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MATHEMATICAL MODELLING AND DESIGN EXPERIMENTS IN BIOVENTING SUBSOIL DECONTAMINATION

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Summary. Bioventing is a subsoil bio-remediation technique which improves the activity of bacteria to transform contaminants into less hazardous compounds by inflating air through wells. The mathematical model describes the bacteria population dynamics and the dynamics of a multiphase, multicomponent fluid in porous media and in this paper a simple version of it will be described. A critical point of the design problem is to choose well positions and air flow rates to optimise the biodegradation process. The numerical simulation and some initial optimisation design results for the simple model proposed will be reported. The decontamination time required for different flow rates and for different well spatial configurations will be compared.

1 INTRODUCTION

Bioventing is a technique used to decontaminate polluted subsoil by exploiting the action of bacteria which biodegrade the pollutant and it is an *in situ* method since no soil removal is required.

The bacteria biodegradation activity requires oxygen and air – or oxygen – circulation is induced in the subsoil by means of injection and/or extraction wells.

The mathematical model reported in this paper provides for the presence, in the subsoil, of air and pollutants; moreover the dynamics of the population bacteria and the pollutant biodegradation are described. A more general model is in [10] and this paper reports a very simple model, useful for simulation and optimal design aims.

2 THE SIMPLIFIED MATHEMATICAL MODEL

The mathematical model is based on the classical continuum approach for the fluid flows in porous media [1], [4]; multi phase and multi component fluids are considered and the presence and the activity of bacteria is also described.

The following simplifying hypotheses are adopted: three different phases are present in the system: the *air* gas phase, the *pollutant* phase and the *bacteria* phase. The water phase is not considered: it is absent or, alternatively, it is present in a very small quantity and it is supposed to be immobile. The pollutant phase is unmiscible and immobile. The gas phase is mobile and is formed of two components, an oxygen part and a non–oxygen part. A classical population dynamics mathematical model [8] is used to describe bacteria diffusion and growth; we suppose that bacteria do not take up significant room in the void space of the porous media and, therefore, their presence do not change the volume of the pore space. Bacteria concentration is a function which depends on space and time.

2.1 Introductory definitions and notations

In order to describe the model some definitions are required: there are quantities which only depend on the space domain and some others vary in time and space. The following notation will be adopted:

- $\Phi(x)$ is the total volume of the pore space
- $\Phi_C(t,x)$ is the volume of the phase pollutant in the pore space
- $\Phi_G(t,x)$ is the volume of the phase gas in the pore space

and, therefore, we have:

$$\Phi = \Phi_C + \Phi_G \tag{1}$$

Now, we can define the saturation of the gas and pollutant phases. The pollutant saturation is:

$$C(t,x) = \frac{\text{volume of the phase } \textit{pollutant}}{\text{pore space volume}} = \frac{\Phi_C}{\Phi} \tag{2}$$

The gas saturation is:

$$G(t,x) = \frac{\text{volume of the phase } \textit{gas}}{\text{pore space volume}} = \frac{\Phi_G}{\Phi} \tag{3}$$

Then, the following equality holds:

$$C + G = 1 \tag{4}$$

We suppose that the gas phase consists of air only; in the air, we will distinguish two components: the *oxygen* part and the *non–oxygen* part. Therefore, for the air gas phase, we denote with the space dependent variable $X_O(t,x)$ the oxygen mass fraction in the gas phase:

$$X_O(t,x) = \frac{\text{oxygen density in the gas phase}}{\text{gas phase density}} \tag{5}$$

and with the space dependent variable $X_N(t,x)$ the non–oxygen mass fraction in the gas phase:

$$X_N(t,x) = \frac{\text{density of non–oxygen components in the gas phase}}{\text{gas phase density}} \tag{6}$$

From the definition of X_O and X_N, in each point of the space domain we have that:

$$X_O + X_N = 1 \tag{7}$$

2.2 Phase and component equations

The continuity equations and the generalized Darcy law for multi phase flow are used to write the equations of the model. The pollutant saturation C is an unknown and, since pollutant is not subject to movement, we have the following equation:

$$\frac{\partial}{\partial t}(\Phi C \rho_C) = q_C \tag{8}$$

where q_C is the pollutant reactive source term.

The gas phase involves four unknowns G, X_O, X_N and p_G (the pressure of gas phase). We have two equations, the first for the oxygen part of the air:

$$\begin{aligned}\frac{\partial}{\partial t}(\Phi G X_O \rho_O) &= \mathbf{div}\left(X_O \rho_O \frac{k_g}{\mu_G}\boldsymbol{K}(\mathbf{grad}\ p_G)\right) + \\ &\quad \mathbf{div}\ (\Phi G \boldsymbol{D}_O \quad \mathbf{grad}\ X_O \rho_O) + q_O + r_O\end{aligned} \tag{9}$$

and the second equation for the non oxygen part of the air:

$$\begin{aligned}\frac{\partial}{\partial t}(\Phi G X_N \rho_N) &= \mathbf{div}\left(X_N \rho_N \frac{k_g}{\mu_G}\boldsymbol{K}(\mathbf{grad}\ p_G)\right) + \\ &\quad \mathbf{div}\ (\Phi G \boldsymbol{D}_N \quad \mathbf{grad}\ X_N \rho_N) + r_N\end{aligned} \tag{10}$$

where q_O is the oxygen reactive source term and r_O, r_N represent air external source terms.

In order to write the equation describing the bacteria population dynamics we suppose that the micro–organisms which biodegrade the pollutant are not subject to convective movements but they are only subject to *Fick*ian diffusion; their growth and death are regulated by appropriate coefficients. Thus, their spatial concentration, denoted by B (an unknown), satisfies the following diffusion and reaction continuity equation [8]:

$$\frac{\partial}{\partial t}B = D_B \boldsymbol{\Delta} B + gB - dB \tag{11}$$

where $\boldsymbol{\Delta}$ is the Laplace operator; g and d will be subsequently defined and they represent the microorganism growth and decay rate, respectively.

In equations (8), (9), (10) and (11) the following constant parameters appear:

$\boldsymbol{K}$ the intrinsic permeability tensor;

k_G the relative permeability of the gas phase;

μ_G the dynamic viscosity of the gas phase;
ρ_C the pollutant density ;
ρ_O the oxygen density ;
ρ_N the non-oxygen part of air density ;
$\boldsymbol{D}_O$ the dispersion tensor of the oxygen in the gas phase;
$\boldsymbol{D}_N$ the dispersion tensor of the non oxygen part in the gas phase;
D_B the bacteria diffusion coefficient;

In bacteria equation (11) we assume that d – the death rate – is a positive constant: it means bacteria death proportionally to their concentration in each point of the spatial domain.

In order to define the growth rate g in equation (11) we assume that bacteria grow only where both oxygen and hydrocarbon are available and, also, their spatial concentration is subject to a logistic type limitation. Then, g is based on the product of three factors:

$$g(C_T, O_T) = \frac{\beta_C C_T}{K_C + C_T} \frac{\beta_O O_T}{K_O + O_T} \frac{B_{max} - B}{B_{max}} \tag{12}$$

where $C_T = \Phi \rho_C C$ denotes the pollutant spatial concentration and $O_T = \Phi \rho_O X_O G$ denotes the oxygen spatial concentration. The first of the three factors in (12):

$$\frac{\beta_C C_T}{K_C + C_T} \tag{13}$$

is of Monod type and it becomes zero as C_T approaches zero. The constant β_C is the hydrocarbon *asymptotic maximum specific growth rates*, that is for large values of C_T the factor tends to β_C. Moreover in (13) K_C denotes the pollutant *half specific velocity constants* : for $C_T = K_C$ then (13) assumes the value $\beta_C/2$. The second factor in (12) is the oxygen Monod term and the oxygen *asymptotic maximum specific growth rates* β_O and the oxygen *half specific velocity constants* K_O play, in that factor, the same role as β_C and K_C in the first factor. The third term in (12) is a logistic limiting factor: when B increases and tends to B_{max} then the factor tends to zero: B_{max} represents the maximum bacteria spatial concentration supported by the environment.

For a complete description of the equations (8) and (9), it is necessary to define their reactive source terms. During the decontamination intervention the spatial concentration of pollutant and oxygen change and the terms q_C, q_O in (8) and (9) give a modelling description of the phenomenon. We suppose that part of pollutant and oxygen are converted into bacteria cell mass that is, in a time unit, in each point of the domain an increase of B corresponds to a decrease of C and O. Moreover, oxygen and pollutant are used in the microbial endogenous metabolism, that is, in a time unit, in each point of the domain the presence of B consumes C and O. Then the pollutant decay term in (8) is:

$$q_C = -\frac{1}{Y_C} g(C_T, O_T) B - M_C O_T C_T B \tag{14}$$

where the function $g(C_T, O_T)$ is defined in (12); the constant parameters Y_C and M_C are the hydrocarbon *yield coefficient* and *metabolic consumption constant*, respectively. In (9) the oxygen reactive decay term is:

$$q_O = -\frac{1}{Y_O}\{g(C_T, O_T) - d\}\, B - M_O\, O_T\, C_T\, B \tag{15}$$

where Y_O and M_O are, respectively, the oxygen *yield coefficient* and *metabolic consumption constant*. The presence of the constant d in (15) means that when bacteria die, some oxygen is released into the environment.

In (9) and (10) r_O and r_N are time dependent external gas source terms. They represent the air injection or extraction wells and they are defined in all the points of the spatial domain of the model and vary in time. We have:

$$r_O = p\Sigma(\boldsymbol{x}, t) \qquad \text{and} \qquad r_N = (1-p)\Sigma(\boldsymbol{x}, t) \tag{16}$$

where p is the oxygen fraction of the air in the atmosphere and $\Sigma(\boldsymbol{x}, t)$ is the time and spatial domain dependent function describing the source air flow. In particular, in order to represent wells located in a fixed finite number of points in the space domain, the function $\Sigma(\boldsymbol{x}, t)$ assumes the following form:

$$\Sigma(\boldsymbol{x}, t) = \rho_G \sum_{i=1}^{N} Q_i(t)\ \delta(\boldsymbol{x} - \boldsymbol{x}_i) \tag{17}$$

where the $\boldsymbol{x}_i$ $(i = 1, ..., N)$ are the spatial positions of the wells. The function $\delta(\cdot)$ is the Dirac delta function and, for $i = 1, ..., N$, Q_i is the volumetric flow rate of the well in position $\boldsymbol{x}_i$; a positive value of Q_i indicates an injection well and a negative value indicates an extraction well. The constant ρ_G is the gas phase density and it is defined as $\rho_G = \rho_O X_O + \rho_N X_N$;

In conclusion, the simplified mathematical model is formed by the spatial time evolution equations (8), (9), (10), (11) and from the relations (1),(4). The unknowns are C, G, X_O, X_N, p_G and B.

3 SIMULATION RESULTS

The simulation experiments reported in this paper do not refer to a real case but they are useful for verifying the functionality of the model. We suppose that the spatial domain is a two dimensional circular domain with radius 75 and centered in $(75, 75)$; therefore, from the modelling point of view the injection wells are point sources (see eq. (17)). In practice, in the simulation, the wells are treated as small hole inside the domain, with assigned flow boundary conditions.

In the computations, further reductions are introduced in comparison with the model shown in Section 2: we suppose that the pollutant saturation is relatively small compared with the gas saturation and, therefore, $G(t, x) = 1$. Moreover, if we suppose that pure oxygen is inflated in the subsoil, then $X_N = 0$ and equations (9) and (10) can be substituted by the single oxygen equation (9) with $X_O = 1$. In this situation the classical ideal gas state law permits expression of the gas pressure p_G in terms of ρ_O: so in the equation (9) the only unknown remains ρ_O.

Therefore, the model is reduced to a system of three partial differential equations of reaction diffusion type describing: pollutant, oxygen and bacteria spatial evolution; the three equations are only coupled by the source reactive terms. The system has been solved using the software COMSOL Multiphysics© (transient analysis of the diffusion module).

In all simulations the soil characteristics – porosity and permeability – are homogeneous isotropic and constants; the initial spatial distribution of the pollutant is:

$$C_0(x, y) = 10e^{-\frac{(x-65)^2+(y-75)^2}{225}} + 10e^{-\frac{(x-85)^2+(y-75)^2}{225}} \tag{18}$$

The initial bacteria concentration is 0.1 uniformly in the spatial domain and the initial spatial oxygen concentration is zero. For bacteria, oxygen and pollutant, zero flux boundary conditions are considered. The following values are assigned to the constants in the reactive terms: $\beta_C = \beta_O = K_C = K_O = 1$, $B_{max} = 1$, $d = 0.01$, $Y_O = Y_C = 1$, $M_O = 0.08$, $M_C = 0.01$.

We will define the *decontamination time* as the time required to reduce the pollutant subsoil concentration to below a fixed required level in all the points of the domain: that is we will control the maximum concentration value in the spatial domain.

Starting from some fixed initial conditions, the *decontamination times* corresponding to different well configurations and/or flow rates have been compared. In particular three significant experiments are reported; we suppose that it is required to reduce the pollutant concentration to below a level of the order of 10^{-2}. Figure 1 shows the spatial pollutant concentration before the decontamination intervention. In the first experiment only one injection well with flow rate equal to 50 is located in the center of the circle and the time required to achieve the pollutant security level is $t = 391$ and Figure 2 shows the spatial pollutant concentration at time $t = 391$. The second experiment is similar to the first but the flow rate is equal to 100 and the decontamination time is $t = 293$, see Figure 3. In the third experiment two injection wells are located in $(65, 75)$ and $(85, 75)$ each one of them with flow rate equal to 50 and the decontamination time is $t = 237$. For this experiment Figures 4, 5 and 6 show pollutant, bacteria and oxygen spatial concentrations, respectively. Comparing the first and the second experiment we can see that there is a reduction in the decontamination time of one third but the flow rate is doubled. In the third experiment there is a time reduction using the same flow rate as the second experiment.

4 CONCLUSIONS AND FINAL NOTES

In this paper a simple mathematical model for a bio-remediation system has been described and the results of some simulation have been reported.

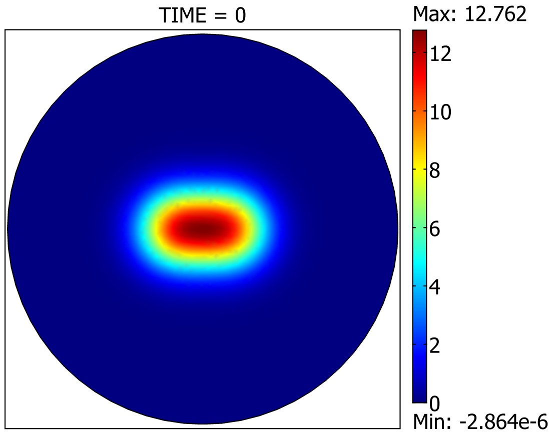

Figure 1: Initial pollutant concentration

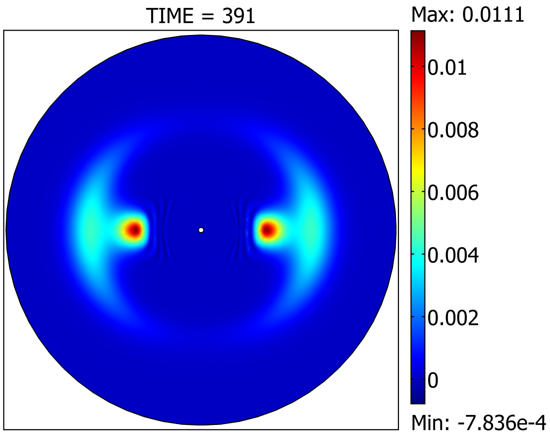

Figure 2: One well: final pollutant concentration, flow = 50

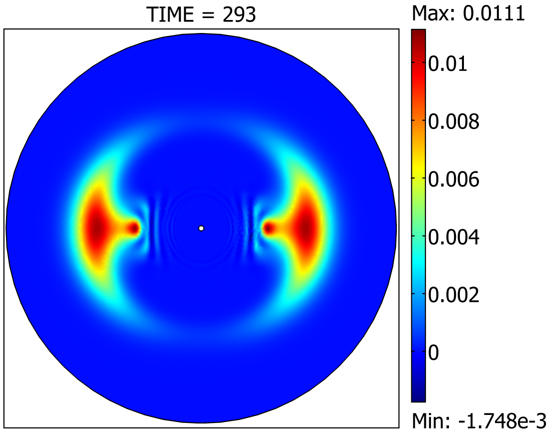

Figure 3: One well: final pollutant concentration, flow = 100

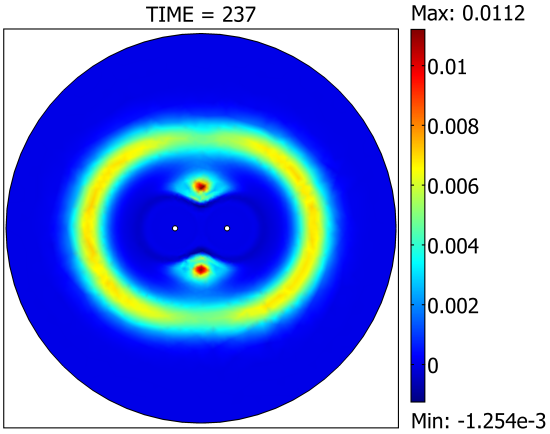

Figure 4: Two wells: final pollutant concentration, total flow = 100

In different situations, the times required for the decontamination intervention have been compared: in this case the minimization of the intervention time – with assigned limited resource, that is the total flow rate – is considered to be the design objective. Other choice are possible for the design objective: minimising the cost and so on.

As regards the model used in the simulations, further developments are: to simulate the complete model exhibited in section 2 and to consider a non-homogeneous subsoil.

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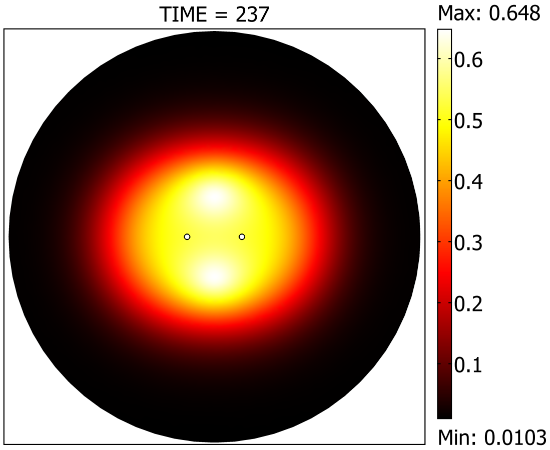

Figure 5: Two wells: final bacteria concentration, total flow = 100

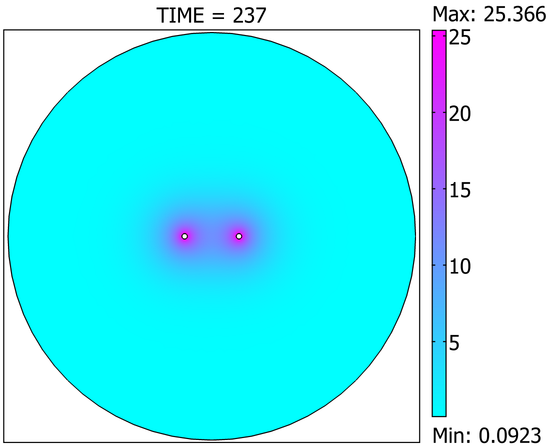

Figure 6: Two wells: final oxygen concentration, total flow = 100

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