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Mathematical Modelling of Atmospheric Pollution in an Industrial Region with a View to Design an Information System Software for Ecological Situation

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Abstract

The paper deals with the issues of information system for monitoring and assessing the ecological situation in an industrial region, based on the mathematical modelling of atmospheric pollution. Our model allows collecting live data and evaluating the possibility of pollution spread. The research object is the air composition changes that occurred under the natural and anthropegenus factors. The purpose of our research is to design an information system software for monitoring and assessing the ecological situation in an industrial region. A mathematical model, based on the hydro-thermodynamics equations, is applied to study the local atmospheric processes that occur in the boundary layer. The following were taken as original equations: equation of motion, continuity equation, heat flow equation and the equation of specific humidity. A modular software system was designed to implement the herein investigated methods and algorithms of solving the problem of the boundary and surface layers and the transfer of impurities.

Keywords: hydro-thermodynamics, atmospheric pollution, monitoring

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INTRODUCTION

The current level and scale of global environmental changes necessitate the identification and understanding of the reasons behind these changes. Collecting information related to the ecological situation and processing it with mathematical methods is the basis of environmental monitoring, which implies a continuous recording and monitoring of environmental indicators. This problem can be solved efficiently with an information system that would automatically collect and process information and support decision making in the management of the ecological situation in a certain region. Nowadays, technical means allow collecting the necessary information regarding the current situation in real time. Up-to-date information regarding the ecological situation in various regions allows drawing conclusions regarding the effect of various factors that pollute the atmosphere, water, soil, and the ecosystem in general. Modern means of collecting environmental information, combined with their automated software processing, are the most promising approach to managing the state environmental security (Ravshanov and Tashtemirova 2017, İnci et al. 2018).

The problems related to the development of environmental monitoring systems are covered extensively in the literature. They include various areas: investigating the state of the air, water, agricultural resources, etc. Numerical models, designed from the models of interaction between the atmospheric layers, form the background of information systems that could be applied to monitor the ecological situation. Statistical cluster analysis method was designed to evaluate the background pollution in the urban areas. The following models have been recently applied to investigate air pollution and record the pollution differences between regions: spatial-temporal model, hybridization model, empirical mode decomposition, modified cuckoo

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search and differential evolution algorithms. The Durbin's spatial model has been applied to study how air pollution affects the health of the population.

Systems, oriented on microprocessors, mobile technologies Kharlamova et al. (2012) and wireless transfer of data [8, 16, 19], are of note. Mathematical models are applied for the environmental information processing Godø et al. (2014) and for aggregating data from many sources. The principles of information systems design Kachinsky and Agarkova (2013) and the effectiveness of these systems should be taken into account for environmental monitoring. Despite the already implemented software solutions, there is still a relevant problem of designing mathematical models that would take into account the combination of non-homogenous factors and meet the following requirements: coherent process description at various modelling stages, continuity, and adaptation capability of models/software to new conditions.

The purpose of our research is to improve the information systems of ecological monitoring and forecast by developing models and algorithms for numerical modelling of dispersion of hazardous impurities in the lower atmospheric layers. The purpose of the research requires achieving the following interrelated objectives: simulating the transfer of hazardous impurities in the surface atmospheric layer, developing the general structure and main input data for the computer-aided model implementation, implementing the information system (Paine et al. 2014).

MATERIAL AND METHODS

Simulation Procedures

Determining the regularities in the generation of ecological hazards and the peculiarities of their manifestation should be the basis for designing an ecological security management system. One of the main ways to maintain environmental security is to prevent pollution by predicting and undertaking necessary conservational measures. In this case, mathematical modelling is a powerful tool for studying the processes occurring in the ecosystem. We have built mathematical models of the boundary atmospheric layer with a free outer fringe. The main mathematical models of atmospheric processes were built with regard to the real hydro-thermodynamic regimes, the mechanism of phase transition of water, planetary boundary layer processes, radiation effect, turbulent energy transfer, condensation, thermodynamic changes in a non-homogenous atmosphere that modify circulation, geophysical properties of the Earth, the Coriolis force and orographic data. In previous studies, including Abramic et al. (2015) we have:

1. Built some models of heat gain as an important factor for baroclinic transformation dynamics, changes in pressure in a humid atmosphere and for abnormal changes in pressure without condensation. Forecast models of compressed atmosphere were offered to determine averaged meteorological elements.
2. Assessed the role of turbulent diffusion and horizontal turbulent transfer of mechanical energy in a cyclone dynamics, most significantly for the final stage of development (Omanović et al. 2015).
3. Built mathematical models of vertical movement dynamics for saturated and humid unsaturated cloudy atmosphere.
4. Built numerical models of atmospheric dynamics, base models of atmospheric circulation and a numerical finite-difference scheme of baroclinic atmospheric processes, and a mathematical model of stationary atmospheric processes.
5. Built mathematical models of transfer and dispersion of hazardous substances with a variable velocity profile (Srbinovska et al. 2015).

We have applied a mathematical model, based on the system of hydro-thermodynamics equations, to study the local atmospheric processes that occur in the boundary layer (8). Since horizontal dimensions of the considered meso-meteorological processes are relatively small (50x50 km), the system of hydro-thermodynamics equation is written in the Cartesian coordinate system x, y, z. The following were taken as original equations: the equation of motion, the continuity equation, the heat flow equation, the equation of specific humidity, etc. These equations include the sought functions of velocity vector, temperature, potential temperature, pressure, density, specific humidity, viscous stress tensor of flow, heat, and humidity, which are coordinate and time functions that were obtained in Toro et al. (2015) for real atmospheric processes.

The software system was designed to allow connecting a certain block that is required to solve a specific problem by setting input parameters of the model. Let us consider the system of hydro-thermodynamics equations of – motion:

$$\frac{du}{dt} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + lv + \frac{\partial \tau_{11}}{\partial x} + \frac{\partial \tau_{12}}{\partial y} + \frac{\partial \tau_{13}}{\partial z} \quad (1)$$

$$\frac{dv}{dt} = -\frac{1}{\rho}\frac{\partial p}{\partial y} - lu + \frac{\partial \tau_{21}}{\partial x} + \frac{\partial \tau_{22}}{\partial y} + \frac{\partial \tau_{23}}{\partial z} \quad (2)$$

$$\frac{dw}{dt} = -\frac{1}{\rho}\frac{\partial p}{\partial z} - g + \frac{\partial \tau_{31}}{\partial x} + \frac{\partial \tau_{32}}{\partial y} + \frac{\partial \tau_{33}}{\partial z} \quad (3)$$

- Continuity:

$$\frac{\partial p}{\partial t} + div\rho\vec{u} = 0 \quad (4)$$

- Phase (Clayperon):

$$p = \rho RT \quad (5)$$

- Heat flow:

$$\frac{d\theta}{dt} = \frac{L_w}{c_p}F + Q_r + \frac{\partial H_1}{\partial x} + \frac{\partial H_2}{\partial y} + \frac{\partial H_3}{\partial z} \quad (6)$$

- Specific humidity:

$$\frac{dq}{dt} = -F + \frac{\partial Q_1}{\partial x} + \frac{\partial Q_2}{\partial y} + \frac{\partial Q_3}{\partial z} \quad (7)$$

$$\theta = T\left(\frac{1000}{p}\right)^{\frac{AR}{c_p}} \quad (8)$$

where:

$$\frac{d\varphi}{dt} = \frac{\partial \varphi}{\partial t} + u\frac{\partial \varphi}{\partial x} + v\frac{\partial \varphi}{\partial y} + w\frac{\partial \varphi}{\partial z} \equiv \frac{\partial \varphi}{\partial t} + \vec{U}grad\varphi$$

$$\varphi = (u, v, w, \theta, q)$$

and

$$F = i\frac{c_p}{L_w}(\gamma_a - \gamma_b)W$$
$$i = \begin{cases} 1 & q \geq q_n \\ 0 & q < q_n \end{cases} \quad (9)$$

Where: γ_a is the dry adiabatic gradient, γ_b is the humid adiabatic gradient, calculated by the following equation:

$$\gamma_b(P,T) = \gamma_a \frac{p + 0{,}622\frac{L_w E}{RT}}{p + 0{,}622\frac{L_w^2 E}{c_p R_n T^2}} \quad (10)$$

where: t is time; u, v, w, – components of wind velocity vector; T – temperature; θ –potential temperature; p – pressure; q – specific humidity; ρ – density; R – universal gas constant; L_w – latent heat of condensation; c_p – specific heat capacity of the air at steady pressure; Q_r – radiation component of the heat flow; A – thermal energy equivalent; g –gravitational acceleration; l – Carioles parameter; $\tau_{i,j}$, ($i = \overline{1,3}$, $j = \overline{1,3}$) – Reynolds viscous stress tensor; H_i, Q_i, $i = \overline{1,3}$ – flows of heat and humidity in directions x, y, z, respectively. The type of summands $\tau_{i,j}$, H_i, Q_i is specified separately.

The system of equations (1-10) is considered with the following initial and boundary conditions:

$$u' = 0, v' = 0, \theta' = 0, q' = 0,$$
$$H(x,y) = H^0(x,y) \text{ at t=0} \quad (11)$$

$$\frac{\partial u\prime}{\partial x} = 0, \frac{\partial v\prime}{\partial x} = 0, \frac{\partial \theta\prime}{\partial x} = 0, \frac{\partial q\prime}{\partial x} = 0 \; at x = \pm X \quad (12)$$

$$\frac{\partial u\prime}{\partial y} = 0, \frac{\partial v\prime}{\partial y} = 0, \frac{\partial \theta\prime}{\partial y} = 0, \frac{\partial q\prime}{\partial y} = 0 \; at y = \pm Y \quad (13)$$

$$u' = 0, v' = 0, \theta' = \alpha\Delta T, q' = 0,$$
$$\pi' = 0, w' = \frac{dH}{dt} at z = H(x,y,t) \quad (14)$$

$$u = 0, v = 0, \theta' = f(x,y,t), w = \frac{d\delta(x,y)}{dt},$$
$$q' = \tilde{Q}(x,y,t) \; at z = \delta(x,y) \quad (15)$$

where: $\Delta T = T_{HOT} - T_{COLD}$, $H^0(x,y)$ is the initial set height of the inversion layer.

$$q_{sum} = \frac{1}{K_{ce}}\sum_{j=1}^{n}(q_{sf.j} - q_{b.j}) = \frac{1}{K_{сд}}\sum_{j=1}^{P}\frac{C_{sf.j} + C_{b.j}}{TLV_j} < 1 \quad (16)$$

where: $C_{sf.j}$ is the surface concentration of substance j, $C_{b.j}$ is the background concentration of substance j, K_{ce} is the combined hygienic effect coefficient of the group of substances.

$$q_{sum\,j} = q_{sf.j} - q_{f.j} = \frac{C_{sf.j} + C_{b.j}}{TLV_j} < 1 \quad (17)$$

In this case, we well get a boundary atmospheric layer problem with air mass movement over a thermally and topographically non-homogenous surface with a free outer fringe, taken into consideration for boundary conditions. The decision support system (DSS) allows supporting multi-objective decision-making in a complex information ecology. The DSS solves two main problems: choosing the most efficient decision out of many possible ones (optimizing and ordering possible decisions) by relevance (ranking). The information technology of decision support provides for a qualitatively new method of organizing interaction between an individual and a computer. Decision-making (main goal of the DSS) that results from the iterative process can be shown schematically as follows (**Fig. 1**) (Goulart et al. 2017).

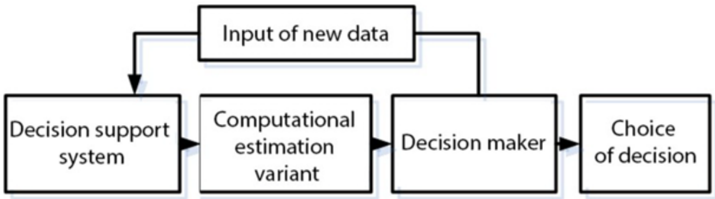

Fig. 1. Iterative process of decision support

A modular software system was designed to implement the herein investigated methods and algorithms of solving the problem of boundary and surface layers and impurities transfer. This simplified the development of the main computational programs by compiling them out of separate module programs.

The developed software system includes modules that implement the main methods and algorithms described in paper. The software calls all parametric procedures and performs temporal integration for a set period (days). The software blocks and algorithms are as follows:

- Regional climate-setting block.
- Input information setting and identifying block;
- Output information organizing block – isograms and tables (this block implies service programs of mathematical support of plotters and visualization systems
- Algorithm of solving the hydro-thermodynamics equations in a curvilinear coordinate system ;
- Algorithm of solving equations for the quasi-homogenous surface layer;
- Algorithm of calculating the temperature and moisture on the ground;
- Algorithm of solving the equation of turbulent transfer of impurities in the atmosphere;
- Algorithm of calculating vertical and horizontal turbulent exchange coefficients;

The main input parameters required to simulate the microclimate of a local area are the following: geographic coordinates and land area; discrete domain parameters; day time; solar zenith angle and declination; surface properties (terrain, roughness, albedo, thermal and physical properties of the soil); background fields of meteorological elements: velocity vector, temperature, and humidity. This list also includes the artificial heat (humidity and impurity) sources distribution and capacity; estimation period in days; number, location, elevation, and capacity of sources both with a continuous effect and generating abnormal emissions at a set time increment. Additional read information includes the vertical profile of pressure, three-dimensional temperature fields, dew point, and wind speed at cellular mesh points, obtained from the objective analysis of these meteorological elements, etc (Qiua et al. 2018).

All values set in the input information are functions of spatial coordinates. Background values for meteorological fields and impurities can be obtained from either atmospheric observations or a large-scale model of atmospheric dynamics. Time and space increments are set based on the specific requirements of the problem (Deardorff 1970).

The software system provides the following output information: spatial fields of meteorological elements and impurities at any specified time, fields of integral concentration of impurities. Output information is presented as numerical values of fields of meteorological elements and impurities all across the area, its parts and sections; their isograms in various sections; fields of velocity vectors for various sections of the area. The procedure also outputs charts with isograms, density of deposited pollutants and surface concentrations. The developed software can be used for numerical forecasting experiments when simulating the transfer of atmospheric impurities from sources with varying intensity and pollutant density. An adapted version of this software can be applied when studying the transfer of hazardous impurities in the boundary and surface atmospheric layers.

We have also applied the requirements of the Ministry of Healthcare for the presence of several hazardous substances in the atmosphere, when the hygienic effect of hazardous substances depends on the combination of substances with a “summative effect”. We have applied them to calculate the conditions for the hazardous substances to go into the atmosphere, depending on particular substance emitted from a source. The computation ceased if conditions (16) and (17) were met. Mathematical dependencies that

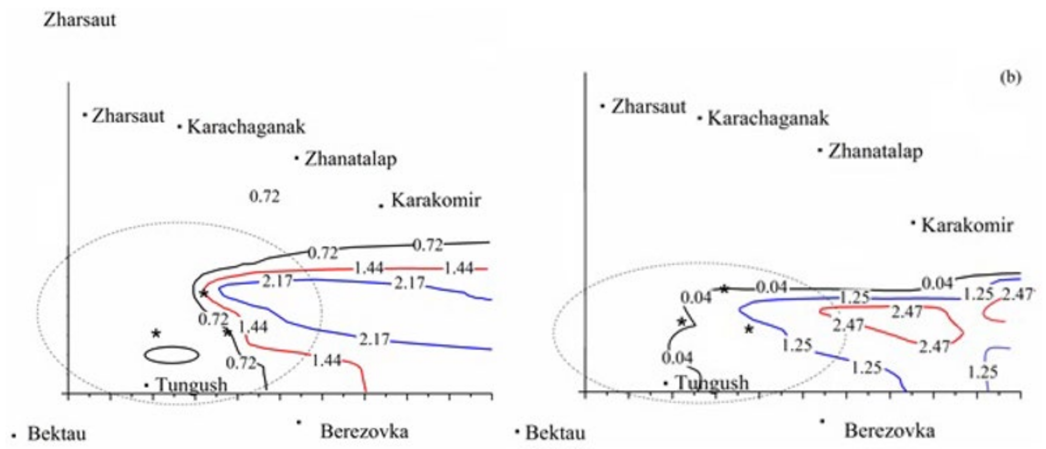

Fig. 2. Isograms of CO_2 concentration in percentage of TLV at 10 m height, a) max CO_2 – 2.89, b) max CO_2 – 3.69

describe the specific types of heat and humidity flows, viscous stress tensor and ecological state are the following include a universal gas constant, latent heat of condensation, specific heat capacity of air at steady pressure, radiation component of heat flow, energy, gravitational acceleration, and the carioles parameter. The formation rate of the liquid phase is calculated up to turbulent elements and expressed with dry adiabatic and humid adiabatic gradients (Gomez-Losada et al. 2018).

RESULTS AND DISCUSSION

Problems related to atmospheric pollution, remedial measures, prediction and assessment of possible risks are covered extensively (The handbook for integrated water resources management in transboundary basins of rivers, lakes and aquifers. International Networking of Basin Organization) (Fritz et al. 2015). Geo-information monitoring systems are applied in order to analyse the consequences of pollution, as they allow analysing large amounts of data and considering many ecological influence factors. In terms of the impact that industrial disasters have on the environment, scientists analyse the spread and effect of various chemical substances, as well as the use of various air treatment technologies. In general, all dispersion models fall within one of the following groups: requiring a full-scale experiment, related to physical modelling, semi-empirical models, and computational fluid dynamics models.

Setting mathematically correct and physically consistent initial and boundary conditions for the system of hydro-thermodynamics equations is an important aspect when it comes to solving the boundary atmospheric layer problems. Therefore, it is expedient to consider some remarks: in the considered models, initial conditions at t=0 are set by measurement data, and thus, are related to the input parameters. However, obtaining detailed physical information regarding the initial mesoscale fields is difficult in practice. Therefore, the initial field is considered as zero when estimating numerically this type of atmospheric circulation. In this case, problem solution at small time values will describe the adaptation of meteorological fields to conditions when turbulence comes into play (Keller et al. 2015). Let us consider the calculation results obtained by our numerical model of impurity spread for the next model situation. We assume that in a region with spatial dimensions of $X=Y=70000$ m and H=1700 m, there is a source of a passive impurity located at the H_s=250 m height ($X=Y=0$), m with the following coordinate increments: $\Delta x=\Delta y=4$ km, $\Delta z=50$ m at $z \leq 200$ m, where wind speed is equal u=2 m/s, $v = w = 0$. The time integration was carried out over an interval of 24 h. **Fig. 2a** shows the results of calculating the moderate concentration, integrated perpendicular to the wind direction and normalized to $\frac{Q}{Hu}$, where Q is the emission rate from the source. The level of the moderate concentration is expressed as percentage of the threshold limit value (TLV). Figure analysis reveals that the torch axis (max concentration line) descends near the source and reaches the underlying surface.

Figs. 2-4 show the isotherms of gas cconcentration, expressed as percentage of TLV under stable atmospheric conditions, when wind speed is 2 m/s in the surface layer (Kozulya and Belova 2013).

Figs. 5 and **6** are show the spread of impurities under stable atmospheric conditions, when wind speed in the surface layer is 4 m/s:

Input data for calculation are presented in **Table 1**.

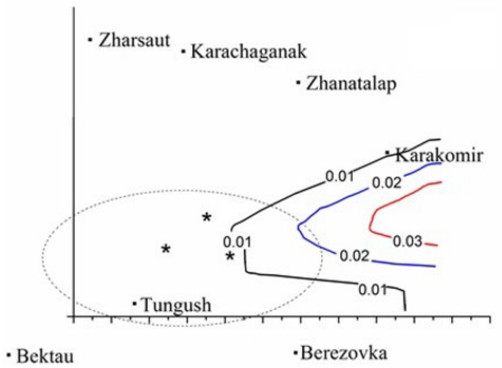

Fig. 3. Isograms of CO_2 concentration in percentage of TLV at 70 m height, max CO_2 – 0.03

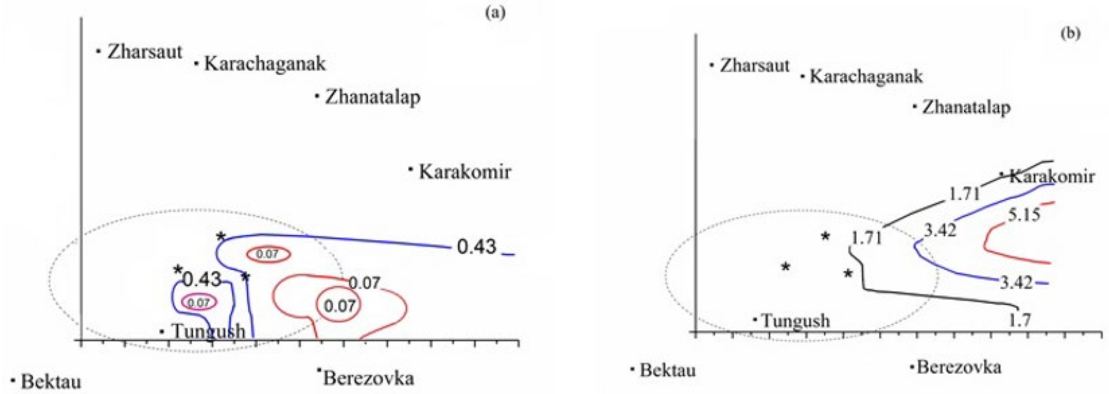

Fig. 4. Isograms of NO_2 concentration in percentage of TLV a) at 10 m height; max NO_2– 1.75, b) at 80 m height; max NO_2– 6.85

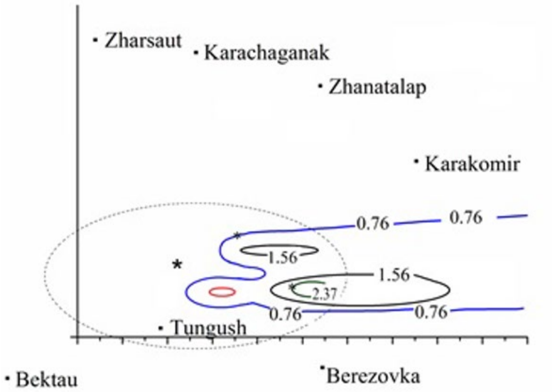

Fig. 5. Isograms of CO_2 concentration in percentage of TLV at 70 m height; max CO_2 – 3.17

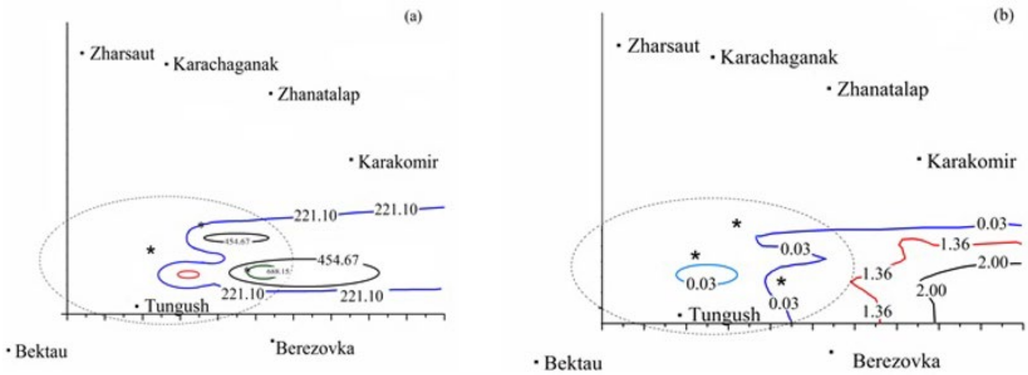

Fig. 6. Isograms of NO_2 concentration in percentage of TLV a) at 70 m height; max NO_2 – 921.63, b) at 80 m height; max NO_2 – 2.82

Table 1. Input data and designations for jet steam calculation

Gas concentration in the well section	T_s Temperature in the well section
Air	293.0° K
Air	700.0° K
Air	1000.0° K
Air	1300.0° K
$C_{CO} = 0.2$	1300.0° K
$C_{O2} = 0.2$	1300.0° K
$C_{H2} = 0.6$	1300.0° K
$C_{CO} = 0.2$	1300.0° K
$C_{H2} = 0.8$	1300.0° K

Calculation was carried out at the time of complete air washing (40 km in length).

As from the **Figs. 4b** and **6b** can be seen, hazardous substances are spreading faster outside the region, as the wind speed is increasing. The effective emission height is maximal for UKSP-16 installations (70-100 m) and near the upper boundary of the surface layer (10-20 m) for other sources of pollution. Since the most powerful sources have a relatively large effective height, the maximum deposition of impurities in the surface layer is found at a great distance from the sources due to inversion conditions (**Fig. 5**). Impurities spread in the wind direction. At that, changes in the direction with changes in height (left turn), in accordance with the Ekman model Yang and Wang (2017) were also found under convectional conditions. It is also worth noting the more intensive NO_2 pollution at heights that are close to the effective height of emission. In **Fig. 5b**, the threshold limit value s exceeded by more than a hundred times (Chen et al. 2017).

This is explained by the lack of upward air currents and weak vertical turbulence under inversion conditions, which causes a localization of emissions near their respective sources. In addition, a strange, at first glance, effect was found during the analysis of calculations with the simplest model under stable conditions, when an increase of wind produced more intensive a pollution near the ground and at a set height of about 70 m. This is related to a similar factor – increase in wind speed with unchanged meteorological parameters significantly reduces the effective height of emission, which, in turn, draws the smoke plume axis closer to the ground. Thus, it is possible to conclude that the noted meteorological situation, together with the commonly known hazardous meteorological conditions that are created with inversion and its combination with lull, is also among the most hazardous ones (Ferdoush and Li 2014).

A number of important scientific and technological problems are still unsolved for most monitoring information systems, for example:

1. Inclusion of physical and geographical features of the region (rugged terrain, large water bodies, other surface non-homogeneities) in the atmospheric transfer models.
2. Automated input of up-to-date meteorological information to predict the development of the situation in real time.
3. Inclusion of a block for assessing the parameters of the atmospheric emission source:
    a. A set of standard design basis scenarios and accidents for a given type of object;
    b. Calculation programs for modelling the development of the accident, which characterize the atmospheric emission.
4. A set of calculation models for calculating substances concentration in the air and their precipitation on the ground.
5. The subsystem should allow assimilating the monitoring data to specify the characteristics of local pollution and the parameters of the emission source in real time.

A stationary DSS should allow:

- Taking into consideration the instability of meteorological conditions and parameters of the emission source in the computations of the atmospheric transfer of emissions;
- Taking into account the effect of non-homogeneity;
- Assimilating live measurement data to specify emission parameters with regard to the actions performed by the accident management personnel.

It is worth noting that up-to-date meteorological information is critical for forecasting the emission spread within the framework of DSSs. In particular, the following data from meteorological measurements is required for stationary subsystems to function:

- Vertical profiles of meteorological parameters in the region;

- Atmospheric parameters near the ground (Castell et al. 2015).

Unlike the forecasting model based on the space-time concentration field, our mathematical model of impurity transfer in the surface atmospheric layer, implemented in a software system, calculate the live spread of impurities. An important feature of the obtained solution is that the software system allows simulating various meteorological conditions and conducting experiments with the model while changing such parameters as wind speed, land area, pollution height, air temperature, etc (Akhmetov and Aitimov 2015, Zaurbekov et al. 2018).

In addition, the developed mathematical technique enables assessing the risk of pollution with several types of pollutants with regard to features that are obtained in the process.

Unlike other studies, for instance, [40] or [41], the herein offered models take into consideration several types of pollution sources and determine requirements to monitoring data. The introduced solution allows assessing the ecological pollution risks in real time by means of the introduced models. In other words, it is possible to collect necessary live data under accurate requirements to input information and to assess the probability of pollution spread and possible danger in the shortest possible period if a pollution source is discovered. This will improve the efficiency of decision making in the field of population and ecological protection.

The following practical and theoretical problems related to local circulation in a limited area was solved with the set of models:

- Analysing the effect of modifications made for ground properties (thermal, dynamic, moisture, etc.) on the dynamics of the boundary atmospheric layer in the Karachaganak gas condensate field;
- Studying the regularities of pollutant spread with the hydro-thermodynamic processes development under various weather conditions (inversion, lull, upward air current, etc.) and with regard to changes in the ground properties in the region;
- Assessing and managing atmospheric pollution and industrial regions;
- Carrying out a numerical simulation of the regional hydro-meteorological regime.

CONCLUSIONS

1. A mathematical model of hazardous impurity transfer in the surface atmospheric layer was developed.
2. The simulation of atmospheric circulation and spread of impurities in the surface atmospheric layer provided systems of equations for the quasi-homogenous surface layer, heat flow and ground moisture; in addition, the system of hydro-thermodynamics equations was closed with regard to the turbulent transfer operator (Delamo et al. 2015).
3. Equations of the block model of hazardous impurity transfer in the surface atmospheric layer were deduced; interaction between blocks w described.
4. Numerical schemes of the block model of hazardous impurity transfer in a baroclinic atmosphere were developed.
5. The general structure and main input data for the implementation of the atmospheric transfer model were determined. A class of practical and theoretical problems of studying local circulation in a limited area was solved, based on a set of models. Requirements to models, output information technique, meteorological information, and computations of surface concentration of specific ingredients in a group of sources were determined.
6. Numerical computations of hazardous substance transfer in the surface atmospheric layer were carried out with regard to the effect of the ground roughness.
7. Geo-ecological maps of hazardous substance transfer under inversion were obtained.

The developed diffusion-model-based program can be used to calculate in real time the area of emission spread from a certain group of sources and to assess their effect on nearby settlements. A small amount of input information and information regarding the parameters of sources (only the emission volume changes) allow quickly conducting numerical experiments with the following view of results (Wu et al. 2016).

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