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A Free Boundary Problem Related to the Location of Volcanic Gas Sources

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Abstract—A mathematical model of general gas emitting systems is derived, and a sample of relevant mathematical results is offered. The present paper indicates that shallow subsurface gas sources in typical volcanic areas can be located if appropriate physico-chemical measurements are made on the Earth's surface and put to use.

Key words: Subsurface source, surface measurement, partial differential equations of parabolic type, free boundary, obstacle problem, *a priori* bound.

1. Introduction

Locating gas sources ranks among high priority goals of volcanic surveillance. In this work we explore the potential of making the grade via physico-chemical surface methods. Roughly speaking, we address ourselves to the following question. Assume that gas moves out of some extended underground source and travels towards the soil with vertical velocity through some homogeneous porous-permeable medium — much as it happens in typical volcanic areas. Assume that both physical and chemical observations are made on the soil: namely, bulk gas flow is sampled at the Earth's surface over time and source gas concentration is measured at and beneath the Earth's surface. Can the gas source be located?

This paper demonstrates that — under suitable hypotheses, which are detailed below—the answer is *yes*, in principle.

Locating subsurface gas sources by surface methods results in a typical *inverse problem*. Inverse problems are currently intensively worked on both in mathematics and in geophysics, and occur in such areas of geophysics as, e.g., locating masses and heat sources based on gravity and temperature fields (see, e.g., GLASKO, 1984; GOSH ROY, 1991; MENKE, 1984; TARANTOLA, 1987). However, the present case has received no attention thus far, to the best of the authors' knowledge.

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Our work was spurred by the alert condition declared during springtime 1988 over the Island of Vulcano and the ensuing Summer 1988 Crash Programme by the Italian Gruppo Nazionale di Vulcanologia (see, e.g., SUNDRY AUTHORS, 1991).

2. *Derivation of a Mathematical Model*

We model the affairs as follows. The natural system of concern is idealized as a layer of some homogeneous porous-permeable medium sandwiched from above and from below by two bodies of different gases: the Earth's atmosphere, consisting of air, and an extended gas reservoir beneath, containing mainly carbon dioxide. The upper boundary of the layer is a reference plane that faces air and represents the Earth's surface; the lower boundary is a geometric two-dimensional surface that may uprise and subside over time, and represents the roof of the gas reservoir—i.e., the subsurface gas source. The former is bound to host data, the latter must be determined. The layer itself includes no sources or sinks of gas, and is filled up by a mixture of air and subsurface gas with varying composition—air percolates downward; the subsurface gas flows upward; both slowly move through the medium.

We assume the system is isothermal and the equation of perfect gases is in force. We choose to give prominence to diffusion and advection, and to ignore any extra process that might occur in fixing the configuration of our system.

We call *time* t, call space coordinates x, y and z, and let x stand for *depth* throughout. As usual, $\nabla =$ *gradient* with respect to x, y and z; $\cdot =$ scalar product of vectors; div $= \nabla\cdot$, the divergence operator; $\Delta =$ div ∇, Laplace operator.

Let P and u denote the *total gas pressure* and the *concentration of the subsurface gas*, respectively. For convenience, we assume P is the ratio between the actual total pressure and the atmospheric pressure—dimensionless.

Let ρ, ρ_1 and ρ_2 denote the total gas density, the density of air and the density of the subsurface gas, respectively. We have

$$\rho_1 = \rho(1-u) \quad \text{and} \quad \rho_2 = \rho u \tag{1}$$

since (concentration of air) + (*concentration* of the subsurface gas) = 1.

A form of *Fick's law* ensures that

$$\text{diffusive flow rate of constituent no.} i = -(D/P)\nabla\rho_i \tag{2}$$

for some positive constant D (which depends on the medium). On the other hand,

$$\text{advective flow rate of constituent no.} i = \rho_i \mathbf{W} \tag{3}$$

provided $\mathbf{W} =$ *bulk gas velocity*. Therefore the flow rate of constituent no i, caused by diffusion and advection, amounts to $-(D/P)\nabla\rho_i + \rho_i\mathbf{W}$. The conservation of mass implies

$$\frac{\partial \rho_i}{\partial t} = \operatorname{div}\left(\frac{D}{P}\nabla \rho_i - \rho_i \mathbf{W}\right). \tag{4}$$

We deduce successively

$$\frac{\partial \rho}{\partial t} = \operatorname{div}\left(\frac{D}{P}\nabla \rho - \rho \mathbf{W}\right) \tag{5}$$

and

$$\rho \frac{\partial u}{\partial t} = D \operatorname{div}\left(\frac{\rho}{P}\nabla u\right) + \left(\frac{D}{P}\nabla \rho - \rho \mathbf{W}\right) \cdot \nabla u. \tag{6}$$

As the temperature is constant, ρ is a constant multiple of P. Hence

$$\frac{\partial P}{\partial t} = \operatorname{div}\left(\frac{D}{P}\nabla P - P\mathbf{W}\right) \tag{7}$$

and

$$P \frac{\partial u}{\partial t} = D\Delta u + \left(\frac{D}{P}\nabla P - P\mathbf{W}\right) \cdot \nabla u. \tag{8}$$

Darcy's law tells us that

$$-\mathbf{W} = \Pi \nabla P \tag{9}$$

for some positive constant Π (which depends on the medium and includes permeability, porosity, tortuosity and viscosity).

The following equations

$$\frac{\partial P}{\partial t} = \Delta\left(D \ln P - \frac{\Pi}{2} P^2\right), \tag{10}$$

$$P \frac{\partial u}{\partial t} = D\Delta u + \nabla\left(D \ln P + \frac{\Pi}{2} P^2\right) \cdot \nabla u \tag{11}$$

are established. They encode the essentials of *gas transport* within the considered system — the former describes changes in bulk gas distribution; the latter accounts for chemical composition.

Boundary conditions can be appended. First, our model applies in the absence of gas surges, i.e., when total gas pressure near the ground is close to atmospheric pressure and bulk gas flow is weak enough to enable atmospheric circulation disposal. Therefore

$$P = 1 \quad \text{at} \quad x = 0, \tag{12}$$

and

$$u = 0 \quad \text{at} \quad x = 0. \tag{13}$$

Secondly, we ask that gas composition be analyzed at diverse depths in the subsoil. Therefore we let

$$[0, T] = \text{life span of the relevant observation} \tag{14}$$

and

$$\frac{\partial u}{\partial x} = \text{a given datum for } x = 0 \text{ and } 0 \leq t \leq T. \tag{15}$$

Thirdly, we think of the subsurface gas reservoir as the place where no air is present and pure subsurface gas occurs. In other words, the subsurface gas source plays the role of a *free boundary* in the present framework, and

$$u = 1 \text{ at the subsurface gas source.} \tag{16}$$

In case suitable extra conditions are met, the classical WKBJ method (see LUNENBURG, 1964; or VAINBERG, 1989, for instance) enables us to simplify the model in hand considerably. Surmise the medium is *fairly permeable* and the subsurface gas source is *shallow*. Then Π is considerably larger than D, total gas pressure can be regarded as nearly constant, and the following arguments apply.

Let

$$\lambda = D/\Pi. \tag{17}$$

Let D remain constant,

$$\lambda \to 0 \tag{18}$$

and the following asymptotic expansions

$$\begin{aligned} P &\simeq 1 + \lambda P_1 + \lambda^2 P_2 + \dots \\ u &\simeq u_0 + \lambda u_1 + \lambda^2 u_2 + \dots \end{aligned} \tag{19}$$

hold—the relevant coefficients are bound not to depend on λ. These expansions, (10) and (11) return a system of equations that determines $P_1, P_2, \dots$ and $u_0, u_1, \dots$ recursively; the beginning of such a system reads

$$\operatorname{div}(D\nabla P_1) = 0 \tag{20}$$

and

$$\frac{\partial u_0}{\partial t} = D\Delta u_0 + (D\nabla P_1) \cdot \nabla u_0. \tag{21}$$

The same Ansatz and Darcy's law tells us that bulk gas flow $\mathbf{W}$ obeys

$$-\mathbf{W} \simeq (D\nabla P_1) + \lambda(D\nabla P_2) + \dots; \tag{22}$$

in particular, $-\mathbf{W}$ approaches $(D\nabla P_1)$ asymptotically.

$$\operatorname{div} \mathbf{W} = 0; \tag{23}$$

concentration of subsurface gas obeys

$$\frac{\partial u}{\partial t} = D\Delta u - \mathbf{W} \cdot \nabla u. \tag{24}$$

Equations (23) and (24) can be conveniently treated under the additional hypothesis that *one-dimensional geometry prevails*, i.e., bulk gas velocity is purely vertical and both bulk gas velocity and the concentration of subsurface gas are invariant under horizontal space translations. In fact, such a hypothesis and (23) imply that the horizontal components of **W** vanish and

$$\text{-(vertical component of } \mathbf{W}) = F, \tag{25}$$

a function of time only. As a consequence, bulk gas velocity becomes an *observable* in the present setting—it takes at any depth the same value that it takes *at the Earth's surface*. Moreover, (24) can be recast thus

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - F(t)\frac{\partial u}{\partial x}. \tag{26}$$

In conclusion, *equation (26) governs gas composition within the considered system* under suitable hypotheses. Under the same hypotheses F represents bulk gas flow at the Earth's surface, hence it can be viewed as a datum. Assembling equation (26) and boundary conditions (13), (15) and (16) results in a mathematical problem that will be examined in the next section.

3. Analysis of the Mathematical Model

Motivated by foregoing arguments, in the present section we are concerned with the mathematical problem of determining a function

$$L : [0, T] \to]0, +\infty[\tag{27}$$

(depending upon time), with the physical meaning

$$L = \text{depth of the subsurface gas source}, \tag{28}$$

and a sufficiently smooth map

$$u : \{(t,x) \mid 0 \le t \le T, 0 \le x \le L(t)\} \to [0,1] \tag{29}$$

(depending upon both time and depth) that obey the following conditions

$$(P)\begin{cases} u_t = Du_{xx} + F(t)u_x & \text{for } 0 < t < \mathrm{T} \text{ and } 0 < x < \mathrm{L(t)}, \\ 0 < u(t,x) < 1 & \text{for } 0 < t < \mathrm{T} \text{ and } 0 < x < \mathrm{L(t)}, \\ u(t,0) = 0 & \text{for } 0 < t < \mathrm{T}, \\ u_x(t,0) = g(t) & \text{for } 0 < t < \mathrm{T}, \\ u(t,L(t)) = 1 & \text{for } 0 < t < \mathrm{T}. \end{cases} \tag{30}$$

where D, T, F, g are given (D and T are positive constants, F and g are sufficiently smooth functions of time).

Recall that D is a diffusion coefficient, T is the time span of observations, F stands for bulk gas flow, and u stands for concentration of subsurface gas.

Problem (P) can be advantageously approached by the following recipe. Let G be the *maximal monotone graph* defined by

$$G(r) = \begin{cases}]-\infty, 0] & \text{if } r=0, \\ \{0\} & \text{if } 0<r<1, \\ [0, +\infty[& \text{if } r=1, \\ \text{the empty set} & \text{if either } r<0 \text{ or } r>1. \end{cases} \tag{31}$$

Consider the problem of determining a sufficiently smooth function

$$u : \{(t,x) | 0 \leq t \leq T, 0 \leq x < \infty\} \to]-\infty, \infty[\tag{32}$$

such that

$$(OP) \begin{cases} u_t = Du_{xx} + F(t)u_x + G(t) \ni 0 & \text{for } 0<t<T \text{ and } 0<x<\infty, \\ u(t,0) = 0 & \text{for } 0<t<T, \\ u_x(t,0) = g(t) & \text{for } 0<t<T. \end{cases} \tag{33}$$

Let u be a solution to (OP) that develops *a coincidence set* , i.e., obeys

$$\{(t,x) | 0 \leq t \leq T, 0 \leq x < \infty, u(t,x) = 1\} \text{ is not empty,} \tag{34}$$

and define L by

$$L(t) = \inf\{x \in [0, +\infty[| u(t,x) = 1\} \tag{35}$$

for every t from $[0, T]$. Then the pair comprised of L and a self-evident restriction of u is a solution to (P).

The first line in (OP) measures up to a *differential inclusion.* (OP), resembls the so-called *obstacle problems* that are studied in wide-spread mathematical literature (see, for instance, RODRIGUES, 1987). However, (OP) departs from standards, since it involves a pair of Cauchy conditions on the boundary segment where $x = 0$ and involves no initial condition.

The following result gives conditions regarding physical and chemical data, ensuring that a subsurface gas source is present. Its proof will appear in a forthcoming paper by the authors.

Theorem 1. *Assume*

$$F(t) \leq M = \text{ constant} \tag{36}$$

and

$$g(t) \geq N = \text{constant} \tag{37}$$

for every t from $[0, T]$; *assume M and N satisfy*

$$N > \max(M, 0) + (\pi DT)^{-1/2} \exp\left(-\frac{M^2}{4D^2}T\right). \tag{38}$$

Then any solution u to problem (OP) develops a coincidence set.

A feature which problem (P) shares with other problems for partial differential equations of parabolic type is *ill-posedness*. First, a small perturbation of data need not result in a small perturbation of solutions; secondly, stability can be restored if solutions themselves are suitably constrained *a priori*. A relevant result can be found in BACCHELLI (1997); the following result is a consequence of FRANCINI (2000).

Theorem 2. *Let* g_1 *and* g_2 *be two copies of* g, *let* (u_1, L_1) *and* (u_2, L_2) *be the corresponding solution pairs to problem* (P) *above. Assume* M, α, β, γ *are positive constants; assume*

$$|F(t)| \leq M \tag{39}$$

for every t from $[0, T]$, *and*

$$\alpha \leq L_i(t) \leq \beta, \quad |L_i'(t)| \leq \gamma \tag{40}$$

for every t from $[0, T]$ *and* $i = 1, 2$. *Let* $0 < a < b \leq T$. *Then a positive constant C exists such that*

$$\sup\{|L_1(t) - L_2(t)| : a \leq t \leq b\} \leq C\left(\log\frac{1}{\varepsilon}\right)^{-0.1} \tag{41}$$

provided

$$\sup\{|g_1(t) - g_2(t)| : 0 \leq t \leq T\} \leq \varepsilon \tag{42}$$

and ε *is sufficiently small.*

A detailed analysis of problem (P) was made in SGHERI *et al.* (1993), and TALENTI and TONANI (1995), in the case where depth L of the subsurface gas source happens to be constant in time and can be summarized thus. Let a function

$$U : \{(l, t, x) | 0 < l < \infty, 0 \leq t \leq T, 0 \leq x \leq l\} \to]-\infty, \infty[\tag{43}$$

(depending upon time, depth and an extra parameter l) obey

$$\begin{cases} U_t = DU_{xx} + F(t)U_x & \text{for } 0 < t < T \text{ and } 0 < x < l, \\ U(l, t, 0) = 0 & \text{for } 0 < t < T, \\ U(l, t, l) = 1 & \text{for } 0 < t < T, \\ u(l, 0, x) = x/l & \text{for } 0 < x < l, \end{cases} \tag{44}$$

a standard boundary value problem for a standard partial differential equation. Such a function U can be computed and plotted via available algorithm and *FORTRAN* code. *Ad hoc* arguments show that $U_x(l,t,0)$ decreases strictly from $+\infty$ to 0 as l increases from 0 to $+\infty$ and t is fixed. Consequently, the following equation

$$U_x(l,T,0) = g(T) \tag{45}$$

has exactly one positive root l which can be routinely computed. The root in hand is an estimate of the source depth which becomes increasingly accurate as the time span of the observation enlarges. The following result appears in the papers quoted above.

Theorem 3. *Let*

$$|F(t)| \le M = \text{constant} \tag{46}$$

for every t from $[0,T]$ *let problem* (P) *have a solution pair such that*

$$L = \text{ constant}, \tag{47}$$

and let l be the unique root of (45). Assume $L_{\max}$ *is an upper bound for both L and l. Then*

$$\frac{|l-L|}{L_{\max}} \le 147\exp\left(-\frac{\pi^2 \cdot D}{L_{\max}}T + 2.3\frac{L_{\max}}{D}M\right), \tag{48}$$

provided T is large enough.

4. Conclusions

The mathematical model proposed here applies in circumstances (such as those met in specimen areas of Vulcano Island) where *one-dimensional geometry* prevails, the considered layer is *fairly permeable*, the subsurface gas source is *shallow*, and bulk gas velocity is *low*. Our results can be summarized accordingly;

(i) Simple conditions on the data are available, allowing one to predict whether a subsurface gas source does exist.

(ii) Detecting a subsurface gas source via surface measurements is an *ill-conditioned* problem, i.e., the solution is extremely sensitive toward errors on data. However, stability can be restored, i.e., gross data can be potentially handled, provided reasonable hypotheses are made and pathological configurations of the gas source are ruled out.

(iii) An easy algorithm is available in the case where the subsurface gas source is presumed to be constant in time.

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