# Working Paper

## The Verification of Air Pollution Episodes in Industrialized Regions

*Vladimir Kovgar*
*YSSP Participant 1996*

WP-96-121
December 1996

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# Contents

# Abstract

There are two approaches for the protection of ambient air against the violation of the admissible threshold values and pollution impacts in large industrial regions.

The first approach is the so-called “technological way”. This approach leads to “green” technologies supporting the lowest level of a harmful pollutant emission. It would be the best solution for the FSU countries, but, unfortunately, this approach is difficult to implement. Many industrial enterprises in these countries are presently utilizing outdated technology, and it is a real problem to modify them quickly in the near term.

The second approach provides control for an emission activity of main pollution sources. The main idea is to control the air pollution level in a region at standard values. The technical basis for this approach is a measurement system and appropriate mechanisms for estimating of the pollution source characteristics, assuming that sources may cheat an agency.

In this paper we analyze the problem of the detection of sources’ characteristics and propose to divide the corresponding framework into two main stages. For each stage we use analytical methods based on the ill-posed problems' theory.

The five-phase decision making procedure based on proposed algorithms is suggested. Numerical examples from real observations in Kiev (Ukraine) show satisfactory results.

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# THE VERIFICATION OF AIR POLLUTION EPISODES IN INDUSTRIALIZED REGIONS

*Vladimir B. Kovgar*
*YSSP Participant 1996*[1]

## Introduction

The atmospheric pollution takes place in various regions of Central and Eastern Europe. Although the seriousness of environmental problems is widely recognized, there are many factors that are likely to delay their solution. These include the high costs of pollution control, and inadequate environmental management. At the same time, the threat to public health from severe air pollution demands that action should be taken as soon as possible to reduce the exposure of the population and properties to dangerous levels of pollutants. An appropriate near term policy should emerge to enforce the immediate protection of public health from the greatest and most obvious environmental hazards using readily available measures. Inter alia, these measures are smog alarm systems that alert the public to impending or occurring air pollution episodes[2] and, in some cases, specify measures to counter the sources and impacts of these episodes (see Breiling, Alcamo [1]). Such measures, in spite of their evident advantage, only treat the symptoms rather than the cause of the region's environmental problems.

FSU countries have agencies which are responsible for monitoring and control of environment (in particular air) pollution sources, but even for them it is difficult or impossible to answer the basic questions:

- How much public money and effort are optimal for detection of violations and caring through the punishment process?
- Which punishment is fair for generating an optimal rate of compliance?
- How much damage can a violation cause - either directly, or indirectly when an unpunished violator encourages others to defy the law?
- How will sources react to the prospect of uncertain punishments that will be determined by a complicated set of probabilities of detection, prosecution and conviction?
- How much detection probability is increased by increases in monitoring budgets?

Thus, even the simple questions about monitoring efforts may lead to a number of complicated problems, resulting in failure to find violations and identification of false violation. In fact, unfortunately, violations are rarely discovered and almost never punished. In developing an appropriate framework it is especially important to keep in mind that firms

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[2] The episode is the case, when the violation of ambient pollution standards at receptor takes place, in other words, when exceeding a threshold value fixed by a monitoring station. The problems (concerning episodes) usually appear in industrialized regions, especially in cases, where the region contains a boundary between different countries.

try to cheat an agency (so-called “problem” sources, which can remain out of compliance for a long time without apparent adverse consequences).

An existing verification methodology is costly and cumbersome. Current monitoring techniques require either an additional equipment installation just at the sources or unexpected visits to enterprises. These techniques require additional investments or special institutions, and does not use “inexpensive” data obtained from remote measurement sensors.

The experts' opinion (see Russel [2], Courtney, Frank, and Powell [3]) is that the research on monitoring technology should be redirected toward developing easy and less expensive detection mechanisms of real pollution emissions by using existing remote monitoring equipment. That mechanism should help the agency to answer the question: “Who is responsible for the episode?”.

The data from existent measurement systems contains much information about a real pollution process history. By nature, the pollutant distribution processes are a physical phenomenon: they agree with the physical laws, and can be described by appropriate differential equations. It means that we can use the set of formal mathematical models (see Marchuk [4]) for the detection of violators' characteristics. Models using estimates of emissions, combined with the observed meteorological condition could simulate the actual concentration. The analysis given in this paper shows a possibility to verify the real sources’ emission values within reasonable errors. It can be done by solving the inverse problem for differential equations, keeping track of the pollutant propagation process. This process includes pollutant diffusion, transport, absorption and emission phenomena.

Thus, we can formulate the problem as follows:

- Develop the verification methodology based on analytical methods to confirm the emission standard violation.
- The methodology should be based on a minimally needed set of measurements of the pollution process history.

Due to the complexity of the problem the proposed framework contains two main stages. In industrial regions, an atmospheric pollution measurement system usually has only a few measurement stations gathering data on pollution at discrete moments of time. It concerns especially the FSU countries, which do not have and will not have sophisticated measurement systems in the near term due to high expenses.

The first stage provides the detection of a small group of suspected violators among all possible violators in a large region. For this purpose, we use the conjugate function method based on the so-called “differential form” of the gaseous admixture propagation model.

The second stage provides the detection of violators among the identified group of sources by using analytic methods based on the so-called “integral form” of the pollutant distribution model.

## 1. The formal description of the problem

Typically the atmospheric pollution monitoring system for industrial regions has only a few measurement points gathering pollution data. Moreover, the data is usually obtained at discrete moments of time and the quality of the measurement data depends on the quality of the measurement devices. It concerns especially the former Soviet Union (FSU) region, that does not have, and will probably not have sophisticated measurement systems in the near term.

Concomitantly with the above mentioned reasons, the high complexity of the problem is due to a measurement data sparseness and their uncertainty. The verification procedure can be separated into two main stages.

During the first stage, the so-called “large scale” detection is provided. It means first of all, that the original emission values of a small group of sources (three or four) among all possible violators in a large region can be estimated. It is reasonable, because practically we have only a poor set of data from stationary monitoring stations, which contains usually 20-30% measurement errors. The main idea is to calculate the difference between the estimated and admissible emission values. The mentioned difference shows the local district of the region, which certainly contains the group of suspected violators. This calculation is based on a differential form of models, which keeps track of the real propagation process under the given conditions: meteorological, geographical, etc. The model is described in the next section.

At the second stage, the detection of violators among the identified group of suspected violators is provided. The detected pollution sources are characterized by the intensity of emission, geographical location, etc. It is easier to estimate the real values of the pollution sources' characteristics inter alia the small group of separated sources. However, there is a number of different cases depending on a particular situation. This means that further analysis of the reasons pertaining to the episode is retained. The analysis based on utilizing the so-called integral form of the pollutant distribution model is also described in the next section.

### 1.1. The models of the admixture propagation process.

It is well known that the air flow at time moment $t$ is characterized by wind field $u(\bar{x},t)$ at each point $\bar{x}=(x_1,x_2,x_3)$ of the spatial domain $\Omega\subset R^3$ (see Marchuk [4]). The gaseous admixture is characterized by concentration $q(\bar{x},t)$. Generally, the propagation of harmful gaseous impurities in an atmosphere is mathematically described by the following equations

$$\frac{\partial q}{\partial t}+div\,uq+dq=\frac{\partial}{x_3}\nu\,\frac{\partial q}{\partial x_3}+\mu\Delta_{x_1,x_2}q+f\,, \tag{1.1}$$

where $\Delta$ is the Laplace operator, $u$ is the wind speed vector, $\nu,\mu\geq 0$ are the vertical and horizontal diffusion coefficients, correspondingly, $d$ is the impurity absorption coefficient and $f$ is the pollution source function or so-called forcing function. The boundary conditions are:

$$q = q_S\,,\ x \in \partial\Omega\,,\ (\bar{u}_n, \bar{n}) < 0\,,$$
$$\frac{\partial q}{\partial n} = 0\,,\ x \in \partial\Omega\,,\ (\bar{u}_n, \bar{n}) \geq 0\,. \qquad (1.2)$$

Here $\partial\Omega$ is the vertical boundary of cylindrical spatial domain $\Omega$; $\bar{n}$ is the normal vector to the lateral surface of domain $\Omega$.

Time $t$ varies over $t \in [0, T]$, the initial concentration is fixed as

$$q(x,0) = q_0(x)\,. \qquad (1.3)$$

From a practical point of view it is more suitable to utilize the two-dimensional approach (2-D model) of the model (1.1-1.3) by vertical averaging of the 3-D model. It gives the possibility to obtain the solution with appropriate numeric precision. As a result the 2-D model is

$$\frac{\partial q}{\partial t} + \frac{\partial u_1 q}{\partial x_1} + \frac{\partial u_2 q}{\partial x_2} + dq = \mu \Delta_{x_1, x_2} q + f\,, \qquad (1.4)$$
$$q(x,0) = q_0(x)\,, \qquad (1.5)$$
$$q = q_S\,,\ x \in \partial\Omega\,,\ (\bar{u}_n, \bar{n}) < 0\,,$$
$$\frac{\partial q}{\partial n} = 0\,,\ x \in \partial\Omega\,,\ (\bar{u}_n, \bar{n}) \geq 0\,, \qquad (1.6)$$

where $\bar{x} = (x_1, x_2) \in \Omega, \Omega \subset R^2$, $t \in [0, T]$.

Generally, there is a considerably complex form of the pollution source function $f$, which represents various kinds of sources. For instance, it may be a set of point sources with emission: 1) accidental or 2) continuous or it may be 3) a group of distributed or linear sources.

For some special cases it is more suitable to utilize the integral form of the model

$$q(\bar{x}, t) = \int_0^T \int_\Omega G(x, \xi, t, \tau) f(\xi, \tau) d\xi d\tau\,, \qquad (1.7)$$

where $G(\cdot)$ is the regularity Green function. This model can be used for detection of characteristics of the point source.

## 1.2. The generalized formulation of the problem

There are different factors that lead to an episode when a high concentration of harmful ingredients is emitted. These factors are essential for elaboration of efficient verification procedures.

An episode may be due to:
1) The increase of industry, domestic heating and traffic emissions.
2) The unfavorable meteorological conditions.
3) The local geography leading to aggrevation of pollution episodes.

From a mathematical point of view, the identification of sources' characteristics is equivalent to the identification of the force function for equation (1.1-1.3) on the basis of discrete measurements (see Marchuk [4]). As it is true for many problems of mathematical physics, such inverse problem is ill-posed in a classical sense. For solving this problem, the Tikhonov’s regularization theory can be used (see Tikhonov and Arsenin [5]). The main idea of this approach is the following. Assume we have to find the approximate solution $f_\eta$ of the problem

$$q(x,t) = Af,\, q \in Q,\, f \in F,\, x \in \Omega, \Omega \subset R^n, \tag{1.8}$$

under the given set of data $\{A_h, q_\delta, \eta\}$, $\eta = (\delta, h)$. Here $Q$ and $F$ are the Hilbert spaces, $A$ is the problem operator, $\delta \geq 0$ is the inaccuracy for $q$, that is $\|q_\delta - q\| \leq \delta$, $q = Af$, $A, A_h : F \to Q$, at that $\|A - A_h\| \leq h$, $h \geq 0$. Let us denote $f_\eta^\alpha$ as the solution of (1.8), minimizing the functional

$$M^\alpha[f] = \|A_h f - q_\delta\|^2 + \alpha\|f\|^2. \tag{1.9}$$

The generalized residual principle (see Goncharskii, Leonov, and Yagola [6]) can be used to define the regularization parameter $\alpha$. To this end the residual $\rho_\eta$ is calculated by

$$\rho_\eta(\alpha) = \|A_h f_\eta^\alpha - q_\delta\|^2 - \left(\delta + h\|f_\eta^\alpha\|\right)^2. \tag{1.10}$$

The advantage of this principle in contrast to conventional techniques is that its numeric realization does not require the detection of compliance degree of equation (1.8) with the given measurement data.

## 2. Identification of the group of sources: stage 1

First, it is necessary to consider the case when various sources are taken into account. This case usually takes place in a big city or in a large industrial region. There may be many different sources such as a complicated set of points, as well as linear or distributed pollution sources. At this stage, we use the mathematical model (1.4-1.6). This large scale model keeps track of the gaseous admixture propagation process in the whole region. Formally it is necessary to estimate the sources function $F(\bar{x},t)$ for partial differential equation

$$\frac{\partial q}{\partial t}+\sum_i\left[u_i\frac{\partial q}{\partial x_i}-\frac{\partial}{\partial x_i}\left(k_i\frac{\partial q}{\partial x_i}\right)\right]+dq=F(\bar{x},t), \tag{2.1}$$

$$q(x,0)=q_0(x),\ q=q_S,\ x\in\partial\Omega,\ (\bar{u}_n,\bar{n})<0;\ \frac{\partial q}{\partial n}=0,\ x\in\partial\Omega,\ (\bar{u}_n,\bar{n})\ge 0,$$

$$\bar{x}\in\Omega,\ \Omega\subset R^n,\ n=2,3,\ t\in[0,T].$$

by using available observation of state function $q$ with errors at discrete sets of measurement points. This observation we denote as $\tilde{q}$ .

Unfortunately, this problem is ill-posed and it is necessary to analyze the appropriate conditions of the problem solvability (see Tikhonov, Arsenin [5]).

### 2.1. The analysis of the solvability conditions

The model (2.1) can be rewritten in the following form

$$A(x,t,f)q=0,\ x\in\Omega,\ t\in]0,T]. \tag{2.2}$$

Here $A$ is the differential operator containing the initial and boundary conditions, $q(x,t)$ is the admixture concentration, $f(x,t)$ is the searching source function. Assume that operator $A$ provides the classical correctness for the (2.2) problem and has the conjugate operator $A^*$ .

The identification criterion is the functional

$$J(f)=\int_{\Sigma'}I(\rho)d\Sigma', \tag{2.3}$$

$$\rho(x,t)=q(x,t)-\tilde{q}(x,t),\ x,t\in\Sigma'\subset\Sigma,$$

where $q$, $\tilde{q}$ are respective solutions of (2.1) and the observed admixture concentration, $\Sigma=\Omega\times]0,T]$ and $I(\rho)$ is a smooth function.

The criterion (2.3) can be minimized by using various iterative procedures. To this end, it is necessary to have the precise data and the adequate differential operator of the system. In practice, unfortunately, such conditions are impossible, because 1) the measurement devices have uncertainty, 2) the numeric calculations have the error. Therefore the convergence of the iterative numeric procedure is guaranteed if conditions providing the well-posed property of the problem are satisfied.

In accordance with the ill-posed problem theory (see Tikhonov, Arsenin [5]) it is reasonable to search the correct solution on compact restrictions of sets $\{f\}$ and $\{q\}$. Therefore we assume further that the sets $\{f\}$ and $\{q\}$ are compacts and the solution of the identification problem (2.2, 2.3) exists in $F=\{f\}$.

The residual error of $\tilde{q}$ is always observed with some uncertainty $\delta$. Considering such residual error, it is possible to estimate only the approximate value of function $\tilde{f}\in F^*(\delta, f^0,\alpha)$, where $F^*=\{f:\inf|\rho|=\delta\}$ is a neighborhood of the exact solution $\bar{f}$ depending on 1) the uncertainty $\delta$, 2) the initial solution $f^0$ and 3) the regularization parameter $\alpha$.

**Remark.** *Any point* $\tilde{f}\in F^*$ *can be accepted as approximate solution. Therefore we can define the uniqueness of solution (2.2)* $\tilde{f}$ *as* $\tilde{f}\to\bar{f}$ *if* $\delta\to 0\ \forall f^0\in F$.

***Theorem 1.*** *The solution of the identification problem (2.2, 2.3) is unique in the sense mentioned above, if the condition of Theorem 1 is fulfilled and the function* $I(\rho)$ *has single minimizing solution in the set of residual errors under* $f\in F$.

For proof see the Appendix

***Corollary 1.*** *The function* $I=\rho^2$ *guarantees the identification of the unique solution f (in the sense mentioned above).*

Thus, the identification of solution $f$ is the well-posed problem if the conditions of theorem 1 are satisfied. So, the following formulation of the problem is well posed.

*Determine the value of the pollutant emission function* $f$ *for the admixture propagation process*

$$\hat{A}q - f = 0\,, \tag{2.4}$$

$$\hat{A}(\cdot)\equiv\left(\frac{\partial}{\partial t}+\sum_{i=1}^{2}\left[u_i\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_i}\left(k_i\frac{\partial}{\partial x_i}\right)\right]+d\right)(\cdot)$$

*minimizing criterion of identification*

$$J=\int_0^T\int_\Omega C(q-\tilde{q})^2\,d\Omega dt\,. \tag{2.5}$$

*The feasible set of solution is defined as*

$$F=\begin{Bmatrix}(f;q)\,|\,(f;q)\ \textit{is linked by}\ (4);\ \alpha< f(x,t)<\beta\ \ \forall(x,t)\in\Omega\times[0,T],\\ \alpha>0,\ \beta\le+\infty;\quad q(x,t)\ge 0,\ \forall(x,t)\in\Omega\times[0,T];\quad \partial q/\partial f\ne 0\end{Bmatrix}.$$

For the solution of optimization problem (2.4-2.5) it is possible to use the Lagrange technique (see Vasil’ev [7]).

Let

$$L(q, f, p) = J + \left(\hat{A}q - f, p\right) \tag{2.6}$$

Here, the gradient $L_f^k(x,t)$ can be defined by means of the conjugate function $p(x,t)$ satisfying the well-posed conjugate problem

$$-\frac{\partial p}{\partial t} + \sum_{i=1}^{2}\left[u_i \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i}\left(k_i \frac{\partial p}{\partial x_i}\right)\right] + dp = 2C(\tilde{q} - q),$$

with corresponding initial and boundary conditions. That conditions are obtained by using the classical variational principles under the variation of (2.6) with respect to $q$.

Notice that the conjugate function is contained in Lagrangean (2.6) linearly. Therefore,

$$\frac{\partial L(p)}{\partial p} = \frac{\partial q}{\partial t} + \sum\left[u_i \frac{\partial q}{\partial x_i} - \frac{\partial}{\partial x_i}\left(k_i \frac{\partial q}{\partial x_i}\right)\right] + dq - f(x,t) = 0,$$

We can differentiate (2.6) with respect to $f$ taking into account

$$L(f + \partial f) - L(f) = \left(\frac{\partial L(f)}{\partial f}, \partial f\right) + o(f, \partial f), \ \forall \delta f \in W_2^1.$$

So, the corresponding expression for derivative (2.6) with respect to $f$ is

$$L_f = \frac{\partial L}{\partial f} = -p(x,t).$$

We can use now the gradient procedure

$$f^{k+1} = f^k - \alpha^k L_f^k \tag{2.7}$$

where $k$ is an iteration number and $\alpha^k$ is a step-size multiplier, and $L_f^k$ is the gradient of the identification criterion.

The defined gradient procedure permits to estimate the real value for the original field of the pollution sources in a whole region. It gives the possibility to compare results with the standard (admissible) value of sources. The detailed description of algorithm is given in the next section.

### 2.2. A principle structure of the algorithm

As noted above, the calculation algorithm is based on the gradient procedure (2.7). The iterative regularization principle (see Bakushinskii and Goncharskii [8]) can be used to provide the stability of the adequate iterative procedure

$$f^{k+1} = \left(1+(1+k)^{-p}\right)^{-1}\left(f^k - \alpha^k L_f^k\right), \qquad (2.8)$$
$$0 < p < 1,\ 0 < \alpha^k \le 2/N,\ \left\|L_{ff}\right\| \le N.$$

Taking into account that the problem operator (2.4) and admixture concentration measurements are given with error $\|q-\tilde{q}\| \le \delta$, the iterative process (2.8) should have condition

$$\lim \frac{\delta}{\varepsilon_n} = 0,$$

where $\varepsilon_n = \varepsilon_n(\delta)$ is some function (see Bakushinskii and Goncharskii [8]).

Let us denote a neighborhood of $f$ as $F_0$ under condition $\operatorname{sgn} L_f \ne const$. Take the initial approximation $f^0 \notin F_0$ ($\operatorname{sgn} L_f = const$). Let us require the same conditions for the first approximation by means of adequate $\alpha^k$: $f^1 \in F,\quad L^1 < L^0$. Let the same requirements hold for several next iterations $k, k \ge 2$ until $f^k \in F_0$. On the first iterations $f^k \in F_0$ the gradient of the functional $L$ can be represented as

$$L_f^k = \frac{L^k - L^{\Delta k}}{f^k - f^{k+1}}, \qquad (2.9)$$

where $L^{\Delta k}$ is a bound for the antigradient at the $k-$iteration.

The expression (2.9) can be written as follows

$$f^{k+1} - f^k = -L_f^k \sigma \left(I_F^k L_F^k\right)^{-1} I_F^k, \quad \sigma = 1 - L^{\Delta k}/L^k. \qquad (2.10)$$

Comparing the expressions (2.9) and (2.10) we can obtain

$$\alpha^k = L_f^k \sigma \left(I_F^k L_F^k\right)^{-1}.$$

### 2.3. The computational results

The value of $\tilde{q}$ is the sum of noise and solution $q$ of equation (2.4) under the “true value” of the source function $\bar{f}$ shown in Fig. 1.

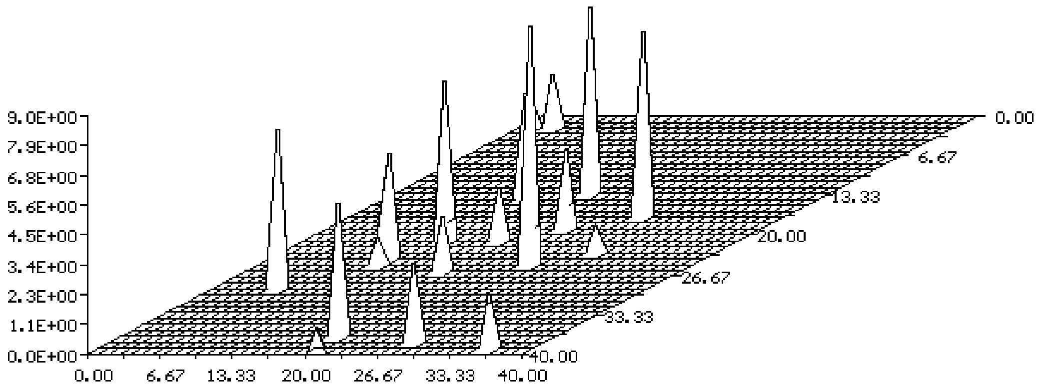


Fig. 1. The "true value" of the source function $\bar{f}$ .

The data was obtained at the measurement points for different "meteorological conditions". The identification process have been carried out under the "initial value" of the emission field

$$f(x,0) = f_0(x)$$

and it is shown in Fig. 2. Under the level of noise $\Delta q\,(10\%)$, the "true value" of $f$ was restored after 5 iterations with error $\Delta f\ (5\%)$.

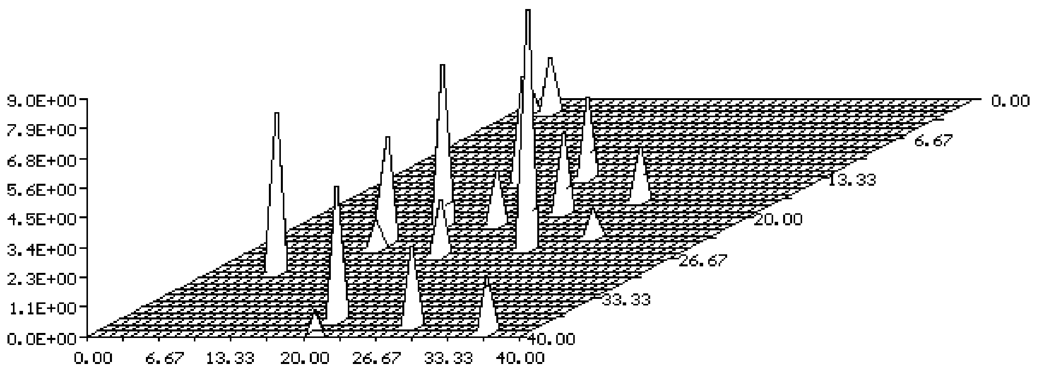


Fig. 2. The "initial value" of the emission field $f(x,0) = f_0(x)$.

The dynamics of the identification process is shown in Fig. 3. Curve (1) shows the dynamics of algorithm described in the previous section; curve 2 presents the case, when the parameter $\alpha$ does not depend from $x$. In such a case, the "true value" of the emission field $f$ was restored with the error of the estimation $\Delta f$ $(15-25\%)$ under the same measurement error value $\Delta q$ $(10\%)$.

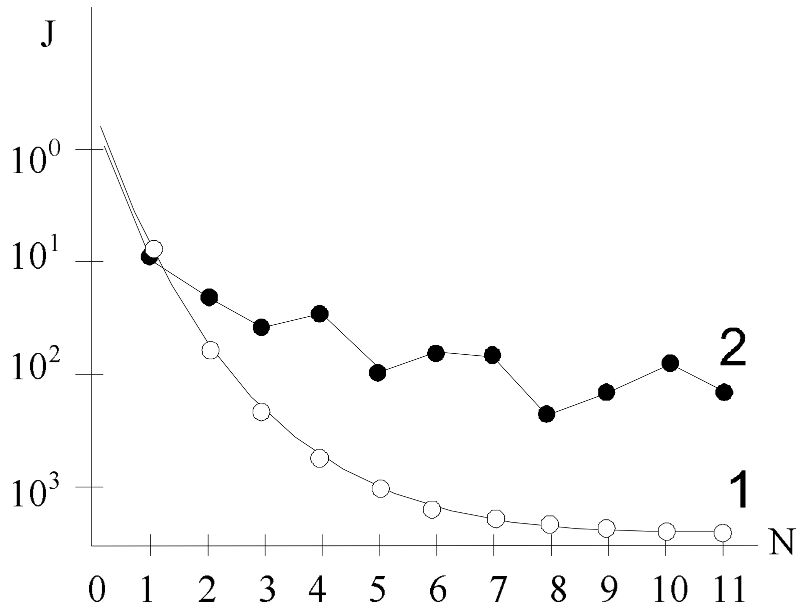


Fig. 3. The dynamics of the identification process.

The dependence of the estimation error $\Delta f$ for restoring of $f(x,0)$ under the measurement error $\Delta q$ is shown in Table 1.

Table 1. The dependence of errors

| Measurement error: $\Delta q(\%)$ | Estimation error: $\Delta f(\%)$ |
|---|---|
| 0 | 0 |
| 5 | 3 |
| 10 | 5 |
| 20 | 7 |
| 30 | 11 |
| 50 | 30 |

The numerical calculations show that the additional a priori information about 1) number of sources, 2) their locations, etc., improves the convergence rate.

## 3. Identification of characteristics of sources: stage 2

The determination of characteristics of separate air pollution sources is a particular case of (1.8). Of utmost importance for the practicable use is to determine a minimal set of the measurement data. It is important, because additional installation of measurement equipment is expensive. In particular, it is interesting to know: how much measurement data is needed to restore the history of emission intensity of the source or its location? So, to this end it is important to determine a minimal set of the measurement data. The problem is also ill-posed, but it is possible to find the particular conditions for which the problem is still solvable. Let us consider these conditions below.

### 3.1. The minimization of measurements

Assume, there is a point source located at point $x^0$ and described by

$$f(x,t) = f(t)\delta(x - x^0) .$$

Here, $f(t)$ is an intensity function of a source emission, $\delta(\cdot)$ is the Dirac function.

Let us first consider the case when it is necessary to estimate the source location. Any 3 points at lend-surface, which are not on the same line, can be used to obtain the minimal set of measurement data. The measurements should be obtain at time T simultaneously. The next theorem affirms it in a formal way.

***Theorem 2.*** *Let* $f(t)$ *be non-negative continuous function* $t > 0$ *and* $\{x^l \in R^2, l = \overline{1,3}\}$ *consist of three different points that do not lie at the same line:* $x^1 \notin (x^2, x^3)^1$*,* $q^l, l = \overline{1,3}$ *are the measurements at those points, and* $x^l \neq x^0$*. Then the solution* $x^0$ *of the inverse problem*

$$q(x^l, T) = \int_0^T G(x^l, x^0, T-\tau) f(x^0, \tau) d\tau ,$$

*with additional conditions* $q|_{t=0} = q_0$*,* $q(x^l, T) = q^l, l = \overline{1,3}$ *is unique.*

For proof see the Appendix.

In practice, the location of the pollution source $x^0$ is often known. In this case we have to find the intensity function for the source's emission $f(t)$. Assuming that $f(t)$ is a continuous function the following theorem can be proof.

***Theorem 3.*** *Let* $f(t)$ *be continuous bounded function and* $x^0, x^1 \in R^2$ *be fixed and* $x^0 \neq x^1$*. Then the solution of the inverse problem*

$$q(x^1, t) = \int_0^t G(x^l, x^0, t-\tau) f(\tau) d\tau , \qquad (3.1)$$

*with additional conditions* $q|_{x=x^1} = q(x^1, t)$ *is unique.*

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[1] Let this notation denote the line in $R^2$ that contains $x^2$ and $x^3$.

For proof see the Appendix.

Taking into account that equation (3.1) has the special form, the Fourier transform technique can be used to solve this problem. The problem is now conditionally well posed for the identification of $f(t)$. In general, due to uncertainty of data, the problem can be solved by using the Tikhonov's regularization technique (see Tikhonov and Arsenin [5]).

Worthy of special attention is the practical case, with the task to determine the number of the pollution sources and their characteristics simultaneously. Special interest, of course, is to find the minimal set of measurement data that allows to solve this problem. The solution of this could be based on the theorem that is the logical corollary of the theorems 2-3.

***Theorem 4.*** *Let* $\left\{x^s \in R^2 \middle| \, s = \overline{1,3}\right\}$ *consist of three different points that do not belong to the same line:* $x^1 \notin \left(x^2, x^3\right)$. *Then, the solution of the problem for simultaneous identification of characteristics* $x^0$ *and* $f(t)$ *is unique under the following conditions* $q(x^1, t) = y(t)$, $q(x^s, T) = y^s$, $l = 2,3$, $T > 0$, *where*

$$q(x,t) = \int_0^t G(x, x^0, t-\tau) f(\tau) d\tau \ . \tag{3.2}$$

The proof follows from proofs of theorems 2 and 3 under the assumption that $f(t)$ is an analytical function.

### 3.2. A conceptual structure of the algorithms

Let us consider the 2-D model of the air admixture propagation. Assume that we have a point source located at $x^0$ and its intensity function is $f(t)$. Then, the admixture concentration field satisfies the conditions

$$\frac{\partial q}{\partial t} + div\, uq - \mu \Delta_{x_1, x_2} q + dq = f(t) \delta\left(x - x^0\right), \tag{3.3}$$

$$-\infty < x_1, x_2 < +\infty\,,\ t > 0\,,\ q(x,0) = q_0(x)\,.$$

Accordingly, the state of the process $q(x,t)$ linked with source parameters $x^0$ and $f(t)$ by relation

$$q(x,t) = \int_0^T G(x, x^0, t-\tau) f(\tau) d\tau \ , \tag{3.4}$$

where $x = (x_1, x_2)$ and $G(\cdot)$ is the Green function of (3.3) problem.

#### 3.2.1. The identification of the source location

The conditions from theorem 4 mean that the concentration data is perfectly known. In most cases, unfortunately, such data contains some measurement noise. To find the approximate solution of this problem it can be reformulated in the following way.

*Find solution* $x^0$ *for*

$$J(x^0) = \sum_{l=1}^{L} \left(q\left(x^l, T, x^0\right) - \tilde{q}\left(x^l, T\right)\right)^2 \qquad (3.5),$$

*where* $\left\{q^l = \tilde{q}\left(x^l, T\right) \middle|\, l = \overline{1, L}\right\}$ *is the set of the measured admixture concentration in time* $T$*, and L is the number of measurement stations.*

The least square method can be used to obtain $x^0$ for (3.5). In this case the condition on location is similar to the condition of theorem 4. The condition will be satisfied if the measurement points are placed into nodes of a square grid determining by parameters $S$ and $h$ (grid size and step, accordingly).

Assume a priori that the source of emission is located at finite distance from the measurement points $x^l$. Assumption $\|x^0\| < K, \quad K < \infty$ allows to introduce the stabilizer $\Omega$.

$$\Omega\left[x^0\right] \equiv \sum_{l=1}^{L} \left(x^0 - x^l\right)^2 .$$

So, any algorithm of minimization of smooth function (see also (1.9))

$$M^{\alpha}\left[x^0\right] \equiv J\left(x^0\right) + \alpha\Theta\left[x^0\right] = \sum_{l=1}^{L} \left(\bar{q}\left(x^l\right) - \tilde{q}\left(x^l\right)\right)^2 + \alpha \sum_{l=1}^{L} \left(x^0 - x^l\right)^2 \qquad (3.6)$$

can be used as solution algorithm for such regularized problem.

The value of regularization parameter $\alpha = \alpha(\delta)$ is chosen by using generalized residual principles (see Goncharskii, Leonov, and Yagola [6]).

The state of the pollution process $q$ depends on $x^0$ nonlinearly. A gradient procedure for minimization of function (3.6) may be used. In this case, the values of the gradient are explicitly defined by derivation (3.6) with respect to parameter $x^0$.

### 3.2.2. The identification of the emission intensity

In practice, the following situation often takes place. The location of the source $x^0$ and concentration value in a few measurement points $\{q(x^1, t),\ q(x^2, t), \ldots\}$ are given, but the data of the real level of the emissions is unfortunately missing. Since the measurement data $\tilde{q}^l = \tilde{q}\left(x^l\right)$ contains uncertainty, the conditions of theorem 3 are not satisfied. Therefore, the estimation of the function $f^0(t)$ is also an ill-posed problem. Taking into account the specific form of equation (3.1), the identification of the intensity function can be carried out by using convolution equation techniques.

Let us represent (3.1) as follows

$$Af = \int_0^t G(t-\tau) f(\tau) d\tau = q(t), t = \overline{0,t}, \qquad (3.7)$$

$$A: W_2^1[0,t] \to L_2[0,t]$$

For this case, the operator $A$ can be given exact or with errors. Let us use even grid along $t$ and $\tau$ :

$$t_k = \tau_k = k\Delta t, \Delta t = T/n, k = \overline{1, n-1}$$

We can approximate (3.7) as

$$\sum_{j=0}^{n-1} G(t_k - \tau_j) f(\tau_j) \Delta t = q(t_k).$$

Denote $q_k = q(t_k)$, $f_j = f(\tau_j)$, $G_{k-j} = G(t_k - \tau_j)$ and define the discrete Fourier transformation for $f_k$ function under discrete variable $k$, $(f_{k+n} = f_k \ \forall k)$ :

$$\tilde{f}_m = \sum_{k=0}^{n-1} f_k e^{-i\omega_m t_k} = \sum_{k=0}^{n-1} f_k e^{-i2\pi(mk/n)}, \quad m = \overline{0, n-1},$$

where $\omega_m = m\Delta\omega, \Delta\omega = 2\pi/T$ .

The inverse Fourier transformation is

$$f_k = \frac{1}{n} \sum_{k=0}^{n-1} \tilde{f}_m e^{i\omega_m t_k}, \quad k = \overline{0, n-1}.$$

Then, finite-difference approximation of smooth functional (1.9) for equation (3.7) has the form

$$\hat{M}^\alpha [f] = \sum_{k=0}^{n-1} \sum_{j=0}^{n-1} \left( G_{k-j} f_j \Delta t - q_k \right)^2 \Delta t + \alpha \sum_{k=0}^{n-1} f_k^2(t_k) \Delta t + \alpha \sum_{k=0}^{n-1} \left( f'(t_k) \right)^2 \Delta t,$$

where

$$f(\tau) = \frac{1}{n} \sum_{k=0}^{n-1} \tilde{f}_m e^{i\omega_m \tau}.$$

Here $\tilde{f}_m$ is the discrete Fourier transformation form $f_k$. Then for the coefficients of discrete Fourier transformation of $f'(t_k)$ we shall have

$$f'(t_k) = \frac{1}{n}\sum_{m=0}^{n-1} i\omega_m \tilde{f}_m e^{i\omega_m t_k},$$
$$\tilde{f}'(t_k) = \frac{1}{n} i\omega_m \tilde{f}_m, \quad k,m = \overline{0,n-1}.$$

So, the functional $\hat{M}^{\alpha}[f]$ approximating the $M^{\alpha}[f]$ can be presented in form

$$\hat{M}^{\alpha}[f] = \frac{\Delta t}{n}\sum_{m=0}^{n-1}\left(\left|\tilde{G}_m\right|^2 (\Delta t)^2 \tilde{f}_m \tilde{f}_m^* - 2\Delta t \tilde{G}_m \tilde{q}_m \tilde{f}_m^* + \left|\tilde{q}_m\right|^2 + \alpha(1+\omega_m^2)\tilde{f}_m \tilde{f}_m^*\right).$$

From the foregoing it is clear that the minimum of $\hat{M}^{\alpha}[f]$ is reached on a vector with the coefficients of discrete Fourier transformation

$$\tilde{f}_m = \frac{\tilde{G}_m^* \tilde{q}_m \Delta t}{\left|\tilde{G}_m\right|^2 (\Delta t)^2 + \alpha(1+(2\pi/T)^2\, m^2)}, \quad m = \overline{0,n-1}.$$

Carrying out the inverse Fourier transformation, we can find $f_{\eta}^{\alpha}(\tau)$ at the grid points $\tau_k$.

### 3.2.3. The detection of sources' contribution

Considering the algorithms and facts, which have been shown above, the procedure for identification characteristics of sources (location and intensity) can be created. Such aggregated procedure combines the previous algorithms.

Let $x_{(0)}^0$ and $f_{(0)}^0(t)$ be some initial approximations of the values $x^0$ and $f^0(t)$. Assume that $x_{(S-1)}^0$ and $f_{(S-1)}^0(t)$ are already obtained. So, $f_{(S)}^0(t)$ is detected by identification algorithm of the emission intensity described above. Then, $x_{(S)}^0$ under known $f_{(S)}^0(t)$ can be detected by above identification algorithm of the source location. The stopping rule of this procedure is the coincidence of two consecutive approximations with given accuracy.

Assuming that the existing measurement system is not perfect, we need to take into account measurement uncertainty. In the light of the above reasoning, it is apparent that the identification criterion here is as follows

$$J = \int_0^T \left(q(x^1,t) - \tilde{q}(x^1,t)\right)^2 dt + \sum_{s=2}^{3}\left(q(x^s,T) - \tilde{q}(x^s,T)\right)^2,$$

where $q$ is the solution of equation (3.4), $\tilde{q}$ is the measured value of concentration.

In this case the equation (3.2) has no solution due to the continuity $G$ along $x$ and t and stochastic discontinuity of the field $\tilde{q}$. If even that solution exists, then $q(t,x)$ is the integral of the function $f(t)$, which is insensitive to sharp local changes. It means we have again an ill-posed inverse problem.

To transfer this problem into a well-posed one, the qualitative information can be used. Assume that $f(t)$ is the smooth and bounded function (in time interval $[0,T]$) function and $x^0$ is a bounded vector. The well-posed problem is achieved by using the stabilizer

$$\Theta[f] \equiv \int_0^T \left( (f'(t))^2 + f^2(t) \right) dt, \quad \Theta[x^0] \equiv \left( x^0 - x^l \right)^2 .$$

Let us represent the source of the emission as a sum of point sources

$$F(x,t) = \sum_{i=1} f_i(t) \delta(x - x_i^0) ,$$

where $f_i(t)$ is the emission power, $x_i^0$ is the coordinate of $i$ -th source, accordingly, and $l$ is the number of the sources.

Any algorithm for the minimization of smooth function

$$M_l^\alpha \left[x^0, f\right] \equiv J_l + \alpha\left(\Theta[f] + \Theta\left[x^0\right]\right), \tag{3.8}$$

$$J_l \equiv \sum_{i=1}^{l} \left( \int_0^T \left( q(x_i^1, x_i^0, f_i, t) - \tilde{q}(x_i^1, t) \right)^2 dt + \sum_{j=2}^{3} \left( q(x_i^j, x_i^0, f_i, T) - \tilde{q}(x_i^j, T) \right)^2 \right).$$

can be used as regularization algorithm for finding the problem solution. The generalized residual principle mentioned above can be used for choosing $\alpha = \alpha(\delta)$ assuming the set $\{ f(t): \Theta[f] \leq h, h > 0 \}$ is a compact set in $C[0,T]$.

Now we can create the next procedure.

*1. The number of sources $l$ is initially equal 1.*

*2. The criterion (3.8) is minimized for cases $l$ and $l+1$ for $f_i(t$*