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## The Solution of Semi-Empirical Equation of Turbulent Diffusion in Problems of Polluting Impurity Transfer by Gauss Approach

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### Abstract

The analysis of the solution of the semi-empirical solution of turbulent diffusion in problems of polluting impurity transfer is carried out by Gauss approach. It is assumed that there is a certain occupied industrial point, which has one or several sources of the pollution, the arrangement of which is determined by coordinates  $x$ ,  $y$ ,  $z$ . For calculation of average impurity concentration from a point source the solution of semi-empirical equation by Gaussian function of impurity distribution, obtained by a method of Green's function was used. Furthermore, the normalization of the key parameters of the problem is carried out and the initial data are defined. By means of the obtained equation, the model of quantity assessment of the aerosol polluting substances arriving from a source with final and continuous duration of action is made. Thus, the considered computational and analytical model of methodology of assessing the concentration of polluting substances is applicable for applied problems of operational control of the condition of industrial region. Proposed model can be adapted to the air pollution monitoring robotic system.

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**Keywords:** air quality; concentration; Gauss function; equation of turbulent diffusion; pollution monitoring robot system.

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### 1. Introduction

Development of energy, engineering, chemistry and transport in the XX century led to the fact that human activity became comparable in scale with natural energy and material processes occurring in the biosphere. Anthropogenic effects lead to disruption of virtually all natural biogeochemical cycles, including those that contain heavy metals. Currently, all major industrial centers are in need of constant monitoring of emissions, caused by both stationary and mobile sources of pollution. Modeling the monitoring of ecological status of the industrial region requires an adequate mathematical model, following which it is possible not only to calculate the concentration of pollutants, but also to build a forecast of the concentrations for the coming periods. The considered diffusion equation is one of the quality and adequate mathematical models for solving the problem [1].

To solve above mentioned problem the infological model was build (see Fig. 1.). The model reflects the real world in a human-friendly concept is completely independent of the parameters of the storage environment The semantic data model that maps the semantic content of our system was build and distinguished essential entities, their attributes and the relationships between them were also defined. The essence of "Observation Point" and "Substance" are related attitude, because it is the observation point of the atmosphere provides control for harmful substances into the atmosphere, and determine their concentration.

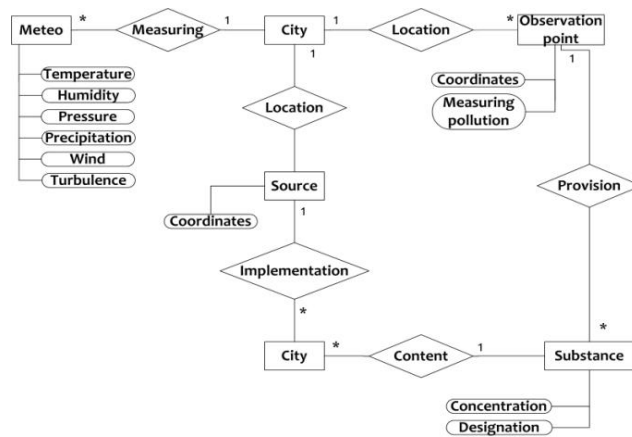


Fig. 1. Infological domain model.

### 2. Modeling the system using UML instruments

In order to well understood by the person, the model should be organized hierarchically and all the entities, should leave at each level of a small number of entities.

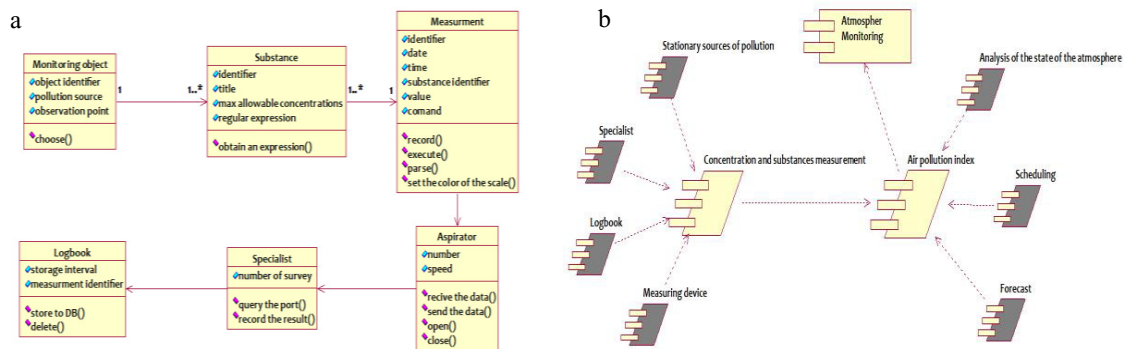


Fig. 2. (a) Static Structure diagram; (b) Component diagram.

This Static Structure diagram should be considered from a conceptual point of view, since it simulates the subject area of the project. All the classes of the diagram are related regarding the direction of association, which corresponds to the presence of a relationship between classes. All classes: "The object of observation", "Substance", "Measurement", "Logbook", "Specialist", "Aspirator" built with the logical chain of the functioning of the system and have their own attributes and operations (see Fig. 2(a)). "Object monitoring" class refers to a specific industrial facility, which hosts emission measurement from stationary sources of pollution. This class is associated attitude of "one-to-many" with the class of "Substance", because in the one studied industrial centre made froze several major pollutants, or rather the most toxic for evaluating the state of the atmosphere. In turn, the class of "substance" is associated with the association of "one-to-many relationship" with class "Measurement", as the measurement is performed several times for a variety of pollutants. Produced substances measurements done by special devices, such as gas analyzer or aspirators. Collected evidence from the devices are handled by specialists, are recorded in the database.

Component diagram - static structural diagram showing a software system partition on the structural components and connections (dependence) between components. As a physical component may act files, libraries, modules, executables, packages, and so on. The basis of atmospheric monitoring is the calculation of the index of air pollution, which in turn depends on the measurement of the concentration of pollutants. The component "Concentration and substance measurement" is associated with its constituent parts: "Stationary sources of pollution", "Specialist", "Logbook", "Measuring device." Next, on the basis of the calculations are based API (air pollution index) concentrations change schedules, the analysis of the data, as well as considering the behavior of the APS over an extended period of time, one can predict the concentration of substances in the near future. In accordance with the distribution component "Air pollution index" attitude associated with the components of "Forecast", "Scheduling", "Analysis of the state of the atmosphere," see Fig. 2(b).

### 3. The Solution of Semi-Empirical Equation of Turbulent Diffusion

Let  $q(P, t)$  – function, which value at time  $t$  at point  $P(x, y, z)$  coincide with the values of instantaneous concentration of impurity, carried by air currents in the atmosphere. It is assumed that the function  $q(P, t)$  is continuously differentiable with respect to  $x, y, z, t$ . Semi-empirical equation of turbulent diffusion is written as follows [3]:

$$\frac{\partial q}{\partial t} + V_x \frac{\partial q}{\partial x} + V_y \frac{\partial q}{\partial y} + V_z \frac{\partial q}{\partial z} = \frac{\partial}{\partial x} K_x \frac{\partial q}{\partial x} + \frac{\partial}{\partial y} K_y \frac{\partial q}{\partial y} + \frac{\partial}{\partial z} K_z \frac{\partial q}{\partial z} + S, \quad (1)$$

where  $S$  is the source of impurity, situated at point  $P_0 (x_0, y_0, z_0)$  and generating instantaneous discharge of pollutants at time  $t_0$  in the amount  $Q_0$ .

To calculate the average of the impurity concentration in the boundary layer of the atmospheric from an instantaneous point source the solution of the equation is used (1):

$$q(x_0, y_0, z_0, t_0) = \frac{Q(x_0, y_0, z_0, t_0)}{[K_x K_y K_z]^{\frac{1}{2}} [4\pi(t-t_0)]^{\frac{3}{2}}} \cdot \exp\left\{\frac{[(x-x_0)-V_x(t-t_0)]^2}{4K_x(t-t_0)}\right\} \cdot \exp\left\{\frac{[(y-y_0)-V_y(t-t_0)]^2}{4K_y(t-t_0)}\right\} \cdot \exp\left\{\frac{[(z-z_0)-V_z(t-t_0)]^2}{4K_z(t-t_0)}\right\}, \quad (2)$$

Called Gaussian function of impurity concentration distribution. The solution for (2) is obtained by the method of Green's functions. To calculate the aerosol concentration in the observation point it is necessary, first of all, to determine and set values of the initial data and conduct normalization of the key parameters and parameterization of the problem. The initial data for the equation (2) are:

- the time when the source generates emissions of polluting substances (PS) –  $t_0$ ;
- the source coordinates  $P_0 (x_0, y_0, z_0)$  (m);
- the distance from the source to the observation point  $R$  (m) – distance from the point  $P_0$  – source of emissions of polluting substances to the point  $P$  – point of observation;
- $Q_0$  ( $10^{-3}$  kg/sec) – the amount of polluting substances ejected by the source at the initial time  $t_0$ ;
- the turbulence of the atmosphere in the boundary layer, characterized by the coefficient of turbulent diffusion  $K = \{K_x, K_y, K_z\}$  ( $m^2/sec$ );
- the wind speed  $V = \{V_x, V_y, V_z\}$  (m/sec).

Apart from the initial data, it is also necessary to calculate the following parameters of the problem: the

coordinates of the observation point P, which hosts measurements of concentration of polluting substances coming from the source:

$$x = \frac{1}{\sqrt{2}}R; \quad y = \frac{1}{\sqrt{2}}R \tag{3}$$

e) Then we carry out the rationing of the variables of the problem. Suppose that

$$q(P_0, P, t_0, t) = Q_0 \cdot q(P_0, P, t_0, t), \tag{4}$$

where

$$\tilde{q}(P_0, P, t_0, t) = \hat{q} \cdot \hat{q}(\hat{P}_0, \hat{P}, \hat{V}, \hat{R}, \hat{t}_0, \hat{t}), \tag{5}$$

$\hat{q}, \hat{P}_0, \hat{P}, \hat{V}, \hat{R}, \hat{t}_0, \hat{t}$  – normalized values with values in the range (0,1). We normalize the variables and the distributions of the problem look as follows:  $\hat{P}_0(\hat{x}_0, \hat{y}_0, \hat{z}_0)$  where  $\hat{x}_0 = \frac{x_0}{R}$ ;  $\hat{y}_0 = \frac{y_0}{R}$ ;  $\hat{z}_0 = \frac{z_0}{R}$ . Similarly, we obtain  $\hat{P}(\hat{x}, \hat{y}, \hat{z})$ , where  $\hat{x} = \frac{x}{R}$ ;  $\hat{y} = \frac{y}{R}$ ;  $\hat{z} = \frac{z}{R}$ . The coefficients of turbulent diffusion and wind speed are normalized as usual:

$$\hat{R} = \{R_x, R_y, R_z\}; \quad R_x = \frac{K_x}{K^*}; \quad R_y = \frac{K_y}{K^*}; \quad R_z = \frac{K_z}{K^*}, \tag{6}$$

where  $K^* = \max\{K_x, K_y, K_z\}$ ;

$$\hat{V} = \{V_x, V_y, V_z\}; \quad V_x = \frac{V_x}{V^*}; \quad V_y = \frac{V_y}{V^*}; \quad V_z = \frac{V_z}{V^*}, \tag{7}$$

where  $V^* = \max\{V_x, V_y, V_z\}$ .

Then, we normalize the variables

$$\hat{t}_1 = \frac{t_1}{T}; \quad \hat{t}_0 = \frac{t_0}{T}; \quad \hat{t}_2 = \frac{t_2}{T}; \quad \hat{t}_1 \leq \hat{t} \leq \hat{t}_2 \tag{8}$$

$T = t^* - t_0$  – time interval, during which the point of observation will be receiving contamination.

Based on the above equation (5) can be written as follows:

$$\hat{q}(\hat{P}_0, \hat{P}, \hat{V}, \hat{R}, \hat{t}_0, \hat{t}) = \frac{1}{[4\pi(\hat{t}-\hat{t}_0)]^{\frac{3}{2}}[R_x, R_y, R_z]^{\frac{3}{2}}} \cdot \exp\left\{-\frac{[(\hat{z}-\hat{z}_0)-\hat{V}_z(\hat{t}-\hat{t}_0)]^2}{4R_z(\hat{t}-\hat{t}_0)}\right\} \cdot \exp\left\{-\frac{[(\hat{x}-\hat{x}_0)-\hat{V}_x(\hat{t}-\hat{t}_0)]^2}{4R_x(\hat{t}-\hat{t}_0)}\right\} \cdot \exp\left\{-\frac{[(\hat{y}-\hat{y}_0)-\hat{V}_y(\hat{t}-\hat{t}_0)]^2}{4R_y(\hat{t}-\hat{t}_0)}\right\}, \tag{9}$$

Let us consider the case, where the source for a finite time interval  $[\zeta, \zeta_0 + T]$  is working at point  $P_0(x_0, y_0, z_0)$  and process of accumulation of polluting substances is taking place at the observation point  $P(x, y, z)$  the. It is assumed that measurements (reception) of concentration of received impurities from sources at times  $t \in [t_1, t_2]$  are carried out at the observation point. The function  $S(P_0, \zeta)$  means the intensity of the source, whereas the function  $S(P_0, \zeta) \Delta\zeta$  ( $10^{-3}$  kg/m<sup>3</sup>) determines the amount of substance emitted into the atmosphere for a simple time interval  $\Delta\zeta$  in the neighborhood  $\zeta$ . According to the considered theory, perturbation impulse of polluting substances  $S(P_0, \zeta)$  will be received at point  $P$  in the range of  $[t_\zeta^* - \tau_1, t_\zeta^* + \tau_2]$ . For this reason, the initial perturbation  $S(P_0, \zeta)$  will be received at point  $P$  at time  $(t_0^* - \tau_1, t_0^* + \tau_2)$  and the last perturbation at time  $(t_T^* - \tau_1, t_T^* + \tau_2)$ . The union of these intervals gives the interval  $(t_0^* - \tau_1, t_T^* + \tau_2)$ . Thus, it becomes evident that the interval  $[\zeta, \zeta_0 + T]$  corresponds to the interval  $(t_0^* - \tau_1, t_T^* + \tau_2)$ . The times  $\zeta$  and  $t_\zeta^*$  are associated with simple transformation:

$$t_\zeta^* = t^* + \zeta, \tag{10}$$

and therefore, the interval  $[\zeta, \zeta_0 + T]$  corresponds to the interval  $\zeta_0 + t^* - \tau_1 \leq t \leq \zeta_0 + T + t^* + \tau_2$ . As a result, we have:

$$\zeta_0 + t^* - \tau_1 \leq t \leq \zeta_0 + T + t^* + \tau_2 \tag{11}$$

Inequality (11) determines the time of a possible reception of perturbation impulse of polluting substances or, in other words, the passage of perturbation impulse of polluting substances through point  $P$  – the observation point.

Now, we need to build an integrated form  $Q(P_0, P, t)$ , defining the amount of polluting substances that have accumulated over time in the source at point  $P$ . To do this, we choose point  $\zeta_k$  and interval  $\Delta\zeta_k$  in the interval  $[\zeta_0, \zeta_0 + T]$  as follows:

$$\zeta_k = \zeta_0 + k\Delta\zeta \tag{12}$$

where  $k = \overline{0, m}$  and  $\Delta\zeta_k = \zeta_{k+1} - \zeta_k$ . Then, we consider the point  $\zeta'_k = \frac{\zeta_k + \zeta_{k+1}}{2}$  and receive the emission at point  $P_0$ :

$$Q(P_0, \zeta'_k) = S(P_0, \zeta'_k)\Delta\zeta_k \tag{13}$$

Then, the reaction at point  $P$  will be as follows: [3]

$$Q(P, t) = Q(P_0, \zeta'_k)\tilde{q}(P_0, P, \zeta'_k, t). \tag{14}$$

As a result, we can write:

$$Q(P_0, P, t) = \sum_{k=0}^{m(t)} Q(P_0, \zeta'_k)\tilde{q}(P_0, P, \zeta'_k, t). \tag{15}$$

It is the integral sum, what is left is to pass to the limit at  $\Delta\zeta \rightarrow 0$  and make changes  $m(t) \rightarrow \zeta(t)$ , when we get:

$$Q(P_0, P, t) = \int_{\zeta_0}^{\zeta(t)} S(P_0, \zeta)\tilde{q}(P_0, P, \zeta, t)d\zeta, \tag{16}$$

where  $\zeta_0 \leq \zeta < \zeta_0 + T$ ,  $\zeta_0 + t^* - \tau_1 \leq t \leq \zeta_0 + T + t^* + \tau_2$  or  $t_1 \leq t \leq t_2$ , if

$$\begin{aligned} t_1 &= \zeta_0 + t^* - \tau_1; \\ t_2 &= \zeta_0 + T + t^* + \tau_2; \zeta(t) = t - t^*. \end{aligned} \tag{17}$$

Next, let us consider the case where the source is operated continuously, and the amount of polluting substances within a certain period of time  $[t_1, t_2]$  are detected at point  $P$ . It is necessary to define

$$\bar{Q}(P_0, P) = \frac{1}{(t_2 - t_1)} \int_{t_1}^{t_2} Q(P_0, P, t)dt. \tag{18}$$

Expression (18) specifies the average value of the concentration of polluting substances per one cubic meter and accumulated over time  $[t_1, t_2]$ . In the given case, interval  $[t_1, t_2]$  is set and it is needed to determine the corresponding interval  $[\zeta_1, \zeta_2]$ . According to (13)  $t_1 = \zeta_0 + t^* - \tau_1$ ,  $t_2 = \zeta_0 + T + t^* + \tau_2$ . Hence, we find  $\zeta_0 = t_1 + \tau_1 - t^*$  and  $\zeta_0 + T = t_2 - t^* - \tau_2$ . We mark  $\zeta_1 = \zeta_0$  and  $\zeta_2 = \zeta_0 + T$ . As a result, we obtain  $\zeta_1 = t_1 + \tau_1 - t^*$  and  $\zeta_2 = t_2 - t^* - \tau_2$ . Thus, we have the following formulas:

$$\bar{Q}(P_0, P, t_1, t_2) = \frac{1}{(t_2 - t_1)} \int_{t_1}^{t_2} Q(P_0, P, t)dt, \tag{19}$$

$$\bar{Q}(P_0, P, t) = \int_{\zeta_1}^{\zeta_2(t)} S(P_0, \zeta)\tilde{q}(P_0, P, \zeta, t)d\zeta \tag{20}$$

$$\begin{aligned} \zeta_1 &= t_1 + \tau_1 - t^*; \\ \zeta_2 &= t_2 - t^* - \tau_2; t_1 \leq t \leq t_2. \end{aligned} \tag{21}$$

We would like to calculate the concentration of impurities entering the observation point. For that, it is necessary, first of all, to set initial data and carry out the normalization of key variables and fields of the problem. We then need to calculate the arrival of P – maximum of polluting substances coming from the source. Then we set the partition of the interval  $[t_1, t_2]$  and form an array  $\{t_l\}$ ,  $l = \overline{1, n}$ ,  $t_{l+1} = t_1 + hl$ ;  $h = \frac{(t_2 - t_1)}{n}$  [4]. After the normalization of variables  $\hat{t}_1 = \frac{t_1}{T - t_0}$ ;  $\hat{t}^* = \frac{t^*}{T - t_0}$ ;  $\hat{t}_0 = \frac{t_0}{T - t_0}$ ;  $\hat{t}_2 = \frac{t_2}{T - t_0}$ ;  $\hat{t}_0 \leq \hat{\zeta} \leq \hat{t} - \hat{t}^*$ ;  $\hat{\zeta} = \frac{\zeta}{T - t_0}$ ;  $d\zeta = (T - t_0)d\hat{\zeta}$  we can write the following:

$$q(\hat{P}, \hat{\zeta}, \hat{t}) = \frac{1}{[4\pi(\hat{t} - \hat{\zeta})^2]^{3/2} [R_x R_y R_z]^3} \cdot \exp\left\{-\frac{[(\hat{x} - \hat{x}_0) - \hat{v}_x(\hat{t} - \hat{\zeta})]^2}{4R_x(\hat{t} - \hat{\zeta})}\right\} \cdot \exp\left\{-\frac{[(\hat{y} - \hat{y}_0) - \hat{v}_y(\hat{t} - \hat{\zeta})]^2}{4R_y(\hat{t} - \hat{\zeta})}\right\} \cdot \exp\left\{-\frac{[(\hat{z} - \hat{z}_0) - \hat{v}_z(\hat{t} - \hat{\zeta})]^2}{4R_z(\hat{t} - \hat{\zeta})}\right\} \tag{22}$$

Next, we consider the source function. Let us assume that

$$S(P_0, \zeta) = S_0 \hat{S}(\hat{P}_0, \hat{\zeta}) = S_0 \cdot \eta(\hat{x}_0, \hat{y}_0, \hat{z}_0, \hat{\zeta});$$

$$\eta(\hat{x}_0, \hat{y}_0, \hat{z}_0, \hat{\zeta}) = (1 + a \cdot \sin(b \cdot \hat{x}_0 + c)) \cdot (1 + a \cdot \sin(b \cdot \hat{y}_0 + c)) \times$$

$$\times (1 + a \cdot \sin(b \cdot \hat{z}_0 + c)) \cdot (1 + a \cdot \sin(b \cdot \hat{\zeta} + c)) \tag{23}$$

As a result, we have [3]:

$$Q(P, t) = \hat{Q}^*(P, t) \cdot \hat{Q}(\hat{P}, \hat{t}); \tag{24}$$

$$\hat{Q}(\hat{P}, \hat{t}) = \int_{\hat{t}_0}^{\hat{t}-\hat{t}^*} \hat{S}(\hat{P}_0, \hat{\zeta}) \hat{q}(\hat{P}_0, \hat{P}, \hat{t}, \hat{\zeta}, \hat{V}, \hat{R}) d\hat{\zeta}; \tag{25}$$

$$\hat{Q}^* = T \cdot S_0 \cdot q^*; \quad S_0 = Q_0. \tag{26}$$

Thus, we illustrated the possibility of practical application of the developed computational and analytical methodology of assessing the concentration of polluting substances in applied problems of operational control of the condition of industrial region, which makes it possible to carry out its ecological forecast [1].

#### 4. Implementation of the model (algorithm and software)

Based on the proposed model, the algorithm (see Fig. 3a) was distinguished, after that "Atmosphere Monitoring" software was created. The program opens by running the executable file IZA.exe. The interface of the program is shown in Fig.3b.).

The necessary initial data will be added after the program launched: the amount of pollution sources, the initial wind speed, date, measurements of pollutants, the coordinates of the source of pollution, the height of the observation point. After that one can calculate the air pollution index for each type of pollutant and see a graph of that calculation.

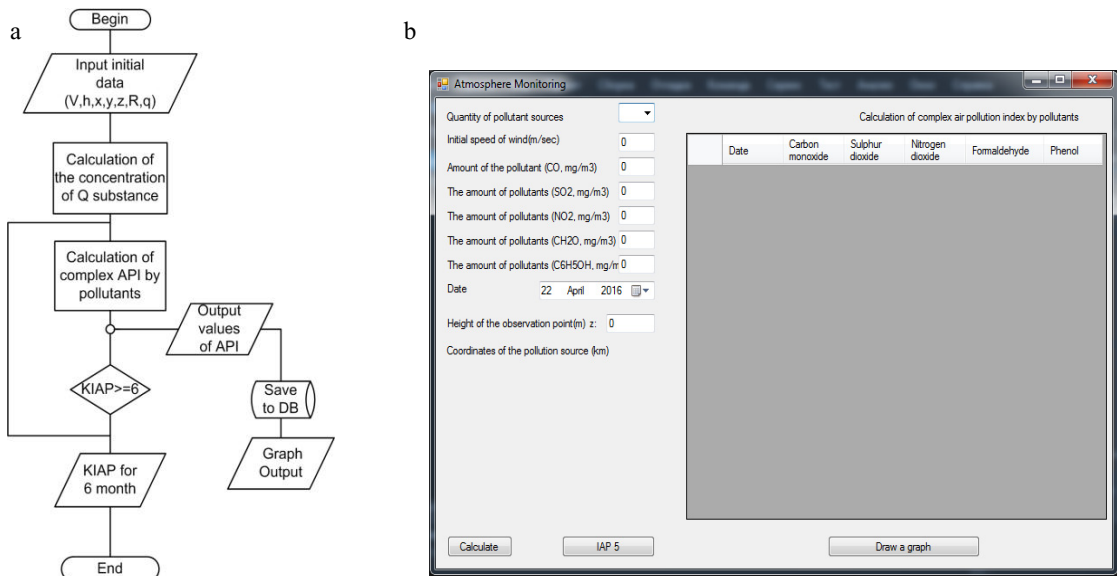


Fig. 3. (a) The algorithm of the system; (b) Main window of the program.

The command "Draw a graph" shows a graph of API values in a new window that clearly illustrates which

substances cause air pollution the most (see Fig. 4).



Fig. 4. The graph of API.

The IAP5 index is used to assess the state of the atmosphere. It is a comprehensive indicator of air pollution in five major pollutants. The IAP5 can be calculated for the last 6 and 12 months by the command "Show IAP5" in the main window of the program.

## 5. Conclusion and future work

Environmental pollution by industrial enterprises and transport vehicles, that causes degradation of the environment and detrimental to human health, remains the most acute environmental problem, which have a priority social and economic importance. Air is mostly polluted by automobile exhaust, emissions from the factories and power plants and by huge fires. In particular, the atmosphere receives too much carbon dioxide from the burning of oil, gas and coal that the Earth will start to get very warm because of the greenhouse effect.

Every year heating systems in the private sector are improving, the emissions of which are released into in ground layer of the atmosphere over the territory of the industrial centers. The new technologies for controlling harmful emissions are developing, but, despite this, the air quality is still poor. Therefore, the development of methodologies for reducing pollutant emissions (pollutants), tools for monitoring and control of pollution levels in order to reduce anthropogenic impacts on the atmosphere are substantial at the moment.

Solving the problem of environmental monitoring is impossible without the use of modern means of measurement, communication and new computer technologies. The integration of all components into a single monitoring technology minimizes the cost of their dock, reducing the time for data exchange and transformation; eliminate data loss, thus increasing the reliability and efficiency of established systems. The open architecture of hardware and software allows one to increase the composition of the measuring equipment and introduce new algorithms for environmental monitoring, also to develop and upgrade the already installed systems.

This paper presents an analysis and comparison of existing mathematical models and numerical methods in issues of environmental monitoring of the atmosphere. The data on indicators of the concentration of pollutants in the atmosphere of Almaty city was collected; an integrated calculation of air pollution index was determined based on solutions for the semiempirical equation of turbulent diffusion. The obtained data can be used in the field of ecology and environmental protection to further carry out the work on the development of air quality in populated areas.

The research results of this paper can be interesting to project organizations, which develop projects on transport infrastructure and general plans of cities for urban development. Also, the obtained information can be useful for

comparison of sanitary - epidemiological bodies, to track the degree of pollutions in order to ensure the environmental safety of the population. The reliability of the results is justified by a large amount of input data for the considered years and confirmed with the correct choice of research methods, with the use of modern mathematical and statistical methods for processing the raw material.

The presented "Atmospheric Monitoring" system has a copyright certificate [6]. This software has been implemented to control emissions of stationary industrial facilities and to improve the quality of the surface air layer over a given settlement. Based on algorithm the "Atmosphere Monitoring" has been implemented as a software – to develop this program we used C Sharp (C #) programming language, on Visual Studio 2012 - Windows Form Application, for the database we took SQL Server 2012. As a future work we are planning to consider networked robotic monitoring system [7-13], where all robots will be equipped with such system for monitoring the environment in industrial areas.

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