Soil venting

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Abstract

Soil venting is a technique for remediation of soils contaminated by NAPLs (non aqueous phase liquids, often called VOCs, i.e., volatile organic compounds). During the operation of soil venting systems the vapor phase of the nonaqueous phase liquid NAPL is being removed by imposing a convective air stream and thus enhancing the evaporation of the fluid phase of the NAPL in contaminated regions of the soil.

In mathematical terms, this multi-phase multi-component process is described by a system of nonlinear parabolic equations. The variables therein are mass and volume fractions of the chemical components involved and the pressures of the different phases. Assuming that the mathematical model has been chosen appropriately, two major steps have to be performed:

“Calibration” of the model. This can be done only for each case separately, since the geological structure of the soil and the spatial distribution of the contaminants have to be taken into account. In addition, due to lack of data and to measurement errors, simulations are possible only in a statistical sense, i.e., conditional Monte-Carlo simulations have to be performed.

“Optimization” of the remediation procedure. The control variables are the number and position of extraction wells (and/or injection wells) and the extraction rates. Since the whole process may take many years, even “sub-optimal” strategies could be of great value.

Keywords

Multi-phase and multi-component transport, porous media, soil venting, remediation

1 INTRODUCTION

In recent years, contamination of ground water by industrial waste has become a serious problem. Benzene, mineral oil, solvents, or other organic compounds entering the subsurface may be a serious and potentially long-term hazard for the environment, e.g., soils and

Figure 1 Contaminated soil

ground water systems, see figure 1. For removing volatile organic compounds (VOCs) from the water-unsaturated zone of contaminated soils commonly the vapor extraction method is used. During the operation of soil venting systems the vapor phase of the nonaqueous phase liquid VOC is being removed by imposing a convective air stream and enhancing the evaporation of the fluid phase of the VOCs in contaminated regions of the soil. Frequently, soil venting systems are designed empirically, using extensive experimental studies and observations.

The major problems that the *engineer* has to solve are these:

1. *Exploration and Installation:* This means, he has to find out and describe the spatial distribution of the pollution and the geology, i.e., the soil properties of the site. And he has to decide which type of the clean-up procedure should be chosen.
2. *Monitoring and Maintenance:* He has to monitor the extraction rates and maintain the machinery and equipment. And he has to decide on modifications, if necessary.
3. *Stopping Criteria:* He has to decide at what time the remediation process may be stopped.

The major problems that the *scientist*, i.e. the mathematician, soil physicist, or soil chemist has to solve are these:

1. *General Model:* An appropriate mathematical physical chemical model has to be found.
2. *Model Calibration:* For each individual remediation site the model has to be calibrated taking the geology and the distribution of the pollution into account. If necessary, modifications may have to be made.
3. *Optimal Control:* The choice and the design of the procedure have to be optimized considering duration and costs of the remediation process.

2 A REMEDIATION SITE

On one of the remediation sites in Germany an estimated 100 tons of VOCs have seeped to the upper three to four meters of the soil in an area of about 20,000 m^2 . This area contains several buildings with basements. Its surface is partially sealed by an asphalt

layer of 5...10 cm, see figure 2. The measured concentrations (in units of mg/m^3) of two

Figure 2 Boreholes, i.e., points where measurements are taken (in the shaded domains there are buildings with basements)

selected VOCs, namely Tetrachlorethen and 1,1,1-Trichlorethan, are shown in figure 3. These plots show only parts of the remediation site, since probes were made only at the points indicated by black dots.

Figure 3 Concentrations of VOCs: Tetrachlorethen and 1,1,1-Trichlorethan

3 A GENERAL PHYSICAL MODEL

Theoretical approaches and simulation models for optimization of the design and the operation of venting systems are often based on narrow physical and simplified mathematical descriptions of the key processes and, furthermore, relatively inefficient numerical methods are frequently applied for the solutions of systems of differential equations.

Most models have been restricted to two-dimensional vertical sections (Kaluarachchi and Parker (1989, 1990), Kuppusamy, Sheng, Parker and Lenhard (1987)) and vertically integrated models (Hochmuth and Sunada (1985), Kaluarachchi, Parker and Lenhard (1990)). Abriola and Pinder (1985) presented a computational model which became a basis for many other papers. Baehr and Corapcioglu (1987) presented a multi-component transport model including oxygen-limited biodegradation. Most papers are based on the assumption of local equilibrium between various phases when describing contaminant volatilization during the soil vapor extraction (Baehr, Hoag and Marley (1989); Rathfelder, Yeh and Mackay (1991)). Non-equilibrium phase models have been presented by Sleep and Sykes (1989), Wilkins, Abriola and Pennell (1995). Mayer, Miller, Poirer-McNeill (1990) presented a comparison between equilibrium and non-equilibrium oil-water models.

3.1 Balance laws

Multi-component and multi-phase transport in porous media is considered (Russell (1995)). Four different phases are taken into consideration: solid (*s*), liquid (water) (*l*), gas (*g*) and contaminant (*o*). The following four components are considered: soil (*s*), air (*a*), water (*w*) and volatile contaminant (*v*) capable of crossing phase boundaries.

The macroscopic mass balance for component *i* in phase α is written as

$$\partial_t(\rho^\alpha \varepsilon^\alpha \omega_i^\alpha) + \nabla \cdot (\rho^\alpha \mathbf{q}^\alpha \omega_i^\alpha) - \nabla \cdot \mathbf{J}_i^\alpha = \rho^\alpha \varepsilon^\alpha [f_i^\alpha + e_i^\alpha] \quad (1)$$

where $\rho^\alpha \left[\frac{kg}{m^3} \right]$ is the mass density of the phase α ; $\varepsilon^\alpha [1]$ is the volume fraction occupied by the phase α ; $\mathbf{q}^\alpha \left[\frac{m}{s} \right]$ is Darcy's velocity of the phase α ; $\omega_i^\alpha [1]$ is the mass fraction of component *i* in the α phase; $\mathbf{J}_i^\alpha \left[\frac{kg}{m^2 s} \right]$ is the flux vector representing the diffusive flux of component *i* in the phase α ; $f_i^\alpha \left[\frac{1}{s} \right]$ is the source of component *i* in the phase α ; $e_i^\alpha \left[\frac{1}{s} \right]$ is the gain of mass of component *i* due to phase change.

Equation (1) is written under the following constraints:

$$\sum_i \omega_i^\alpha = 1, \quad \sum_\alpha \varepsilon^\alpha = 1, \quad \sum_\alpha \rho^\alpha \varepsilon^\alpha e_i^\alpha = 0. \quad (2)$$

Each component could appear in different phases at the same time, thus the macroscopic mass balance for component *i* is derived from (1) by summing over all phases, taking into account the last equation of (2)

$$\sum_\alpha [\partial_t(\rho^\alpha \varepsilon^\alpha \omega_i^\alpha) + \nabla \cdot (\rho^\alpha \mathbf{q}^\alpha \omega_i^\alpha) - \nabla \cdot \mathbf{J}_i^\alpha] = \sum_\alpha \rho^\alpha \varepsilon^\alpha f_i^\alpha. \quad (3)$$

Analogously, one can derive the macroscopic mass balance for phase α

$$\sum_i [\partial_t (\rho^\alpha \varepsilon^\alpha \omega_i^\alpha) + \nabla \cdot (\rho^\alpha \mathbf{q}^\alpha \omega_i^\alpha) - \nabla \cdot \mathbf{J}_i^\alpha] = \rho^\alpha \varepsilon^\alpha \sum_i [f_i^\alpha + e_i^\alpha]. \quad (4)$$

This is the general framework of multi-phase multi-component transport. To make this operational, special assumptions have to be introduced.

3.2 Special assumptions

We adopt the following assumptions in order to simplify the calculations.

- The soil matrix is rigid, i.e. incompressible and immobile. There is no mass exchange across a solid-fluid interface.
- The temperature field is given; no freezing occurs.
- Water appears in the liquid phase l only.
- Air may be present in phase g only.
- The volatile organic component appears in two phases o, g .
- There are no distributed sources for water and for the organic component.
- Darcy's law for phase α is adopted in the following form (Forchheimer's law is compared with Darcy's law below in the text)

$$\mathbf{q}^\alpha = -\frac{\mathbf{k} k_r^\alpha}{\mu^\alpha} \cdot (\nabla p^\alpha - \rho^\alpha \mathbf{g})$$

where $\mathbf{k}$ [m^2] is the permeability; k_r^α [1] - relative permeability of phase α ; μ^α [$\frac{kg}{ms}$] - dynamic viscosity of phase α ; p^α [$\frac{N}{m^2}$] - pressure of phase α .

The local non-equilibrium is assumed to obey a linear phase change law of volatile contaminant between phases o and g , namely

$$e_v^g = \frac{\varepsilon^o}{\varepsilon^g} \lambda_v^{og} (\omega_{v,sat}^g - \omega_v^g) \text{ and } e_v^o = -\frac{\rho^g}{\rho^o} \lambda_v^{og} (\omega_{v,sat}^g - \omega_v^g)$$

where λ_v^{og} [$\frac{1}{s}$] is the phase change rate between both phases, $\omega_{v,sat}^g$ [1] - mass fraction of volatile contaminant v in the phase g at saturation. The continuity equation

$$\rho^g \varepsilon^g e_v^g + \rho^o \varepsilon^o e_v^o = 0$$

is satisfied.

3.3 Equation summary

The general laws of section 3.1 and the assumptions of section 3.2 lead to the following eight equations with eight unknowns: mass fractions (ω_v^g, ω_v^o), volume fractions ($\varepsilon^l, \varepsilon^g, \varepsilon^o$), and pressures (p^l, p^g, p^o).

1. Water conservation

$$\partial_t(\rho^l \varepsilon^l) + \nabla \cdot (\rho^l \mathbf{q}^l) - \nabla \cdot \mathbf{J}_w^l = 0$$

2. Volatile component conservation for the gaseous phase

$$\partial_t(\rho^g \varepsilon^g \omega_v^g) + \nabla \cdot (\rho^g \mathbf{q}^g \omega_v^g) - \nabla \cdot \mathbf{J}_v^g = \varepsilon^g \lambda_v^{og} \rho^g (\omega_{v,sat}^g - \omega_v^g)$$

3. Volatile component conservation for the organic phase

$$\partial_t(\rho^o \varepsilon^o \omega_v^o) + \nabla \cdot (\rho^o \mathbf{q}^o \omega_v^o) - \nabla \cdot \mathbf{J}_v^o = -\varepsilon^o \lambda_v^{og} \rho^g (\omega_{v,sat}^g - \omega_v^g)$$

4. Air conservation

$$\partial_t(\rho^g \varepsilon^g) + \nabla \cdot (\rho^g \mathbf{q}^g) - \nabla \cdot \mathbf{J}_a^g = 0$$

$$5. \omega_v^g + \omega_a^g = 1$$

$$6. \varepsilon^s + \varepsilon^l + \varepsilon^g + \varepsilon^o = 1$$

$$7. p^l - p^g = p^{lg}(\varepsilon^l, \varepsilon^g)$$

$$8. p^o - p^g = p^{og}(\varepsilon^o, \varepsilon^g)$$

If the full problem of coupled water, NAPL, and air transport is to be modelled, this nonlinear system of four differential and four algebraic equations has to be solved simultaneously, together with appropriate initial and boundary conditions. At the moment, it is a challenging task to solve this system in 2D or 3D.

3.4 Turbulent flow

In general, Darcy's law is valid for laminar flow (the Reynolds number $Re < 1 \dots 10$). Here the viscous forces are predominant. As the velocity of flow increases, Darcy's law is no longer valid; at higher values of Re (say $Re > 150 \dots 300$) the flow becomes turbulent. Forchheimer's law

$$-\nabla p = \frac{\mu}{k} \mathbf{q} + \frac{\rho \alpha}{k^{1/2}} |\mathbf{q}| \mathbf{q}$$

presents one of the generalizations of Darcy's law (α is the viscosity resistance coefficient), where gravity effects for gas have been omitted. Putting this into the mass balance equation for air

$$\partial_t(\rho \theta) + \nabla \cdot (\rho \mathbf{q}) = 0$$

and using a gas law of the form $\rho = \beta p^\gamma$ (where β is the inertia coefficient, and γ is the adiabatic coefficient $0 \leq \gamma \leq 1$), one gets

$$\partial_t(\beta \theta u^{\gamma/(1+\gamma)}) - \nabla \cdot (F(|\nabla u|) \nabla u) = 0$$

Figure 4 Darcy - Forchheimer

with

$$F(s) = \frac{\mu}{2\alpha k^{1/2}} \left[\left(1 + \frac{4\alpha\beta k^{3/2}}{(1+\gamma)\mu^2} s \right)^{1/2} - 1 \right] \frac{1}{s}.$$

This differential equation is degenerate for $u \rightarrow 0$ and for $u \rightarrow \infty$; there are special numerical tools for dealing with such degeneracies (cf. Jäger and Kačur (1994)); in practical soil remediation problems the regime of these degeneracies is not reached. We have compared Darcy and Forchheimer's law for a steady state, one well, radially symmetric case. The equipotentials are drawn in figure 4. In spite of high discharge of the well the difference between both cases is small and thus this kind of nonlinearity is practically not significant.

4 THE GAS FLOW FIELD

In practical applications it has turned out that an important piece of information is the gas flow field. Even if this is not being used as part of the full system of section 3.3, this knowledge as such is relevant to estimate the operation of the pumping strategy. If the spatial distribution of the pollutant has been found out, one obviously should try to generate a high gas stream in those domains where the NAPL concentration is large. In this section we describe an approach for calculating the air flow field for the remediation site described in section 2.

4.1 Air permeability

Compressible flow in porous media has been a subject of investigations for many years. Mathematical models of air movement in unsaturated porous media have been calibrated using air pressure data in several investigations in order to determine the air permeability. When considering the standard two-phase model of flow in unsaturated porous media (air and water), the soil consists of the porous matrix, the water and the air phase. Thus one

Layer	$\theta_r[-]$	$\theta_s[-]$	$K_s [10^{-12}m^2]$	$\alpha[cm^{-1}]$	$l[-]$	$n[-]$
Coarse Sand	0	0.449	655.87	0.4976	0.5	3.551
Middle Sand	0	0.426	10.28	0.2789	0.5	1.596
Fine Sand 1	0	0.457	6.57	0.2501	0.5	1.422
Fine Sand 2	0	0.419	6.00	0.1729	0.5	1.912

Table 1 Van-Genuchten parameters for water ($m = 1 - \frac{1}{n}$)

can write

$$\theta_{gas} + \theta_{water} + \theta_{matrix} = 1$$

for the saturations. We suppose that the domain is insulated on all sides and there exist active and passive air-wells; this means pumps generating a certain under-pressure are used at the active wells, and the passive wells are allowed to function as sources of air. In this situation the flux of air will be determined by the pumping rates at the active wells. There are no distributed sink/source for water and we consider the water saturation as a given function of position (x, y, z) . We have used van-Genuchten formula for describing the relation between pressure head h and the saturation θ_{water}

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + (\alpha h)^n)^m}.$$

The parameters are given in the table 1. The relationships $h - \theta$ are plotted in figure 5 for different layers. The air permeability k_{gas} varies in the different layers and it is given by the formula

$$k_{gas} = k_{water} \frac{\mu_{water}}{\mu_{gas}},$$

where μ_{water} and μ_{gas} are the dynamic viscosities of water and air, respectively. In this way one obtains K_{gas} as a function of the position (x, y, z) .

4.2 Horizontal flow in 2D

In many cases the domain for which the model has to be developed is essentially two-dimensional. Here we consider a situation in which the vertical thickness is small compared with the horizontal lengths. Then the numerical calculations can be significantly simplified by averaging over the vertical axis (see Gilding (1988)). This methodology is explained here for steady-state compressible gas flow. In three-dimensional space, conservation of mass is given by

$$\nabla \cdot (\rho_{gas} \mathbf{q}_{gas}) = f_{gas}$$

Figure 5 $h - \theta$ relationships for different layers (the full line corresponds to air and the dashed line to water)

where ρ_{gas} is the gas density, q_{gas} denotes the specific discharge vector, and f_{gas} a distributed source, if there is any. According to the ideal gas law, Darcy's law and for constant temperature, one obtains

$$\nabla \cdot (\tilde{k}_{gas} \nabla p_{gas}^2) = f_{gas}.$$

Under the assumption that the gas flow is essentially horizontal, one integrates between the soil surface at $z = z_2$ and the water table at $z = z_1$ (below $z = z_1$ the soil is water saturated, thus there is no gas flow) and gets

$$\nabla \cdot (T_{gas} \nabla u) = \overline{f_{gas}} \quad (5)$$

where u is the two-dimensional average of p_{gas}^2 , T_{gas} is the transmissivity

$$T_{gas}(x, y) = \int_{z_1}^{z_2} \tilde{k}_{gas}(x, y, z) dz$$

and $\overline{f_{gas}}$ is the average of the source

$$\overline{f_{gas}}(x, y) = \int_{z_1}^{z_2} f_{gas}(x, y, z) dz.$$

Equation (5) has to be considered in a two-dimensional domain Ω . In principle, this is a straightforward and well known method. In practical applications - of course - there is only a limited number of measurements available. In most cases the variable T_{gas} is known at a relatively small number of points that are non-uniformly distributed in the domain Ω . A method that is used very frequently in the geosciences is "Kriging" (see, e.g., Journel and Huijbregts (1978)). The basic idea is that one considers the variable in question - here $T = T_{gas}$ - as a random variable in space and assumes that the measurements T^i taken are realizations of this random field. In a first step one assumes that the field is stationary and estimates its spatial auto-covariance structure. In a second step an "interpolation" $\tilde{T}(\mathbf{X})$ of the T^i at an arbitrary point $\mathbf{X}$ is calculated as a convex combination

$$\tilde{T}(\mathbf{X}) = \sum_i \lambda_i(\mathbf{X}) T^i.$$

of the T^i . The weights $\lambda_i(\mathbf{X})$ are determined by the requirement that the variance of the deviation $T(\mathbf{X}) - \tilde{T}(\mathbf{X})$ is as small as possible. As a consequence, for each point $\mathbf{X}$ where the "interpolant" $\tilde{T}(\mathbf{X})$ is needed a linear system with a symmetric matrix has to be solved for the weights $\lambda_i(\mathbf{X})$. A modified conjugate gradient (CG) methods proves to be useful in this context.

4.3 Wells in 2D

Wells are used for extracting gas from the soil during the venting process. For the mathematical model special care has to be taken when incorporating them into the equations. There are two different cases:

1. The radius of the wells is sufficiently **large**. Then one may consider the boundary of the well as part of the boundary of the domain Ω . In this case it may be crucial to use local refinements of a finite element grid in the vicinity of the well, because one expects large gradients of the pressure and thus large discharges there.
2. The radius of the wells is **small** compared to the diameter of the domain Ω . In this case, it is reasonable to approximate the wells as point sources (or sinks).

Here we study the second case. Assuming that the discharge of each well is known, one considers the boundary value problem

$$\begin{cases} -\nabla \cdot (T(\mathbf{X}) \nabla u) = \sum_{j=1}^N s_j \delta(\mathbf{X} - \mathbf{X}_j) & \text{in } \Omega \\ u = u_D & \text{on } \Gamma_D \\ -T(\mathbf{X}) \nabla u \cdot \nu = q_N & \text{on } \Gamma_N. \end{cases} \quad (6)$$

where $\mathbf{X} = (x, y)$ is the space variable, $\mathbf{X}_j \in \Omega$; $j = 1, \dots, N$ are the locations of the sources/sinks in the domain Ω , δ is the Dirac delta-function, s_j is the specific discharge

of the well at the point $\mathbf{X}_j$, and u_D and q_N are given boundary data on Γ_D and Γ_N , resp. Assuming that the transmissivity T is constant $T_j = T(\mathbf{X}_j)$ in the vicinity of each of the wells, the local behavior of the solution u is given by a multiple of the fundamental solution

$$\omega_j(\mathbf{X}) = -\frac{1}{2\pi} \ln |\mathbf{X} - \mathbf{X}_j|.$$

The idea is to synthesize the solution u of the boundary value problem (6) in the form

$$u = \tilde{u} + \sum_j \frac{s_j}{T_j} \omega_j.$$

The function $\tilde{u}$ solves the equation

$$-\nabla \cdot (T(\mathbf{X}) \nabla \tilde{u}) = \sum_j \nabla \cdot \left([T(\mathbf{X}) - T_j] \nabla \left(\frac{s_j}{T_j} \omega_j \right) \right).$$

Therefore, $\tilde{u}$ is determined as the solution of the following boundary value problem.

$$\begin{cases} -\nabla \cdot (T(\mathbf{X}) \nabla \tilde{u}) = -\sum_j \frac{s_j}{2\pi T_j} \nabla \cdot \left[(T(\mathbf{X}) - T_j) \frac{\mathbf{X} - \mathbf{X}_j}{|\mathbf{X} - \mathbf{X}_j|^2} \right] & \text{in } \Omega \\ \tilde{u} = u_D + \sum_j \frac{s_j}{2\pi T_j} \ln |\mathbf{X} - \mathbf{X}_j| & \text{on } \Gamma_D \\ -T(\mathbf{X}) \nabla \tilde{u} \cdot \nu = q_N - T(\mathbf{X}) \sum_j \frac{s_j (\mathbf{X} - \mathbf{X}_j) \cdot \nu}{2\pi T_j |\mathbf{X} - \mathbf{X}_j|^2} & \text{on } \Gamma_N. \end{cases}$$

Since the singularities at the wells are subtracted from the function u , the auxiliary function $\tilde{u}$ is smooth.

If the discharges s_j of the wells are unknown, a modification of the approach described so far has to be made. Here we assume that values u_j for u at the boundaries of the wells are prescribed. Then we impose the condition

$$u = \frac{1}{2\pi R_j} \int_{|\mathbf{X} - \mathbf{X}_j| = R_j} u \, d\sigma = u_j$$

where R_j is the “effective radius” of the well at $\mathbf{X}_j$ and σ is the arc length. Now the discharges s_j have to be determined such that this condition is satisfied; in other words, we have to consider an augmented system of equations where the s_j are additional unknowns.

4.4 Numerical examples

Several test calculations were carried out for the remediation site shown in figure 2. First we have chosen homogeneous Neumann boundary conditions at the boundaries of the domain Ω and the same discharges for all active wells. The resulting pressure field (in units of Pa) is shown in the figure 6. The pressure together with the flow field (the lengths of the flux vectors are taken to be proportional to the logarithm of their moduli) can be found in figure 7. A scenario with a different number and modified locations of the active and passive wells is shown in figure 8.

As a comparison we have also taken Dirichlet boundary conditions at the boundary of

Figure 6 Zero Neumann boundary conditions: Pressure

Figure 7 Zero Neumann boundary conditions: Pressure & Log Mass Flux

Figure 8 Modified location of wells: Zero Neumann boundary conditions: Pressure & Log Mass Flux

Ω , namely atmospheric pressure. Again, the discharges are the same for all active wells. The resulting fields are shown in figures 9 and 10.

5 OPTIMIZATION

The optimal control aspect of soil venting consists of optimizing the remediation process with respect to its efficiency. There are several conflicting goals: (i) One wants to extract as much VOCs as possible, (ii) the duration of the process should be short, (iii) the costs should be low, and (iv) restrictions with respect to the available technical equipment have to be fulfilled. It is by no means obvious how to formulate an appropriate mathematical objective/cost functional that adequately takes all these points into account (the choice of the “objective” function is highly “subjective”).

Another basic difficulty arises when applying the tools from mathematical control theory. The distribution of the pollution and the geological properties of the soil are only partly known. This means that there is quite an uncertainty in an optimal control approach. Recently Unger, Sudicky, and Forsyth P. A. (1995) have addressed the problem of robustness of a remediation strategy with respect to spatial heterogeneities of the soil. Here we describe another methodology, namely we study - as a model problem - a random elliptic control problem. This means, we consider the coefficient (here this is the transmissivity) of the elliptic equation as a random field.

Figure 9 Atmospheric Dirichlet boundary conditions: Pressure

Figure 10 Atmospheric Dirichlet boundary conditions: Pressure & Log Mass Flux

5.1 A model problem

We study a typical problem where the control variables u_j are the pressures that are 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 (8)) that is produced at some other part of the boundary and also the costs (using Ψ in equation (8)) that are caused when generating the pressures u_j . In principle, such a problem is in the framework of well known theory for optimal control of partial differential equations. First we describe the problem in its deterministic version. We consider an elliptic boundary value problem of the form

$$\begin{cases} -\nabla \cdot (K \nabla y) &= f, & x \in \Omega \\ y &= g + Bu, & x \in \Gamma_D \\ q_\nu &= h, & x \in \Gamma_N \end{cases} \quad (7)$$

Here K is a strictly positive bounded function in the bounded domain $\Omega \subset \mathbb{R}^2$ the piecewise smooth boundary of which is $\Gamma = \Gamma_D \cup \Gamma_N$ with $\Gamma_D \cap \Gamma_N = \emptyset$. The functions f , g , and h are given boundary data, and the quantity $q_\nu = -\nu \cdot K \nabla y$ is the flux in normal direction on Γ . The *state* variable is $y(u)$, and the *control* variable is $u \in U$. The operator $B : U \rightarrow H^{1/2}(\Gamma)$ is assumed to be linear from the Hilbert-space U into $H^{1/2}(\Gamma)$. Its adjoint $B^* : H^{-1/2}(\Gamma) \rightarrow U$ is given by

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

The *cost functional* is chosen as

$$\boxed{J(u) = \int_{\Gamma_D} \Phi(q_\nu(y(u)))\mu \, d\Gamma + \Psi(u)} \quad (8)$$

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

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

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

where $r_\nu = -\nu \cdot K \nabla p(u)$ is the normal boundary flux belonging to the adjoint p . We get the following formula for the differential of the cost functional.

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

Proof: Following the methodology of Lions (1971), chapter II.4, we get

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

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

$$\begin{aligned}
& \int_{\Omega} \nabla \cdot (K \nabla p(u))(y(v) - y(u)) \, d\Omega - \int_{\Gamma} \nu \cdot K \nabla p(u)(y(v) - y(u)) \, d\Gamma \\
&= \int_{\Omega} \nabla \cdot (K \nabla (y(v) - y(u))p(u)) \, d\Omega - \int_{\Gamma} \nu \cdot K \nabla (y(v) - y(u))p(u) \, d\Gamma
\end{aligned}$$

Since $\nabla \cdot (K \nabla p(u)) = 0$ in Ω , $y(v) - y(u) = Bv - Bu$ on Γ_D , $r_\nu = 0$ on Γ_N , $\nabla \cdot (K \nabla (y(v) - y(u))) = 0$ on Ω , and $q_\nu(y(v)) - q_\nu(y(u)) = 0$ on Γ_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.

Now we specialize more and assume $\Gamma_D = \Gamma_I \cup \Gamma_O$ with $\Gamma_I \cap \Gamma_O = \emptyset$. Further, we assume $B(U) \subset H^{1/2}(\Gamma_I)$. Let $U = \mathbb{R}^k$, and $\Gamma_j \subset \Gamma_I$ pairwise disjoint open subsets; for $u = (u_1, \dots, u_k) \in U$ 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 $r \in H^{-1/2}(\Gamma_I)$, where $1_j(x) = 1$ for $x \in \Gamma_j$ and $1_j(x) = 0$ for $x \in \Gamma_I \setminus \Gamma_j$. Let $\mu = 0$ on Γ_I . In addition, let $f = 0$, $g = 0$, and $h = 0$. For $\Phi(z) = \frac{z}{2}(z - 2)$ we get $\Phi'(z) = z - 1$. If $\Psi(u) = \frac{1}{2}|u|^2$, we have $\partial_u \Psi = id$. Finally, we take $\mu = 1$ in the lower half of Γ_O and $\mu = 0$ in the upper half.

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., $u = -B^* r_\nu(p(u))$. Since in our situation 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_I is the left vertical boundary, Γ_O is the right vertical boundary, and Γ_N consists of the two - lower and upper - horizontal boundaries. Results that were obtained using a hybrid mixed finite element method can be seen in figures 11 and 12. A transmissivity field K was chosen such that its values are either 1 (light areas) or 100 (dark areas). The meaning of this is that the soil described here contains very highly conducting "holes".

The main point of this numerical study is a Monte-Carlo experiment where we have used 100 realizations of a transmissivity field each of which had a similar geometric structure as the one of figure 11; the sizes and locations of the "holes" were chosen randomly. Now we have made the following comparison: (a) We have determined the optimal solution for each individual realization; the resulting optimal controls u (as functions Bu on the left boundary of the unit square) are plotted in the left part of figure 13. As one can see, the optimal u has quite a large variation. The right part of this figure shows the control for the example of figures 11 and 12 (zig-zag solid line) and also the arithmetic average (dotted line) of all 100 optimal controls u , together with (b) the solution of the "averaged" optimal control problem (dashed line)

$$\inf_U E J(u), \tag{9}$$

Figure 11 Transmissivity and flux of the state variable for one of the optimal control problems

Figure 12 Discharge (on a logarithmic scale) of the state variable for one of the optimal control problems

Figure 13 Optimal controls for 100 samples of a Monte-Carlo simulation experiment and averages

where E denotes the *expectation* (in the sense of Monte-Carlo simulations). The monotone curve in the right part of figure 13 shows (c) the optimal solution of the deterministic problem (smooth solid line) for the “effective” (constant) transmissivity K which was determined by solving 100 boundary problems (with constant boundary values) for the state equation.

The left part of figure 14 shows the cumulative distribution function of the objective function; the small vertical line indicates the value of the objective function for the problem with the effective transmissivity. The right part shows the normal flux on the lower half of the right boundary Γ_O for the case of figures 11 and 12 (zig-zag solid line), the arithmetic average (dotted line) of all 100 fluxes of the Monte-Carlo experiment, and the flux of the problem with the effective transmissivity (smooth solid line).

The fact that the three “averages” differ significantly is of great importance for practical applications. Care must be taken when one tries to deal with the influence of the stochastic aspects of optimal control problems. In particular, the often used “effective” parameters prove to be of only limited value for this type of problems.

6 CONCLUSION

The problem of soil remediation presents many difficulties: mathematical, physical, numerical, statistical, and experimental. We can say that the first two are almost solved by many works during the last 40 years. In this paper we deal with the third and the fourth

Figure 14 Distribution of the objective function and fluxes

aspect, we use efficient numerical methods such as the “Mixed Finite Element Method”, and we show how the random aspect of the problem can make the numerical results - in some cases - useless. The experimental part and the model calibration are still extremely difficult.

For projects of the type described here all important areas of Applied Analysis come into play, namely Partial Differential Equations, Numerical Analysis, Stochastics, Geostatistics, Inverse Problems, and Optimal Control. In addition, methods from Soil Physics, Soil Chemistry, Thermodynamics, Parallel Computing, and Computer Graphics are being used extensively. The consequence is that projects of this kind require interdisciplinary cooperation and teams of researchers that are large enough to deal with very complex problems.

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