Numerical approximation of an identification problem in porous media

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When the ground is accidentally polluted with a volatile organic contaminant, it is important to know the amount of this contaminant in liquid form, in this paper it is shown that the concentration in the liquid phase of the volatile organic contaminant can be identified by analyzing the gaseous phase and using inverse problem. In order to do that we consider an inverse problem.

Key words : :mass transfer, identification of coefficients, inverse problem

I. INTRODUCTION

The mathematical model developed in this work can be used in the context of the industrial or accidental pollution of a soil with a liquid volatile organic pollutant. A relevant question for determining a possible remediation senarii is the ability to haracterize the level of the pollution in a short time. In this study, we consider a simple mathematical model for the rate limited mass transfer model between the liquid and the gaseous phase, we show that the pollutant concentration in the liquid phase at t=0 can be identified if the pollutant concentration in the gaseous phase is known at any positive time T. Let us consider a column of polluted soil, assumed to be a rigid porous medium, in which flows down fresh air. The gaseous phase is analysed at the bottom of the column.

The speed v of the flow is assumed to be small such that the volume fractions of liquid and gaseous phases θ_w and θ_a can be considered constant. The adsorption is neglected, and we denote by C_a, respectively by C_w the concentration of the pollutant in the gaseous, and in the liquid phases. Hereafter the positive constants H, C* and D stand respectively for the Henry constant, the saturation concentration in gas and for the effective diffusion coefficient.
A 1-D mathematical model for the mass transfer between the two phases reads (see [3], [4], [6], [10] and [12]) :

$$\begin{cases} \partial_t C_a - D\partial_x^2 C_a + \partial_x(vC_a) = (HC_w - C_a) in Q_T \\ \partial_t C_w = -\dfrac{\theta_a}{\theta_w}(HC_w - C_a) in Q_T \\ \partial_x C_a(-1,t) = 0, C_a(1,t) = C^* in (0,T) \\ C_a(x,0) = C_a^0(x), C_w(x,0) = C_a^0(x) in (-1,1) \end{cases} \qquad (1)$$

The functions C^0_a and C^0_w are initial concentrations.

Set $\alpha = \dfrac{\theta_a}{\theta_w}$, I=(-1,1), Q_T = (-1,1) x (0,T); the Function C_w is then given by:

$$C_w(x,t) = C_w^0(x)e^{-\alpha Ht} + \alpha\int_0^t e^{-\alpha H(t-s)}ds \qquad (2)$$

$\forall (x,t) \in Q_T$

using the representation formula (2) for the function C_w , Equation $(1)_1$ is transformed in

$$\partial_t C_a - D\partial_x^2 C_a + \partial_x(vC_a) = HC_w^0(x)e^{-\alpha Ht} + \alpha H\int_0^t e^{-\alpha H(t-s)}C_a(x,s)ds - C_a in Q_T \qquad (3)$$

and Equation $(1)_2$ is eliminated.
We can then consider the inverse problem :
for any T>0, if C_a satisfies (3) and $(1)_3$-$(1)_4$ and if $C_a(.,T)$ is given, does it determine uniquely the function C^0_w?

Our next goal is to have a time independent function to be identified in the right end side of Equation (3), we consider the following change of unknown functions. Set

$$u(x,t) = \frac{1}{H}e^{\alpha Ht}C_a(x,t); f(x) = C_w^0(x);$$

$$u_0(x) = \frac{1}{H}C_w^0(x); \gamma(t) = \frac{C^*}{H}e^{\alpha Ht}$$

$\forall (x,t) \in Q_T$

and define the space differential operator A by :

$$A = -D\partial_x^2. + v\partial_x. + (1 - \alpha H + \partial_x v)Id.$$

With these notations, the inverse Problem P can be written:
For T>0 and given functions γ ,u_0 and h_T find (u,f) verifying :

$$P\begin{cases} P_1\begin{cases} \partial_t u + Au = f + \alpha H\int_0^t u(s)d\sin Q_T \\ \partial_x u(-1,t) = 0 in (0,T) \\ u(1,t) = \gamma(t) in (0,T) \\ u(x,0) = u_0(x) in (-1,1) \end{cases} \\ u(x,T) = h_T(x) in (-1,1) \end{cases}$$

To study the inverse Problem P we use a generalization of the method proposed by Isakov in [8] which consists in expressing theinverse Problem P like a Fredholm equation at the final time T.

Let us end this introduction by specifying the hypothesis that we assume to be satisfied:

H) $v \in C^2(\bar{I}); u_0 \in H^1(I)$ with $u_0(1) = \gamma(0)$

II. INVERSE PROBLEM P

In order to approximate the pollutant concentration C_W we consider an inverse problem, in [8] Isakov suggests this method but his approach uses the Sobolev spaces, our formulation uses the Hilbert space L^2 which permits to prove the uniqueness of the solution and to approach this solution easily. Now we are going to show the existence and the uniqueness of a solution to the inverse Problem P, and we follow the method proposed by Isakov in [8] which is transposed in the setting of the Hilbert space L^2. This functional framework allows us to get uniqueness of the solution of the inverse Problem P for more general parabolic operators, and is more convenient for numerical applications.

Theorem 1:

Assume that the hypothesis (H) is satisfied and let h_T be in $H^2(I)$ such that $\frac{d}{dx}h_T(-1) = 0$ and $h_T(1) = \gamma(T)$, then the Problem P has a unique solution $(u,f) \in W \times L^2(I)$. Where

$$W = \left\{\varphi \in L^2(0,T;H_1(I)); \frac{d}{dt}\varphi \in L^2(0,T;L^2(I)) \right\}$$

For the proof of the theorem1 the reader is referred to [1] ,[2]. We have the existence and the uniqueness of the solution of the inverse problem P which permits to determine (C_a,C^0_W) where C_a is the concentration of the pollutant in the gaseous phase and C^0_W is the initial concentration of the pollutant in liquid phase.

III. IDENTIFICATION OF C^0_W

In order to compute C^0_W, we have to find (λ,φ) solution of the following problem:

$$\begin{cases} -D\varphi^n + v\varphi' = \lambda\varphi in I \\ \varphi(1) = 0, \varphi'(-1) = 0 \end{cases} \quad (4)$$

and set $\lambda_0 = \frac{-v^2}{4D}$, then we have the following result :

Lemma 1:

The eigenvalues and the eigenfunctions of the problem (4) $\{\lambda_n, e_n\}_{n\geq 1} \subset]\lambda_0,\infty[\times C^\infty(\bar{I})$ are respectively given by:

$$\lambda_n = \frac{v^2}{4D} + \frac{D}{4}\omega_n^2 \quad (5)$$

$$e_n = \exp(\frac{v}{2D}x)\left\{C_{1n}\cos(\frac{\omega_n}{2}x) + C_{2n}\sin(\frac{\omega_n}{2}x)\right\} \quad (6)$$

where ω_n is a sequence of positive real numbers satisfying:

$$\frac{v}{D}\tan(\omega_n) = \omega_n \quad (7)$$

The constants C_{1n} and C_{2n} are arbitrary.

Lemma 2:

A normalized orthonormal base of $L^2(I,\mu)$ with its associated sequence of eigenvalues $\{e_m, \lambda_m\}_{m\geq 1}$ solution of the problem (4)$ is given by :
$\forall m \geq 1$

$$e_m(x) = \frac{\exp(\frac{v}{2D}x)}{\sqrt{1-\frac{D}{v}\cos^2(\omega_m)}}\sin(\frac{\omega_m}{2}(x-1)). \quad (8)$$

In order to compute the solution of the inverse problem, we have to compute the orthonormal basis $\{e_m\}^M{}_{m=1}$ with its associated eigenvalues $\{\lambda_m\}^M{}_{m=1}$. Then we use the Galerkin approximation to show that there exists a solution of the problem (P_1). Let $e_i \in V, i \in IN$ be a family of functions such that for all M, e_1,......,e_M are linearly independent, the finite linear combinations of the e_i are dense in $L^2(I)$. Such a sequence exists because V is separable (see [9]).

For each integer M, we seek an approximate solution u_M in the form $u_M = \sum_{k=1}^M g_k(t)e_k$.

Hence we obtain for the unknowns the following expression: $(u_M, f_M) = \left(\sum_{k=1}^M g_k(t)e_k, \sum_{k=1}^M f_k(t)e_k\right)$

Lemma 3:

Assume that hypothesis (H) holds true , then for $1 \leq k$ the components f_k of f are given by:

$$f_k = -\frac{D}{\lambda_k(1-\exp(-\sqrt{\Delta_k}T)}(+r_k - (\frac{\beta+\lambda_k}{2})\times$$
$$\exp(-\sqrt{\Delta_k}T))(u_0''/e_k) + \frac{v}{\lambda_k(1-\exp(-\sqrt{\Delta_k}T)}\times$$
$$(+r_k - (\frac{\beta+\lambda_k}{2})\exp(-\sqrt{\Delta_k}T))(u_0'/e_k)$$
$$-\frac{D\sqrt{\Delta_k}\exp(-+r_kT)}{\lambda_k(1-\exp(-\sqrt{\Delta_k}T)}(h''_T/e_k) +$$
$$\frac{v\sqrt{\Delta_k}\exp(-+r_kT)}{\lambda_k(1-\exp(-\sqrt{\Delta_k}T)}(h'_T/e_k)$$

With :

$$\Delta_k = 4\alpha H + (\beta+\lambda_k)^2$$
$$\pm r_k = \frac{-(\beta+\lambda_k)\pm\sqrt{\Delta_k}}{2}.$$

For the proof the reader is referred to [1].

IV. NUMERICAL APPROACH

The numerical approach of (u,f) is possible using as a data the final concentration in the gaseous phase $C_a(x,T)$. The computation of (u,f), solution of the inverse problem (P) is down in two parts:

In the first part we solve the direct problem (P_1) by the finite difference method, hence we choose an arbitrary function f(x) for the space discretization we use the finite difference method and for the time discretization we use the retrograde Euler schema.

Algorithm1:

Step1: discretization of I=[-1,1] and computation of x(i)=x(0)+2(i-1)h, i=1...,n with x (0) = -1 and h= 1/(n-1)

Step2: discretization of (0,T) and computation of $t(j) = (j-1)\tau,\ j = 1,...,m$ with $\tau = \frac{T}{m-1}$.

Step3: solution of the system AU=B using the tridiagonal algorithm for linear systems.

In order to test the proposed method we used a simple example which his exact solution is known let be $f(x)=C^*/H + e_1(x)$, the exact solution of the problem (P_1) is:

$$u(x,t) = \frac{1}{\sqrt{\Delta_1}}\left[\exp(+r_1t) - \exp(-r_1t)\right].$$

The second part consists in the computation of the components of the function f on the spectral base $\{e_k\}$, in order to do that we have to compute numerically the eigenvalues λ_k and the eigenfunctions e_k.

$$\lambda_k = \frac{v^2}{4D} + \frac{D}{4}\omega^2,$$

$$e_k(x) = \frac{\exp(\frac{v}{2D}x)}{\sqrt{1-\frac{D}{v}\cos^2(\omega_k)}}\sin(\omega_k(x-1))$$

where ω_k is a sequence of positive real numbers satisfying:

$$\frac{v}{D}\tan(\omega_k) = \omega_k$$

We compute ω_k using the Newton method, the components f_k of f on the base e_k are:

$$f_k = (f - f(1)/e_k) = \sqrt{\Delta_k}\frac{\exp(-+r_kT)}{1-\exp(\sqrt{\Delta_k}T)}(h_T - h_T(1)/e_k)$$

$$f = \frac{C^*}{H} + \sum_{k=1}^{\infty} f_k e_k, et\|f - f(1)\|^2_{L^2(I,\mu)} = \sum_{k=1}^{\infty} f_k^2$$

The scalar products

$$(h_T - h_T(1)/e_k) = \int_I (h_T - h_T(1))e_k\exp(-\frac{v}{d}x)dx$$

are computed by using a Simpson formula.

Algorithm2:

Step1: discretization of I=[-1,1] like in the step1 of the algorithm1

Step2: computation of the eigenvalues and the eigenfunctions using the Newton method.
We do a boucle on the numbers of the eigenfunctions.

Step3: computation of the scalar products (h_T-h_T (1)/e_k) by the Simpson method.

Step4: computation of the components f(k) of f on the base e(k).

Step5:computation of $f(x_i) = \sum_k f(k)w_k(x_i)$

V. NUMERICAL RESULTS

In the numerical example, u_0=C*/H, the parameters used are given in Tab.1 (see [11])

V(m/min)	D(m^2/min)	T(min)	$\frac{\theta_a}{\theta_w}$
1.3	1.3	1.5	0.708
H	C*(Kg/m^3)	h	τ
0.04	0.248	1.25E-003	10 E-002

Tab.1

Using the proposed algorithm we use:
$f(x) = e_1(x)\cos(2\pi(1-x))$; for other examples see [1] .

In what follows some numerical examples are carried out in order to test the numerical algorithm to the solution of the inverse problem, hence we consider that the function f(x) is a data and we compute u(x,t) solution of the problem (P_1), so we have the value of u(x,T) on the final time T considered and we have the punctual values of $h_T(x)=u(x,T)$. These values $h_T(x_i)$ will be used for solving the inverse problem (P) and computing the components of f(x).

We end the presentation of the numerical results by two figures, in figure 1 we plot the function $h_T(x)$, in figure2 the exact (squares) and identified (points) functions are plotted as functions of x , for the case:
$f(x) = e_1(x)\cos(2\pi(1-x))$ and M=50.

The oscillation of the identified function for x=-1 is probably due to the Newman boundary condition.

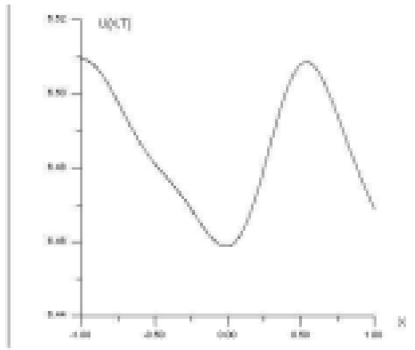

FIG 1

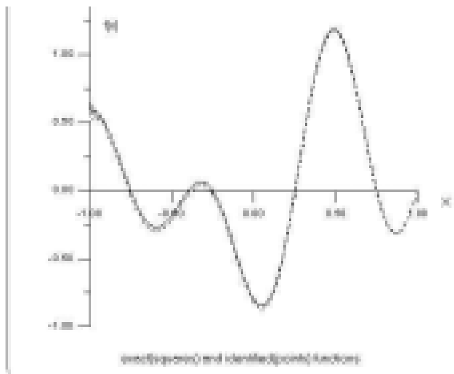

FIG 2

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In Tab2, the ten first components of f are reported.

f_k	f_k computed
5.1846 E-002	5.1722 E-002
-4.9701 E-001	-4.9657 E-001
-6.8298 E-002	-6.8274 E-002
5.1090 E-002	5.1070 E-002
4.9470 E-001	4.9460 E-001
-1.4567 E-002	-1.4569 E-002
4.9380 E-003	4.9327 E-003
-2.3281 E-003	-2.3308 E-003
1.2832 E-003	1.2791 E-003
-7.7814 E-003	-7.8016 E-003

Tab.2

VI. CONCLUSION

We have considered a simple mathematical model for the rate limited mass transfer model between the liquid and the gaseous phases, in order to identify a parameter of the model when some gas phase experimental data are available.

We introduced an inverse problem, hence we obtain the existence and the uniqueness of a solution to this problem and we proposed a numerical method to identify the initial concentration of the pollutant in the liquid phase. We have done different tests using 20, 50,100 and 200 eigenfunctions, the results obtained show that the convergence is so fast, we reach an error in the order 10E-2 from 50 eigenfunctions.

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