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Inverse problem of estimation of emission source parameters in the atmospheric boundary layer*

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The inverse problem of the reconstruction of the effective source height and the strength from observed data of ground-level pollutant concentration is considered by solving the semiempirical equation of turbulent diffusion. Hanna's parametrization under conditions of the intensive exchange is used to describe the vertical profile of the eddy diffusivity in the atmospheric boundary layer. The vertical profile of the wind velocity in the surface layer was approximated by logarithm function of the height and higher this layer the wind speed was taken equal to the constant. The efficient method for solving the inverse problem and numerical construction of optimal observation design is suggested. This method is based on the utilization of the dual representation of linear functionals dependent on concentration by way of solutions of the direct and adjoint problems. The proposed model of the observation design and the estimation of the source parameters was verified on the measured data of SO_2 concentrations obtained around the Dickerson power station. Comparison of the experimental parameters with corresponding values estimated by the proposed model shows their satisfactory agreement.

1. Introduction

Mathematical models of the dynamics of atmosphere and ocean contain some parameters such that, whether their values are unknown or setted approximately and require further the improvement of these parameters by solving related inverse problems, using *a priori* information and observation data. In particular the problem of this type is the estimation of a strength of a source of heat and pollutants, using the results of circumstantial observations.

By present time in this direction some theoretical and applied studies devoted to both the qualitative validation of statements of the inverse problem and the numerical methods for solving these problems have been fulfilled [1, 2].

It should be pointed out that planning of the observations is an important stage of solving the problem of the estimation and the improvement of model parameters. Since the solutions of inverse problems, as a rule, are nonlinear

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dependent on initial parameters, this case places specific requirements on the numerical methods and procedures of planning of the observations.

In the given paper the model of the estimation of the effective height and the strength of stationary source in the atmospheric boundary layer is presented using torched observations of pollutant concentration. It is properly the development of studies [3, 4]. The semiempirical equation of the turbulent diffusion is used to describe the air pollution. The quality criterion of the estimates of parameters is the meansquare deviation between measured pollutant concentrations and computed by the atmospheric diffusion model. The use of the superposition and the duality principle for the representation of functionals dependent on concentration in terms of the direct and adjoint problems permits to suggest the effective method of solving the inverse problem. The method of the numerical construction of the optimal design of the observation is realized by the sequential procedure of parameter estimation.

To verify the proposed models of the estimation using experimental data obtained in neighborhoods of the Dickerson power station the test is performed. Hanna's parametrization corresponding to the conditions of the intense mixing is used to describe the profile of vertical turbulent exchange coefficient in the atmospheric boundary layer. The wind vertical profile is approximated by the logarithmic function in the surface layer but higher this layer the wind speed is taken equal to the constant.

The numerical modeling of locally D-optimum designs of observations is developed depending on current meteorology and source parameters. Then the designs, close to optimal designs, were selected by using available experimental data. These designs were used in order the effective height and strength of the source be evaluated. The comparison of the experimental source parameters with calculated indicates their satisfactory accord.

2. Statement of the problem

For the stationary and horizontal uniform atmospheric boundary layer the gas-aerosol pollutant concentration is given by [5]:

$$q(\vec{x},\vec{\theta}) = Q \cdot R(x,y) \cdot \Psi(x,z,H), \tag{1}$$

$$R(x,y) = \frac{1}{\sqrt{2\pi}\sigma(x)} \exp\Big[-\frac{y^2}{2\sigma^2(x)}\Big]. \tag{2}$$

Here $\vec{x} = (x,y,z)$, $\vec{\theta} = (Q,H)$, Q is the strength of the emission source located at the height H with the coordinates $x = 0$, $y = 0$, x is the downwind distance from the source, y is the cross-wind distance from the plume axis, z is the vertical distance from the underlying surface, $\sigma^2(x)$ is the dispersion of plume spread in the cross-wind direction, $\Psi(x,z)$ is the function characterizing the pollutant vertical distribution.

In the approximation of the semiempirical K-theory of turbulent diffusion in the atmospheric boundary layer, having the thickness of h, the problem of the definition $\Psi(x,z)$ is of the form

$$L\Psi \equiv u(z)\frac{\partial\Psi}{\partial x} - w\frac{\partial\Psi}{\partial z} - \frac{\partial}{\partial z}\nu(z)\frac{\partial\Psi}{\partial z} = 0, \tag{3}$$

with the boundary conditions

$$\left(\nu\frac{\partial\Psi}{\partial z} + w\Psi\right)\Big|_{z=0} = 0, \quad \nu\frac{\partial\Psi}{\partial z}\Big|_{z=h} = 0, \quad u\Psi\Big|_{x=0} = \delta(z-H), \tag{4}$$

where the axis x is directed downwind, $u(z)$ is the wind speed, w is the speed of the aerosol particle sedimentation, $\nu(z)$ is the vertical eddy diffusivity, $\delta(z-H)$ is the delta-function.

Assume that the measurements of the ground-level concentration are given by

$$r_k = q(x_k, y_k, \vec{\theta}) + \xi_k, \quad E[\xi_k] = 0, \quad E[\xi_k\xi_j] = \delta_{kj}\sigma_k^2, \quad k,j = \overline{1,N}. \tag{5}$$

Here E is the operation of the mathematical expectation, δ_{kj} is the Kroneker symbol. The estimates of the method of least squares (MLS-estimates) and the function $\hat{q}_N = q(\vec{x}, \hat{\vec{\theta}})$ will be regarded as the solution to inverse problem (1)–(5).

MLS-estimates supply the minimum of the squared functional

$$J_N(\vec{\theta}) = \sum_{k=1}^{N} \sigma_k^{-2}[r_k - q(\vec{x}_k, \vec{\theta})]^2. \tag{6}$$

3. Method of the solution

The solution to problem (1)–(6) can be discovered by the common way using the method of the Lagrange multipliers and the iterative procedures for the determination of the local minima of the function (6). This may require to solve numerically a large number of the problems (1)–(4). In the given case, it is advisable to use the properties of the pollutant distribution model (1)–(4), allowing the superposition of solutions and duality principle for the representation of the functionals dependent on the concentration in terms of the direct and adjoint problems.

Let us consider the following sequence of the relations:

$$\begin{aligned} q(\vec{x_k}, \vec{\theta}) &= Q \cdot R(x_k, y_k) \int_0^h \int_0^X \Psi(x,z,H)\delta(z-z_k) \cdot \delta(x-x_k)\, dxdz \\ &= Q \cdot R(x_k, y_k) \int_0^h \int_0^X \Psi(x,z,H) \cdot L^*\Psi_k\, dxdz \\ &= Q \cdot R(x_k, y_k) \int_0^h \int_0^X \Psi_k^*(x,z) \cdot L\Psi(x,z,H)\, dxdz \end{aligned}$$

$$
\begin{aligned}
&= Q \cdot R(x_k, y_k) \int_0^h \int_0^X \Psi_k^*(x,z) \cdot \delta(z-H)\delta(x)\, dx dz \\
&= Q \cdot R(x_k, y_k) \cdot \Psi_k^*(0, H), \qquad k = \overline{1,N}.
\end{aligned}
\tag{7}
$$

Here $X > x_k$, Ψ_k^* are the solutions to the set of the adjoint problems

$$
L^*\Psi_k^* \equiv -u(z)\frac{\partial \Psi_k^*}{\partial x} + w\frac{\partial \Psi_k^*}{\partial z} - \frac{\partial}{\partial z}\nu(z)\frac{\partial \Psi_k^*}{\partial z} = \delta(x - x_k, z - z_k), \tag{8}
$$

$$
\begin{aligned}
&\left(-\nu(z)\frac{\partial \Psi_k^*}{\partial z} + w\Psi_k^*\right)\bigg|_{z=0} = 0, \\
&\nu\frac{\partial \Psi_k^*}{\partial z}\bigg|_{z=h} = 0, \quad u\Psi_k^*\big|_{x=X} = 0, \quad k = \overline{1,N},
\end{aligned}
\tag{9}
$$

in the domain $0 < z < H$, $x < X$.

L^* is the adjoint operator relative to the operator L in sence of Lagrange. With regard of (7) the functional (6) takes the following form

$$
J_N(\vec{\theta}) = \sum_{k=1}^{N} \sigma_k^{-2}\left[r_k - Q \cdot R(x_k, y_k) \cdot \Psi_k^*(0,H)\right]^2. \tag{10}
$$

Thus, it is sufficient to solve adjoint problems (8)–(9), to define the functional (10), and the search of the minimum of the functional $J_N(\vec{\theta})$ in the form (10) is the typical problem of the nonlinear programming [7, 8].

Remark 1. In the case when all the measurements are made at the same height $z = h_1$ it is sufficient to solve one problem

$$
\begin{aligned}
&L^*\Psi^* = 0, \\
&\left(-\nu\frac{\partial \Psi^*}{\partial_z} + w\Psi^*\right)\bigg|_{z=0} = 0, \\
&\nu\frac{\partial \Psi^*}{\partial_z}\bigg|_{z=h} = 0, \quad u\Psi^*\big|_{x=X} = \delta(z - h_1),
\end{aligned}
\tag{11}
$$

instead of N problems (8)–(9). Then, the functions Ψ_k^* are defined by the corresponding shift of the function Ψ^* along the axis x:

$$
\Psi_k^*(0,H) = \Psi^*(X - x_k, H).
$$

Remark 2. For the number of measurements $N = 2$ the solution of problem (1)–(6) can be represented in the explicit form. In fact, in this case, the determination of the minimum of function (10) is equivalent to the solution of the system

$$
\begin{aligned}
Q \cdot R(x_1, y_1) \cdot \Psi_1^*(0,H) &= r_1 \\
Q \cdot R(x_2, y_2) \cdot \Psi_2^*(0,H) &= r_2.
\end{aligned}
$$

Hence, excepting Q, we obtain the equation for the determination of H.

4. Design of observations

Since the air pollution is assumed stationary, i.e., the concentration is time-independent then the union of quantities

$$\varepsilon_N = \left\{ \begin{matrix} \vec{x}_1, & \vec{x}_2, & \ldots, & \vec{x}_n \\ p_1, & p_2, & \ldots, & p_n \end{matrix} \right\},$$

will be regarded as the design of observations, where $p_i = S_i/N$, S_i is the number of observations in the point $\vec{x}_i$, N is the general number of observations.

For definiteness we restrict our consideration to D-optimal designs that maximizing the determinant of the informative matrix $M(\varepsilon, \vec{\theta})$

$$M(\varepsilon, \vec{\theta}) = F \cdot F^T,$$

where

$$F = \|\vec{f}(\vec{x}_1, \vec{\theta}), \ldots, \vec{f}(\vec{x}_n, \vec{\theta})\|, \quad f^T = \|f_1, f_2\|,$$

$$f_1(\vec{x}, \vec{\theta}) = R(x, y) \cdot \Psi(x, z, H), \quad f_2(\vec{x}, \vec{\theta}) = Q \cdot R(x, y) \cdot \frac{\partial \Psi(x, z, H)}{\partial H}.$$

By virtue of the nonlinear dependence $q(\vec{x}, \vec{\theta})$ on $\vec{\theta}$ *a priori* construction of optimal design is impossible in general. So we shall restrict the construction of locally optimal designs with the help of the procedure of the sequential analysis and planning of observations [9, 10].

1. Let the experiment involving $N-1$ observations was carried out by the nonsingular plan ε_{N-1} (i.e., $|M(\varepsilon_{N-1}, \hat{\vec{\theta}})| \neq 0$). The point $\vec{x}_N$ is found so that

$$d(\vec{x}_N, \varepsilon_{N-1}, \hat{\vec{\theta}}_{N-1}) = \max_{\vec{x} \in \Omega} d(\vec{x}, \varepsilon_{N-1}, \hat{\vec{\theta}}_{N-1}),$$

where

$$d(\vec{x}, \varepsilon_{N-1}, \vec{\theta}_{N-1}) = \vec{f}^T(\vec{x}, \vec{\theta}) M^{-1}(\varepsilon_{N-1}, \vec{\theta}) \cdot \vec{f}(\vec{x}, \vec{\theta})\Big|_{\vec{\theta} = \hat{\vec{\theta}}_{N-1}}.$$

2. In the point $\vec{x}_N$ the additional observation $r_N = q(\vec{x}_N)$ is performed.

3. The MLS-estimates $\hat{\vec{\theta}}_N$ by N observations are calculated according to the design

$$\varepsilon_N = \frac{N-1}{N} \varepsilon_{N-1} + \frac{1}{N} \varepsilon(\vec{x}_N),$$

where $\varepsilon(\vec{x}_N)$ is the singlepoint design.

After the realization of Item 3 we turn to Item 1 and etc. These operations are repeated until

$$|M^{-1}(\varepsilon_N, \hat{\vec{\theta}}_N)|/N$$

becomes less than some given value.

Remark 3. With the approximate estimates H, Q the procedure 1–3 may be replaced by the following two steps [1]:

- to construct the optimal design ε by the existing preliminary estimates and to make the observations according to this plan;
- to evaluate H, Q, using the measurements obtained according to the plan ε.

5. Numerical experiments and conclusions

In this section let us present the results of the numerical experiments for evaluating of the source effective height and its strength by using the field data obtained in the vincinity of the Dickerson power station.

Since the existing data do not permit immediately to use the sequential planning procedure for the search of the locally optimal design of measurements then, let us restrict ourselves to the construction of observational schemes according to Remark 3. The source geometric height is taken as the approximate estimate of the effective height of the emission source. We next choose the twopoint plans, close to obtained plans. The final estimation of H and Q is developed by using these plans.

The numerical experiments for evaluating of the source parameters include solving the direct (3)–(4) and adjoint (8)–(9) problems. The numerical solution of these problems for the case of fine-particle pollutant has been obtained by using the known scheme similar to the implicit scheme for the heat equation for which the stability takes place at the norm C. For the given scheme in view of the condition $\frac{\partial q}{\partial z}|_{z=h} = 0$ the finite difference analog of the mass conservation law is performed. The scheme has the second order of the approximation with respect to z and the first order with respect to x. This scheme complemented by the approximation of boundary conditions is realized by the Thomas algorithm.

The meansquare deviation in formula (2) is calculated depending on the stability class, the source height, the time of taking samples as [12]

$$\sigma(x) = b_0(H) \cdot \left(\frac{T}{20}\right)^{0.2} x,$$

where T is the time of taking samples of the air.

The profile of the wind velocity in (3) has been approximated by the following relation:

$$u(z) = \begin{cases} \dfrac{\bar{u}\log\left(\frac{z}{z_0}\right)}{\log\left(\frac{100}{z_0}\right)} & \text{at } z \leq 100, \\ \bar{u} & \text{at } 100 < z \leq h, \end{cases}$$

where z_0 is the roughness, h is the height of the mixed layer, $\bar{u}$ is the mean wind velocity.

The vertical eddy diffusivity is evaluated by the relation proposed by Hanna [13], and corresponding to the intense mixing conditions in the atmospheric boundary layer

$$\nu(z) = 0.15\sigma_w\lambda_{mw}, \qquad \lambda_{mw} = 10\,T_L^w\sigma_w,$$

where σ_w is the vertical component of the turbulent energy, λ_{mw} is the wave length, T_L^w is the Lagrange time scale. The parameters σ_w, T_L^w have been calculated by Irwin's and Panofsky's formula [14]:

$$\frac{\sigma_w}{w_*} = 0.96\left(3\frac{z}{h} - \frac{L}{h}\right)^{1/3} \quad \text{at } \frac{z}{L} < 0.03,$$

$$\frac{\sigma_w}{w_*} = \min\left[0.96\left(3\frac{z}{h} - \frac{L}{h}\right)^{1/3}, 0.763\left(\frac{z}{h}\right)^{0.175}\right] \quad \text{at } 0.03 < \frac{z}{L} < 0.4,$$

$$\frac{\sigma_w}{w_*} = 0.722\left(1 - \frac{z}{L}\right)^{0.207} \quad \text{at } 0.4 < \frac{z}{L} < 0.96,$$

$$\frac{\sigma_w}{w_*} = 0.37 \quad \text{at } 0.96 < \frac{z}{L} < 1.$$

From these formulae it follows that the turbulent energy under the unstable stratification is completely defined by the values of h, L, w_*, where L is the Monin–Obuchov length, w_* is the convective velocity. For T_L^w in unstable conditions the following relations were used [14]:

$$T_L^w = 0.01\frac{z}{\sigma_w}\frac{1}{[0.55 + 0.38(z - z_0)/L]} \quad \text{at } \frac{z}{L} < 0.1, \ -\frac{z - z_0}{L} < 1,$$

$$T_L^w = 0.59\frac{z}{\sigma_w} \quad \text{at } \frac{z}{L} < 0.1, \ -\frac{z - z_0}{L} > 1,$$

$$T_L^w = 0.15\frac{L}{\sigma_w}\left[1 - \exp\left(-\frac{5z}{L}\right)\right] \quad \text{at } \frac{z}{L} > 0.1.$$

Table 1 presents the results of the numerical modeling of optimal desings of measurements for the weak, mean and relatively high wind velocity with regard to the restrictions on the permissible domain of allocation of observations. In the calculations of characteristics of optimal desings the mean pollutant strength was equal 1000 gs^{-1}. About the quality of the obtained designs one can judge in Figures 1, 2, which illustrate that constructed

Table 1. Optimal plans of measurements of the ground-level concentration of fine-particle pollutant for $H = 122$ m

Current meteorology			Area of design	Points of plan		Determinant of informative matrix
u m/s	w_* m/s	h m	km	x_1 km	x_2 km	$M(\varepsilon, H)$
3.5	1.8	900	[2, 10]	2.0	3.4	$0.23 \cdot 10^3$
			[7.5, 8.9]	7.5	8.9	$0.42 \cdot 10^{-1}$
7	1.6	900	[1.7, 5.7]	1.7	2.9	$0.14 \cdot 10^5$
			[5.7, 14.6]	5.7	9.9	$0.11 \cdot 10^1$
			[1, 10]	1.0	2.0	$0.28 \cdot 10^6$
11	2	1100	[1, 10]	1.0	2.3	$0.34 \cdot 10^5$
			[3.1, 5.3]	3.1	5.1	$0.12 \cdot 10^3$

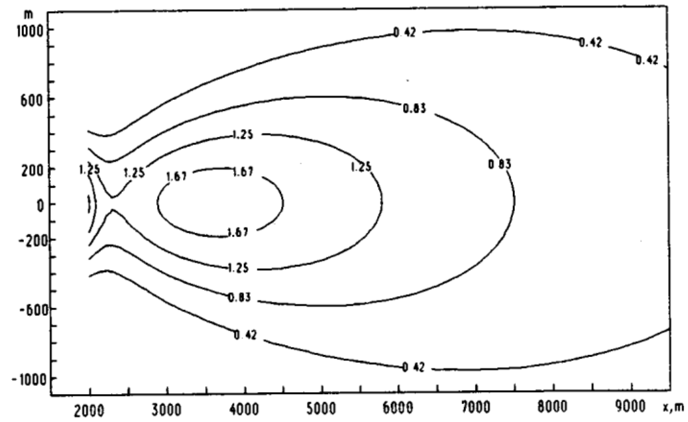

Figure 1. Dispersion of concentration of fine-particle pollutants at $x \geq 2$ km ($u = 3.5$ ms^{-1}, $w_* = 1.8$ ms^{-1}, h=900 m)

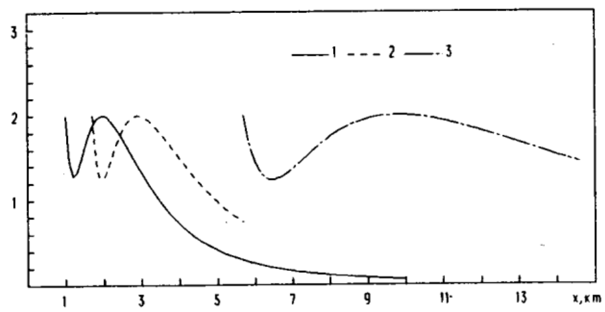

Figure 2. Dispersions of axial concentrations with downwind distance on the optimal plans ($u = 7$ ms^{-1}, $w_* = 1.6$ ms^{-1}, $h = 900$ m): (1) $x \in [1, 10]$ km; (2) $x \in [1.7, 5.7]$ km; (3) $x \in [5.7, 14.6]$ km.

designs are close to optimal plans since the values of locally maxima of concentration dispersions are close to 2, i.e., to the number of evaluated parameters. Then, the optimum of simulated designs of observations follows according to the theorem of the equivalence of D-optimal and minimax designs. The analysis of Table 1 shows that varying the wind velocity and the boundaries of the domain of observations the points of the optimal plan can essentially change their location relatively to the position of the emission source.

The restrictions on the planning domain reduce the information of obtained designs according to the D-optimum criterion.

Table 2. Estimates of the strength and the effective source height for the Dickerson data set

No. realization	Current meteorology			Points of plan	Measurements	Calculation	Estimates of parameters		
	u m/s	w_* m/s	h m	x km	r $\mu g/m^3$	q $\mu g/m^3$	Q	H m	$\frac{H}{H_{exp}}$
1	3.3	1.42	891	9.7	110	115	0.95	400	1.4
	3.2	1.92	1091	2.0	458	615			
2	3.5	1.88	1091	8.9	64	67.1	0.98	510	2.6
	3.7	1.97	1191	7.5	64	68.8			
3	7.6	1.65	841	5.7	121	153	1.04	310	2.3
	7.8	2.03	1091	1.7	212	542			
4	7.6	1.65	841	5.7	121	153	1.01	340	2.5
	6.6	1.45	891	14.6	50	46.7			
5	11.2	2.01	1091	8.7	30	58.2	0.64	290	2.3
	11.5	2.06	1191	3.1	72	255			
6	10.0	1.99	1041	5.3	97	90.5	2.2	460	3.7
	11.5	2.06	1191	3.1	72	255			

The decrease of the information is sufficiently traced in Table 2 by the quality of the Q, H estimates if we compare the 2-th, 4-th, 6-th realizatios with the 1-th, 3-th, 5-th realizations respectively. From Table 2 it follows that the precision of the estimation of Q, H is determined mainly by two factors: the choice of the observation design and the degree of the correspondence between observed concentrations and calculated by the dispersion model. On the measurement designs, close to the optimal designs, the values of parameter estimates are completely satisfactory if we take into account significant deviations of calculated and observed concentrations. It should also be noted that the strength estimates in the considered realizations were derived essentially nearer to the experimental ones than the effective height estimates. This circumstance indicates on the smaller sensitivity of the strength estimates to deviations of calculated and observed concentrations and observation designs.

Figure 3 presents the axial ground-level concentration of SO_2 for the restored and experimental values of Q, H in the first realization. This figure shows that the degree of influence of the error of the H estimate for given meteorological inputs is essentially in the nearly and is decreasing sharply at the considerable distance downwind from the source.

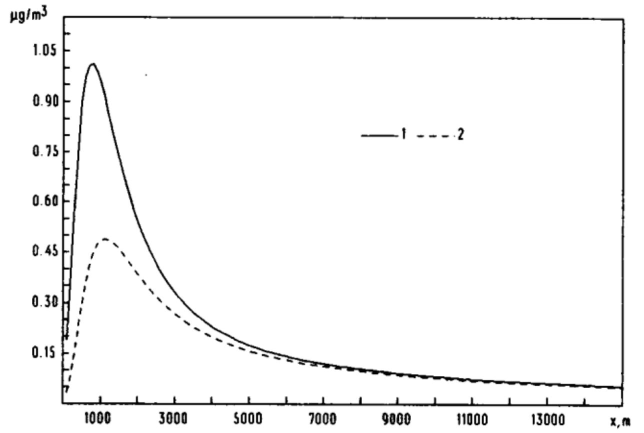

Figure 3. Axial relative concentration of SO_2 (u = 3.3 ms^{-1}, h = 891 m, w_* = 1.42 ms^{-1}): (1) for measured values of the source strength (M = 1) and the effective height (H = 286 m); (2) for evaluated values (M = 0.95, H = 400 m)

This study permits to come to the following conclusions:

- the agreement of measured parameters and model parameters derived on the designs, close to optimal plans, by solving the inverse problem is satisfactory;
- the choice of optimal allocation of air sampling points effectes essentially on the quality of the reconstruction;
- the numerical algorithms for solving the inverse problem and constructing of the plans of observations are completely effective and require negligible computing resources. It will allow their operative utilization under conditions of sequential planning and the analysis of observations;
- attraction of *a priori* information about meteorology, source characteristics, permissible domains for making observations are of the important significance.

The principal moment for solving the inverse problem of the source parameter estimation is the choice of the dispersion model. The use of the semiempirical turbulent diffusion equation provides some advantages from the point of view the generality of processes describing the transport of pollutant. The lacks of the model used are the following: the problem of its use at sufficiently short distances from the source, the complexities due to the specification of inputs. To overcoming these difficulties it is possible to use some transport models describing in more details the process of pollutant dispersion at various distances from the source, and also the introduction of the information about the efficiency of describing of pollutant dispersion in the procedure of observation designing. For practical aims the adaptation of proposed methods of analysis and planning of observations to most expanded procedures of the calculation of pollutant dispersion is advisable [15].

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