REVISTA MATEMÁTICA COMPLUTENSE
Volumen 11, número 2: 1998

Optimal control of fluid flow in soil 1. deterministic case.

Youcef KELANEMER

*In memory of Professor Ulrich Hornung**

Abstract

We study the numerical aspect of the optimal control of problems governed by a linear elliptic partial differential equation (PDE). We consider here the gas flow in porous media. The observed variable is the flow field we want to maximize in a given part of the domain or its boundary. The control variable is the pressure at one part of the boundary or the discharges of some wells located in the interior of the domain. The objective functional is a balance between the norm of the flux in the observation region and the costs due to the control variables. We consider several geometric configurations of the control and the observation variables, and we make use of different objective functionals. We take advantage of the linearity of the flux w.r.t. the control variable to significantly reduce the computational effort and to deduce the optimal controls of wide class of objective functionals. In this paper we consider the deterministic case where the model parameters are given in the whole domain.

1 Introduction

Stationary fluid transport in porous media and heat transfer in conducting materials are governed by a well-known second order elliptic

*Professor Ulrich Hornung was of a big help to this work.

Mathematics Subject Classification: 49J20, 35J25, 35Q35.
Servicio Publicaciones Univ. Complutense. Madrid, 1998.

differential equation [Bea79]. In general, this equation is the combination of the mass conservation and Darcy laws for the mass transfer, or the energy conservation and Fourier laws for the heat transfer. In this paper we will refer to the gas flow in porous media, but the study and the results are directly applicable to other problems like water transport and heat transfer. The model is two-dimensional and results from a vertical averaging. Together with appropriate boundary conditions which are in our case the Dirichlet boundary condition on one part and the Neumann one on the other part, the boundary value problem (BVP) of gas transfer can be written as

$$\begin{cases} -\nabla \cdot (K \nabla y) & = f, \quad x \in \Omega \\ y & = g, \quad x \in \Gamma_D \\ q_\nu & = h, \quad x \in \Gamma_N. \end{cases} \tag{1}$$

Here K is a strictly positive-bounded function in the bounded domain $\Omega \subset \mathbb{R}^2$ and called transmissivity. We assume that there are two constants c_1 and c_2, such that $0 < c_1 \leq K \leq c_2 < \infty$. The functions f and the boundary data g and h are given. The flux $q = -K\nabla y$ is the gas velocity in the medium and the quantity $q_\nu = q \cdot \nu$ is the flux in the outer normal direction on Γ. The *state* variable y is for the compressible gas the square of the air pressure.

When dealing with soil remediation, several strategies are used. The one we consider here is the soil venting. Pump and treat (PAT) technique, which consists of extracting air using pumps located in a contaminated soil and treat it with filters, has widely been used [RM94], [Bru91] and [NG91]. The pumps are called wells and are sources when they introduce air in the domain and sinks when they extract the air out of it. The air movement induces a convection which removes the diluted pollutant to the exterior part of the contaminated porous media. Instead of introducing or extracting air using some wells in the domain, other applications need to do this from the boundary.

2 The Optimization Problem

The procedure of air pumping is very costly and the remediation takes many years. Therefore the optimization of the soil venting technique is very important. When we observe this technique, we see that the discharges of the pumps or the under-pressures produced at some places are the mean control variables. The cost and the result of the remediation depend strongly on them. Designing cost-effective and reliable remediation schemes is a difficult task. In groundwater quality management, Wagner and Gorelick [WG87] [WG89] and Gorelick [Gor90] minimize the discharges of some wells subject to a reduction of contaminant concentration to acceptable level. In soil venting one would maximize the extracted contaminant subject to some constraints on the discharges. Both problems are rather complicated: multiphase and multicomponent transport governing laws are not obvious and the big number of unknown parameters make the prediction and the optimization hard tasks. Therefore, a simplification of the problem is to reduce it to maximization of the air flow in the region of high volatilization.

Here we describe our optimal control problem.

1. The observation is the flux we want to maximize in one region of the domain or through one part of the boundary.

2. The control variable is the pressure prescribed on the boundary and represented by the Dirichlet condition or the discharges of the wells at some locations and represented by a source term of Dirac type. The control variable is notated here by u and belongs to the space $\mathbb{R}^n$.

3. The objective functional called J, is a balance between the profit of the strategy, function of the norm of the flux in the interesting region, and the costs of this strategy, function of the norm of the control variable. We have to minimize the difference between the costs and the profits.

4. Due to technical and physical reasons, the optimization is subject to some constraints. The equipment works under restrictions and the change rate in pollutant phase is too small, such that a moderate air pumping will remove almost as much pollutant as will do a strong one. Nevertheless, large discharges u will give high values for J and avoid the explicite use of the constraints in many cases.

In this paper we study three optimal control problems which correspond to three different configurations, namely:

1. Boundary observation and Dirichlet boundary condition control variable. We look for the Dirichlet condition on one part of the boundary which produces the "best" flux observed on another part of it. In this first part we study the maximization of the flux through different segments on the right side of the unit square. We will see that due to the diffusion and the geometrical considerations, the effect of the control variable on the observation may be small.

2. Distributed observation and Dirichlet boundary condition control variable. The only difference between this second problem and the first one is that the flux is observed in one region of the domain instead of one part of the boundary. The control variable is still the Dirichlet boundary condition. In opposite to the first formulation, when the region of the observation is located near the control variable, we see that the optimization makes sense and the solution is not always the more intuitive one.

3. Distributed observation and the discharges of Dirac type sources control variable. In the third problem we change the nature and the locations of the control variable. We also optimize the discharges of some wells located inside the domain in order to produce a strong flux in a given region. This third formulation makes one more step than the second one. Then it is clear that the optimization of the discharges when combined with optimization of the positions must produce the "best" "optimal" of all. The last step, namely the optimization of the positions, is still to be done in future work.

2.1 Boundary Observation and Dirichlet Condition Control

We study a typical problem where the control variables u_j are the pressures generated at some part of the boundary of a remediation site Ω, and the cost functional $J(u)$ simultaneously measures the normal flux (using Φ in equation (3)) that is produced at some other part of the boundary and also the costs (using Ψ in equation (3)) that are caused when generating the pressures u_j. In principle, such a problem is in the

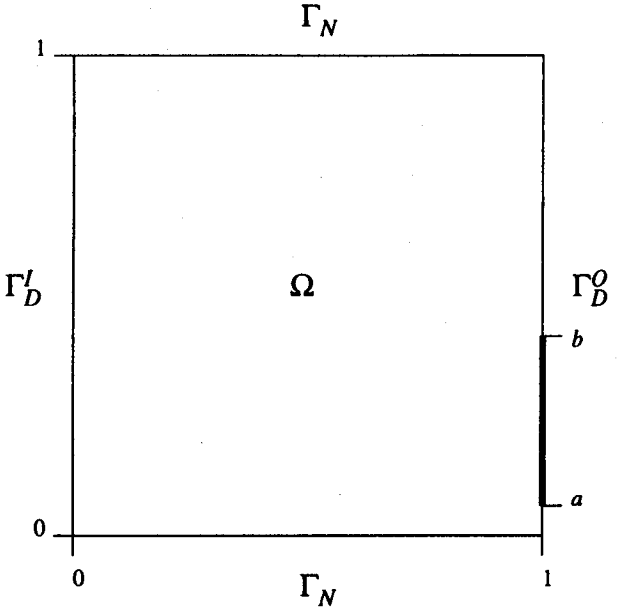

Figure 1: The domain, the boundary types and the observation segment (a, b)

framework of a well-known theory for optimal control of partial differential equations [Lio71]. We consider an elliptic boundary value problem of the form

$$\begin{cases} -\nabla \cdot (K \nabla y) & = f, \quad & x \in \Omega \\ y & = g + Bu, \quad & x \in \Gamma_D \\ q_\nu & = h, \quad & x \in \Gamma_N. \end{cases} \tag{2}$$

Here K is a strictly positive-bounded function in the bounded domain $\Omega \subset \mathbb{R}^2$ the piecewise smooth boundary of which $\Gamma = \Gamma_D \cup \Gamma_N$ with $\Gamma_D \cap \Gamma_N = \emptyset$ as shown in Figure 1. The *state* variable is $y(u)$, and the *control* variable is $u \in U$. The operator $B : U \to H^{1/2}(\Gamma)$ is assumed to be linear from the Hilbert-space U into $H^{1/2}(\Gamma)$. Its adjoint $B^* : H^{-1/2}(\Gamma) \to U$ is given by

$$\langle B^* r, v \rangle = \langle r, Bv \rangle \; \forall r \in H^{-1/2}(\Gamma), \; v \in U.$$

The *cost functional* is chosen as

$$\boxed{J(u) = \int_{\Gamma_D} \Phi(q_\nu(y(u))\mu)\ d\Gamma + \Psi(u)} \tag{3}$$

where Φ is a differentiable convex function on $\boldsymbol{R}$, $\mu \in L^\infty(\Gamma)$ is a weight function on Γ, and Ψ is a differentiable convex functional on U.

Adjoint problem. We introduce the *adjoint* variable p as the solution of the elliptic problem

$$\begin{cases} -\nabla\cdot(K\nabla p(u)) & = 0, & x\in\Omega \\ p(u) & = \Phi'(q_\nu(y(u))\mu)\mu, & x\in\Gamma_D \\ r_\nu & = 0, & x\in\Gamma_N \end{cases}$$

where $r_\nu = -\nu\cdot K\nabla p(u)$ is the normal boundary flux belonging to the adjoint p. The interest of the adjoint state p consists of simplifying the integral in the functional J. We get the following lemma.

Lemma 2.1. *The differential of the cost functional J is given by*

$$\boxed{\partial_u J(u) = B^* r_\nu(p(u)) + \partial_u\Psi(u).} \tag{4}$$

Proof. Following the methodology of Lions [Lio71], chapter II.4, we get

$$\begin{aligned}\langle\partial_u J(u), v-u\rangle &= \int_{\Gamma_D}\Phi'(q_\nu(y(u))\mu)(q_\nu(y(v)) \\ &- q_\nu(y(u)))\mu\ d\Gamma + \langle\partial_u\Psi(u), v-u\rangle\end{aligned}$$

for any $v\in U$. Green's formula gives

$$\int_\Omega \nabla\cdot(K\nabla p(u))(y(v)-y(u))\ d\Omega - \int_\Gamma \nu\cdot K\nabla p(u)(y(v)-y(u))\ d\Gamma$$

$$= \int_\Omega \nabla\cdot(K\nabla(y(v)-y(u))p(u)\ d\Omega - \int_\Gamma \nu\cdot K\nabla(y(v)-y(u))p(u)\ d\Gamma.$$

Since

$$\nabla\cdot(K\nabla p(u)) = 0 \text{ in } \Omega,$$

$$y(v)-y(u) = Bv - Bu \text{ on } \Gamma_D,$$

$$r_\nu = 0 \text{ on } \Gamma_N,$$

$$\nabla \cdot (K\nabla(y(v) - y(u)) = 0 \text{ on } \Omega,$$

and

$$q_\nu(y(v)) - q_\nu(y(u)) = 0 \text{ on } \Gamma_N,$$

we get

$$\int_{\Gamma_D} p(u)(q_\nu(y(v)) - q_\nu(y(u)))\, d\Gamma = \int_{\Gamma_D} r_\nu B(v-u)\, d\Gamma,$$

and from this we obtain

$$\langle \partial_u J(u), v-u \rangle = \langle B^* r_\nu, v-u \rangle + \langle \partial_u \Psi(u), v-u \rangle$$

and thus the conclusion. Q.E.D.

Equation (4) gives a theoretical tool to compute the functional J. In discrete form, one can compute the images $B^* r_\nu$ and then the cost functional for the basis vectors. Therefore the quadratic functional J can be expressed in matrix form with the dimension of the control variable.

2.1.1 Finite Element Discretization of the PDE

In this paper the domain Ω is taken to be the unit square in $\mathbb{R}^2$. It is clear that in order to compute the state variable and the flux, problem (2) should be solved numerically. To discretize this elliptic problem, we make use of the mixed-hybrid finite element method (MHFEM). The original mixed method leads to an indefinite matrix, a difficulty which is overcome by hybridization using Lagrange multipliers. This method computes the state variable and flux simultaneously and has the advantage to conserve the mass balance cell by cell. For more details about the theoretical and numerical aspects of the MHFEM, the reader is invited to see [Tho77] and [BF91]. More details about the basis functions and methods of assembling the matrices can be found in [KH90]. It is to be mentioned that in this optimization formulations, the flux is a linear function with respect to the control variable and thus the elliptic PDE has to be solved for the basis vectors only. Also the domain is subdivided to a finite set of triangles. In our case the triangulation of the unit square is uniform and contains 3200 elements. This corresponds to a 40 segments in in each of the two directions and ensures the super-convergence of the discretization, i.e. the L^2-norm of the error in the pressure is of order the square of the edge size. We approximate the pressure by piecewise constant functions and the flux in the lowest order Raviart-Thomas space. The discret flux is therefore linear in each triangle and with continuous normal component across the inter-element boundaries (the edges). As mentioned before, we introduce Lagrange multipliers on the edges of the triangulation to make the solution of the linear system more convenient. This last one is done using conjugate gradient method, preconditioned by cholesky factorization.

Discrete Variational Formulation. We give here the discrete formulation which correspond to the MHFEM. We define

- $\mathcal{T}_h$ the regular triangulation of Ω. $\mathcal{T}_h$ is then the set of triangles which form by their union $\bar{\Omega}$ and satisfy the two following conditions
  - Conformity: Intersection of two different triangles is empty, one common edge or one common vertex.
  - Regularity: The minimal angle (taken over all triangles $\mathcal{T}$ in $\mathcal{T}_h$) is bounded from below by a strictly positive constant.
- $E_h = \bigcup_{\mathcal{T}\in\mathcal{T}_h} \partial\mathcal{T}$,
- $RT^0(\mathcal{T}) = \{(a + bx_1, c + bx_2), a, b, c \in \mathbb{R}\} \subset (P_1(\mathcal{T}))^2$, where $\mathcal{T} \in \mathcal{T}_h$, $P_1(\mathcal{T})$ is the four dimensional space of the linear functions in x_1 and x_2.
- $RT^0_{-1}(\mathcal{T}_h) = \{\phi \in (L^2(\Omega))^2, \phi_{|\mathcal{T}} \in RT_0(\mathcal{T}), \forall\mathcal{T} \in \mathcal{T}_h\}$,
- $M^0_{-1}(\mathcal{T}_h)$ the space of piecewise constant functions on $\mathcal{T}_h$ (constant on each element),
- $M^0_{-1}(E_h)$ the space of piecewise constant functions on E_h (constant on each edge),
- $M^0_{-1,D}(E_h) = \{\lambda \in M^0_{-1}(E_h) | \lambda = 0 \text{ on } \Gamma_D\}$.

The hybrid version of the lowest order Raviart-Thomas mixed method for problem (2) is given by: Find $(q, y, \lambda) \in RT^0_{-1}(\mathcal{T}_h) \times M^0_{-1}(\mathcal{T}_h) \times M^0_{-1,D}(E_h)$ such that

$$\begin{cases} \displaystyle\int_\Omega (K^{-1}q)\cdot v \\ \displaystyle\quad -\sum_{T\in\mathcal{T}_h}\left(\int_T y\nabla\cdot v - \int_{\partial T}\lambda v\cdot\nu_T\right) = -\int_{\Gamma_D}(g+Bu)v\cdot\nu & \forall v\in RT^0_{-1}(\mathcal{T}_h) \\ \displaystyle\int_\Omega \nabla\cdot q\psi = -\int_\Omega f\psi & \forall\psi\in M^0_{-1}(\mathcal{T}_h) \\ \displaystyle\sum_{T\in\mathcal{T}_h}\int_{\partial T}(q\cdot\nu_T)\mu = \int_{\Gamma_N} h\mu & \forall\mu\in M^0_{-1,D}(E_h) \end{cases} \tag{5}$$

for given control variable u and parameters g, f, and h. Let us choose the bases for the spaces $RT^0_{-1}(\mathcal{T}_h)$, $M^0_{-1}(\mathcal{T}_h)$ and $M^0_{-1,D}(E_h)$ as described in Kaasschieter and Huijben [KH90]. The discrete variational formulation (5) leads to a linear system of the form

$$\begin{cases} Aq \; +B^t y \; +L^t\lambda = G \\ Bq = F \\ Lq = H \end{cases} \tag{6}$$

Solving the Linear System (6). We want to determine the unknowns q, y, λ in (6). First, using the formal elimination, we compute λ, then y and at the end q. We describe briefly all steps (cf. Kaasschieter and Huijben [KH90]). Let us note that the matrix A is block diagonal. Each block is 3×3 and positive definite. Thus its inverse A^{-1} can be easily computed.

- Solve the system

  $$[L[Id_A - MB]A^{-1}L^t]\lambda = L[-MB + Id_A]A^{-1}G + LMF - H$$

  for λ, where $M = A^{-1}B^t[BA^{-1}B^t]^{-1}$. The matrix $L[Id_A - MB]A^{-1}L^t$ is sparse, symmetric, and positive definite. One can effectively solve it using a preconditioned conjugate gradient method.

- Solve the system

  $$[BA^{-1}B^t]y = (-F + BA^{-1}G - BA^{-1}L^t\lambda)$$

for y. Now $[BA^{-1}B^t]$ is a positive definite diagonal matrix which makes its inversion trivial.

- After getting λ and y solve

$$q = A^{-1}[G - B^t\, y - L^t\lambda]$$

for q.

2.1.2 Application

Now we specialize more and assume $\Gamma_D = \bar{\Gamma}_D^I \cup \bar{\Gamma}_D^O$ with $\Gamma_D^I \cap \Gamma_D^O = \emptyset$, as shown in Figure 1. Further, we assume $B(U) \subset H^{1/2}(\Gamma_D^I)$. Let $U = \mathbb{R}^k$, and $\Gamma_j \subset \Gamma_D^I$ pairwise disjoint open subsets, such that $\bar{\Gamma}_D^I = \bigcup_1^k \bar{\Gamma}_j$; for $u = (u_1, \ldots, u_k) \in U$ let $B(u)(x) = u_j$ whenever $x \in \Gamma_j$. In this case we get $(B^*r)_j = \langle r, 1_j \rangle$ for $r \in H^{-1/2}(\Gamma_D^I)$, where $1_j(x) = 1$ for $x \in \Gamma_j$ and $1_j(x) = 0$ for $x \in \Gamma_D^I \setminus \Gamma_j$. Let $\mu = 0$ on Γ_D^I. In addition, let $f = 0$, $g = 0$, and $h = 0$. For $\Phi(z) = z(z-\gamma)$, we get $\Phi'(z) = z - \gamma$. If $\psi(u) = \frac{\alpha}{\beta}\sum_j |u_j|^\beta$, we have $(\partial_u \psi(u))_j = \alpha u_j |u_j|^{\beta-2}$. The parameters α, β and γ are positive numbers. Finally, we take $\mu = 1$ on the segment (a, b) of Γ_D^O (Figure 1) and $\mu = 0$ otherwise. The support of μ is called the region of observation.

For an unconstrained control problem, i.e.

$$\inf_U J(u),$$

the necessary and sufficient optimality condition of first order is $\partial_u J(u) = 0$, i.e., $u = -B^* r_\nu(p(u))$. If we consider the case $\beta = 2$, then the problem is quadratic with respect to the control variable u, one efficient way of solving this numerically is the CG method. We have applied this technique to a problem in the unit square of $\mathbb{R}^2$; here Γ_D^I is the left vertical boundary, Γ_D^O is the right vertical boundary, and Γ_N consists of the two - lower and upper - horizontal boundaries.

Lemma 2.2. *For $\beta = 2$ and $\gamma \neq 0$, let $\theta \in \mathbb{R}$ and define the class of objective functionals*

$$J_\theta(u) = \int_{\Gamma_D} \Phi_\theta(q_\nu(y(u))\mu)\; d\Gamma + \Psi(u)$$

where $\Phi_\theta(z) = z(z - \theta\gamma)$. Then

- $J_\theta(\theta u) = \theta^2 J_1(u)$.
- *If* u *is the minimizer of* J_1*, then* θu *is the minimizer of* J_θ.
- *The minimizers of* J_θ*, for* $\theta \in \mathbb{R}$*, form one-dimensional vectorial space.*

Proof. For the proof one needs only the linearity of the flux q w.r.t. the control u. Q.E.D.

Though, the optimal problem does not use a fixed constraints, this simple lemma 2.2 is a flexible way to find the optimal control with the acceptable price or the suitable norm (see also lemma 2.5).

2.1.3 Results

In this application, we consider the quadratic case $\beta = 2$. Thus the minimizer exists and is unique. For $\gamma = 100$ and $\alpha = 0.01$ we try to

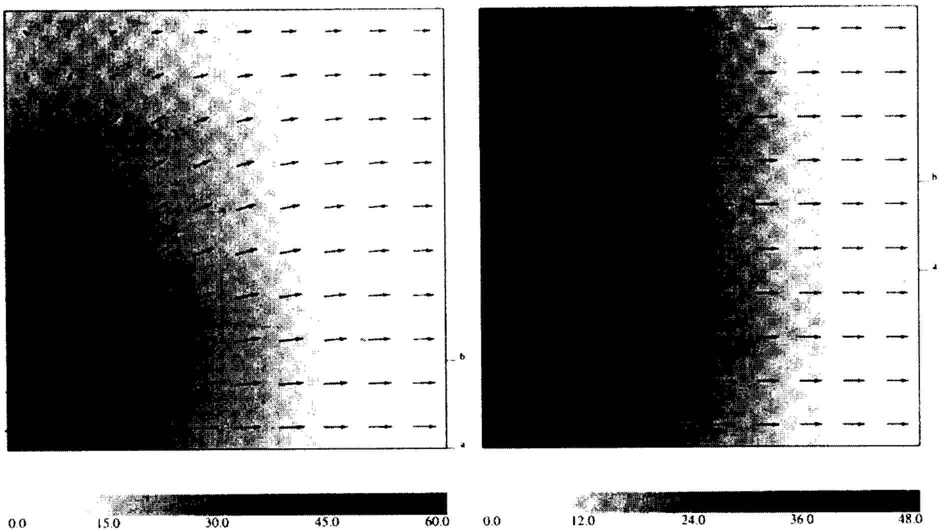

Figure 2: Optimal solution, state variable (gray) and flux (arrows): $\alpha = 0.01$, $\beta = 2$ and $\gamma = 100$, (left): $(a, b) = (0, 0.2)$, and (right): $(a, b) = (0.4, 0.6)$

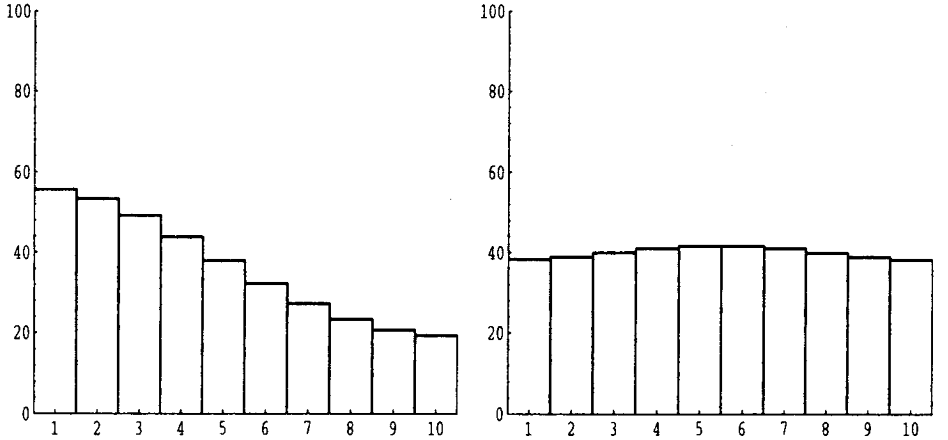

Figure 3: Optimal control, pressure on Γ_D^I :
$\alpha = 0.01$, $\beta = 2$ and $\gamma = 100$, (left): $(a, b) = (0, 0.2)$, and (right): $(a, b) = (0.4, 0.6)$

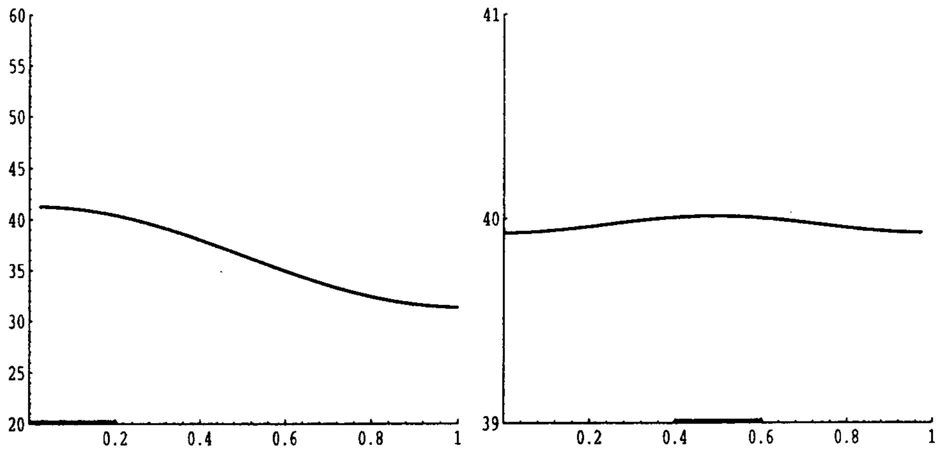

Figure 4: Optimal flux on the right boundary:
$\alpha = 0.01$, $\beta = 2$ and $\gamma = 100$, (left): $(a, b) = (0, 0.2)$, and (right): $(a, b) = (0.4, 0.6)$

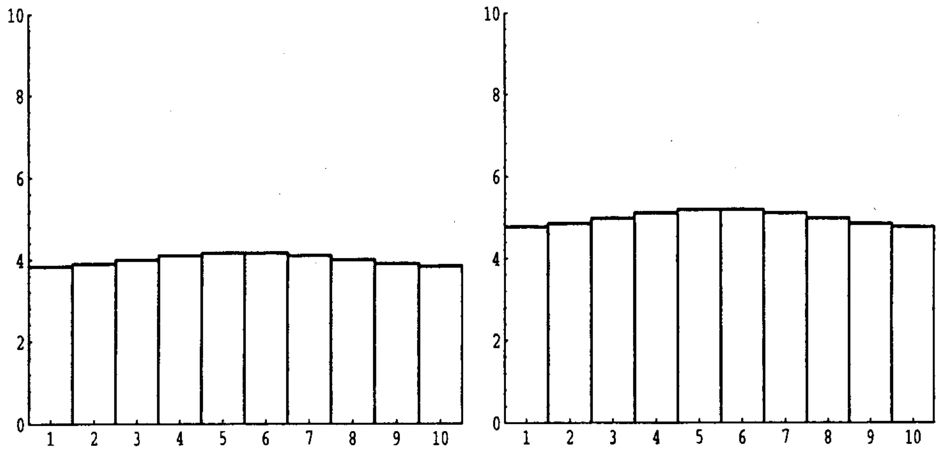

Figure 5: Optimal control, pressure on Γ_D^I :
$(a,b) = (0.4,\ 0.6)$, $\beta = 2$ and $\gamma = 10$, (left): $\alpha = 0.01$ and (right): $\alpha = 0.0001$

to maximize the flux through the segment $S_1 = 1 \times (0, 0.2)$ or $S_2 = 1 \times (0.4, 0.6)$. Figure 2 shows the state variable and the flow field for the case of S_1 and S_2. This variables correspond to the optimal control represented in Figure 3. The correspondent fluxes on Γ_D^O are shown in Figure 4. We do the same when the observation of the flux is done on the segment S_2. It is clear that the optimization in the case where the observation is on the segment S_1 is more meaningful than the case of S_2. This is due to two things: The first one is that the diffusion plays the role of dilution of the control effect. The second reason is that the segment S_1 lies down near the insulated side $(0, 1) \times 0$ which avoids the diffusion in the down direction. One can see in Figure 4 that the flux on Γ_D^O is almost uniform for the case of S_2 while for the case of S_1, the flux has a visible difference between the down and upper parts. We have tried to play with the parameters γ and α but the situation remained the same as shows Figure 5. We conclude this first part by the following remark.

Remark. In many field applications, the parameters of the flow model, namely K, f, g and h are not available. Neverthless, if the normal flux on the segment of observation can be measured when using the basis control variables, then the optimization is realizable.

2.2 Distributed Observation and Dirichlet Condition Control

2.2.1 Formulation

Now we consider an optimal control problem where the observation is distributed and the control variable is given as Dirichlet boundary condition. We consider an elliptic boundary value problem of the form

$$\begin{cases} \nabla \cdot q & = 0, & x \in \Omega \\ q & = -K\nabla y, & x \in \Omega \\ y & = Bu, & x \in \Gamma_D \\ q_\nu & = 0, & x \in \Gamma_N. \end{cases} \tag{7}$$

Here K is the previously defined transmissivity field in the bounded domain $\Omega \subset \mathbb{R}^2$ the smooth boundary of which is $\Gamma = \bar{\Gamma}_D \cup \bar{\Gamma}_N$ with $\Gamma_D \cap \Gamma_N = \emptyset$. The *control* variable is $u = (u_1, ..., u_n) \in \mathbb{R}^n$.

The *cost functional* is

$$J(u) = \int_\Omega \Phi(x, q(y(u)))\, d\Omega + \Psi(u), \tag{8}$$

where $\Phi(x, \cdot)$ is a differentiable functional on $\mathbb{R}^2$ and Ψ is a differentiable functional on $\mathbb{R}^n$. Here we take

$$\Phi(x, q) = -\frac{\mu(x)}{2}|q|^2 \text{ and } \Psi(u) = \frac{1}{\beta}\sum_j |u_j|^\beta \tag{9}$$

where $\mu \in L^\infty(\Omega)$ is a weight function on Ω and $\beta > 2$, a given real number.

What we want to find are minimizers of J, i.e., $u \in U_{ad} \subset \mathbb{R}^n$, such that

$$J(u) \leq J(v)\ \forall v \in U_{ad}.$$

Lemma 2.3. *For $\beta > 2$, one can deduce that*

1. ***Φ is quadratic functional of u,***

2. *the functional $J(u)$ is not quadratic and not convex but of regularity at least C^1,*

3. *$J(u) \to \infty$ when $|u| \to \infty$ i.e. $\forall\ A > 0$, $\exists M > 0$, such that, $|u| > M \ \Rightarrow J(u) > A$,*

4. *$J(0) = 0$ and $\partial_u J(0) = 0$,*

5. *$J(u) < 0$ for $|u|$ small enough and different of 0,*

Lemma 2.4. *Using lemma 2.3, we conclude that*

1. *J is bounded from below and has one global minimum, i.e. it exists (not necessarily unique) $u \in \mathbb{R}^n$, such that*
$$J(u) \leq J(v)\ \forall v \in \mathbb{R}^n,$$

2. *Since the functional J is of regularity at least C^1, we can say that it is convex near any minimizer u and satisfies the equation*
$$\partial_u J(u) = 0,$$
where
$$\langle \partial_u J(u), w\rangle = -\int_\Omega K\partial_q \Phi(x, q(y(u))) \cdot \nabla \bar{y}(w)\ d\Omega + \langle \partial_u \Psi(u), w\rangle$$
for all $w \in \mathbb{R}^n$.

Lemma 2.5. *Let u_0 be a global minimizer of J defined by (8) and (9) for $\beta > 2$ and $\mu \neq 0$. Define $\Phi_\theta(x,q) = -\theta\frac{\mu(x)}{2}|q|^2$ and $J_\theta(u) = \int\limits_\Omega \Phi_\theta(x, q(y(u)))\ d\Omega + \Psi(u)$ where $\theta \in \mathbb{R}_+$, then*

- *$\tilde{u} = \theta^{\frac{1}{\beta - 2}} u_0$ is a global minimizer of $J_\theta(u)$ and $J_\theta(\tilde{u}) = \theta^{\frac{\beta}{\beta - 2}} J(u_0)$*

Proof. We have $J_\theta(0) = 0$, $\partial_u J_\theta(0) = 0$ and q is linear w.r.t. u, therefore the lemma can be proved using substitutions only. Q.E.D.

This lemma which is similar to lemma 2.2 has also an important application: Increasing the weight function by a constant factor without modifying the costs of the control variable leads to a multiplication of the optimal solution by another factor.

2.2.2 Numerical Optimization

We propose here to apply the Newton method to find the variables u for which the gradient of the objective functional vanishes. This method is well adapted to this case because the Hessian matrix of J is easy to compute. The algorithm is well known but to make it easier and time-effectiver, we compute its tools as

1. Solve the state systems

$$\begin{cases} \nabla \cdot q_0 & = 0, & x \in \Omega \\ q_0 & = -K\nabla y_0, & x \in \Omega \\ y_0 & = 0, & x \in \Gamma_D \\ \nu \cdot q_0 & = 0, & x \in \Gamma_N \end{cases}$$

and for $j = 1, \ldots, n$

$$\begin{cases} \nabla \cdot q_j & = 0, & x \in \Omega \\ q_j & = -K\nabla y_j, & x \in \Omega \\ y_j & = Be_j, & x \in \Gamma_D \\ \nu \cdot q_j & = 0, & x \in \Gamma_N. \end{cases}$$

Determine the matrix

$$\mathcal{D}_{ij} = -\int_\Omega \mu(x) q_i \cdot q_j \, d\Omega, \tag{10}$$

the constant vector

$$b_j = -\int_\Omega \mu(x) q_0 \cdot q_j \, d\Omega, \tag{11}$$

and the constant real

$$c = -\int_\Omega \frac{\mu(x)}{2} |q_0|^2 \, d\Omega. \tag{12}$$

2. For a given $u = (u_j)_{j=1,\dots,n} \in \mathbb{R}^n$, one can compute the functional J, its differential $\partial_u J(u)$ and its Hessian $\mathcal{H}$ using the matrix $\mathcal{D}$, the vector b and the constant c given by (10), (11), and (12) without to make use of the fluxes; Using (17) and (18) we get the functional

$$J(u) = \frac{1}{2} u \cdot \mathcal{D}\, u + u \cdot b + c + \Psi(u) \tag{13}$$

the differential

$$\partial_u J(u) = \mathcal{D}\, u + b + \nabla\Psi(u) \tag{14}$$

and the Hessian

$$\mathcal{H}_{i\,j} = \begin{cases} \mathcal{D}_{i\,j} & \text{if} \quad i \neq j \\ \mathcal{D}_{i\,j} + \alpha(\beta - 1)|u_j|^{\beta-2} & \text{if} \quad i = j \end{cases} \tag{15}$$

Therefore it is not necessary to solve the PDE for each control variable in order to compute the Hessian matrix since all the information is stored in $\mathcal{D}$, b and c. At each iteration of the Newton method, one needs to update the term $\alpha(\beta - 1)|u_j|^{\beta-2}$ on the diagonal of the Hessian. In this case of non-quadratic functional, there exist in general more than one minimizer. The difficulty is that the Newton algorithm is a local search and depends on the initialization. To avoid that the solution given by the Newton algorithm is one maximizer or one saddle point, as the one given in Figure 7, we run the algorithm with some hundreds of random initial data. We have seen that most of the solutions to which the Newton method converges are the global minimizer or its opposite ($J(-u) = J(u)$). The dimension of the control variable is rather small (≤ 10). Thus the numerical solution of the linear system (the Hessian) can be done by many ways. We have chosed the LU-factorization.

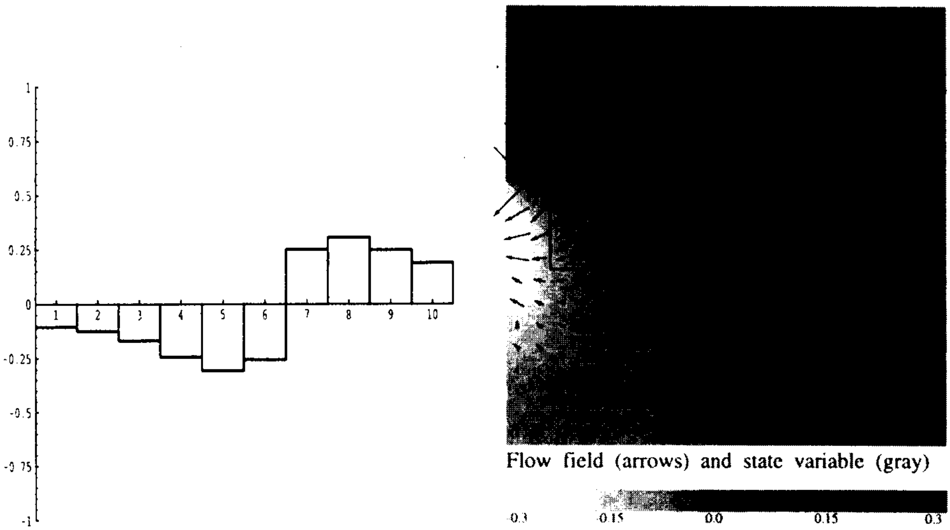

Figure 6: Optimal control, state variable and flux: Box = (0.1, 0.2) × (0.4, 0.8), $\beta = 4$

2.2.3 Application and Results

Figures 6, 9 and 10 represent the optimal solution (left), and the state variable and the flow field (right) with $\beta = 4$, $\beta = 8$ and $\beta = 2.5$, respectively. For these three cases we have optimized the flux in $\text{box}_1 = (0.1, 0.2) \times (0.4, 0.8)$. Also, $\mu = 1$ in box_1 and $\mu = 0$ outside it, except for the case $\beta = 2.5$. In this case when β is not much larger than 2, the minimizer becomes very small and in order to avoid this we make use of lemma 2.3 and we put $\mu = 10$ in box_1. The number of iterations depends on the initialization and the tolerated error on the solution. For a random initializations in $[-10, 10]^n$ and for stopping criterion for Newton algorithm of 10^{-10} the average number of iterations over 100 initializations (minimizations) is 12, 33, 60, 102, 160 and 151 for $\beta = 2.5$, 4, 6, 8, 10 and 12 respectively. One remark that the rate of convergence is highly related to the value of β. For $\beta = 2.5$, we are rather near

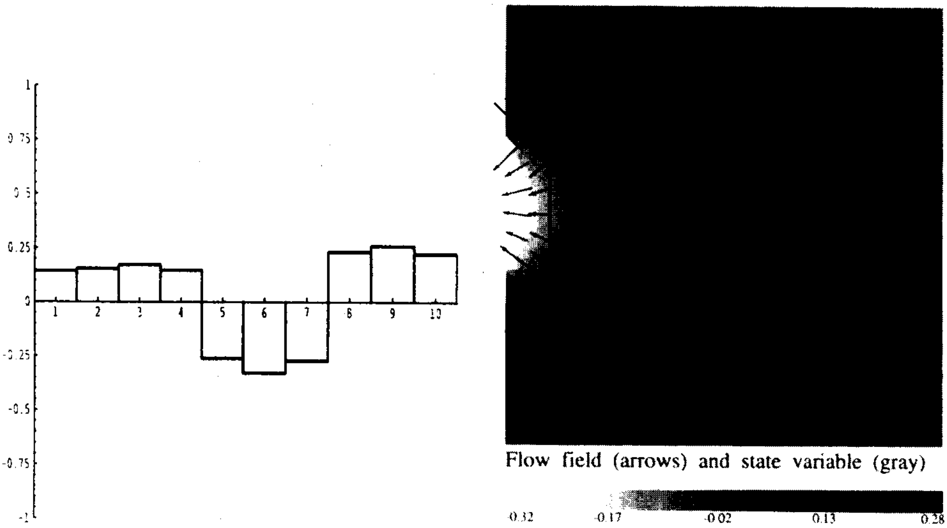

Figure 7: Optimal solution, state variable and flux: Box = $(0.1,\ 0.2)\times(0.4,\ 0.8)$, $\beta = 4$

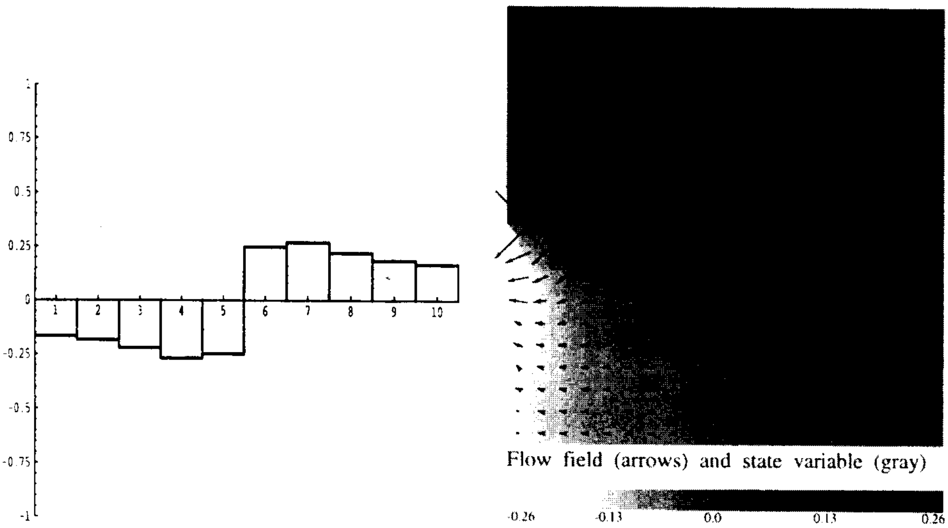

Figure 8: Optimal solution, state variable and flux: Box = $(0.1,\ 0.4)\times(0.4,\ 0.6)$, $\beta = 4$

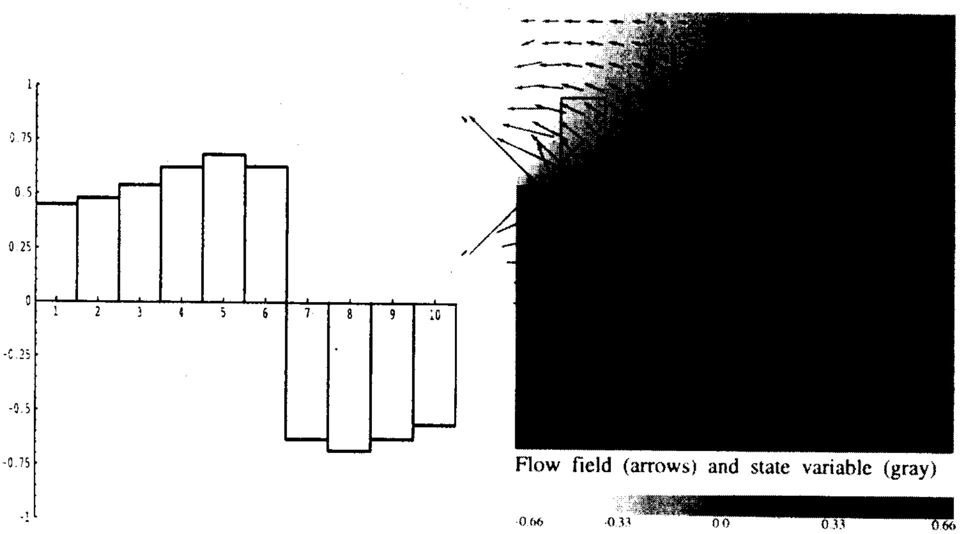

Figure 9: Optimal solution, state variable and flux: Box = (0.1, 0.2)×(0.4, 0.8), $\beta = 8$

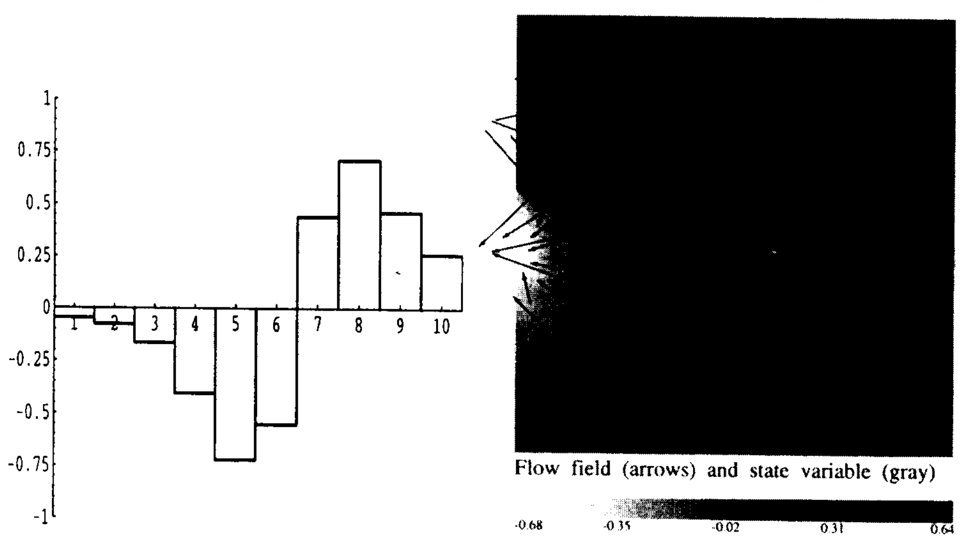

Figure 10: Optimal solution, state variable and flux: Box = (0.1, 0.2) × (0.4, 0.8), $\beta = 2.5$

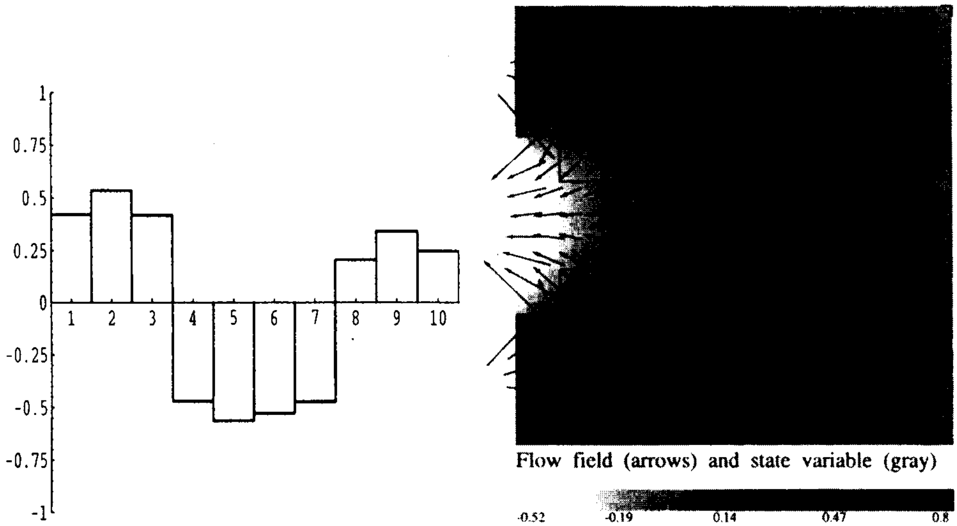

Figure 11: Optimal solution, state variable and flux, observation in two boxes: Box1 = (0.1, 0.4) × (0.2, 0.4), Box2 = (0.1, 0.2) × (0.6, 0.8), $\beta = 2.5$

the quadratic case and the rate is the highest. The flux for $\beta = 4$ (Figure 6)and especially for $\beta = 2.5$ (Figure 10) are strong near the box and small elsewhere. For $\beta = 8$ (Figure 9) the flux is still strong far from the box. The reason is that the β-norm or the functional Ψ for β large tends to the infinity norm which says that the price you pay for one control variable is the price you pay for its maximum value. This is also the reason why the absolute value of the optimal control variable does not vary too much in the case $\beta = 8$, as shows Figure 9-(left), contrary to the case $\beta = 4$ and $\beta = 2.5$ as present Figure 6-(left) and 10-(left). Note that the saddle point solution given in Figure 7 would be the intuitive solution in many cases: one would prescribe a large under-pressure on the opposite of the centre of the box to extract the contaminants. Figure 8 presents one optimal solution where we have changed the location of the box to $(0.1, 0.4) \times (0.4, 0.6)$. One can see that if the observation is not close enough to the control variable, the optimization leads to rather poor strategies.

In this second case, where the observation is distributed in one region of the domain and if this region is not too far from the control variable, the optimization gives a meaningful answer to the question of existence of a best choice of ventilation strategy. We remind the reader that this answer was not so clear in the case of the boundary observation considered in Section 2.1. The strong dependence between the locations of the control and the observation shown in the two first optimal control problems is a logical motivation to the next formulation.

2.3 Distributed Observation and the Discharges of Dirac Type Sources Control

2.3.1 Formulation

In this third and last part we change the problem a little bit more and we permit the control variable to enter the domain, too. We are interested in solving an optimal control problem where the observation is distributed and the control function is given as sources or sinks located in the domain. We consider the elliptic boundary value problem

$$\begin{cases} \nabla \cdot q & = \sum_{j=1}^{n} u_j \delta_j, & x \in \Omega \\ q & = -K\nabla y, & x \in \Omega \\ y & = 0, & x \in \Gamma_D \\ \nu \cdot q & = 0, & x \in \Gamma_N. \end{cases} \tag{16}$$

Here the *control* variable is $u = (u_1, ..., u_n) \in \mathbb{R}^n$ and δ_j is the Dirac function at $x_j \in \Omega$ the position of the well j: $\delta_j(x) = \delta(x - x_j)$.

The *cost functional* is

$$J(u) = \int_{\Omega} \Phi(x, q(y(u)))\, d\Omega + \Psi(u), \tag{17}$$

where $\Phi(x, \cdot)$ and Ψ are two differentiable functionals on $\mathbb{R}^2$ and $\mathbb{R}^n$, respectively. Here we take Φ exponentially decreasing of q which is more realistic because the quantity of extracted pollutant from the soil increases but converges exponentially to a maximal value. The functional Ψ is a penalty term taken equal to the β-norm;

$$\Phi(x, q) = \mu(x) exp(\frac{-\lambda}{2}|q|^2) \text{ and } \Psi(u) = \frac{\alpha}{\beta} \sum_j |u_j|^\beta, \tag{18}$$

where $\mu \in L^\infty(\Omega)$ is a weight function on Ω. The two real numbers $\beta \geq 1$ and $\alpha > 0$ are given. The weight function is zero outside an observation box in the unit square and in a small and fixed vicinity of each well, and equal to 1 in the rest of the domain. The flux, solution of problem (16) does not belong to the Hilbert space $L^2(\Omega)$, and to avoid any ambiguity, we cut off a fixed vicinity from the support of μ. This vicinity will not depend on the discharge of the well or the space discretization. We have

Lemma 2.6.

1. *The functional Φ decreases with the norm of q but is still positive. It means that a very strong flux will not help much more than a moderate one.*

2. *The functional Ψ increases with the norm of the discharges u. For small values of u and $\beta > 2$, Φ dominates Ψ and thus the minimizer should not be 0. For $\beta < 2$ the norm of the minimizer depends on α.*

For large u and $\beta > 1$ the functional J is also large and diverges to ∞ with u and therefore we have the existence of a global minimizer of J, i.e., $u \in U_{ad} \subset \mathbb{R}^n$, such that

$$J(u) \leq J(v) \ \forall v \in U_{ad}.$$

2.3.2 Numerical solution of the BVP

The right-hand side in problem (16) is the sum of functions with regularity less than $H^{-1}(\Omega)$. To solve it we proceed as follows. We assume that the conductivity is Lipschitz in a vicinity of each well and we define the functions of the Hilbert space $L^2(\Omega)$

$$y_j(x) = \frac{-u_j}{2\pi K_j} \ln |x - x_j|. \tag{19}$$

Therefore

$$\nabla \cdot (K_j \nabla y_j) = -u_j \delta_j,$$

then the function $\tilde{y} = y - \sum_{j=1}^{n} y_j$ satisfies the BVP

$$\begin{cases} -\nabla \cdot (K\nabla\tilde{y}) &= \sum_{j=1}^{n} \nabla \cdot ((K - K_j)\nabla y_j) & \text{in } \Omega \\ -K\nabla\tilde{y}\cdot\nu &= \sum_{j=1}^{n} K\nabla y_j \cdot \nu & \text{on } \Gamma_N \\ \tilde{y} &= -\sum_{j=1}^{n} y_j & \text{on } \Gamma_D. \end{cases} \tag{20}$$

The right-hand side in problem (20) is in this case a divergence of a function in $L^2(\Omega)$, and thus we can deduce a variational formulation which has a unique solution for (20) in $H^1(\Omega)$. Therefore, we apply the finite element discretization to problem (20) and by adding the fundamental solutions $y_j, j = 1, \ldots, n$ defined by (19), we get the solution of problem (16).

2.3.3 Application and Results

In this case of non-convex functional one can make use of global optimization techniques like stochastic search or genetic algorithm [Gol89] because the computation of the functional is rather cheap and there may exist many local minimizers. These two global search methods are especially suitable for non-regular functional with control variable of high dimension. The dimension of the control variable is in our case low which makes the number of minimizers low, too. In the other hand the functional is of high regularity and thus we think that Newton algorithm is still applicable. Due to the form of the objective functional (Figure 13), the Newton method slowly converges for β being larger than 2 and may diverge for β being smaller than 2. Therefore some modifications are in order: For example for $\beta < 2$ one can introduce a relaxation factor in the iteration to avoid a big change in the solution. One can also initialize this iteration with the solution of a larger β. One has to take care of the vicinity of zero for $\beta < 2$ because Ψ will not be differentiable to the order 2. We try to see the impact of the parameter β on the optimal control. We have taken $\alpha = 0.002$, $\lambda = 1$, and β varies between 1.2 and 12. We suppose that the pollutants are located in the region given by the box $(0.4, 0.8) \times (0.4, 0.8)$. Figure 12represents the optimal solutions which correspond to $\beta = 2$ and $\beta = 3$ and Figure 14 shows the behaviour of the optimal control function of the parameter β. The best solution in term of positions of the wells for $\beta = 2$ is to put all the discharge on the well located in the centre of the pollution. This is not the case, if β becomes large. For $\beta > 4$ the wells share the discharges in an equitable way. For soil remediation it is important to have negative total discharge which is the case shown in Figure 12.

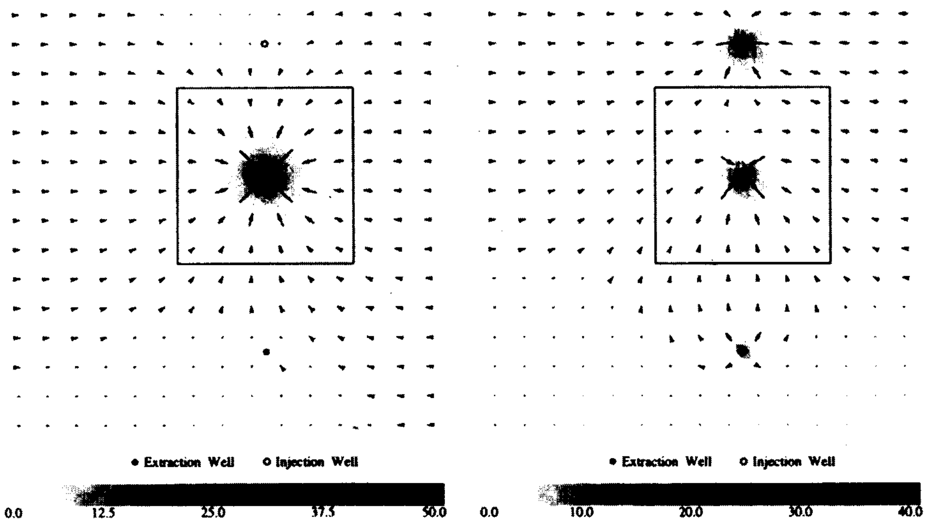

Figure 12: Optimal solution: flow field, Box(0.4, 0.8) × (0.4, 0.8), the location of the wells are (0.6, 0.2), (0.6, 0.6) and (0.6, 0.9), (right): $\beta = 2$ and (left): $\beta = 3$

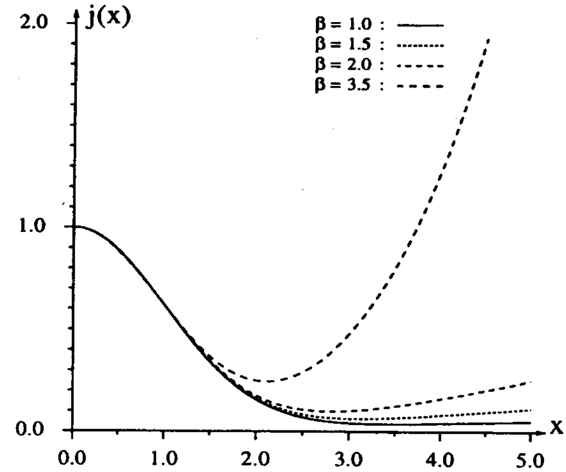

Figure 13: 1-D representation of the functional J when varying β : $j(x) = e^{-x^2/2.} + 0.01 * x^\beta$

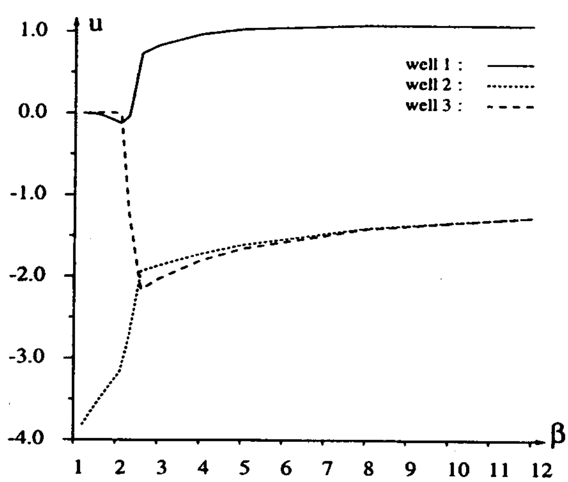

Figure 14: Optimal solutions: Discharges of the three wells respectively functions of β, wells locations respectively: $(0,6,\ 0.2)$, $(0.6,\ 0.6)$ and $(0.6,\ 0.9)$.

3 Conclusion

In this paper, we have considered some aspects of optimization of flow essentially governed by a second order elliptic differential equation. The control variable was the pressure on one part of the boundary for the first and the second formulations, and the discharges of some wells located in the domain for the third one. We would say that the first formulation is rather hard in the sense that the unique optimal solution does not always produce a very good strategy. This is due to the fact that the control and the observation locations are distant and the diffusion of the fluid avoids any strong relation between them. In the second formulation, where the region of observation moves towards the control variable, the situation becomes better and the optimal solutions seem to treat the problem of soil venting in a clear way. This is better than the first formulation but one cannot imagine that a polluted soil "moves" towards the ventilation equipments. Thus the third formulation seems to be the best approach. The control variable should move in the domain to find the positions which permit to treat the problem of optimization of the discharges. As future work we plan to treat the optimization of the positions and the discharges of the wells simultaneously. Another advantage of this third strategy is that the extracted air leaves the domain at a small area which make the treatment of this air easier. The injection wells can be also used to introduce heated air to enhance remediation in some cases [LD90].

Another point we have to mention is the spacial variability of the soil properties, namely the transmissivity. Recently Unger, Sudicky, and Forsyth [USF95] have addressed the problem of robustness of a remediation strategy with respect to spatial heterogeneities of the soil. This variability of the transmissivity has to be considered and the optimal control problem depends strongly on it. Without this effort the optimization gives in general highly uncertain results in term of remediation [Gor90].

Another aspect of the optimization of soil venting is the pollutant transport in the soil. This brings many complications to the problem, namely the numerical solution of the convection-diffusion transport equation, the parameters of this equation which are almost unknown but offers the possibility to define the objective functional in a more direct way. In this case, one should maximize the quantity of the extracted pollutants under some physical and technical restrictions. This has to be done and to be compared with the optimization considered in this paper.

Aknowledgements The author whishes to thank to Professor Enrique Zuazua for his help and advices. This work was supported by the BMBF (German Federal Ministry for Education, Science, Research and Technology) Grant Number 03-HO7BWM.

References

[Bea79] J. Bear. *Hydraulics of Groundwater.* McGraw-Hill Series in Water Resources and Environmental Engineering, 1979.

[BF91] F. Brezzi and M. Fortin. *Mixed and Hybrid Finite Element Methods.* Springer-Verlag, New York, 1991.

[Bru91] M. L. Brusseau. Transport of organic chemicals by gas advection in structured or heterogeneous porous media: Developement of a model and application to column experiments. *Water Resour. Res.*, 27.12:3189–3199, 1991.

[Gol89] D. E. Goldberg. *Genetic Algorithms in Search, Optimization, and Machine Learning.* Addison-Wesley Publishing Company, INC, New York, 1989.

[Gor90] S. M. Gorelick. Large scale nonlinear deterministic and stochastic optimization: Formulations involving simulation of subsurface contamination. *Mathematical Programming*, 48:19–39, 1990.

[KH90] E. F. Kaasschieter and A. J. M. Huijben. Mixed hybrid finite element and streamline computation for the potential flow problem. Technical Report Report PN 90-92-A, TU Delft, 1990.

[LD90] S. Lingineni and V. K. Dhir. Modeling of soil venting processes to remediate unsaturated soils. *Journal of Environmental Engineering*, 118.1:135–151, 1990.

[Lio71] J. L. Lions. *Optimal Control of Systems Governed by Partial Differential Equations.* Springer, Berlin, 1971.

[NG91] M. Nahold and K. Gottheil. Ckw-schadensfälle - die optimierung von bodenluftabsaugungen. *WLB Wasser, Luft und Boden*, 11.12:83–86, 1991.

[RM94] A. J. Rabideau and C. T. Miller. Two-dimensional modeling of aquifer remediation influenced by sorption nonequilibrium and hydraulic conductivity heterogeneity. *Water Resour. Res.*, 30.5:1457–1470, 1994.

[Tho77] J. M. Thomas. *Sur l'analyse numérique des méthodes d'éléments finis hybrides et mixtes.* PhD thesis, University Pierre et Marie Curie, Paris, 1977.

[USF95] A. J. A. Unger, E. A. Sudicky, and P. A. Forsyth. Mechanisms controlling vacuum extraction coupled with air sparging for remediation of hetereogeneous formations contaminated by dense nonaqueous liquids. *Water Resour. Res.*, 38.1:1913–1925, 1995.

[WG87] B. J. Wagner and S. M. Gorelick. Optimal groundwater quality management under parameter uncertainty. *Water Resour. Res.*, 23.7:1162–1174, 1987.

[WG89] B. J. Wagner and S. M. Gorelick. Reliable aquifer remediation in the presence of spacially variable hydraulic conductivity: from data to design. *Water Resour. Res.*, 25.10:2211–2225, 1989.

Department of Computer Science,
University of the Federal Armed Forces Munich,
D-85577 Neubiberg,
Germany.

Recibido: 10 de Junio de 1997
Revisado: 11 de Enero de 1997