Scaling Up of Sources Terms with Random Behavior in a Diffusion Convection equation

A. Bourgeat [a] O. Gipouloux [a,b,*] F. Smai [a]

[a] *Université de Lyon, Université Lyon1, CNRS, UMR 5208 Institut Camille Jordan, Batiment du Doyen Jean Braconnier, 43, blvd du 11 novembre 1918, F - 69200 Villeurbanne Cedex, France*

[b] *Département de mathématiques, Faculté des Sciences et Techniques, Université de Saint Etienne 23 Rue Paul Michelon 42023 Saint Etienne Cedex, France*

Abstract

We are interested to study the evolution in time of the concentration of a pollutant which is transported by diffusion and convection from a "sources site" made of a large number of similar "local sources". Assuming the release curve (source emission vs. space and time), of each local source, being random, our aim is to give a mathematical model describing the global evolution of such a system and numerical simulations illustrating the theoretical results.

Key words: Partial differential equation, Homogenization, Numerical simulations.

Introduction

We consider a transport diffusion model given by a partial differential equation describing the temporal evolution of a quantity (the concentration of a radionuclear pollutant for example) in a parallelepipedic porous domain. The partial differential equation source term is constituted by spatially periodically distributed sources lying on the porous medium median plane. Each of these sources are identical parallelepipeds. The behavior of each source is spatially homogeneous but their time dependence is uncertain. Our aim is to give a mathematical model describing the global evolution of such a system

* Corresponding author

Email addresses: bourgeat@mcs.univ-lyon1.fr (A. Bourgeat), gipoul@mcs.univ-lyon1.fr (O. Gipouloux), smai@mcs.univ-lyon1.fr (F. Smai).

and to perform numerical simulations to illustrate the theoretical results. The deterministic case where all the sources are leaking at the same time with the same "leaking curve" has been studied in [5,6]. In the first section, we successively describe the geometry of the porous medium, the equations and the uncertainty of the source terms. In the second section, we give the theoreticals results on the homogenization processes. The third section is devoted to numericals tools used in the last section. Finally, in the last section, numerical simulations are performed to illustrate the theoretical results.

1 Setting the problem

1.1 Description of the geometry

We consider an open bounded domain $\mathcal{D} \subset \mathbb{R}^d$, with $d = 2$ or $d = 3$, such that $\mathcal{D}^+ = \{x = (x_1, \cdots, x_d) \in \mathcal{D} : x_d > 0\}$ and $\mathcal{D}^- = \{x = (x_1, \cdots, x_d) \in \mathcal{D} : x_d < 0\}$ are nonempty domains. Let $L > 0$ be the typical length of the repository containing the sources, we suppose that $\mathcal{D}$ contains $\Sigma = [0; L]^{d-1} \times \{0\}$ (See Figure 1). Let ε be a small positive number, we denote the "global variable" $x = (x_1, \cdots, x_d)$ and the "local variable" $x/\varepsilon = (x_1/\varepsilon, \cdots, x_d/\varepsilon)$. The support K^ε of a source in the local variables (see Figure 2) is defined by :

$$K^\varepsilon = [0; s_1] \times \cdots \times [0; s_{d-1}] \times [-\varepsilon^{\gamma-1} s_d/2; \varepsilon^{\gamma-1} s_d/2], \tag{1}$$

with $0 < s_i < 1$ for $i \in \{1, \cdots, d-1\}$ and $\gamma > 0$. The global periodic support is given by :

$$\begin{aligned} \tilde{B}^\varepsilon &= \bigcup_{\mathbf{j} \in \mathbb{N}^{d-1}} \varepsilon L(K^\varepsilon + (\mathbf{j}, 0)) \quad \text{, in global variables and} \\ \tilde{B} &= \bigcup_{\mathbf{j} \in \mathbb{N}^{d-1}} K^\varepsilon + (\mathbf{j}, 0) \quad \text{, in local variables.} \end{aligned}$$

Here, ε measures the adimensionalised spatial period of the source supports and for simplicity we assume that $1/\varepsilon = N \in \mathbb{N}$. So the whole source site support (see Figure 3) is defined by :

$$\begin{aligned} B^\varepsilon &= \tilde{B}^\varepsilon \cap \mathcal{S}, \text{ or also,} \\ &= \bigcup_{\mathbf{j} \in I} \varepsilon L(K^\varepsilon + (\mathbf{j}, 0)), \end{aligned}$$

with $\mathcal{S} = [0; L]^{d-1} \times \mathbb{R}$ and $I = \{1, \cdots, N\}^{d-1}$, then B^ε contains N^{d-1} distinct sources. In the following, we also use the notation

$$B^\varepsilon_{\mathbf{j}} = \varepsilon L(K^\varepsilon + (\mathbf{j}, 0)).$$

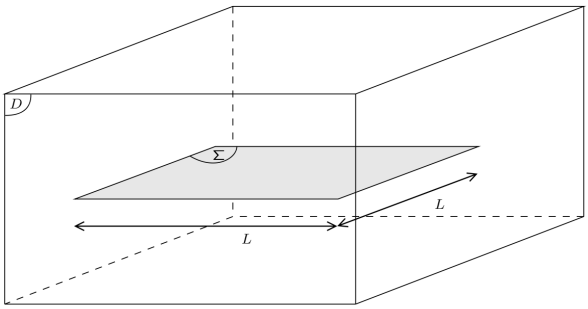

Fig. 1. Global domain

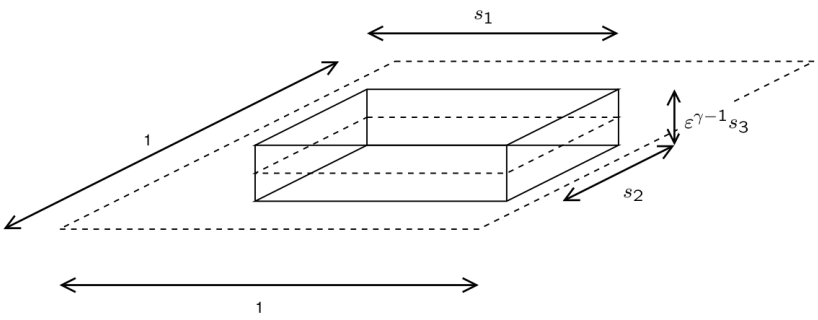

Fig. 2. One source in the local scale

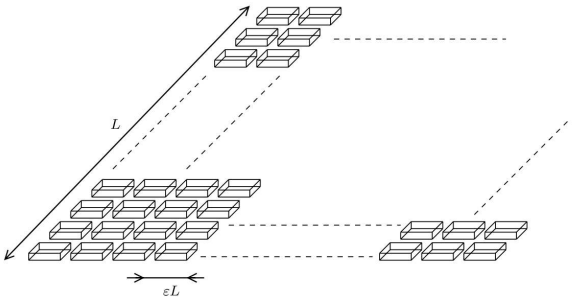

Fig. 3. Global configuration of sources

1.2 Description of the randomness

Let $(\Omega, \mathcal{F}, \mathbf{P})$ be a standard probability space. To describe the randomness dependancy in space, we define on this probability space the random ergodic dynamical system (T_z). Moreover, assuming without loss of generality that each source term is spatially homogeneous, the dynamical system is assumed to be discrete, *i.e.* $z \in \mathbb{Z}^{d-1}$. Then, by definition, the random ergodic dynamical system (T_z) is a collection of measurable maps $T_z : \Omega \to \Omega$ such that T_z

- has the group properties, $T_{z_1+z_2} = T_{z_1} \circ T_{z_2}$, $T_0 = \mathrm{Id}$;
- preserves the measure $\mathbf{P}$ for all $z \in \mathbb{Z}^{d-1}$;
- is ergodic, *i.e.* the relation $\mathbf{P}(\mathcal{A})(1 - \mathbf{P}(\mathcal{A})) = 0$ holds for any invariant set $\mathcal{A} \in \mathcal{F}$.

1.3 Description of the equations

Under the above assumptions, we are now considering the convection-diffusion problem, with a random source term Q^ε :

$$\partial_t u^\varepsilon - \nabla(a(x)\nabla u^\varepsilon - \mathbf{b}(x)u^\varepsilon) + \lambda u^\varepsilon = Q^\varepsilon \quad \text{in}[0;T] \times \mathcal{D} \tag{2a}$$

$$u^\varepsilon = 0 \quad \text{in}\{0\} \times \mathcal{D} \tag{2b}$$

$$(a(x)\nabla u^\varepsilon - \mathbf{b}(x)u^\varepsilon) \cdot \mathbf{n}(x) = 0 \quad \text{in}[0;T] \times (\partial\mathcal{D} \setminus \Gamma_d) \tag{2c}$$

$$u^\varepsilon = 0 \quad \text{in}[0;T] \times \Gamma_d \tag{2d}$$

where u^ε (the concentration) is a scalar field of $[0;T] \times \mathcal{D}$, λ (the radioactive decay constant) is a non negative constant, $a(x)$ (the diffusion tensor) is a uniformly positive definite smooth matrix-function, $\mathbf{b}(x)$ (the convection field) is a smooth given divergence free vector field, $\mathbf{n}$ is the external normal of domain $\mathcal{D}$ and Γ_d is a subset of $\partial\mathcal{D}$. To simplify notations of equation (2a), let's introduce the linear operator A defined by :

$$Au \equiv -\nabla(a(x)\nabla u - \mathbf{b}(x)u) + \lambda u.$$

Concerning the random source term, as usual in "probability literature", we will not show explicitly the dependency in ω and write the random variable:

$$Q^\varepsilon(t,x) = \mathbb{1}_{B^\varepsilon} \frac{1}{\varepsilon^\gamma} f(T_{[x'/L\varepsilon]}\omega, t), \tag{3}$$

where x' denotes the restriction to $\mathbb{R}^{d-1}$ of x :

$$\begin{array}{ccc} \mathbb{R}^d & \longrightarrow & \mathbb{R}^{d-1} \\ x = (x_1, \cdots, x_d) & \longrightarrow & x' = (x_1, \cdots, x_{d-1}) \ ; \end{array}$$

$[\cdot]$ denotes the floor function extended to $\mathbb{R}^p$ by :

$$\begin{aligned} \mathbb{R}^p &\longrightarrow & \mathbb{Z}^p \\ y &\longrightarrow [y] = ([y_1], \cdots, [y_p]) \end{aligned}$$

where $[y_i]$ is the classical floor function in $\mathbb{R}$;
and, for any set $\mathcal{E}$, $\mathbb{1}_{\mathcal{B}} : \mathcal{E} \to \{0, 1\}$ denotes the indicator function of the subset $\mathcal{B} \subset \mathcal{E}$.
Besides, we will assume that the random variable $f(\omega, t)$ is uniformly bounded, i.e. there exists two nonrandom positive constants Λ and C_0 such that

$$\forall \omega \in \Omega \quad \forall t \in [0; T] \qquad |f(\omega, t)| < C_0 e^{-\Lambda t}.$$

A classical result gives that, for each $\varepsilon > 0$ and each $\omega \in \Omega$, problem (2) has a unique solution $u^\varepsilon \in L^2(0, T; H^1(\mathcal{D})) \cap C(0, T; L^2(\mathcal{D}))$ (see [6]).

2 Homogenization of the random problem

In this section, we recall some theoretical results from [1] about convergences of the detailed problem (2) to a homogenized problem. More precisely, in a first part, Theorem 1 gives convergence of the random solution u^ε to a deterministic limit u^0, solution of a problem of the same type but with only one source lying on Σ. Theorem 2 provide an estimation of the rate of this convergence. In a second part, under some assumptions about the source term randomness, Theorems 3 give the rescaled field $\varepsilon^{-(d-1)/2}(u^\varepsilon - u^0)$ convergence in law to Gaussian field and provide the parameters of the limit law.

2.1 Convergence to a deterministic limit

Let $\delta_\Sigma(x)$ denote the surface Lebesgue measure with support Σ, by $\mathbf{E}[f(\cdot, t)]$ the expectation of $f(\omega, t)$ and define :

$$F(t) = \left(\prod_{i=1}^{d} s_i \right) L\mathbf{E}[f(\cdot, t)].$$

It may be proved that the solution u^ε of problem (2) converge, when $\varepsilon \to 0$, to a limit u^0, solution of a similar convection-diffusion problem :

$$\begin{aligned} \partial_t u^0 + Au^0 &= F(t)\delta_\Sigma(x) && \text{in } [0;T]\times\mathcal{D} && \text{(4a)}\\ u^0 &= 0 && \text{in } \{0\}\times\mathcal{D} && \text{(4b)}\\ (a(x)\nabla u^0 - \mathbf{b}(x)u^0)\cdot\mathbf{n}(x) &= 0 && \text{in } [0;T]\times(\partial\mathcal{D}\setminus\Gamma_d) && \text{(4c)}\\ u^0 &= 0 && \text{in } [0;T]\times\Gamma_d && \text{(4d)} \end{aligned}$$

More precisely, the following theorem (proved in [1]) holds :

Theorem 1 *Under the above assumptions*

$$\lim_{\varepsilon\to 0} \|u^\varepsilon - u^0\|_{L^2(0,\infty;H^1(\mathcal{D}))} = 0 \quad a.s.$$

Under natural additional assumptions, this convergence result can be completed by an estimation of the convergence rate. To do this, we introduce the correlation function, R, of f in the local variables :

$$R : [0,T]\times[0,T]\times\mathbb{R}^{d-1}\times\mathbb{R}^{d-1} \to \mathbb{R},$$

such that $\forall t,s\in[0;T] \quad \forall x,y\in\mathbb{R}^d$:

$$R(t,s,x',y') = \mathbf{E}\left[(f(T_{[x']}\cdot,t) - \mathbf{E}[f(T_{[x']}\cdot,t)])(f(T_{[y']}\cdot,s) - \mathbf{E}[f(T_{[y']}\cdot,s)])\right]. \tag{5}$$

We assume that there exists $\bar{R} : \mathbb{R}^{d-1} \to \mathbb{R}_+$ such that

$$\forall t,s\in[0;\infty] \quad \forall x,y\in\mathbb{R}^d \qquad |R(t,s,x',y')| \le e^{-\Lambda\min(t,s)}\bar{R}(x'-y').$$

We define the following conditions on $\bar{R}(y')$:

H1 *There exist $R_0 > 0$ such that*

$$\bar{R}(y') = 0 \quad \text{if } |y'| > R_0.$$

H2

$$\int_{\mathbb{R}^{d-1}} \bar{R}(y')dy' < \infty.$$

H3 *There exists $C_0 > 0$ and $\nu > 2$ such that*

$$\bar{R}(y') \le C_0(1+|y'|)^{-\nu}.$$

Theorem 2 *Under the assumptions of Theorem 1 and one of the additional condition* **H1**, **H2** *or* **H3**, *we have*

$$\mathbf{E}\left[\|u^\varepsilon - u^0\|^2_{L^2(0,T;L^2(\mathcal{D}))}\right] \le C_1(\varepsilon^2 + \varepsilon^{2\gamma}) \tag{6}$$

with C_1 a positive constant independent of ε.

In other terms, considering a fixed $\varepsilon > 0$, Theorem 1 provides the far field approximation, u^0, of the solution, u^ε, of problem (2) : u^0 do not mimic the local oscillatory behaviour of u^ε "near the sources", but give an accurate far field approximation of u^ε far from the source. Notice that u^0 is the solution of problem (4) which differs from the original problem only by the source term : $F\delta_\Sigma$ instead of Q^ε. That implies that u^0 can be computed in the same way as $u^\varepsilon(\omega)$, with a given $\omega \in \Omega$, but the geometry of the new problem (4) may be very less detailed, so numerical computation of u^0 will be faster than for u^ε.

2.2 Convergence in law of the rescaled field

Theorems 1 and 2 give a deterministic approximation, u^0, of the average behavior of the random solution, u^ε, of problem (2), but we are also interested by random fluctuations of u^ε around its homogenized value. In the same way as the Central Limit Theorem, it may be proved, as in [1], under some assumptions, that the rescaled field $\varepsilon^{-(d-1)/2}(u^\varepsilon(t,x) - u^0(t,x))$ converges in law to a Gaussian field.

Denote by $G(t,s,x,y)$ the Green function associated with problem (2) and

$$\bar{\bar{c}}(t,s) \equiv \lim_{N\to\infty} \frac{s_d^2 L^{d+1}}{N^{d-1}} \int_{[0,N]^{d-1}} \int_{[0,N]^{d-1}} R(t,s,y,z) \mathbb{1}_{\tilde{B}}(y) \mathbb{1}_{\tilde{B}}(z) dy dz. \quad (7)$$

Further more, denote $\tilde{f}(t,x') \equiv f(T_{[x']}\cdot, t)$ and consider the following conditions :

H4 *For each $t_0 \geq 0$ the strong mixing coefficient $\alpha_{t_0}(s)$ of $\tilde{f}$ decays fast enough so that*

$$\exists \nu_1 > 2 \quad \exists C_2 > 0 \quad \exists \Lambda_1 > 0 \quad \forall s > 0 \quad \alpha_{t_0}(s) < C_2 e^{\Lambda_1 t_0} (1+s)^{-\nu_1}.$$

Here we define $\alpha_{t_0}(s)$ as follows

$$\alpha_{t_0}(s) = \sup_{G_1, G_2} \sup_{\substack{\mathcal{E}_1 \in \mathcal{F}_{G_1} \\ \mathcal{E}_2 \in \mathcal{F}_{G_2}}} |\mathbf{P}(\mathcal{E}_1 \cap \mathcal{E}_2) - \mathbf{P}(\mathcal{E}_1)\mathbf{P}(\mathcal{E}_2)|$$

with $\mathcal{F}_{G_1}$ and $\mathcal{F}_{G_2}$ are the following sigma-algebra : $\mathcal{F}_{G_1} = \sigma\{\tilde{f}(t_1, y_1') : y_1' \in G_1, t_1 \geq t_0\}$, $\mathcal{F}_{G_2} = \sigma\{\tilde{f}(t_2, y_2') : y_1' \in G_2, t_2 \geq t_0\}$. The first supremum is taken over all sets $G_1, G_2 \subset \mathbb{R}^2$ such that dist$(G_1, G_2) \geq s$.

H5 *For each $t_0 \geq 0$ the maximum correlation coefficient $\beta_{t_0}(s)$ of $\tilde{f}$ decays fast enough so that*

$$\exists \nu_2 > 2 \quad \exists C_3 > 0 \quad \exists \Lambda_2 > 0 \quad \forall s > 0 \quad \beta_{t_0}(s) < C_3 e^{\Lambda_2 t_0} (1+s)^{-\nu_2}.$$

with

$$\beta_{t_0}(s) = \sup_{G_1,G_2} \sup_{\xi,\mu} |\mathbf{E}(\xi\mu)|.$$

Here the second supremum is taken over all random variables ξ and μ wich are respectively $\mathcal{F}_{G_1}$- and $\mathcal{F}_{G_2}$-measurable and satisfy the conditions $\mathbf{E}\xi = \mathbf{E}\mu = 0$ and $\|\xi\|_{L^\infty(\Omega} = \|\mu\|_{L^\infty(\Omega} = 1$. The first supremum is taken over all sets $G_1, G_2 \subset \mathbb{R}^2$ such that dist$(G_1, G_2) \geq s$.

We have a result concerning the pointwise convergence in law :

Theorem 3 *Assume that condition* **H4** *or* **H5** *holds. Then for each $t > 0$ and $x \in \mathcal{D} \setminus \Sigma$, the normalized difference $\varepsilon^{-(d-1)/2}(u^\varepsilon(t,x) - u^0(t,x))$ converges in law toward a Gaussian random variable with zero mean and the covariance σ^2 given by :*

$$\sigma^2(t,x) = \int_0^t \int_0^t \int_\Sigma G(t,s,x,y')G(t,r,x,y')\bar{\bar{c}}(s,r)dy'dsdr. \tag{8}$$

3 Numerical simulations Tools

In this section, we define some tools and approaches used to perform the numerical simulations presented in this article. First, an approach using the problem linearity to compute the random solution u^ε is presented. Second, a way to compute σ^2 (see equation (8)) is presented. Finally, a classical distance is explained in order to evaluate the convergence in law.

3.1 Linearity and randomness : distribution and moment computations

In order to perform numerical computations for validation of the previous results of convergence, we are interested in a method to compute efficiently moments and distribution of u^ε, for a fixed ε. Usual approaches are Monte-Carlo methods which need to compute a large number of realization of the random source term and the corresponding solutions. It leads to numerically solve a large number of detailed problems (2), especially higher than the number of sources. Considering the high computation cost of one resolution, we choose an other approach, based on the linearity of the problem and the particular form (3) of the source term Q^ε. Though this approach uses a Monte-Carlo method to simulate the source randomness, it requires only a number of resolution equal to the number of sources, N^{d-1}.

3.1.1 "Decoupling" the time behavior of sources from their geometry

Let us define, for $\mathbf{i} \in I$, $f_{\mathbf{i}}(\omega, t) = \frac{1}{\varepsilon^\gamma} f(T_{\mathbf{i}}\omega, t)$, thus we can write (3) as

$$Q^\varepsilon(t,x) = \sum_{\mathbf{i}\in I} f_{\mathbf{i}}(\omega,t)\mathbb{1}_{B^\varepsilon_{\mathbf{i}}}(x).$$

Considering furthermore the family of problems indexed by $\mathbf{i} \in I$:

$$\partial_t u_{\mathbf{i}} + Au_{\mathbf{i}} = \delta_0(t)\mathbb{1}_{B^\varepsilon_{\mathbf{i}}}(x) \qquad \text{in } [0;T]\times\mathcal{D} \tag{9a}$$
$$u_{\mathbf{i}} = 0 \qquad \text{in } \{0\}\times\mathcal{D} \tag{9b}$$
$$(a(x)\nabla u_{\mathbf{i}} - \mathbf{b}(x)u_{\mathbf{i}})\cdot\mathbf{n}(x) = 0 \qquad \text{in } [0;T]\times(\partial\mathcal{D}\setminus\Gamma_d) \tag{9c}$$
$$u_{\mathbf{i}} = 0 \qquad \text{in } [0;T]\times\Gamma_d \tag{9d}$$

where $\delta_0(t)$ is the Dirac function in the variable t. We can now define :

$$U(\omega,t,x) = \sum_{\mathbf{i}\in I} \tilde{f}_{\mathbf{i}}(\omega,\cdot) * \tilde{u}_{\mathbf{i}}(\cdot,x)(t), \tag{10}$$

where $*$, the convolution product, is defined for two mappings $g, h : \mathbb{R}^p \to \mathbb{R}$ by :

$$\begin{aligned} g(\cdot) * h(\cdot) = g * h : \mathbb{R}^p &\longrightarrow \mathbb{R} \\ x &\longrightarrow \textstyle\int_{\mathbb{R}^p} g(x)h(x-y)dy. \end{aligned}$$

And where $\tilde{u}_{\mathbf{i}}(t,x)$ and $\tilde{f}_{\mathbf{i}}(\omega,t)$ are the extensions of $u_{\mathbf{i}}(t,x)$ and $f_{\mathbf{i}}(\omega,t)$ respectively on $\mathbb{R}\times\mathcal{D}$ and $\Omega\times\mathbb{R}$ by:

$$\tilde{u}_{\mathbf{i}}(t,x) \equiv \begin{cases} u_{\mathbf{i}}(t,x) & \text{if } t\in[0;T] \\ 0 & \text{otherwise} \end{cases} ; \; \tilde{f}_{\mathbf{i}}(\omega,t) \equiv \begin{cases} f_{\mathbf{i}}(\omega,t) & \text{if } t\in[0;T] \\ 0 & \text{otherwise} \end{cases}.$$

In order to simplify the notations, we will now assimilate $u_{\mathbf{i}}$ and $f_{\mathbf{i}}$ with their extensions when necessary.

Proposition 1 *$U(\omega,t,x)$ given by* (9) *and* (10) *is a solution of problem* (2).

Thus, equation (10) provides a direct expression of the solution u^ε of detailed problem (2) where the random terms $f_{\mathbf{i}}(\omega,t)$ explicitly appears. More precisely, expression (10) gives a splitting between the part coming from the random source behavior and the part coming from the convection-diffusion dynamic and the source geometry.

3.1.2 Distribution of $U(\omega,t,x)$

A numerical estimation of the distribution of $U(\omega,t,x)$ requires a sample of $U(\omega,t,x)$. Considering that U is a solution of the problem (2), a direct approach to obtain this sample could consist in simulating a sample of the source

term Q^ε and solving the problem (2) for each Q^ε sample element. A good sample of Q^ε must respect the variability of Q^ε. So, due to its particular form (3) constituted by N^{d-1} distinct sources, a good sample size is especially higher than N^{d-1}, the number of sources.

By using expression (10) of U and a good sample of Q^ε, we compute the associated sample of $U(\omega, t, x)$ by solving only N^{d-1} partial differential equations (the problem family (9)). With this approach, the Q^ε sample sizes effectively computable are particularly higher than with the previous direct approach since performing a time convolution are less expensive than solving the problem (2).

3.1.3 First order moments

With the expression of detailed problem's solution given by equation (10), we can compute the first moments of U.

Considering, for each $t \in [0;T]$, the stationarity of the "spatial" random process $f_{\mathbf{i}}(\cdot, t)$, we have $\mathbf{E}[f_{\mathbf{i}}(\cdot, t)] = \mathbf{E}[f_{\mathbf{j}}(\cdot, t)]$ for each $\mathbf{i}, \mathbf{j} \in I$. So, by denoting $\mathbf{E}f(t) = \mathbf{E}[f_{\mathbf{i}}(\cdot, t)]$, we can compute the first order moment of $U(\omega, t, x)$ for each $(t, x) \in [0;T] \times \mathcal{D}$:

$$\begin{aligned}\mathbf{E}[U(\cdot, t, x)] =& \sum_{\mathbf{i}\in I} \mathbf{E}[f_{\mathbf{i}}] * u_{\mathbf{i}}(\cdot, x)(t) \\ =& \sum_{\mathbf{i}\in I} \mathbf{E}f * u_{\mathbf{i}}(\cdot, x)(t) \\ =& \mathbf{E}f * \sum_{\mathbf{i}\in I} u_{\mathbf{i}}(\cdot, x)(t).\end{aligned}$$

Second order moment can also be computed by introducing the tensorial product $\otimes$, defined for two mappings $g : \mathbb{R}^p \to \mathbb{R}$ and $h : \mathbb{R}^q \to \mathbb{R}$ as :

$$\begin{aligned}g(\cdot) \otimes h(\cdot) = g \otimes h : \mathbb{R}^p \times \mathbb{R}^q &\longrightarrow \mathbb{R} \\ (x, y) &\longrightarrow g(x)h(y).\end{aligned}$$

Then, we can compute second order moment of U, for (t_1, x_1) and $(t_2, x_2) \in$

$[0;T]\times\mathcal{D}$:

$$\begin{aligned}\mathbf{E}[U(\cdot,t_1,x_1)U(\cdot,t_2,x_2)] =&\mathbf{E}\left[\sum_{\mathbf{i},\mathbf{j}\in I} f_{\mathbf{i}}*u_{\mathbf{i}}(\cdot,x_1)(t_1)f_{\mathbf{j}}*u_{\mathbf{j}}(\cdot,x_2)(t_2)\right]\\ =&\mathbf{E}\left[\sum_{\mathbf{i},\mathbf{j}\in I}(f_{\mathbf{i}}\otimes f_{\mathbf{j}})*(u_{\mathbf{i}}(\cdot,x_1)\otimes u_{\mathbf{j}}(\cdot,x_2))(t_1,t_2)\right]\\ =&\sum_{\mathbf{i},\mathbf{j}\in I}\mathbf{E}\left[f_{\mathbf{i}}\otimes f_{\mathbf{j}}\right]*(u_{\mathbf{i}}(\cdot,x_1)\otimes u_{\mathbf{j}}(\cdot,x_2))(t_1,t_2)\\ =&\sum_{\mathbf{i},\mathbf{j}\in I}\mathrm{Cov}(f_{\mathbf{i}},f_{\mathbf{j}})*(u_{\mathbf{i}}(\cdot,x_1)\otimes u_{\mathbf{j}}(\cdot,x_2))(t_1,t_2)\\ &+\mathbf{E}[U(\cdot,t_1,x_1)]\mathbf{E}[U(\cdot,t_2,x_2)],\end{aligned}$$

with

$$\mathrm{Cov}(f_{\mathbf{i}},f_{\mathbf{j}})(t_1,t_2)\equiv\mathbf{E}\left[f_{\mathbf{i}}(t_1)f_{\mathbf{j}}(t_2)\right]-\mathbf{E}[f_{\mathbf{i}}(t_1)]\mathbf{E}[f_{\mathbf{j}}(t_2)].$$

3.1.4 Expectation of $\|u^\varepsilon-u^0\|^2_{L^2(0,T;L^2(\mathcal{D}))}$

Calculation of second order moments is useful for computation of the error given in Theorem 2. Indeed, we can develop error expression (6) as

$$\begin{aligned}\mathbf{E}\left[\|u^\varepsilon-u^0\|^2_{L^2(0,T;L^2(\mathcal{D}))}\right]=&\underbrace{\mathbf{E}\left[\|u^\varepsilon\|^2_{L^2(0,T;L^2(\mathcal{D}))}\right]}_{=I_1}\\ &-2\underbrace{\mathbf{E}<u^\varepsilon,u^0>_{L^2(0,T;L^2(\mathcal{D}))}}_{=I_2}+\underbrace{\mathbf{E}\left[\|u^0\|^2_{L^2(0,T;L^2(\mathcal{D}))}\right]}_{=I_3},\end{aligned}$$

where I_3 is explicit since u^0 is deterministic, $I_2=<\mathbf{E}u^\varepsilon,u^0>_{L^2(0,T;L^2(\mathcal{D}))}$ and

$$\begin{aligned}I_1=&\int_0^T\int_{\mathcal{D}}\mathbf{E}\left[u^\varepsilon(t,x)^2\right]dxdt\\ =&\int_0^T\int_{\mathcal{D}}\left[\mathbf{E}[u^\varepsilon(t,x)]^2+\left(\sum_{\mathbf{i},\mathbf{j}\in I}\mathrm{Cov}(f_{\mathbf{i}},f_{\mathbf{j}})*(u_{\mathbf{i}}(\cdot,x)\otimes u_{\mathbf{j}}(\cdot,x))(t,t)\right)\right]dxdt\\ =&\|\mathbf{E}u^\varepsilon\|^2_{L^2(0,T;L^2(\mathcal{D}))}\\ &+\int_0^T\sum_{\mathbf{i},\mathbf{j}\in I}\mathrm{Cov}(f_{\mathbf{i}},f_{\mathbf{j}})*\left(\int_{\mathcal{D}}u_{\mathbf{i}}(\cdot,x)\otimes u_{\mathbf{j}}(\cdot,x)dx\right)(t,t)dt,\end{aligned}$$

and finally :

$$\begin{aligned}\mathbf{E}\left[\|u^\varepsilon-u^0\|^2_{L^2(0,T;L^2(\mathcal{D}))}\right]=&\|\mathbf{E}u^\varepsilon-u^0\|^2_{L^2(0,T;L^2(\mathcal{D}))}\\ &+\int_0^T\sum_{\mathbf{i},\mathbf{j}\in I}\mathrm{Cov}(f_{\mathbf{i}},f_{\mathbf{j}})*\left(\int_{\mathcal{D}}u_{\mathbf{i}}(\cdot,x)\otimes u_{\mathbf{j}}(\cdot,x)dx\right)(t,t)dt.\quad(11)\end{aligned}$$

Theorems 3 need to compute the quantity (see (8)) :

$$\sigma^2(t,x) = \int_0^t \int_0^t \int_\Sigma G(t,s,x,y')G(t,r,x,y')\bar{\bar{c}}(s,r)dy'dsdr$$

where (t,x) is a point of $\mathbb{R}_+ \times (\mathcal{D} \setminus \Sigma)$. This quantity require to know the Green function, $G(t,s,x,y)$, of problem (2). For a fixed $(s,y) \in [0;T] \times \mathcal{D}$, the Green function can be defined as the solution of the following problem, parametrized by (s,y) :

$$\begin{cases} \partial_t G(t,s,x,y) + AG(t,s,x,y) = \delta_s(t)\delta_y(x) & \text{for } (t,x) \in [0;T] \times \mathcal{D}, \\ G(t,s,x,y) = 0 & \text{for } (t,x) \in \{0\} \times \mathcal{D}, \\ (a(x)\nabla G(t,s,x,y) - \mathbf{b}(x)G(t,s,x,y)) \cdot \mathbf{n} = 0 & \text{for } (t,x) \in [0;T] \times (\partial\mathcal{D} \setminus \Gamma_d), \\ G(t,s,x,y) = 0 & \text{for } (t,x) \in [0;T] \times \Gamma_d \end{cases}$$

where $\delta_y(x)$ is the space Dirac function at y and $\delta_s(t)$ is the time Dirac function at s.

No explicit formulation of this Green function is known, so it can only be estimated by partial differential equation simulations. Estimating entirely the Green function need to compute and to store a partial differential equation solution for each $(s,y) \in [0;T] \times \mathcal{D}$. This can be extremely costly but it appears that an entire estimation is not necessary to compute σ^2. First, given that equation parameters A, a and $\mathbf{b}$ are constant in time, we have $G(t,s,x,y) = G(t-s,0,x,y)$. Second, equation (8) need to know $G(t,s,x,y)$ only for $y \in \Sigma$. Finally, we are interested to know $G_0(x,t,y) = G(t,0,x,y)$ for x, $t \in [0,T]$ and $y \in \Sigma$. Thus $\sigma^2(t,x)$ can now be written as :

$$\sigma^2(t,x) = \int_\Sigma (G_0(x,\cdot,y') \otimes G_0(x,\cdot,y')) * \bar{\bar{c}}(\cdot,\cdot)(t,t)dy'. \tag{12}$$

For a given value of the parameter y, $G_0(x,t,y)$ is computed by solving one partial differential equation. So, complying with the partial differential equation spatial discretization, G_0 is entirely computed by solving a number of partial differential equation equal to the number of discrete elements constituting Σ.

3.3 Evaluation of the distance between distributions of random variables

In order to illustrate the Theorem 3 result, we are interested to define a quantity characterizing the "distance" between the distribution of two random variables. To do this, we propose to use the Kolmogorov-Smirnov distance (see [3]).

Considering $X, Y : \Omega \to \mathbb{R}^k$ two random variables, we define the cumulative distribution functions of X and Y, F_X and $F_Y : \mathbb{R} \to [0; 1]$, by :

$$\forall \mathbf{x} \in \mathbb{R} \quad F_X(\mathbf{x}) = \mathbf{P}(X^{-1}(M(\mathbf{x}))) \quad \text{and} \quad F_Y(\mathbf{x}) = \mathbf{P}(Y^{-1}(M(\mathbf{x})))$$

where $M(\mathbf{x}) = \{\mathbf{y} \in \mathbb{R} : \mathbf{y} \leq \mathbf{x}\}$. Let us recall the definition of Kolmogorov-Smirnov distance (see [3]) :

Definition 1 *Let $X, Y : \Omega \to \mathbb{R}$ be two random variables, the Kolmogorov-Smirnov distance between the distributions of X and Y is defined by :*

$$D_{KS}(F_X, F_Y) = \|F_X - F_Y\|_{L^\infty(\mathbb{R})}.$$

In the following, this Kolmogorov-Smirnov distance will be used to compare an empirical distribution to a theoretical distribution. In this case, $F_X(\mathbf{x})$ is known and $F_Y(\mathbf{x})$ is estimated by the empirical cumulative distribution function $\hat{F}_Y$ given by :

$$\hat{F}_Y(\mathbf{x}) = \frac{1}{N_s} \sum_{i=1}^{N_s} \mathbb{1}_{M(\mathbf{x})}(\mathbf{y^i})$$

where $\mathbf{x} \in \mathbb{R}$ and $\{\mathbf{y}^i\}_{i=1..N_s}$ is a sample of size N_s of the random vector Y.

4 Numerical results

In this section, our goal is to illustrate by numerical simulations the theoretical results described in section 2. After a description of the test case, we present the comparisons between u^ε and u^0,the solutions of the detailed model (2) and the homogenized model (4). More precisely, we first compute the error defined in Theorem 2 for several ε (Figures 7). Then, we compute, for several ε, a distance between the distributions of $\varepsilon^{-(d-1)/2}(u^\varepsilon(t_j, x_j) - u^0(t_j, x_j))$ and a centered Gaussian distribution with variance (σ^2) (Figure 8).

In the following, all the numerical computations of partial differential equations have been done with the *Cast3m* software (see [4]). This software devel-

oped by the Commissariat à l'Energie Atomique (France) is devoted to numerical resolution of classical mechanics equations. Numerous choice are possible in term of discretization. All the following numerical simulations have been performed with a Mixed Hybrid Finite Element Method for spatial discretization, and an Implicit Scheme for the time discretization.

4.1 Setting test case

The geometry and the physical characteristics considered describe a synthetic case and don't represent a real waste repository. But these results may be useful to better understand real waste depository.

4.1.1 Geometry and equation coefficients

For sake of simplicity, the geometry of the test case is two-dimensional, *i.e.* $d = 2$. The domain $\mathcal{D}$ is taken as a rectangular domain : $\mathcal{D} = [-750\,m; 2250\,m] \times [-400m; 400m]$, Γ_d is taken as the top of the domain : $\Gamma_d = [-750m; 2250m] \times \{400\,m\}$ and the length of the inside repository is $L = 1500\,m$ (see Figure 6). The size of a source in local variables (see (1)) is given by $s_1 = 7\ 10^{-1}$, $s_2 = 5\ 10^{-2}$ and $\gamma = 1$.

The test case is defined with :

- a spatially constant diffusion tensor, $a(x) = 10^{-1} m^2/years$ for each $x \in \mathbb{R}^k$;
- a null convection, $\mathbf{b}(x) = 0\,m/years$ for each $x \in \mathbb{R}^k$;
- a radioactive decay constant fixed to $\lambda = 4.415\ 10^{-8}\, years^{-1}$ (characteristic of a radioactive element such ^{129}I).

4.1.2 Random source term

Let $f : \Omega \times [0, T] \to \mathbb{R}$ be the random function given by :

$$f(\omega, t) = \begin{cases} e^{-\lambda t} M_1/t_1(\omega) & \text{if} \quad 0 < t - t_0 \leq t_1(\omega) \\ e^{-\lambda t} M_2/t_2(\omega) & \text{if} \quad 0 < t - t_0 - t_1(\omega) \leq t_0 + t_1(\omega) + t_2(\omega) \\ 0 & \text{otherwise} \end{cases}$$

where $t_1(\omega)$ and $t_2(\omega)$ are two independent random variables such that $\log(t_1)$ and $\log(t_2)$ are normal random variables respectively with parameters (expectation and standard deviation) of $(m_{Lt_1}, \sigma_{Lt_1})$ and $(m_{Lt_2}, \sigma_{Lt_2})$. The numerical values of all those parameters are given in Table 1.

	$mol.m^{-2}$		$years$	$\log(years)$			
Parameter	M_1	M_2	t_0	m_{Lt_1}	σ_{Lt_1}	m_{Lt_2}	σ_{Lt_2}
Value	$2\ 10^{-3}$	3.998	$4\ 10^3$	2.112	0.7196	13.80	0.7806

Table 1
Numerical values of parameters of f

By defining a such source term, the test case is in accordance with assumptions. Teh expectation and variance of f are plotted on Figure 4 and Figure 5.

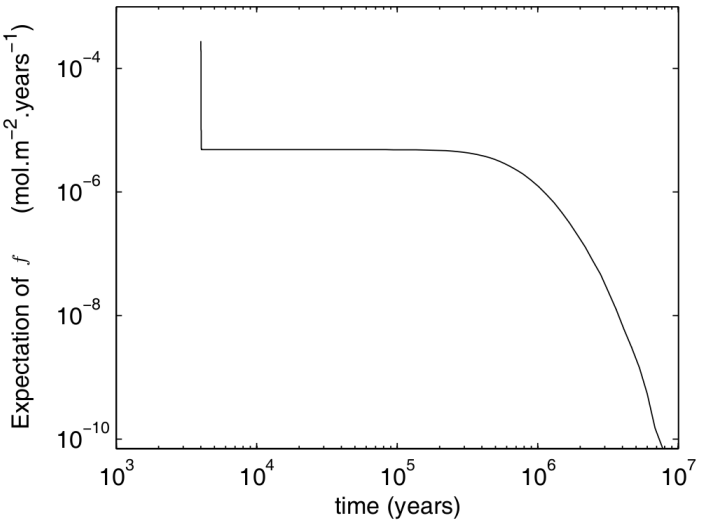

Fig. 4. Time evolution of $\mathbf{E}[f(\cdot,t)]$

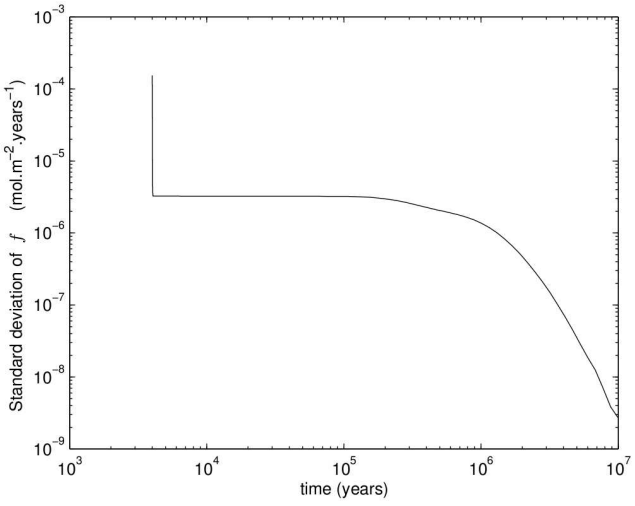

Fig. 5. Time evolution of $\sqrt{\mathrm{Var}[f(\cdot,t)]}$

4.1.3 Observation points

Numerical validation of Theorem 3 result requires to define some points of $\mathbb{R}_+ \times (\mathcal{D} \setminus \Sigma)$, where the field randomness is simultaneously observed. Since the previous homogenization results concern especially the far field, in the following we consider two physical points far from the sources. The first point, $x_A = (750\,m, 200\,m)$, is taken far from the domain boundaries and the second point, $x_B = (750\,m, 350\,m)$, near from the top of the domain (see Figure 6). We also define the two times $t_1 = 10^5$ *years* and $t_2 = 10^6$ *years*. This two times are chosen such that concentrations respectively at points x_A and x_B are non negligible.

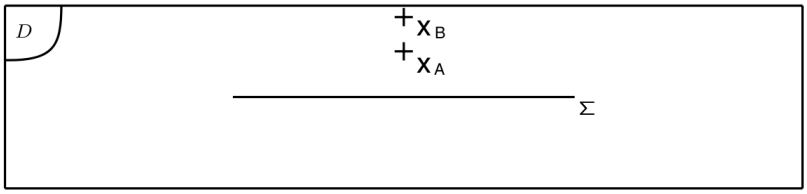

Fig. 6. Test case domain and observation points

4.2 Convergence to u^0

Figure 7, the evolution of $\mathbf{E}\|u^\varepsilon - u^0\|^2_{L^2(0,T;L^2(\mathcal{D}))}$ versus ε is plotted in solid line. The behavior of the Theorem 2 upper bound is plotted in dotted line. Numerical results are in accordance with result (6). More precisely, they suggest a decrease rate in a power of ε greatest than 2.

4.3 Convergence in law

Let X denote the following random variable:

$$X = \varepsilon^{-(d-1)/2}(u^\varepsilon(t_j, x_j) - u^0(t_j, x_j)).$$

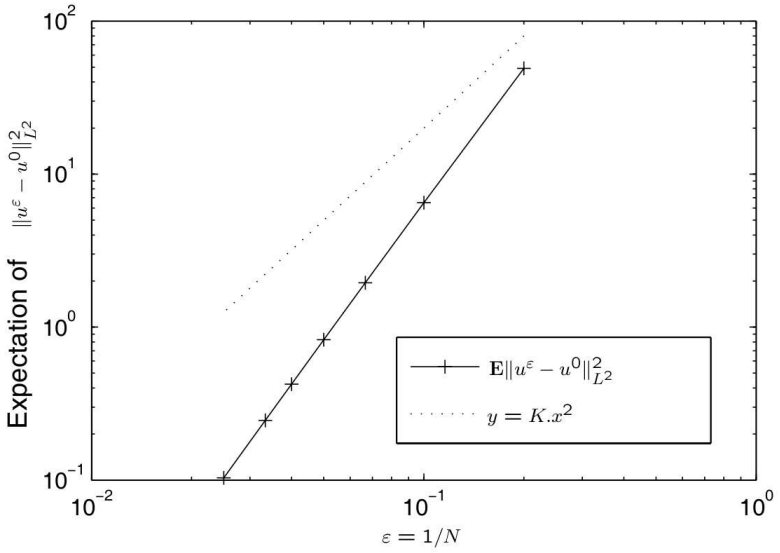

Fig. 7. Evolution of $\mathbf{E}\|u^\varepsilon - u^0\|^2_{L^2(0,T;L^2(\mathcal{D}))}$ vs. ε

Theorem 3 gives the convergence in law of X to a gaussian random variable with zero mean and σ^2 variance (see (8)). This convergence is illustrated by the computation of the Kolmogorov-Smirnov distance.

The time-space observation point sets considered are constituted of the two spatial points x_A and x_B and the two times t_1 and t_2 as defined in section 4.1.3. More precisely, we consider the observation point sets specified in Table 2. The empirical cumulative distribution $\hat{F}_Y$ is estimated on a sample of u^ε. The sample have a size equal to 2000, it is computed by simulating the random source term f and by using Equation (10).

$\{(t_1, x_A)\}$	$\{(t_1, x_B)\}$	$\{(t_2, x_A)\}$	$\{(t_2, x_B)\}$

Table 2
Time-space observation point sets considered for the computation of $D_{KS}(\hat{F}_Y, F_{N_0})$

4.3.1 Statitical noise

Due to a statistical noise, $D_{KS}(\hat{F}_Y, F_{N_0})$ cannot be strictly null, even Y follows also the standard gaussian normal law. It means that, $D_{KS}(\hat{F}_{N_0}, F_{N_0})$ is a positive random variable which can be assimilated with a residual noise of D_{KS} for empirical distributions. This residual noise depends upon the sample size. To include this effect in the following results, 100 samples of N_0 of size 2000 have been simulated . Expectation and variance of the residual noise $D_{KS}(\hat{F}_{N_0}, F_{N_0})$ have been estimated from these simulations and are mentioned in Table 3. In the following figures plotting $D_{KS}(\hat{F}_Y, F_{N_0})$, these noise characteristics will be plotted to visualize the quality of our results.

Expectation	$1.43\ 10^{-2}$	Variance	$0.82\ 10^{-2}$

Table 3
Characteristics of the residual noise $D_{KS}(\hat{F}_{N_0}, F_{N_0})$ for a size sample equal to 2000

Figure 8, evolutions of $D_{KS}(\hat{F}_Y, F_{N_0})$ versus ε are plotted,corresponding to the Theorem 3 configuration. The convergence in law is observed for all observation points. Indeed, for ε small enough, values of $D_{KS}(\hat{F}_Y, F_{N_0})$ decrease with ε to become of residual noise order.

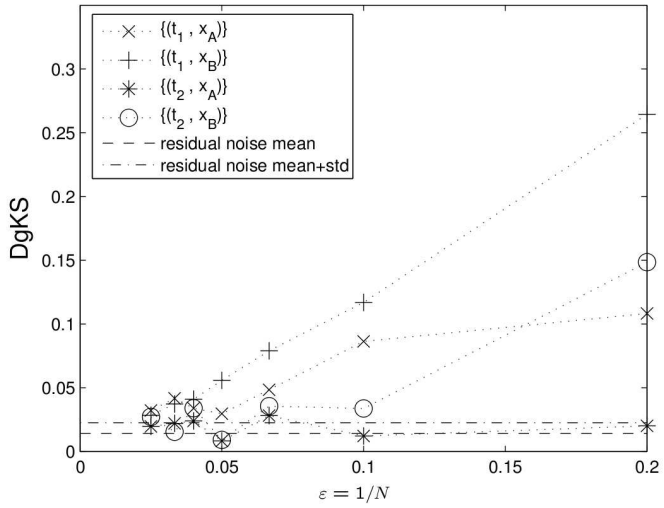

Fig. 8. Evolution of D_{KS} vs. ε

Aknowledgements The work of the authors has been partially supported by the grant from the CNRS/ANDRA/BRGM/CEA/EDF/IRSN GDR 2439, the grant CNRS n° 9588 - IRSN n° CA 31002716 and the European Integrated Project PAMINA n° 036404.

References

[1] Alain Bourgeat and Andey Piatnitski, *Homogenization of a diffusion convection equation, with random source terms periodically distributed*, Preprint Institut Camille Jordan 2008.

[2] J. L. Doob, *Stochastic Processes*, Wiley Publications in Statistics, 1953.

[3] D.R. Cox and D.V. Hinkley, *Theoretical Statisics*, Chapmann and Hall Editors, 1974.

[4] www-cast3m.cea.fr.

[5] A. Bourgeat, E. Marusic-Paloka. A homogenized model of an underground waste repository including a disturbed zone. SIAM J. on Multiscale Modeling and Simulation, Vol.3, Number 4 ; Pages 918 - 939, 2004.

[6] 1. A.Bourgeat, O. Gipouloux, E. Marusic-Paloka. Mathematical Modeling of an underground waste disposal site by upscaling. Math. Meth. Appli. Sci., Volume 27, Issue 4; March 2004, p 381-403.