A free-boundary problem related to the location of volcanic gas sources

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Abstract. A mathematical model of general gas emitting sytems is derived which is suited for locating shallow gas sources in typical volcanic areas via surface measurements. The model involves a partial differential equation of parabolic type and a related free boundary problem. Mathematical results which are available up to now about such a model are presented.

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

1 Introduction and derivation of a mathematical model

Locating gas sources ranks among high priority goals of volcanic surveillance. In this work we investigate the potential of making the grade via physico-chemical surface methods. Roughly speaking, we address ourselves to the following question. Suppose 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. Suppose 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?

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 rise 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 concur in fixing the configuration of our system.
We call 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 scalars and vectors; $\text{div} = \nabla \cdot$, the divergence operator; $\Delta = \text{div}\nabla$, 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 $\rho$, $\rho_1$ and $\rho_2$ denote the total gas density, the density of air and the density of the subsurface gas, respectively. We have

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

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

A form of Fick’s law ensures that

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

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

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

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

$$\frac{\partial \rho_i}{\partial t} = \text{div}(\frac{D}{P} \cdot \nabla \rho_i - \rho_i \cdot \mathbf{W}).$$

We deduce successively

$$\frac{\partial \rho}{\partial t} = \text{div}(\frac{D}{P} \cdot \nabla \rho - \rho \cdot \mathbf{W})$$

and

$$\rho \cdot \frac{\partial u}{\partial t} = D \cdot \text{div}(\frac{\rho}{P} \cdot \nabla u) + (\frac{D}{P} \cdot \nabla \rho - \rho \cdot \mathbf{W}) \nabla u$$

As the temperature is constant, $\rho$ is a constant multiple of $P$. Hence

$$\frac{\partial P}{\partial t} = \text{div}(\frac{D}{P} \cdot \nabla P - P \cdot \mathbf{W})$$

and

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

Darcy’s law tells us that

$$-\mathbf{W} = \Pi \cdot \nabla P$$

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

The following equations
\[
\frac{\partial P}{\partial t} = \Delta(D \cdot \ln P - \frac{\Pi}{2} \cdot P^2),
\]
\[
P \cdot \frac{\partial u}{\partial t} = D \cdot \Delta u + \nabla(D \cdot \ln P + \frac{\Pi}{2} \cdot P^2) \cdot \nabla u
\]
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 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 for atmospheric circulation be able to dispose of it. Therefore

\[
P = 1 \text{ at } x = 0,
\]
and

\[
u = 0 \text{ at } x = 0.
\]

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

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

\[
\frac{\partial u}{\partial x} = \text{a given datum for } x = 0 \text{ and } 0 \leq t \leq T.
\]

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

\[
u = 1 \text{ at the subsurface gas source.}
\]

In case that suitable extra conditions are met, the classical WKBJ method (see [10] or [14], for instance) enables us to simplify the model in hand considerably. Suppose the medium is fairly permeable and the subsurface gas source is shallow. Then \(\Pi\) is much larger than \(D\), total gas pressure can be regarded as nearly constant, and the following arguments apply.

Let

\[
\lambda = D/\Pi.
\]

Let \(D\) remain constant,

\[
\lambda \to 0
\]
and the following asymptotic expansions

\[
P \simeq 1 + \lambda P_1 + \lambda^2 P_2 + \ldots
\]
\[
u \simeq u_0 + \lambda u_1 + \lambda^2 u_2 + \ldots
\]

3
hold—the relevant coefficients are bound not to depend on \( \lambda \). These expansions, (1) and (2) return a system of equations that determines and recursively; the beginning of such a system reads

\[
div(D \cdot \nabla P_1) = 0
\]

and

\[
\frac{\partial u_0}{\partial t} = D \cdot \Delta u_0 + (D \cdot \nabla P_1) \cdot \nabla u_0.
\]

The same ansatz and Darcy’s law tells us that bulk gas flow \( \mathbf{W} \) obeys

\[
-\mathbf{W} \simeq (D \cdot \nabla P_1) + \lambda (D \cdot \nabla P_2) + \ldots;
\]

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

Therefore the following situation emerges in the limit. Total gas pressure \( P \) becomes a perfect constant; bulk gas velocity \( \mathbf{W} \) need not vanish, but becomes solenoidal as if gas were incompressible—in other words,

\[
div\mathbf{W} = 0; \quad (7)
\]

concentration of subsurface gas obeys

\[
\frac{\partial u}{\partial t} = D \cdot \Delta u - \mathbf{W} \cdot \nabla u. \quad (8)
\]

Equations (7) and (8) 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 (7) imply that the horizontal components of vanish and

\[-(vertical\ component\ of\ \mathbf{W}) = F,\]

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, (8) can be recast thus

\[
\frac{\partial u}{\partial t} = D \cdot \Delta u - F(t) \cdot \frac{\partial u}{\partial x}. \quad (9)
\]

In conclusion, equation (9) 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 can be viewed as a datum. Assembling equation (9) and boundary conditions (4), (5) and (6) results in a mathematical problem that will be examined in the next section.

2 Analysis of the mathematical model

Let \( D \) be a positive constant; let \( F \) and \( g \) be two real-valued functions of time, defined in \([0, T]\). Motivated by foregoing arguments, in the present section we are concerned with the problem of determining a map

\[
L : [0, T] \rightarrow ]0, +\infty[
\]
and a sufficiently smooth map 

\[ u : \{(t, x) \mid 0 \leq t \leq T, 0 \leq x \leq L(t)\} \to [0, 1] \]

that obey the following conditions

\[
(P) \quad \begin{cases} 
  u_t = D \cdot u_{xx} + F(t) \cdot u_x & \text{for } 0 < t < T \text{ and } 0 < x < L(t), \\
  0 < u(t, x) < 1 & \text{for } 0 < t < T \text{ and } 0 < x < L(t), \\
  u(t, 0) = 0 & \text{for } 0 < t < T, \\
  u_x(t, 0) = g(t) & \text{for } 0 < t < T, \\
  u(t, L(t)) = 1 & \text{for } 0 < t < T. 
\end{cases}
\]

Recall that \( D \) = diffusion coefficient, \( T \) = time span of physico-chemical surface observations, \( F \) stands for bulk gas flow, and \( u \) = concentration of subsurface gas. Here is the physical meaning of \( L \):

\[ L = \text{depth of the subsurface gas source}. \]

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

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

Consider the problem of determining a sufficiently smooth map

\[ u : \{(t, x) \mid 0 \leq t \leq T, 0 \leq x < \infty \} \to ]-\infty, \infty[ \]

such that

\[
(OP) \quad \begin{cases} 
  u_t = D \cdot u_{xx} + F(t) \cdot u_x + G(t) \geq 0 & \text{for } 0 < t < T \text{ and } 0 < x < \infty, \\
  u(t, 0) = 0 & \text{for } 0 < t < T, \\
  u_x(t, 0) = g(t) & \text{for } 0 < t < T.
\end{cases}
\]

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

\[
\{(t, x) \mid 0 \leq t \leq T, 0 \leq x < \infty, u(t, x) = 1\} \text{ is not empty,}
\]

and define \( L \) by

\[
L(t) = \inf \{ x \in [0, +\infty[ \mid u(t, x) = 1 \}
\]

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

The first line in \((OP)\) amounts to a differential inclusion. \((OP)\) bears resemblance with the so-called obstacle problems that are studied in a wide literature — see, \([2, 4, 7, 8, 9, 11]\), for instance. However, \((OP)\) departs from standards, since it involves a pair of Cauchy conditions on the boundary segment where \( x = 0 \), and does not involve any
initial condition. One contribution of the present work consists precisely in treating an obstacle problem in absence of initial conditions.

A detailed analysis of problem $(P)$ was made in [12] and [13] in the case where the depth of subsurface gas source happens to be constant, and can be summarized thus. Let a map

$$ U : \{(l,t,x) \mid 0 < l < \infty, 0 \leq t \leq T, 0 \leq x \leq l\} \rightarrow \mathbb{R} $$

obey

$$
\begin{align*}
U_t &= D \cdot U_{xx} + F(t) \cdot U_x & \text{for } 0 < t < T \text{ and } 0 < x < l, \\
U(l,t,0) &= 0 & \text{for } 0 < t < T, \\
U(l,t,l) &= 1 & \text{for } 0 < t < T, \\
u(l,0,x) &= x/l & \text{for } 0 < x < l.
\end{align*}
$$

—a standard boundary value problem for a standard partial differential equation. Such a map 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

$$ U_x(l,T,0) = g(T) $$

has exactly one positive root $l$, which can be routinely computed. The root in hand is an estimate of the source depth, which gets more and more accurate as the time span of the observation gets larger and larger. The following theorem appears in the papers quoted above.

**Theorem 1.** Let

$$ |F(t)| \leq M = \text{Constant} $$

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

$$ L = \text{Constant}, $$

and let $l$ be defined as above. Suppose $L_{\text{max}}$ is an upper bound for both $L$ and $l$. Then

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

provided $T$ is large enough.

A feature, which problem $(P)$ shares with Cauchy 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 [1]; the following theorem is a corollary of [6].

**Theorem 2.** Let $g_1$ and $g_2$ be copies of $g$, let $(u_1,L_1)$ and $(u_2,L_2)$ be the corresponding solution pairs to problem $(P)$ above. Assume $M, \alpha, \beta, \gamma$ are positive constants; assume

$$ |F(t)| \leq M, \quad |F'(t)| \leq M $$

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

$$ \alpha \leq L_1(t) \leq \beta, \quad |L_1'(t)| \leq \gamma $$

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

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

provided

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

and $\varepsilon$ is sufficiently small.

The following theorem gives conditions on physical and chemical data ensuring that a subsurface gas source acts below. Its proof will appear in a forthcoming paper [5].

**Theorem 3.** Assume

$$F(t) \leq M = \text{Constant}$$

and

$$g(t) \geq N = \text{Constant}$$

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

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

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

**References**


