is the parameter which define the method. Thus, an implementation derive of (35) where $\boldsymbol{\nu}$'s are unnecessary are given by:

$$(\mathbf{M}+\alpha\Delta t\mathbf{K})\mathbf{w}_{n+1} = (\mathbf{M}-(1-\alpha)\Delta t\mathbf{K})\mathbf{w}_n+\Delta t(\alpha\mathbf{F}_{n+1}+(1-\alpha)\mathbf{F}_n), \tag{36}$$

where is well-known that to $\alpha = 0, 0.5$ or 1 we have the Foward Euler, Crank-Nicolson or Backward Euler method, respectively.

5 NUMERICAL EXPERIMENTS

In this section, we present some numerical experiments to illustrate the methodology used in cases (A) and (B) of the Section (3), showing its potential. In each case, in order to avoid inverse crimes, we pollute the p^i_{exp} data with Gaussian white noise, i.e., we take $\hat{p}^i_{exp} = p^i_{exp} + \varepsilon^i(0, \sigma)$, where $\varepsilon^i(0, \sigma) \sim N(0, \sigma^2)$. Thus, we take into account the first and the second order topological asymptotic expansion of functional (8): $\Psi_\varepsilon(u_\varepsilon) \approx \Psi(u_o) + \gamma_1(\varepsilon)\mathcal{T}$ and $\Psi_\varepsilon(u_\varepsilon) \approx \Psi(u_o) + \gamma_1(\varepsilon)\mathcal{T} + \gamma_2(\varepsilon)\mathcal{T}^2$ to obtain the estimates ε_1 and ε_2, respectively, for the retention coefficient ε and compare the results.

Since the problem is severely ill-posed, it is necessary to impose some kind of regularization. To avoid adding an artificial regularization term in the functional (8), we choose to take the greatest value of a sample of thirty repetitions of the experiment.

5.1 Case A

In these experiments, we wish to obtain an estimated value for ε by first and second order topological derivatives formulas given by Eq. (15) and Eq. (16), respectively. We consider the diffusion coefficient $D = 2 \times 10^{-4}$ and the standard deviation $\sigma = 0.02$, which means considering up to 4% noise in the data. The time interval t was assumed to vary from 5 to 95, with a time step $\Delta t = 1$. Thus we obtain 90 experimental data from a sensor positioned at $x = 0.5$ coordinate for different values of ε. Here, we do not consider the influence of the spatial numerical approaches because we know the analytical solutions of unperturbed and perturbed initial value problems, given by (10) and (11), respectively.

Table 1: First (ε_1 – Eq. (15)) and second order (ε_2 – Eq. (16)) topological estimated ε for 4% noise data

exact	ε_1	ε_2
5.0×10^{-5}	2.1479×10^{-5}	3.3203×10^{-5}
1.0×10^{-5}	0.5029×10^{-5}	0.9045×10^{-5}
5.0×10^{-6}	3.0163×10^{-6}	4.9201×10^{-6}
1.0×10^{-6}	2.2828×10^{-6}	1.1014×10^{-6}
5.0×10^{-7}	4.7840×10^{-7}	5.0446×10^{-7}
1.0×10^{-7}	2.2785×10^{-7}	1.0118×10^{-7}

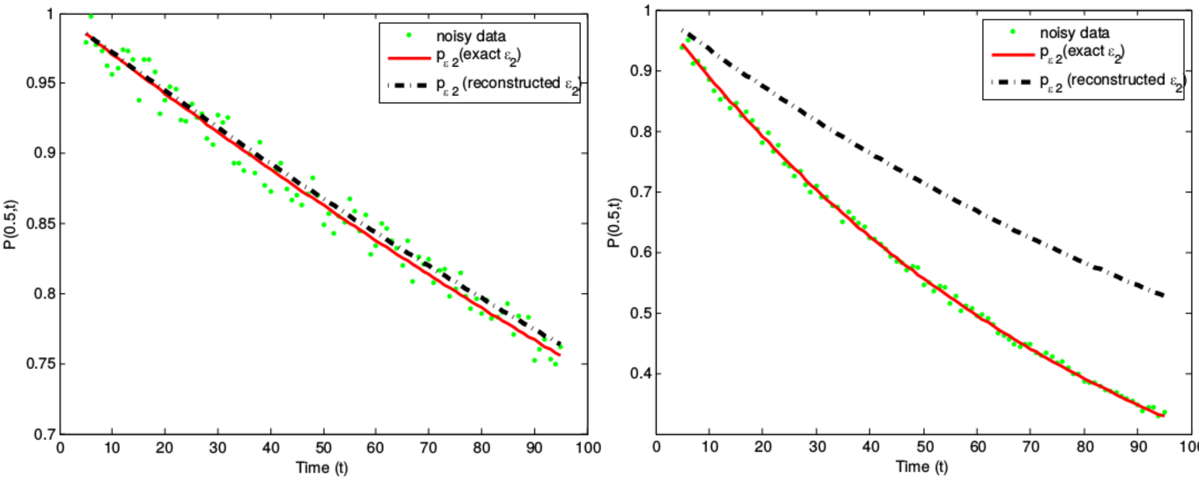
A set of results are shown in Table 1, where the first column includes the exact values of ε parameter and the second and third columns include an estimate for ε parameter, using the first ε_1 and second order ε_2 topological asymptotic expansion, respectively. Note, by compare first and second column, that the first order topological asymptotic expansion is not a good estimator for retention coefficient, it is because the perturbed operator is the higher order term of equation, and thereby more information of expansion would be required. When we consider the second order term of expansion, all estimates are improved, as we can see in the last column of the table. This confirms our expectation that this (second order) term would be a good estimator to reconstruct the parameter ε. Note that the accuracy is improved to the extent that ε becomes much smaller than D.

Figure 1 shows two different sceneries for noisy data, analytical solution and reconstructed solution, obtained from estimated ε using second order topological derivative. In Fig. 1a the exact $\varepsilon = 1.0 \times 10^{-5}$ was considered and the solution using estimated $\varepsilon = 0.9046 \times 10^{-5}$ was well reconstructed. In Fig. 1b the exact $\varepsilon = 1.0 \times 10^{-4}$ was assumed and the solution using estimated $\varepsilon = 0.4898 \times 10^{-5}$ was not reconstructed accurately; note that the reconstructed solution is out of noise range.

Like Table 1, the Fig. 1 also illustrate the hypothesis that the smaller value of ε give us a more accuracy for reconstructed solution.

5.2 Case B

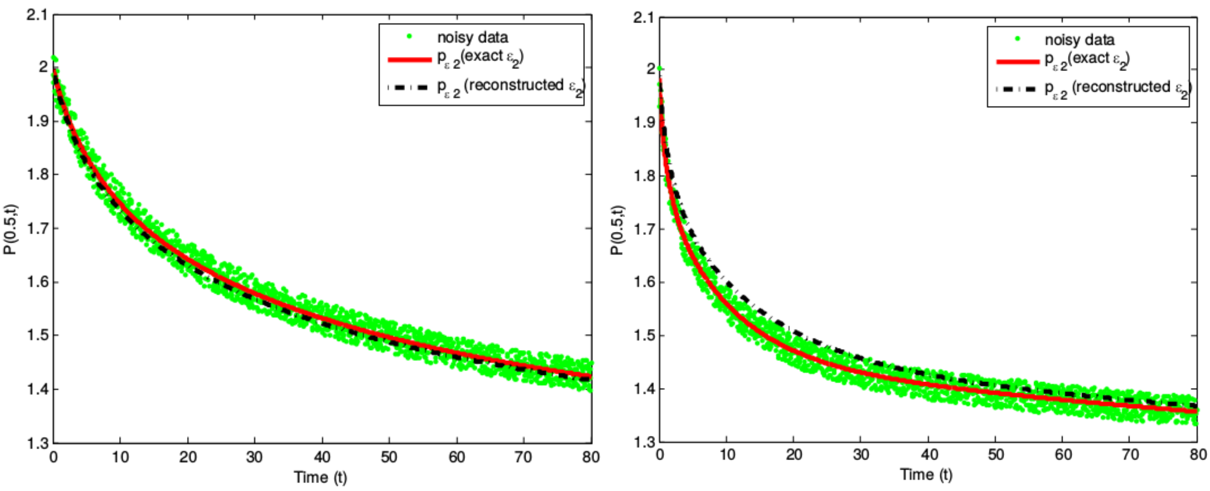
In this case, we will consider the influence of the spatial numerical approaches, so that we disregard the existence of analytical solution for unperturbed and perturbed initial value



(a) (b)

Figure 1: Solution $P_\varepsilon(0.5,t)$ for ε exact and reconstructed, using $f(x) = \sin \pi x$. (a) $\varepsilon = 1 \times 10^{-5}$ (b) $\varepsilon = 1 \times 10^{-4}$.

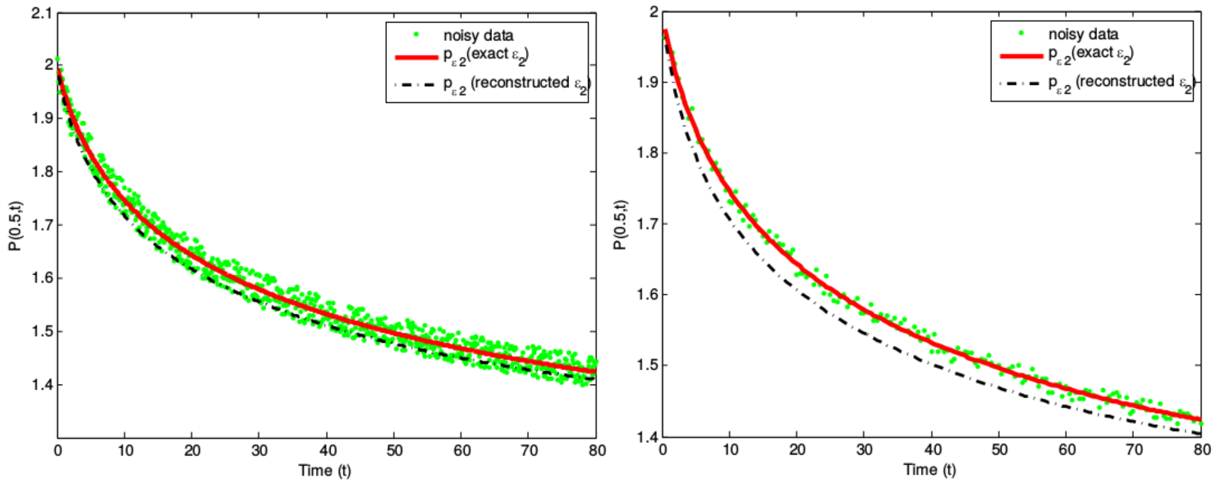
problems. As in Case A, we admitted $D = 2 \times 10^{-4}$ and the standard deviation $\sigma = 0.02$, which means considering up to 4% noise in the data. We assume a time interval $I = [0, 80]$ and spatial domain $\Omega = [0, 1]$, with $x = 0.5$ fixed. Only the second order topological derivative has been used.



(a) (b)

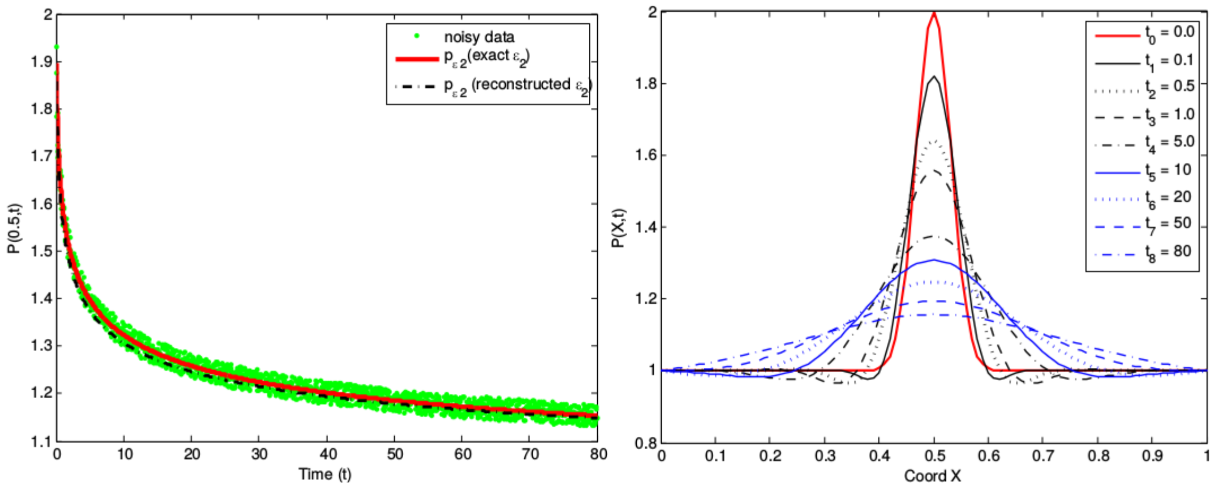
Figure 2: Numerical solution $P_\varepsilon(0.5,t)$ for ε exact and reconstructed, using $f(x) = (\sin \pi x)^{11} + 1$ and $\Delta t = 0.05$. (a) $\varepsilon = 1 \times 10^{-6}$ (b) $\varepsilon = 1 \times 10^{-5}$.

Figure 2 shows two sceneries obtained by numerical simulation, both admitting $f(x) = (\sin \pi x)^{11} + 1$ and boundary conditions $a_0 = a_1 = 1$. Here we used a time step $\Delta t = 0.05$, $\alpha = 0.5$ (Crank-Nicolson) and an uniform spatial partition of 20 elements. In Fig. 2a the exact $\varepsilon = 1.0 \times 10^{-6}$ was considered and the solution using estimated $\varepsilon_2 = 1.2370 \times 10^{-6}$ was well reconstructed. In Fig. 2b the exact $\varepsilon = 1.0 \times 10^{-5}$ was assumed and the solution using estimated $\varepsilon_2 = 6.5298 \times 10^{-6}$ was not reconstructed accurately. This shows that the magnitude of ε definitely influences the methodology used for the parameter reconstruction, regardless of the number of observations and spatial discretization. We have obtained best estimates for smaller ε values. In this particular experiment, the parameter should be less than 10^{-5}.



(a) **(b)**

Figure 3: Numerical solution $P_\varepsilon(0.5, t)$ for ε exact and reconstructed, using $f(x) = (\sin \pi x)^{11} + 1$ and $\varepsilon = 1 \times 10^{-6}$. (a) $\Delta t = 0.1$ (b) $\Delta t = 0.5$.



(a) **(b)**

Figure 4: Numerical solution using $f(x) = (\sin \pi x)^{100} + 1$ and exact $\varepsilon = 1 \times 10^{-6}$. (a) Solution $P_\varepsilon(0.5, t)$ for ε exact and reconstructed (b) Solution $P_\varepsilon(x, t_i)$ for reconstructed ε .

In Fig. 3, we are interested in investigating the influence of the number of measurements for accuracy of reconstructed solution. For this, we obtained $N = 80/\Delta t$ measurements $P_\varepsilon(0.5, x)$, considering $\varepsilon = 1.0 \times 10^{-6}$ and the same initial-boundary conditions and spatial partition of the previous experiment. In Fig. 3a we used a time step $\Delta t = 0.1$, $\alpha = 0.5$ and estimated $\varepsilon_2 = 1.5770 \times 10^{-6}$; in Fig. 3b, $\Delta t = 0.5$, $\alpha = 0.5$ and $\varepsilon_2 = 1.8580 \times 10^{-6}$. We can observe in Fig. 2a,3a and 3b that increasing the number of measurements leads to significant improvement in the accuracy of the reconstructed parameter ε_2. In the case of Fig. 3b, the number of measurements has not been sufficient to maintain the solution within the noise range.

Figure 4 was obtained by assuming an initial condition given by $f(x) = (\sin \pi x)^{100} + 1$, boundary conditions $a_0 = a_1 = 0$, uniform spatial partition of 100 elements, time step $\Delta t = 0.05$ and $\alpha = 0.5$. Furthermore, we consider the exact parameter $\varepsilon = 1.0 \times 10^{-6}$ and obtained the reconstructed solution $\varepsilon_2 = 1.2067 \times 10^{-6}$. Figure 4b presents the solution $P_\varepsilon(x, t_i)$ at the following instants of time $t_i = 0.0, 0.1, 0.5, 1.0, 5.0, 10, 20, 50, 80$. Figure 4a shows that combining the number of observations, the spatial discretization and the size of ε parameter, we obtain a good accuracy for reconstructed solution of complex problem.

6 CONCLUSIONS

Although a large body of literature has been produced over the last two decades, demonstrating that anomalous diffusion can offer a better fit to experimental data, in many diffusive processes, the mathematical study of inverse problems in anomalous diffusion is in an initial stage. Mainly due to the nonlocality of the forward model by fractional differential equations. For a recent review the reader may refer to Jin and Rundell (2015).

In order to avoid this difficulty, we adopt the fourth order PDE model introduced Bevilacqua et al. (2011a). This approach allow us approximate the anomalous diffusion problem (P_ε) by three coupled pure diffusion problems ($p_0, w_1,$ and w_2) given, respectively, by (7, 19 and 21) plus a higher order term, which may be disregarded, in general. This methodology allows us to take advantage of both the theoretical and numerical point of view. In fact, it implies approaching the solution of a new model by classical ones. Further, from the proposed ansätz, given by eq. (17), we derive a new topological asymptotic expansion for (P_ε) problem solution. It was crucial in order to derive first and second order topological derivative in a straightforward way.

In particular, in this paper we used a topological optimization formulation for the inverse problem to reconstruct the unknown ε, i.e., the retention parameter. For this, we assumed that the diffusion coefficient (D) was know and proposed a methodology grounded on the topological derivative to minimize the shape functional (8), that measures the quadratic distance between noisy measurements and simulated data. The results, illustrated by numerical experiments, shows the effectiveness of the second order topological derivative, ensuring a better approximation as the lowest is ε compared with D, i.e., when the retention effect is a small perturbation in the process diffusive. Moreover, as the smaller Δt, more accurate is the numerical reconstruction, as expected due to the increase in the number of observations.

Despite the usefulness of the first order topological derivative in several applications, the results obtained by this approaching are not enough to guarantee a good approximation in the inverse problem under analysis. On the other hand, second order topological derivative proved to be a proper tool for estimate the coefficient related to retention with low computational cost and good results, even for noisy data. Reconstructed solutions are valid if limited by noisy data, which is enough for the inverse problem reconstruction. In this case, the numerical experiments corroborate the efficiency of the second order topological derivative.

In future works, it is interesting to investigate the application of the approach proposed in this work in higher dimensional problems and simultaneous identification of D and ε.

REFERENCES

Bevilacqua, L., ao A.C.N.R, G., Costa, F. P., 2011a. A new analytical formulation of retention effects on particle diffusion processes. An. Acad. Bras. Cienc 83 (4), 1443–1464.

Bevilacqua, L., Galeão, A. C. N. R., Costa, F. P., 2011b. On the significance of higher order differential terms in diffusion processes. Journal of the Brazilian Society of Mechanical Sciences and Engineering 33, 166 – 175.

Eschenauer, H., Kobelev, V., Schumacher, A., 1994. Bubble method for topology and shape optimization of structures. J. Struct. Optim. 8, 42–51.

Hadamard, J., 1902. Sur les problèmes aux dérivées partielles et leur signification physique. Princeton University Bulletin 13, 49–52.

Hughes, T. J. R., 1987. The finite element method : linear static and dynamic finite element analysis. Englewood Cliffs, N.J. Prentice-Hall International.

Jin, B., Rundell, W., 2015. A tutorial on inverse problems for anomalous diffusion processes. Inverse Problems 31 (3), 035003.

Novotny, A. A., Sokołowski, J., 2013. Topological derivatives in shape optimization. Interaction of mechanics and mathematics. Springer, Heidelberg, New York.

Rocha de Faria, J., Novotny, A. A., 2009. On the second order topological asymptotic expansion. Structural and Multidisciplinary Optimization 39 (6), 547–555.

Silva, L. G., Knupp, D. C., Bevilacqua, L., Galeão, A. C. N., Silva Neto, A. J., 2014a. Formulação e solução de um problema inverso de difusão anômala com técnicas estocásticas. Ciência e Natura 36 (Ed. Especial), 82–96.

Silva, L. G., Knupp, D. C., Bevilacqua, L., Galeão, A. C. N., Silva Neto, A. J., 2014b. Inverse problem in anomalous diffusion with uncertainty propagation. In: Proceedings of the of 8nd International Conference on Inverse Problems in Engineering. Cracow, Poland.

Silva, L. G., Knupp, D. C., Bevilacqua, L., Galeão, A. C. N., SIMAS, J. G., Vasconcellos, J. F., Silva Neto, A. J., 2013. Investigation of a new model for anomalous diffusion phenomena by means of an inverse analysis. In: Proceedings of the of 4nd Inverse Problems, Design and Optimization Symposium. Albi, France.

Sokołowski, J., Zochowski, A., 1999. On the topological derivative in shape optimization. SIAM J. Control Optim. 37 (4), 1251–1272.