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Pollution in porous media: non permanent cases

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Abstract

In this work, we focus on pollution transfer in porous media. We prove that the pollutant transfer can be modeling by a non linear evolutive system. We used the mathematical frameworks presented on [5] to solve the non linear problem. And so we build a numerical scheme, based on topological optimization to get the representation of the pollution in the non permanent case. To end the paper, we give some numerical results.

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1 Introduction

In this beginning of the third millennium, we are in front of two major

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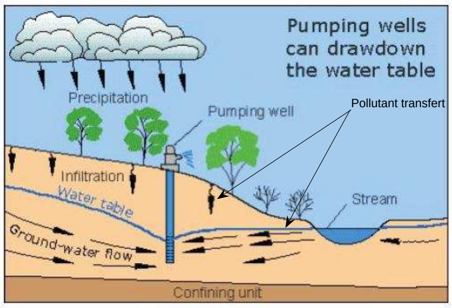

Figure 1: Example of pollutant transfer in porous media

challenges: they are mainly the global warming and the access of the drinkable water for a great part of the population (particularly Subsaharian Africa). Indeed, in one hand, the galloping industrialization favors the rejection (by factories, vehicles, ...) of an important quantity of carbon monoxide (CO_2) in the atmosphere. The latter is in a great part, responsible of the air pollution and consequently of the global warming on the earth. In another hand, the use of chemical manure and pesticides in farming areas involves the infiltration of chemical products (thus of polluters) in the sub-soil which can reach the water layer. It is in this context that we are proposing a mathematical model and resolution method allowing us to study problem of the transfer of pollutants in porous media.

In [5], we studied the distribution of a pollution in a unsaturated porous media. We considered the stationary evolution case of the fluid under some reasonable hypotheses. And in the model, we used strongly some experimental laws accepted by the scientific community to overcome difficulties appeared in the modeling of the pollution phenomena.

And we use mainly topological optimization and some nonlinear techniques in partial differential equations to have theoretical and numerical results.

The goal of the topological optimization problem is to find an optimal design with an a priori poor information on the optimal shape of the structure. The topological optimization problem consists in minimizing a functional

$j(\Omega) = J(\Omega, u_\Omega)$ where the function u_Ω is defined, for example, on a variable open and bounded subset Ω of $\mathbb{R}^n$. For $\varrho > 0$, let $\Omega_\varrho = \Omega \backslash \overline{(x_0 + \varrho\omega)}$, be the set obtained by removing a small part $x_0 + \varrho\omega$ from Ω, where $x_0 \in \Omega$ and $\omega \subset \mathbb{R}^n$ is a fixed open and bounded subset containing the origin. Then, using general adjoint method, an asymptotic expansion of the function will be obtained in the following form:

$$j(\Omega_\varrho) = j(\Omega) + f(\varrho)g(x_0) + o(f(\varrho))$$
$$\lim_{\varrho \to 0} f(\varrho) = 0, \ \ f(\varrho) > 0$$

The topological sensitivity $g(x_0)$ provides information when creating a small hole located at x_0. Hence the function g will be used as descent direction in the optimization process.

The paper is organized us follows: the section 2 deals with the modeling of pollution in porous media. In section 3, we give some mathematical framework to prove that the the non linear problem which arise from the modeling gets a solution . In section 4, we study the problem of pollution transfer as a topological optimization one, in the section 5, we give some numerical results.

2 Modeling

In [5], we presented the modeling of a pollution problem and we study the model under some realistic hypotheses. In order to be completed, we present the model. Our aim in this work is to weaken the hypotheses done in [5] and to get additional results.

Let $\mathcal{D}$ be a porous medium. Let us introduce, for $x \in \mathcal{D}$ and $t \in (0, 1)$. The effective porosity $\varepsilon(t, x)$ is given by

$$\varepsilon(t, x) = \frac{dV_l}{dV_{total}}$$

where dV_l is an element of the volume of the fluid and dV_{total} an element of the total volume ;
$\sigma(t, x)$ the porosity given by

$$\sigma(t, x) = \frac{dV_v}{dV_{total}}$$

where dV_v is an element of the volume of the vacuum and
q the Darcy velocity vector given by

$$q = \varepsilon V$$

where V is the velocity vector of the fluid.
Ω is considered as an elementary domain of a porous domain $\mathcal{D}$.
We have $M(\Omega, t) = \int_\Omega dm;$ dm is an element of the mass of the fluid.
$dm = \rho(t,x)\varepsilon(t,x)$; $\rho(t,x)$ is the fluid density of the solution.
For our model we will use these notations: $\rho_s[kg/m^3]$ the fluid density of the solution given by

$$\rho_s = \frac{dm_{solution}}{dv_{solution}}$$

$W(t,x)$ the fraction of the mass (concentration):

$$W(t,x) = \frac{dm_{solute}}{dm_{solution}}.$$

$dm_{solution}$ is an element of the mass of the solution and dm_{solute} is an element of the mass of the pollutant.

Remark 1. *It is acceptable to consider the same model for the air pollution. In this case, the porosity is a constant.*

2.1 The conservation of the mass of the solution

We have

$$dm_{solution} = \rho_s dv_{solution} = \rho_s \frac{dv_{solution}}{dv_{total}} dv_{toal}$$
$$= \rho_s \varepsilon(t,x) dv_{total}$$
$$M_{solution}(\Omega, t) = \int_\Omega dm_{solution} = \int_\Omega \rho_s \varepsilon dx.$$

The principle of conservation of the mass stipulate that the variation of the mass in Ω is equal to the flux through the boundary of Ω with velocity V.

$$\frac{dM_{solution}(\Omega, t)}{dt} = -\int_{\partial\Omega} \rho_s \varepsilon V \nu d\sigma.$$

Hence,

$$\int_\Omega \frac{\partial}{\partial t}(\rho_s \varepsilon) + \int_{\partial\Omega} \rho_s \varepsilon V \nu d\sigma = 0$$

By the Green formula we obtain

$$\int_{\Omega}(\frac{\partial}{\partial t}(\rho_s\varepsilon) + div(\rho_s\varepsilon V))dx = 0 \quad \forall\, \Omega \subset \mathcal{D}$$

Hence

$$\frac{\partial(\rho_s\varepsilon)}{\partial t} + div(\rho_s q) = 0 \quad \text{in } \mathcal{D} \tag{1}$$

2.2 Conservation of the mass of pollutant liquid

Here, we consider for example that our pollutant liquid is: water + chemical concentration (it is homogeneous). By the formula given $W(t,x)$ we have

$$dm_{solute} = W(t,x)dm_{solution} = W(t,x)\rho_s(t,x)\varepsilon(t,x)dv_{total}$$

$$M(\Omega,t) = \int_{\Omega} dm_{solute} = \int_{\Omega} W\rho_s\varepsilon dx.$$

We use the principle conservation of the mass. This imply that

$$\int_{\Omega}(\frac{\partial}{\partial t}(W\rho_s\varepsilon) + div(W\rho_s q + J))dx \;=\; 0,$$

where J is the flux of dispersion diffusion. Hence

$$\frac{\partial}{\partial t}(W\rho_s\varepsilon) + div(W\rho_s q + J) \;=\; 0 \quad \forall\, \Omega \subset \mathcal{D}$$

$$\frac{\partial}{\partial t}(W\rho_s\varepsilon) + div(W\rho_s q + J) \;=\; 0 \quad \text{in } \mathcal{D} \tag{2}$$

2.3 Conservation of the momentum

If the porous medium is homogeneous the Darcy law is given by

$$q = -\frac{K}{\mu}(\nabla p + \rho_s g e_3);$$

where e_3 is third vector of the canonical basis of $\mathbb{R}^3$; p is the pressure, $ge_3 = \vec{g}$ is the gravity field, K the intrinsic permeability tensor, μ the dynamic viscosity and K/μ hydraulic conductivity.

If we have some weak concentration the flux of dispersion diffusion J is determined by the Fick law

$$J = -\rho_s D \nabla W$$

where D be the tensor of dispersion diffusion.

Finally we have a system of equations

$$\begin{cases} \frac{\partial \varepsilon \rho_s}{\partial t} + div(\rho q) = 0 \\ \frac{\partial(\varepsilon \rho_s W)}{\partial t} + div(\rho_s W q + J) = 0 \\ J = -\rho_s D \nabla W \\ q = -\frac{K}{\mu}(\nabla p + \rho_s g e_3) \end{cases} \tag{3}$$

where ε, ρ_s, W and p are unknowns.

And it is almost impossible to get mathematical solution for the above system. So we are going to introduce in the next two section two approaches to overcome these difficulties, of course, under reasonable hypotheses.

2.4 Preliminaries considerations and some hypotheses

In this subsection, we are beginning by introducing some experimental laws and setting hypothesis. Mainly we introduce laws of the behaviors of the density ρ_s and the effective porosity.

Remark 2. *i-* $\rho_s = \rho_s(T, p, W)$. *For our study we suppose that* ρ_s *satisfy the relation*

$$\rho_s = \rho_0 \exp(\beta_T(T - T_0) + \beta_p(p - p_0) + \gamma W)$$

here β_T, β_p *et* γ *are constants ;* p *designates the pressure of the fluid,* T *the temperature and* W *the concentration.* $\rho_0 = \rho(T_0, p_0, 0)$ *is a reference density;* T_0 *and* p_0 *are respectively the reference temperature and the reference pressure. This expression is used in engineering science see for instance [9].*

ii- The porosity ε *of the medium can be given by many laws. We can quote [12]*

1. *The Garner law(1958) given by*

$$\varepsilon = \frac{\varepsilon_s - \varepsilon_r}{1 + (\alpha h)^\beta} + \varepsilon_r \qquad for \quad h \leq 0$$

$$\varepsilon = \varepsilon_s \qquad for \quad h > 0$$

2. *The Brooks and Correy law (1964) where*

$$\varepsilon = (\varepsilon_s - \varepsilon_r)(\frac{h}{h_0})^\beta + \varepsilon_r \qquad for \quad h \le h_l$$

$$\varepsilon = a.h^5 + bh^4 + \varepsilon_s \qquad for \quad h_l < h \le 0$$

$$\varepsilon = \varepsilon_s \qquad for \quad h > 0$$

3. *The Van Genuchten law (1980) where*

$$\varepsilon = (\varepsilon_s - \varepsilon_r)(1 + (\alpha h)^\beta)^\tau + \varepsilon_r \qquad for \quad h \le 0$$

$$\varepsilon = \varepsilon_s \qquad for \quad h > 0$$

with $\tau = 1 - 1/\beta$.

h is the pressure measured relatively at the atmospheric pressure and expressed in columns of water.

To fix the idea we will use the Van Genuchten law for our model.
Solving these equations in the porous medium is very difficult. To overcome these difficulties, we do the following hypothesis to get some simplification.

- **H-4** ρ_s is a constant.

Replacing q by its expression in the first equation of (3) we obtain the expansion of the divergence

$$\frac{\partial}{\partial t}\varepsilon - div(\frac{K}{\mu}\nabla p) - \rho_s g div(\frac{K}{\mu}e_3) = 0 \quad \text{in} \quad]0,1[\times\Omega \tag{4}$$

Replacing q and J by their expressions in the second equation (3) and after simplifications we have

$$\frac{\partial}{\partial t}(\varepsilon W) - div(W\frac{K}{\mu}\nabla p) - \rho_s g div(\frac{K}{\mu}W e_3) - div(D\nabla W) = 0 \quad \text{in} \quad]0,1[\times\Omega \tag{5}$$

- **H-5** The hydraulic conductivity tensor is a constant positive: $(\frac{K}{\mu} = \beta I_3, \beta > 0)$ and D is a constant positive $(D = aI_3, a > 0.)$
  Using the hypothesis (**H-5**) the equations (4) and (5) become respectively

$$\frac{\partial \varepsilon}{\partial t} - \frac{K}{\mu}\Delta p = 0 \quad \text{in} \quad]0,1[\times\Omega \tag{6}$$

and

$$\frac{\partial}{\partial t}(\varepsilon W) - \frac{K}{\mu}div(W\nabla p) - \rho_s g\frac{K}{\mu}\frac{\partial W}{\partial z} - a\Delta W = 0 \quad \text{in }]0,1[\times\Omega \tag{7}$$

Using the equation (6), the equation (7) becomes

$$\varepsilon\frac{\partial}{\partial t}W - \frac{K}{\mu}\nabla W\nabla p - \rho_s g\frac{K}{\mu}\frac{\partial W}{\partial z} - a\Delta W = 0 \quad \text{in} \quad]0,1[\times\Omega \tag{8}$$

To the equations (6) and (8) we are going to add boundaries conditions adapted to pollution in porous medium. We obtain finally some boundaries and initial value problems given by

$$\begin{cases} \frac{\partial\varepsilon}{\partial t} - \beta\Delta p = 0 & \text{in} \quad]0,1[\times\Omega \\ \varepsilon(0,x) = \varepsilon_0 & \text{in} \quad \Omega \\ \varepsilon = \varepsilon_1 & \text{on} \quad]0,1[\times\partial\Omega\setminus\Gamma_1 \\ \varepsilon = \varepsilon_s & \text{on} \quad]0,1[\times\Gamma_1 \end{cases} \tag{9}$$

and

$$\begin{cases} \varepsilon\frac{\partial W}{\partial t} - \frac{k}{\mu}\nabla W\nabla p - \frac{k}{\mu}\rho_s g\frac{\partial W}{\partial z} - D\Delta W = 0 & \text{in} \quad]0,1[\times\Omega \\ \frac{\partial W}{\partial n} = 0 & \text{on} \quad]0,1[\times\partial\Omega\setminus\Gamma_1 \\ W = V & \text{on} \quad]0,1[\times\Gamma_1 \\ W(0,x) = W_0 & \text{in} \quad \Omega \end{cases} \tag{10}$$

where $\Gamma_1 \subset \partial\Omega$

- **H-6** The evolution is isotherm.

Let us recall that by hypothesis (**H-4**) ρ_s is constant and is given by the expression

$$\rho_s = \rho_0 \exp[\beta_T(T - T_0) + \beta_p(p - p_0) + \gamma W]$$

Using hypothesis (**H-4**) we can find a relation between p the pressure and W the concentration:

$$\log \frac{\rho_s}{\rho_0} = \beta_p(p - p_0) + \gamma W.$$

then

$$p = p_0 + \frac{1}{\beta_p}[\log \frac{\rho_s}{\rho_0} - \gamma W]$$

We deduce

$$\nabla p = -\frac{\gamma}{\beta_p}\nabla W, \quad \textit{and} \quad \Delta p = -\frac{\gamma}{\beta_p}\Delta W$$

Remark 3. *In the particulary case of permanent evolution, applying the hypothesis (**H-4**)-(**H-6**) and replacing ∇p by its value in (9) and (10) we obtain:*

$$\begin{cases} -\Delta p \quad = \quad 0 \quad in \quad \Omega_1 \\ p = \frac{[(\frac{\varepsilon_1 - \varepsilon_r}{\varepsilon_s - \varepsilon_r})^{-\frac{1}{m}} - 1]^{\frac{1}{n}}}{\alpha} \quad on \quad \partial\Omega \setminus \Gamma_1 \\ p = 0 \quad on \quad \Gamma_1 \end{cases} \tag{11}$$

and

$$\begin{cases} \beta|\nabla W|^2 - \beta\rho_s g \frac{\partial W}{\partial z} - \frac{D_0}{\rho_0}\Delta W = 0 \quad in \quad \Omega \\ \frac{\partial W}{\partial n} = V \quad on \quad \partial\Omega\backslash\Gamma_1 \\ W = 0 \quad on \quad \Gamma_1 \end{cases} \tag{12}$$

Here, the boundary condition of (11) is obtained with the Van Genuchten law. This case was studied in [5].

In the follows, we will focus our effort on the two following cases:

1. the $\varepsilon \neq cte$ *and* $\frac{\partial \varepsilon(t,x)}{\partial t} \neq 0$

2. and the case $\varepsilon(t,x) = \varepsilon_0(x)$ and $\exists\ \alpha_0 > 0 : \ \varepsilon_0(x) > \alpha_0, \ \forall x \in \Omega$ then $\frac{\partial \varepsilon(t,x)}{\partial t} = 0$.

In the second case, it follows from the first equation of (9) that $\Delta p = 0 \Rightarrow \Delta W = 0$ and the system (9) writes $\Delta W = 0$ with adequate boundaries conditions.

The second equation of (10) becomes

$$\varepsilon_0 \frac{\partial W}{\partial t} + \frac{\kappa\gamma}{\mu\beta_p}|\nabla W|^2 - \frac{\kappa}{\mu}\rho_0 g \frac{\partial W}{\partial z} = 0$$

We can combine furthermore the systems (10) and (9), and we get

$$\left\{\begin{array}{lcll}\varepsilon_0\frac{\partial W}{\partial t}+\frac{\kappa\gamma}{\mu\beta_p}|\nabla W|^2-\frac{\kappa}{\mu}\rho_0 g\frac{\partial W}{\partial z}+\Delta W & = & 0 &]0,1[\times\Omega \\ \frac{\partial W}{\partial\nu}(0,x) & = & V_0(x) &]0,1[\times\partial\Omega\backslash\Gamma_1 \\ W(t,x) & = & 0 &]0,1[\times\Gamma_1 \\ W(0,x) & = & W(x) & \Omega\end{array}\right. \quad (13)$$

Without losing of generality in the arguments, we suppose that $\frac{\partial W}{\partial z}=0$. As $\Delta W=0$, we can add to the first equation of the above system ΔW and the system (13) writes

$$\left\{\begin{array}{lcll}\frac{\partial W}{\partial t}+\frac{\kappa\gamma}{\varepsilon_0\mu\beta_p}|\nabla W|^2+\frac{D}{\varepsilon_0}\Delta W & = & 0 &]0,1[\times\Omega \\ \frac{\partial W}{\partial\nu}(0,x) & = & V_0(x) &]0,1[\times\partial\Omega\backslash\Gamma_1 \\ W(t,x) & = & 0 &]0,1[\times\Gamma_1 \\ W(0,x) & = & W(x) & \Omega\end{array}\right. \quad (14)$$

In the first case, replacing Δp by $-\frac{\gamma}{\beta_p}\Delta W$, the system (9) writes

$$\left\{\begin{array}{l}\frac{\partial\varepsilon}{\partial t}+\frac{\beta\gamma}{\beta_p}\Delta W=0 \quad \text{in} \quad]0,1[\times\Omega \\ \varepsilon(0,x)=\varepsilon_0 \quad \text{in} \quad \Omega \\ \varepsilon=\varepsilon_1 \quad \text{on} \quad]0,1[\times\partial\Omega\setminus\Gamma_1 \\ \varepsilon=\varepsilon_s \quad \text{on} \quad]0,1[\times\Gamma_1\end{array}\right. \quad (15)$$

In order to solve (10), we suppose that there exists, $\alpha_0>0$ such that $\forall\,\varepsilon(t,x)\in\,]0,1[\times\Omega;\;\; \varepsilon(t,x)\geq\alpha_0>0$ and dividing the first equation of (10) by $\varepsilon(t,x)$, it writes

$$\frac{\partial W}{\partial t}=\frac{\kappa\gamma}{\mu\beta_p}\frac{1}{\varepsilon}|\nabla W|^2-\frac{D}{\varepsilon}\Delta W=0 \quad (16)$$

Setting $\varpi=\frac{\kappa\gamma}{\mu\beta_p}\frac{1}{\varepsilon}$, (14) writes

$$\left\{\begin{array}{lcll}\frac{\partial W}{\partial t}+\varpi(|\nabla W|^2-D\Delta W) & = & 0 &]0,1[\times\Omega \\ \frac{\partial W}{\partial\nu}(x,0) & = & V_0 &]0,1[\times\partial\Omega\backslash\Gamma_1 \\ W(x,t) & = & 0 &]0,1[\times\Gamma_1 \\ W(x,0) & = & W(x) & \Omega\end{array}\right. \quad (17)$$

3 Well posedness of the non linear problem

We give here a mathematical framework which allows us to solve non linear model. The same technique is used in [5, 10] in the stationary case.

Proposition 1. *Let $W(t,x)$ be the solution of (17), setting $u(t,x) := \phi(W(t,x))$, then $u(x,t)$ is the solution of the following partial differential equation,*

$$\left\{\begin{array}{ccccc} \frac{\partial u(t,x)}{\partial t} - \frac{D}{\varepsilon}\Delta u(t,x) & = & 0 & in &]0,1[\times\Omega \\ u(0,x) & = & u_0(x) & on & \Omega \\ \frac{\partial u(t,x)}{\partial \nu} & = & u_1(t,x) & on &]0,1[\times\partial\Omega \end{array}\right. \tag{18}$$

if $\psi(x)$ is a solution of the following ordinary differential equation.

$$\frac{\phi''(s)}{\phi'(s)} = -\frac{\varepsilon\, f(t,x)}{D} \tag{19}$$

Proof. Let $u(t,x) = \phi(W(t,x))$, then

$$\frac{\partial u}{\partial t} = \phi'(W)\frac{\partial W}{\partial t}, \quad \nabla u = \phi'(W)\nabla W, \quad \Delta u = \phi''(W)|\nabla W|^2 + \phi'(W)\Delta W.$$

$$\frac{\partial u}{\partial t} = \phi'(W)\frac{\partial W}{\partial t} = -\phi'(W)\left[f(t,x)|\nabla W|^2 - \frac{D}{\varepsilon}\Delta W\right]$$

$$\frac{\partial u}{\partial t} = -\phi'(W)f(t,x)|\nabla W|^2 + \frac{D}{\varepsilon}\phi'(W)\Delta W$$

$$\frac{\partial u}{\partial t} = -\phi'(W)f(t,x)|\nabla W|^2 + \frac{D}{\varepsilon}\Delta u - \frac{D}{\varepsilon}\phi''(W)|\nabla W|^2$$

$$\Longleftrightarrow \frac{\partial u}{\partial t} - \frac{D}{\varepsilon}\Delta u = -|\nabla W|^2\left[\phi'(W)f(t,x) + \frac{D}{\varepsilon}\phi''(W)\right]$$

It follows that $\frac{\partial u}{\partial t} - \frac{D}{\varepsilon}\Delta u = 0$ since ϕ solves the ordinary differential equation

$$\phi'(W)f(t,x) + \frac{D}{\varepsilon}\phi''(W) = 0 \tag{20}$$

In order to compute ϕ, let us suppose that the integral

$$\int_0^s \frac{\varepsilon f(t,s)}{D}d\sigma < \infty. \quad \forall\, t \ \in \ [0,1], \ \forall s > 0$$

and we set

$$K_s(t,x) = \int_0^s \frac{\varepsilon f(t,x)}{D}d\sigma = s\frac{\varepsilon f(t,x)}{D}$$

(20) implies

$$\int_0^s \frac{\phi''(\sigma)}{\phi'(\sigma)} ds = \ln |\phi'(\sigma)| \Big]_0^s = \ln \frac{\phi'(s)}{\phi'(0)} = -K_s(t,x) \tag{21}$$

It follows that $\phi'(s) = \alpha e^{-K_s(t,x)}$ where $\alpha = \pm\phi'(0)$.

$$\int_0^W \phi'(s) ds = \alpha \int_0^W e^{-K_s(t,x)} ds \ \Rightarrow \ \phi(W) - \phi(0) = \alpha \int_0^W e^{-K_s(t,x)} ds$$

Conversely, if ϕ is in the form (21) and $u(t,x)$ the solution of (18), the function $W(t,x) = \phi^{-1}(u(t,x))$ is solution of (17), see [5] for details. □

4 Topological optimization for the non permanent problem

For all $\varrho \geq 0$, we set $\Omega_\varrho = \Omega \backslash \omega_\varrho$ where $\omega_\varrho = x_0 + \varrho\omega$, $\omega \in \mathbb{R}^n$ in a reference domain and $Q_\varrho =]0,1[\times\Omega_\varrho$. The interior boundary of Q_ϱ is noted Σ_ϱ.

The topological optimization problem consists to minimize the function

$$J(u) = \int_Q |W_\varrho(x,t) - W_d(x,t)|^2 dx \tag{22}$$

where W_ϱ be solution of the problem in the perturbed domain: W_ϱ solves

$$\left\{ \begin{array}{ccccc} \frac{\partial W_\varrho}{\partial t} + |\nabla W_\varrho|^2 + \lambda \Delta W_\varrho & = & 0 & Q_\varrho \\ \Delta W_\varrho & = & 0 & Q_\varrho \\ \frac{\partial W_\varrho}{\partial \nu} & = & 0 &]0,1[\times\partial\Omega\backslash\Gamma_1 \\ W_\varrho(0,x) & = & V_0(x) & \Omega \\ W_\varrho & = & 0 & \Sigma_\varrho \\ W_\varrho(0,x) & = & W_0(x) & \Omega \end{array} \right. \tag{23}$$

and $W_d(t,x)$ is a target function.

In order to get a linearized problem (23), let us consider the same change of variable as in the above section, $u_\varrho = \phi(W_\varrho)$. The system (23) becomes

$$\left\{\begin{array}{rclcc} \frac{\partial u_\varrho}{\partial t} - \Delta u_\varrho & = & 0 & in & Q_\varrho \\ \frac{\partial u_\varrho(t,x)}{\partial \nu} & = & 0 & on &]0,1[\times\partial\Omega\backslash\Gamma_1 \\ u_\varrho(0,x) & = & u_0(x) & on & \Gamma_1 \\ u_\varrho(t,x) & = & 0 & on & \Sigma_\varrho \\ u_\varrho(0,x) & = & u_1(x) & in & \Omega \end{array}\right. . \tag{24}$$

Then the topological optimization problem consists now to get the asymptotic expansion of the functional

$$J_\varrho(u_\varrho) = \int_\Omega |\phi^{-1}(u_\varrho(t,x) - \phi^{-1}(u_d(t,x)|dx \tag{25}$$

where $u_\varrho = \phi(W_\varrho)$ is the solution of (24) and $u_d = \phi(W)$.

The result which gives the existence, the uniqueness and the regularity of u_ϱ is standard partial differential equations theory, for the proof, see for instance [1] and [3].

Theorem 4.1. *Let $u_0(x) \in L^2(\Omega)$ and $u_1(x) \in L^2(\Omega)$, then there exists a unique solution $u_\varrho(t,x)$ of (24) and:*

$$u_\varrho \in \mathcal{C}([0,\infty[, L^2(\Omega_\varrho)) \cap \mathcal{C}([0,\infty[; H^2(\Omega_\varrho) \cap H_0^1(\Omega_\varrho)) \cap \mathcal{C}^1(]0,\infty[, L^2(\Omega_\varrho)). \tag{26}$$

More ever,

$$u_\varrho \in L^2(0,\infty; H_0^1) \cap \mathcal{C}(\overline{\Omega_\varrho} \times [\delta,\infty[), \ \ \forall \ \ \delta > 0 \tag{27}$$

and

$$\frac{1}{2}\|u_\varrho(1)\|^2_{L^2(\Omega_\varrho)} + \int_0^1 \|\nabla u_\varrho(t)\|^2_{L^2(\Omega_\varrho)} = \|u_0\|^2_{L^2(\Omega_\varrho)} + \|u_1\|^2_{L^2(\Omega_\varrho)}. \tag{28}$$

And the associated problem posed on the non perturbed domain has a unique solution u which satisfies:

$$u \in \mathcal{C}([0,\infty[, L^2(\Omega)) \cap \mathcal{C}([0,\infty[; H^2(\Omega) \cap H_0^1(\Omega)) \cap \mathcal{C}^1(]0,\infty[, L^2(\Omega)). \tag{29}$$

More ever,

$$u \in L^2(0,\infty; H_0^1) \cap \mathcal{C}(\overline{\Omega} \times [\delta,\infty[), \ \ \forall \ \ \delta > 0 \tag{30}$$

and

$$\frac{1}{2}\|u(1)\|^2_{L^2(\Omega)} + \int_0^1 \|\nabla u(t)\|^2_{L^2(\Omega)} = \|u_0\|^2_{L^2(\Omega)} + \|u_1\|^2_{L^2(\Omega)}. \tag{31}$$

In order to get the topological derivative of (22) we have to prove the following result.

Theorem 4.2. *Let u_ϱ be solution of (24) and u a solution of the associated problem posed on the non perturbed domain, then there exists a function* $f(\varrho) > 0$, $\lim_{\varrho\to 0} = 0$ *such that*

$$\|u_\varrho(t) - u(t)\|_{L^2(\Omega)} = o(f(\varrho)) \tag{32}$$

Proof. Without lost the generality, we suppose that $\Gamma_s = \emptyset$. Let $u_\varrho(t,x)$ and $u(t,x)$ be solution of

$$\left\{\begin{array}{rclcc} u_t(t,x) - \Delta u(t,x) & = & 0 & in &]0,1[\times\Omega \\ u(t,x) & = & 0 & on &]0,1[\times\partial\Omega\backslash\Gamma_1 \\ u(0,x) & = & u_0(x) & on & \Omega \\ \frac{\partial u(0,x)}{\partial\nu} & = & u_1(x) & in & \Omega\times \end{array}\right. \tag{33}$$

$$\left\{\begin{array}{rclcc} \frac{\partial u_\varrho(t,x)}{\partial t} - \Delta u_\varrho & = & 0 & in & Q_\varrho \\ \frac{\partial u_\varrho(t,x)}{\partial\nu} & = & 0 & on &]0,1[\times\partial\Omega\backslash\Gamma_1 \\ u_\varrho(0,x) & = & u_0(x) & on & \times\Omega \\ u_\varrho(t,x) & = & 0 & on & \Sigma_\varrho \\ u_\varrho(0,x) & = & u_1(x) & in & \Omega \end{array}\right. \tag{34}$$

In order to prove the theorem, we will use homogenization method.

Let

$$A^\varrho(x) = \chi^\varrho_{\Omega_\varrho}(x) = \left\{\begin{array}{c} 1\, if \;\; x \;\in \Omega\backslash\omega_\varrho \\ 0 \;\; if \; x \;\in \omega_\varrho \end{array}\right.$$

It is evident if $\varrho \longmapsto 0$, $A^\varrho \longrightarrow A^0 = \mathbb{I}_\Omega(x)$, the systems (33) and (34) write

$$\left\{\begin{array}{rclcc} u_t(t,x) - div(A^0(x)\nabla u(t,x)) & = & 0 & in &]0,1[\times\Omega \\ u(0,x) & = & u_0(x) & on & \Omega \\ \frac{\partial u(0,x)}{\partial\nu} & = & u_1(x) & in & \Omega \end{array}\right. \tag{35}$$

which variational formulation is

$$\left\{\begin{array}{c} Find\; u \in \mathcal{W}\; such\; that \\ \left\langle \frac{\partial u(t)}{\partial t}, v \right\rangle_{H^{-1}(\Omega), H^1_0(\Omega)} + \int_\Omega A^0(x)\nabla u(t,x)\nabla v(x)dx = 0 \\ in\mathcal{D}'(\Omega),\; \forall v \in H^1_0(\Omega) \\ \frac{\partial u(0,x)}{\partial\nu} = u_1(x), \quad u(0,x) = u_0(x) \end{array}\right. \tag{36}$$

$$\left\{\begin{array}{rcll} \frac{\partial u_\varrho(t,x)}{\partial t} - div(A^\varrho(x)\nabla u_\varrho) & = & 0 & in \quad Q_\varrho \\ u_\varrho(0,x) & = & u_0(x) & on \quad \Omega \\ u_\varrho(t,x) & = & 0 & on \quad \Sigma_\varrho \\ u_\varrho(0,x) & = & u_1(x) & in \quad \times\Omega \end{array}\right. \tag{37}$$

which variational formulation is

$$\left\{\begin{array}{c} Find\ u_\varrho \in \mathcal{W}\ such\ that \\ \left\langle \frac{\partial u_\varrho(t)}{\partial t}, v\right\rangle_{H^{-1}(\Omega),H_0^1(\Omega)} + \int_\Omega A^\varrho(x)\nabla u_\varrho(t,x)\nabla v(x)dx = 0 \\ in\mathcal{D}'(\Omega),\ \forall v \in H_0^1(\Omega) \\ \frac{\partial u_\varrho(0,x)}{\partial \nu} = u_1(x), \quad u_\varrho(0,x) = u_0(x) \end{array}\right. \tag{38}$$

Then we use the result below to conclude □

Theorem 4.3 (Theorem 11.4 of [3]). *Let u_ϱ be the solution of (36) and A^ϱ be defined as above, then the following convergence hold*

$$\left\{\begin{array}{l} i)\ \ u_\varrho \rightharpoonup u \ \ weakly\ \in L^2(\Omega, \\ ii)\ \ A^\varrho\nabla u_\varrho \rightharpoonup \ A^0\nabla u \quad weakly\ \in (L^2(Q))^n \end{array}\right. \tag{39}$$

where u is the solution of (35) and $f(\varrho)$ is given by:

Boundary condition in the hole	$f(\varrho)$	$g(x,t)$
Neumann 2D	$\pi\varrho$	$-2\nabla u(x,t).\nabla v_0(x,t)$
Neumann 3D	$\frac{4}{3}\pi\varrho^3$	$-\frac{3}{2}\nabla u(x,t)\nabla v_0(x,t)$
Dirichlet 2D	$\frac{-2\pi}{log(\varrho)}$	$u(x,t)v_0(x,t)$
Dirichlet 3D	$4\pi\varrho$	$u(x,t)v_0(x,t)$

4.1 Main Result

In this subsection, we use topological optimization tools in order to get the asymptotic expansion of the cost function $J_\varrho(u_\varrho(x,t))$ which is the main result of this section. But we will not focus on the details of theses tools. The reader interested to this tools can refer to [7],[5].

Theorem 4.4. *Let $j(\varrho) = J_\varrho(u_\varrho)$ be given by (25), where $u_\varrho(x,t)$ is solution of (24). Let v_0 be solution of the adjoint problem which weak formulation writes*

$$a_\varrho(v_0,\xi) = -DJ(u)\xi, \quad \forall\ \xi\ \in\ \mathcal{V}$$

where DJ is the derivative of J which respect J and $a(.,.)$ be the weak formulation associated to (13). The J has the following asymptotic expansion

$$J(\varrho) = J(0) + f(\varrho)(\delta_a(u, v_0) + \delta_J(v_0)) + o(f(\varrho))$$

4.1.1 Variation of the cost function

Proposition 2. *Let $J_\varrho(u_\varrho(x,t))$ the functional defined by (25), the J admits the following development:*

$$J_\varrho(u_\varrho) - J(u) = 2\int_Q \langle u - u_\varrho, u_d\rangle dx + f(\varrho)\delta_J + o(f(\varrho)) \tag{40}$$

Proof.

$$J_\varrho(u_\varrho) - J(u) = \int_{Q_\varrho} |u_\varrho - u_d|^2 dx - \int_Q |u - u_d||^2 dx$$

$$= \int_Q \left[|u_\varrho - u_d|^2 - |u - u_d|^2\right] dx - \int_{\Sigma_\varrho} |u - u_d|^2 d\gamma$$

$$= \underbrace{\int_Q |u_\varrho|^2 dx}_{E^\varrho(u_\varrho)} - \underbrace{\int_Q |u|^2 dx}_{E(u)} - 2\int_Q \langle u - u_\varrho, u_d\rangle dx$$

$$- \int_{\Sigma_\varrho} |u - u_d|^2 d\gamma$$

The proof of (40) reduces to prove that $\|E^\varrho(u_\varrho) - E^0(u)\| = o(f(\varrho))$, because, it is well know that $\int_{\Sigma_\varrho} |u - u_d|^2 d\gamma = o(f(\varrho))$, see [11]. Then we conclude by using the following result, which proof can be found in [3]. □

Proposition 3. *Let $E(u_\varrho)$ and $E(u)$ be the energies associated to the systems (37) and (39), then the following estimate holds*

$$\|E^\varrho(u_\varrho) - E^0(u)\|_\mathcal{V} = o(f(\varrho))$$

5 Numerical Results

In the numerical results, we set $\epsilon = 1,\ \theta(x) = 1$ so that,

$$\phi'(x) = e^{-xf(t,x)} \quad \Longrightarrow \quad \psi(t,x) = -\frac{1}{f(t,x)} e^{-xf(t,x)}$$

Thus, we solve numerically

$$\begin{cases} \frac{\partial u(t,x)}{\partial t} - \frac{D}{\epsilon} \Delta u(t,x) & = & 0 & in]0,1[\times \Omega \\ \frac{\partial u(0,x)}{\partial \nu} & = & u_0(x) & in \Omega \\ u(0,x) & = & u_1(x) & in \Omega \end{cases} \tag{41}$$

It follows that

$$W(t,x) = \phi^{-1}(u(t,x)) = -\frac{1}{f(t,x)} \log(-u(t,x) f(t,x)) \tag{42}$$

Remark 4. *As* $\int_{\Sigma_\varrho} |u - u_d|^2 d\gamma = o(f(\varrho))$, *il follows that* $\delta_J = 0$. *When* $\omega = B(0,1)$, $\delta_a(u,v) = 2\pi u(t,x) v_0(t,x)$, *il follows that the topological derivative is given by*

$$g(t,x_0) = 2\pi u(t,x_0) v_0(t,x_0); \quad \forall\ (t,x_0) \in (0,1) \times \Omega.$$

Example 1: here, we impose homogeneous Dirichlet boundary condition ($u(0, x) = 0$ *on* $\partial\Omega$)

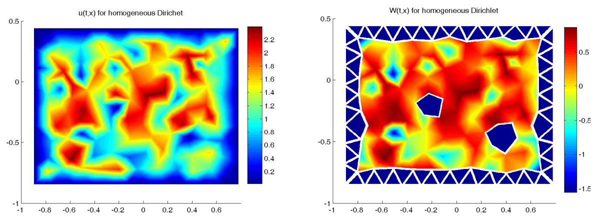

Figure 2: Left: Left: $u(x, t)$, Right: $W(x, t)$

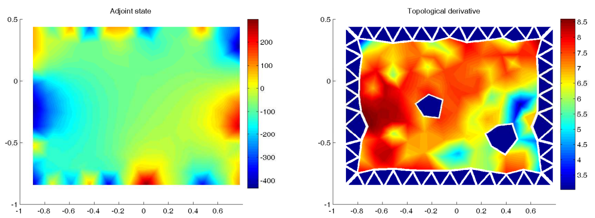

Figure 3: Left: $u(x, t)$ Adjoint state, Right: Topological derivative

Example 2: here, we impose non homogeneous Dirichlet boundary condition ($u(0, x) = 1$ *on* $\partial\Omega$)

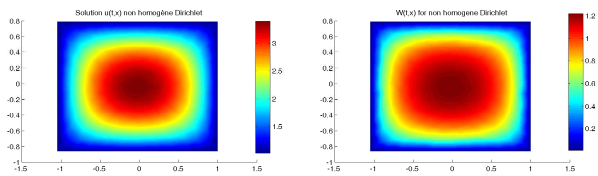

Figure 4: Left: $u(x, t)$, Right: $W(x, t)$

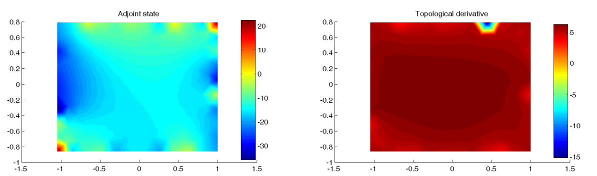

Figure 5: Left: $u(x, t)$ Adjoint state, Right: Topological derivative

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