Mathematical modeling of atmospheric transformation of pollutants considering weather conditions and time of day

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ABSTRACT

This paper is devoted to the problem of propagation of harmful impurities in the atmosphere from point sources, with the photochemical transformation. A list of characteristic pollutants of the atmosphere of an industrial city has been determined. The most common harmful substances, such as NO_2, H_2SO_4, were selected to study the process of transformation of impurities. A scheme for the transformation of pollutants by chemical reactions has been developed.

In order to account for the influence of anthropogenic heat sources and the heterogeneity of the underlying surface on the spread of harmful substances, the model of the boundary layer of the atmosphere and the equation of transport and transformation of impurities are considered. It takes into account the parameter that describes photochemical transformations depending on weather conditions and time of day on the example of the city of Ust-Kamenogorsk.

An application software package has been developed for numerical modelling of atmospheric air pollution, taking into account photochemical transformations and visualizations of corresponding scenarios.

The results of numerical modeling of the distribution and transformation of harmful impurities against the background of mesometeorological processes with the terrain and water surfaces are presented.

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1. INTRODUCTION

The main Atmospheric air pollution remains an acute problem for most cities of the Republic of Kazakhstan. The main pollutants of atmospheric air in Kazakhstan primarily include enterprises of thermal power engineering, ferrous and non-ferrous metallurgy, oil-producing and oil-refining sectors, automobile and railway transport.

Weak implementation of environmental protection measures led to severe air pollution of industrial cities of the Republic of Kazakhstan. Outdated technologies used in thermal power engineering, non-ferrous and ferrous metallurgy, oil and coal mining, construction, automobile and railway transport are the causes of atmospheric air pollution in Kazakhstan.

Every year, seven million people die prematurely from air and indoor air pollution in the world. This is more than from the main diseases with high mortality – malaria, tuberculosis and AIDS – combined.

The problems of atmospheric pollution and the study of air quality began to take on importance after the London fog of 1952, which led to thousands of premature deaths. This is evidenced by reports made by the UK Ministry of Health [1-3].

Today, the leading country with densely populated cities and developed industry is China, where more than 370,000 new industrial enterprises have been built over the past 40 years. In the works of Gautam S., Patra A.K., Kumar P. [4] the state of air pollution, especially $PM_{2.5}$, is considered in 21 cities in China based on chemical characteristics and regulatory data. In the works of Kuerban M., Liu S., Chang Y. et al. [5-8] an assessment of carbon-containing aerosols in Shanghai was carried out.

The results of the study of air quality in industrial cities carried out by foreign and domestic scientists indicate a lack of information about atmospheric pollution and note the need for detailed studies [9-10].

The study [9] assessed additional morbidity and mortality in 21 cities of the Republic of Kazakhstan, due to exposure to fine particles. It was found that due to air pollution in large cities of Kazakhstan, 8134 premature deaths of adults occur annually, with a significant difference between individual cities. At the same time, the authors openly inform that due to the insufficient network of monitoring posts for fine particles, data on the total volume of suspended particles were used in the study. It is noted that the health effects should be recalculated based on the measured concentrations of $PM_{2.5}$ in the atmospheric air of cities when the monitoring network is installed and expanded [9].

The objective of researches [10] was to examine the impact of the COVID-19 quarantine measures implemented in 2020 on the levels of atmospheric pollutants in Almaty. The researchers compared the daily concentrations of pollutants during different periods: before, during, and after the quarantine period. Studies have shown low pollution rates during the quarantine period.

According to the WHO Regional Office for Europe (World Health Organization), well-thought-out and rational measures to combat air pollution can reduce the growth of diseases and the risk of climate change in the long term and, thereby, radically improve the quality of life [11].

Unfortunately, the problem of air pollution has not been solved in any of the country's regions, however, in many European countries, as well as in the USA, Canada and Japan, where strict policy guidelines and regulatory rules have been adopted, as well as regular monitoring systems have been established a noticeable reduction in emissions and a decrease in concentrations of pollutants [12].

Human actions are responsible for the emergence of profound environmental problems in the lowermost layer of the atmosphere. Industries release substantial quantities of chemicals, leading to environmental pollution and adverse impacts on human health. Impurities play a crucial role in chemical changes that take place within the lowest layer of the atmosphere. These impurities can be harmful, diminishing the transparency of the atmosphere to thermal radiation and influencing the condensation of water vapor in the same layer. The concentration of impurities surpasses the equilibrium levels, indicating a troposphere that is chemically active and not in a state of equilibrium [13].

As a result of its historical socio-economic development, the East Kazakhstan region has become one of the most environmentally disadvantaged areas in the country. The city of Ust-Kamenogorsk is a heavily urbanized area that is overwhelmed with a variety of industrial establishments representing different technological orientations. These include non-ferrous metallurgy, nuclear-industrial and rare-metal complexes, thermal power engineering, transportation, food processing industries, and utilities. Furthermore, the pollution in the city is compounded by emissions from both transportation and the private sector. The specific pollutants commonly found in Ust-Kamenogorsk encompass sulfur dioxide, nitrogen dioxide, carbon monoxide, phenol, formaldehyde, chlorine, inorganic arsenic compounds, hydrogen chloride, hydrogen fluoride, sulfuric acid, hydrogen sulfide, ammonia, benz(a)pyrene, as well as six metallic elements: lead, zinc, copper, cadmium, beryllium, and mercury [13]. The city's air pollution is significantly influenced by various sources and is exacerbated by its unique atmospheric circulation resulting from its geographical location, situated in a river valley surrounded by mountains. This topography gives rise to mountain-valley and stagnant winds, leading to unfavorable meteorological conditions such as temperature inversions, calm surface layers, fogs, and unfavorable wind directions. These unfavorable conditions trigger chemical changes in pollutants, with sulfur dioxide, in particular, dissolving in mist droplets and forming toxic sulfuric acid aerosols. The calm conditions combined with fogs and inversions contribute to the highest levels of pollution. Approximately 85% of the fog occurrences happen during periods of calm weather, while the remaining 15% occur when the wind speed ranges from 1-3 m/s [13].

There are a lot of scientific publications devoted to this topic all over the world, including in Kazakhstan, which consider various methods of modeling the propagation of pollutants in the atmosphere. The works of Marchuk G.I. [14], Penenko V.V. [15-18], Aloyan A.E. [19-23], Baklanov A.A.[24-26], Nieuwstadt F. T. M., H. Van Dop. [27-29] are devoted to the mathematical modeling of the process of atmospheric air pollution.

In [30-31], using a probabilistic-statistical approach, an information system for modeling the transfer of harmful impurities in the atmosphere from motor vehicles was created.

Artificial neural networks have proven their effectiveness as accurate predictors for classification and regression tasks. A review of the scientific literature shows that they are used to predict the surface boundary layer of the atmosphere, predict air pollution indicators and simulate the effects of point sources. In recent years, the use of deep machine learning using artificial neural networks has raised the level of scientific research to new heights. Platforms for air monitoring using artificial intelligence and the Internet of Things (IoT) are being developed all over the world [32-36].

Thus, deep learning methods are very fruitful in detecting and predicting atmospheric air pollution and forecasting how different industries will affect the ecological environment [32].

The paper [33] examines the environmental impact of $PM_{2.5}$ in Iraq and Kuwait from 2001 to 2018 using machine learning and remote sensing. Abnormal annual concentrations of $PM_{2.5}$ have been revealed for Kuwait and Iraq.

In [34], researchers have presented a successful application of Internet of Things technology to monitor air pollution levels, specifically using the Malaysia Air Pollution Index (API) as a basis. This affordable and real-time system has the capability to continuously track various common air pollutants, such as Particulate Matter (PM) including $PM_{2.5}$ and PM_{10}, as well as Carbon Monoxide (CO) gas, along with ambient temperature and humidity.

In [35], the authors propose a mobile, cost-effective, and precise system for monitoring air pollution. They achieve this by employing an Arduino microcontroller in combination with gas sensors.

In [36], a typical case of dusty weather was selected and its main mechanism of development in the northeast of the Tibetan Plateau was analyzed, and then six ML methods and a time series regression model were applied to predict the concentration of PM_{10} in this area.

Therefore, the use of machine learning methods is optimal in tasks for which there is no strict mathematical model. The trained system, only with the available expert assessments, is able to reproduce a pattern that is difficult and impossible to formalize.

In [37-38], the order of convergence and the order of approximation accuracy are presented.

In this article, we delve into the issue of impurity dispersion originating from specific point sources. We take into careful consideration the influence of weather conditions and the time of day on the photochemical transformation of these impurities. Our focus is to understand how these factors impact the spread and subsequent transformations of harmful impurities. To shed light on this matter, we present the outcomes of extensive numerical modeling. Our study specifically examines the dynamics of impurity dispersion and transformations, taking into account the prevailing mesometeorological processes in the city of Ust-Kamenogorsk. Through this investigation, we aim to gain insights into the intricate relationship between impurity propagation, photochemical reactions, and local meteorological conditions within the context of this particular city.

2. METHOD

2.1. Understanding the conversion of harmful impurities: a chemical modeling approach

To capture the changes that occur to harmful impurities during their transfer, the method introduced is employed. This approach utilizes the most prevalent types of harmful substances, including CH_2O, CO, CO_2, SO_2, SO_3, HSO_3, NO, NO_2, NO_3, HNO_3, MgO, CaO, H_2SO_4, $MgSO_2$, $CaSO_2$, and their chemical reactions, to simulate photochemical processes (as illustrated in Figure 1).

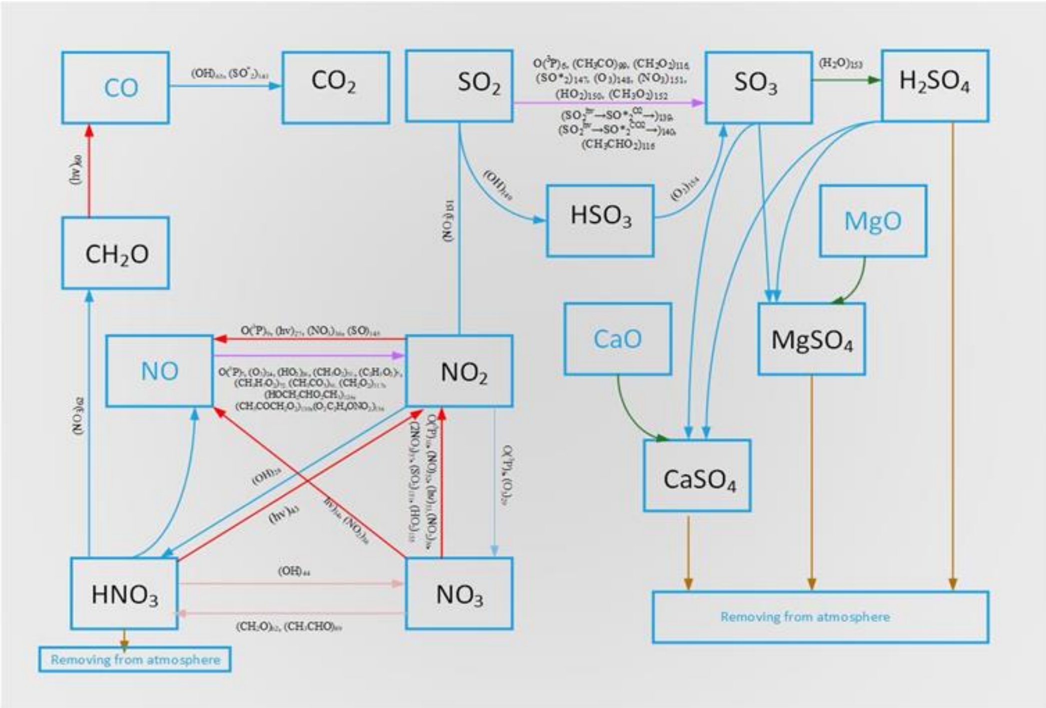

Figure 1. Scheme of the transformation of pollutants

Figure 1 presents a collection of diagrams outlining the transformation of certain substances into impurities under the influence of heat and moisture. Each transformation has a unique rate constant, and the scheme details the process through which the substances are changed into fine solid particles and dust during successive reactions, ultimately leading to their removal from the atmosphere.

As an illustration, when SO_2 molecules absorb solar radiation, they become energized and undergo a reaction with oxygen in an excited state, resulting in the formation of SO_3 and O_3:

$$SO_2 + hv \rightarrow {SO_2}^*$$

$${SO_2}^* + O_2 \rightarrow SO_3 + O$$

Thick smog appears in the city of Ust-Kamenogorsk during adverse weather conditions (AWC).

In nature, there are two distinct types of smog: London type, which is reducing, and Los Angeles type, which is photochemical oxidative. Industrial cities tend to have restorative smog, which is a blend of smoke, soot, and sulfur dioxide. The highest levels of smog are typically observed in the early morning at around 0°C.

Consider the main types of smog: smog formation due to atmospheric pollution by soot or smoke containing sulfur dioxide SO_2 and air pollution by car exhaust gases containing nitrogen oxides.

The second type of smog, known as photochemical smog, requires photochemical reactions to occur, which lead to the formation of ozone (O_3). This reaction is triggered by the presence of hydrocarbons and nitrogen oxides. The concentration of O_3 in the air samples begins to increase when the ratio of NO_2 and NO concentrations is at its maximum. The formation of O_3 in the presence of nitrogen oxides is initiated by solar radiation with a wavelength of less than 580 nm, and it is more intense in air containing NO_2. Solar radiation with wavelengths ranging from 285 nm to 580 nm can reach the Earth's surface.

Sulfur oxidation proceeds in three states: gas, liquid, solid. SO_2 molecules interacting with oxygen O_2 in the atmosphere, forms sulfur trioxide SO_3 and three oxygen O_3:

$${SO_2}^* + O_3 \rightarrow SO_3 + O_2$$

or interacting with carbon monoxide CO forms sulfur oxide SO and carbon dioxide CO_2

$${SO_2}^* + CO \rightarrow SO + CO_2$$

or by reaction involving the third body M:

$${SO_2}^* + CO \rightarrow SO + CO_2$$

For other chemicals, such as CH_2O, CO, CO_2, HSO_3, NO, NO_2, NO_3, HNO_3, MgO, CaO, H_2SO_4, $MgSO_4$, $CaSO_4$, the corresponding reactions are also selected [39].

The chemical transformations shown in the diagram (Figure 1) are described by a system of fifteen differential equations [13]. Some equations, for example, for CH_2O, CO, CO_2 the equations have the following form:

$$\frac{d\varphi_{CH_2O}}{dt} = -k_{60}\varphi_{CH_2O} - k_{62}\varphi_{CH_2O} + f_{CH_2O} \quad (1)$$
$$\frac{d\varphi_{CO}}{dt} = k_{60}\varphi_{CH_2O} - k_{65}\varphi_{CO} - k_{141}\varphi_{CO} + f_{CO} \quad (2)$$
$$\frac{d\varphi_{CO_2}}{dt} = k_{65}\varphi_{CO} - k_{141}\varphi_{CO} + f_{CO_2} \quad (3)$$

Unlike the work [13], this research takes into account the $\gamma_i(p)$ parameter, which is determined depending on weather conditions and time of day, i is the number of the corresponding reaction from Figure 1. In order to uphold the principle of mass conservation, differential equations in the form of (1)-(3) were formulated. These equations consider the transfer of substance fractions, where a fraction is subtracted from its original substance and added to the volume of the newly formed substance during a reaction.

2.2. Mathematical model of the boundary layer of the atmosphere

In order to examine the impact of anthropogenic heat sources, detrimental substances, and surface heterogeneity on the atmosphere of an industrial city, a three-dimensional domain Ω is utilized, following a model of the atmospheric boundary layer. The model is based on previous studies [13-18].

Equations of motions and continuity equation:

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p_i}{\partial x_i} + a_i K_i + \frac{\partial}{\partial x_3}\left(\nu \frac{\partial u_i}{\partial x_3}\right) + \Delta u_i,\ \frac{\partial u_j}{\partial x_j} = 0, i = 1,2,3, \quad (4)$$

where t is time, $p = (p_1, p_2, p_3)$ is pressure, in the second term in the left part and in the continuity equation summation is performed by repeating indices j $(j = 1,2,3)$, $u = (u_1, u_2, u_3)$ is a velocity vector, $x = (x_1, x_2, x_3)$ is Cartesian coordinates, $a = (1, -1, \lambda), K = (u_1, u_2, \theta)$. Heat inflow equation:

$$\frac{\partial \theta}{\partial t} + \frac{\partial u_i \theta}{\partial x_j} + S u_3 = \frac{\partial}{\partial x_3}\left(\nu \frac{\partial \theta}{\partial x_3}\right) + \Delta\theta, i = 1,2,3, \quad (5)$$

here θ is background potential temperature, ν is vertical coefficient of turbulent exchange, S is stratification parameter. Equation of transfer of harmful substances in the atmosphere:

$$\frac{\partial \varphi_q}{\partial t} + u_i \frac{\partial \varphi_q}{\partial x_j} = \Delta\varphi_q + \frac{\partial}{\partial x_3}\left(\nu \frac{\partial \varphi_q}{\partial x_3}\right) + \alpha_q \varphi_q + \beta_q + f_q, \sum_q \varphi_q = 1,\ i = 1,2,3, \quad (6)$$

here $\Delta = \frac{\partial}{\partial x}\mu_x \frac{\partial}{\partial x} + \frac{\partial}{\partial y}\mu_y \frac{\partial}{\partial y}$ is the differential operator of horizontal turbulent diffusion. t - time, x, y, z - Cartesian coordinates, $\vec{U}$- wind velocity vector with components u, v, ω, π - pressure, $\lambda = \frac{g}{T}$- convection parameter or buoyancy parameter,$S = \frac{\partial \theta}{\partial z}$ is a stratification parameter, g - gravity acceleration, T - air temperature, μ_x, μ_y- coefficients of horizontal turbulence for motion and heat transfer, ν - vertical coefficient of turbulent exchange for motion and heat transfer, θ is the background potential temperature, l is the Coriolis parameter.

$\phi_q$is the fraction of the concentration of a harmful substance in the impurity, f_q describes the sources of substances at the level of roughness,$\alpha_q, \beta_q$are coefficients arising from the equations of transformations of impurities in the atmosphere, the index q means the chemical formula of the substance.

In equations (5) and (6) as in equation (4), summation in the second term is performed by the index j.

The following initial and boundary conditions are given for the system of equations (4) - (6):

$$\vec{U}^0(x_1, x_2, x_3), \theta = \theta^0(x_1, x_2, x_3), \phi_q = \phi_q^0(x_1, x_2, x_3) \text{ when } t = 0,$$

$$u_1 = u'_{11}(x_2, x_3, t), u_2 = u'_{21}(x_2, x_3, t), u_3 = 0, \frac{\partial \theta}{\partial x_1} = 0, \phi_q = {\phi_q}^0 \text{when } x_1 = 0, 0 \le x_2 \le Y,$$

$$\frac{\partial u_1}{\partial x_1} = 0, u_2 = 0, u_3 = 0, \frac{\partial \theta}{\partial x_1} = 0, \frac{\partial \phi_q}{\partial x_1} = 0 \text{ when } x_1 = X, 0 \le x_2 \le Y,$$

$$u_1 = u'_{12}(x, z, t), u_2 = u'_{22}(x, z, t), u_3 = 0, \frac{\partial \theta}{\partial x_2} = 0, \phi_q = {\phi_q}^0 \text{when } x_2 = 0, 0 \le x_1 \le X, \quad (7)$$

$$u_1 = 0, \frac{\partial u_2}{\partial x_2} = 0, u_3 = 0, \frac{\partial \theta}{\partial x_2} = 0, \frac{\partial \phi_q}{\partial x_2} = 0 \text{ when } x_2 = Y, 0 \le x_1 \le X,$$

$$u_1 = 0, u_2 = 0,\ u_3 = 0, \theta = 0, \pi = 0, \phi_q = 0 \text{ when } x_3 = H,$$

$$u_3 = 0, h\frac{\partial u_1}{\partial x_3} = a_{u_1} u_1, h\frac{\partial u_2}{\partial x_3} = a_{u_1} u_2, h\frac{\partial \theta}{\partial x_3} = a_\theta(\theta - \theta_0), \phi_{q,0} = \frac{f_q + a_\theta \phi_{q,h} \nu}{\beta + a_\theta \nu_h} \text{ when } x_3 = h,$$

here H is the atmospheric boundary layer height, X, Y - lateral boundaries of the region, $\phi_{q,0}$, $\phi_{q,h}$ - proportions of concentrations of matter q at the level of roughness and the surface layer, θ_0 - roughness level temperature, $a_{u_1} = \frac{\psi_{u_1}(\varsigma_h)}{\eta_{u_1}(\varsigma_h,\varsigma_0)}$ - parameter resulting from the interaction between air flows and the underlying surface friction., $a_\theta = \frac{\psi_\theta(\varsigma_h)}{\eta_\theta(\varsigma_h,\varsigma_0)}$ - a turbulent heat exchange parameter,β - a velocity-based value that characterizes the interaction between impurities and the underlying surface, h - surface layer height, ς_0, ς_h- dimensionless height parameters, ψ_{u_1}, ψ_θ - Businger interpolation functions obtained using experimental data. A comprehensive overview of alternative interpolation formulas suggested by different authors can be found in references [27-29]. In our task, we utilized interpolation functions with the following form:

$$\psi_{u_1}(\varsigma) = 1 + 4.7\varsigma, \quad \psi_\theta(\varsigma) = 0.74 + 4.7\varsigma \text{ when } \varsigma > 0,$$

$$\eta_{u_1}(\varsigma, \varsigma_{u_1}) = \int_{\varsigma_{u_1}}^{\varsigma} \frac{\psi_{u_1}(\varsigma)}{\varsigma} d\varsigma, \quad \eta_\theta(\varsigma,\ \varsigma_0) = \int_{\varsigma_0}^{\varsigma} \frac{\psi_\theta(\varsigma)}{\varsigma} d\varsigma \tag{8}$$

Based on meteorological conditions, the boundary conditions of the type $u = u'_{11}(y,z,t)$, $u_2 = u'_{21}(y,z,t)$ are determined. The similarity theory of Monin-Obukhov and empirical functions from [14] were chosen for modeling the surface layer of the atmosphere at $z = h$. The terrain equation $x_3 = \delta(x,y)$ is taken into account when setting boundary conditions for θ, ϕ_qin the surface layer at $x_3 = h$. The remaining boundary conditions guarantee that perturbations are smooth and that the continuity equation holds at the boundary of the integrable domain.

2.3. The algorithm of numerical implementation

After all the above mathematical investigations, the practical part is considered - the problem of the propagation of harmful impurities in the atmosphere from point sources, taking into account photochemical transformations. The above-stated problems (4)-(7) are solved by the finite difference method and numerically performed by the splitting method for physical processes, which is successfully used in numerical solutions of the equations of aerohydrodynamics in natural variables.

In the area $\Omega = \{0 \le x \le l_1, 0 \le y \le l_2, 0 \le z \le l_3\}$, we introduce the following uniform grids:

$\boldsymbol{\Omega_h} = \{(x_i, y_j, z_k) = (i\boldsymbol{h}_1, j\boldsymbol{h}_2, k\boldsymbol{h}_3),\ i = 0, \rightleftarrows 1, \ldots,\ N_1,\ j = 0,1,\ldots,\ N_2,\ k = 0,1,\ldots\ , N_3\}$,

$\Omega_{x,h} = \{(x_{i-1/2}, y_j, z_k) = ((i - 1/2)\boldsymbol{h}_1, j\boldsymbol{h}_2, k\boldsymbol{h}_3), i = 1,2,\ldots, N_1, j = 0,1,\ldots, N_2, k = 0,1,\ldots, N_3\}$,

$\Omega_{y,h} = \{(x_i, y_{j-1/2}, z_k) = (i\boldsymbol{h}_1, (j - 1/2)\boldsymbol{h}_2, k\boldsymbol{h}_3), i = 0,1, \ldots, N_1, j = 1,2, \ldots, N_2, k = 0,1,\ldots, N_3\}$,

$\Omega_{z,h} = \{(x_i, y_j, z_{k-1/2}) = (i\boldsymbol{h}_1, j\boldsymbol{h}_2, (k - 1/2)\boldsymbol{h}_3), i = 0,1,\ldots, N_1, j = 0,1\ldots, N_2, k = 1,2,\ldots, N_3\}$,

here $\boldsymbol{h}_1 = l_1/N_1$, $\boldsymbol{h}_2 = l_2/N_2$, $\boldsymbol{h}_3 = l_3/N_3$.

When the method of splitting by physical processes is considered, the wind speed u component is determined in the nodes of the grid $\Omega_{x,h}$, the component v in the nodes of the grid $\Omega_{y,h}$, the component ω in the nodes of the grid $\Omega_{z,h}$, a pressure π, temperature θ, the proportion of concentrations of harmful substances ϕ_q in the nodes of the grid Ω_h.

Let the velocity field $\vec{U}_h = (u_h, v_h, \omega_h)$, pressure field π_h^n, for concentrations of harmful substances $\phi_{q,h}^n$, temperature $\theta_h{}^n$be known at the nodal points of the grid regions $\Omega_{x,h}$, $\Omega_{y,h}$, $\Omega_{z,h}$, Ω_h at a time t^n. A splitting scheme is used to determine unknown parameters, such as the velocity field and pressure, temperature, concentration at the time t^{n+1}. This scheme consists of the following stages, the parameter $\gamma_i(p)$ is also taken into account, which is determined depending on weather conditions and time of day:

1. To determine the intermediate values of the velocity $\vec{U}_h^{\,n+1/2}$, taking into account the Coriolis force and the influence of temperature

$$\frac{\vec{U}_h^{n+1/2} - \vec{U}_h^n}{\tau} = -L_h\vec{U}_h^n + \Lambda_h\vec{U}_h^n + \vec{G}_h^n \tag{9}$$

where $L_h\vec{U}_h^{\,n}$, $\Lambda_h\vec{U}_h^{\,n}$ are the difference analogues of convective transport and turbulent exchange, $\vec{G}_h = (lv_h^n,\ -lu_h^n,\ \lambda\theta_h^n)$ is the influence of the Coriolis force and temperature.

At this stage, due to convection, turbulent exchange, coriolis forces and temperature, the amount of movement is transferred.

2. Taking into account the solenoidality of the velocity vector $div_h\vec{U}^{n+1} = 0$, the equation for the pressure field is defined as follows

$$\Lambda_h\pi_h{}^{n+1} = \frac{div_h\vec{U}_h^{n+1/2}}{\tau} \tag{10}$$

3. The transfer of the amount of motion is carried out only due to the pressure gradient and to determine

the velocity $\vec{U_h}^{n+1}$ on the time layer t^{n+1}, thus we have

$$\frac{\vec{U}_h^{n+1}-\vec{U}_h^{n+1/2}}{\tau}=-\nabla_h{\pi_h}^{n+1}, \qquad (11)$$

where $\nabla_h$is the difference analog of the nabla operator $\nabla=(\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z})$.

4. The calculation of temperature transfer and diffusion is carried out according to the following difference scheme according to the velocity fields found

$$\frac{\theta_h^{n+1}-\theta_h^n}{\tau}=-L_h\theta_h^n+\Lambda_h{\theta_h}^n \qquad (12)$$

Further, the transfer and transformation of the fractions of concentrations of harmful substances $\phi_{q,h}^{n+1}$ into impurities is determined.

5. Due to convection and turbulent exchange, the transfer of fractions of concentrations of harmful substances into impurities is determined according to the following difference scheme

$$\frac{\phi_{q,h}^{n+1/2}-\phi_{q,h}^n}{\tau}=-L_h\phi_{q,h}^n+\Lambda_h\phi_{q,h}^n; \qquad (13)$$

6. Influence of external sources the transformation of the concentration fractions of harmful substances into impurities is calculated as follows

$$\frac{\phi_{q,h}^{n+1}-\phi_{q,h}^{n+1/2}}{\tau}=\alpha_q\phi_{q,h}^{n+1}+\beta_q+f_q. \qquad (14)$$

where $\phi_{q,h}^{n+1}$is the fraction of the concentration of the harmful substance q in the impurity on the $n+1$ layer over time, the coefficients α_q,β_q are determined from differential equations (4)-(6).

For example, for the fraction of concentrations of the substance HSO_3 we have:

$$\phi_{HSO_3}^{n+1}=\frac{\phi_{HSO_3}^{n+1/2}+\tau\beta_{HSO_3}+\tau f_{HSO_3}}{1-\tau\alpha_{HSO_3}}$$

where

$\alpha_{HSO_3}=-\gamma_{154}(p)k_{154}\phi_{HSO_3}$,

$\beta_{HSO_3}=\gamma_{149}(p)k_{149}\phi_{SO_2}$,

$\gamma_i(p)$ is a parameter, that is determined depending on weather conditions and time of day.

3. RESULTS AND DISCUSSION (10 PT)

3.1. Numerical results and discussion

The numerical implementation algorithm is presented in [13]. The above model and the developed algorithm were utilized to simulate atmospheric air pollution, taking into account photochemical transformations, at various input parameter values (Table 1). Numerical calculations were performed for an area of 35x35 kilometers and a fixed surface layer height of 3500 meters. The stratification parameter S, which indicates temperature changes with height, was calculated using the vertical temperature gradient during the calculations.

Table 1. Input parameters for atmospheric air modeling taking into account photochemical transformations

Parameter name	Designation	Value
convection parameter	λ	0,16 $m(s\cdot deg)^{-1}$
Coriolis force	l	$10^{-4}s^{-1}$
horizontal coefficient of turbulent exchange	μ_{x_1}	$6\cdot 10^3 m^2 s^{-1}$
vertical coefficient of turbulent exchange	μ_{x_2}	$6\cdot 10^3 m^2 s^{-1}$
characteristic length scale	L	$35000m$
wind	U^*	$10m\ s^{-1}$
speed temperature	θ^*	20^0C

Calculations were carried out on grids 100x100x50, 200x200x100 and 400x400x200. The numerical calculation was carried out on a modern personal computer with the following characteristics of Intel(R) Core(TM)i9-10900F CPU@2.80GHz , 32 GB RAM. The results of numerical calculations are presented using the graphical editor Tecplot and Surfer.

To simulate the dispersion of harmful pollutants in the atmosphere originating from specific emission points while considering photochemical transformations, the following tasks were undertaken:

- Data on harmful substances present in the atmosphere of an industrial city were obtained from the Regional Automated Measuring System of Industrial and Environmental Monitoring (RAMSIEM).
- Information regarding meteorological characteristics and harmful substances in the atmosphere of the industrial city was acquired from the regional branch of the Federal State Enterprise "Kazhydromet" in the East Kazakhstan region.
- A method was selected to account for the transformation of harmful pollutants during their transport.
- A model of the atmospheric boundary layer was employed to incorporate the influence of anthropogenic heat sources and the heterogeneity of the underlying surface on the dispersion of harmful substances. This was done while considering photochemical transformations, using the city of Ust-Kamenogorsk as an example.

During the initial phase of the research, data were gathered from the RAMSIEM. This automated measurement station operates continuously in an online mode, providing data from nine chemical monitoring stations for eight constituents, three radiation monitoring stations, two meteorological parameter stations, and one river water level monitoring station every 20 minutes (72 times per day).

When modeling the chemical transformation of harmful substances in the atmosphere, the following input data of the composition of harmful substances were taken (Table 2).

Table 2. Input parameters for atmospheric air modeling taking into account photochemical transformations

Reaction number	**Amount of harmful substances (mg/hour)**
P_1	$CH_2O = 40$
P_2	$CO = 2$
P_3	$CO_2 = 2$
P_4	$SO_2 = 10$
P_5	$SO_3 = 10$
P_6	$HSO_3 = 2$
P_7	$NO = 10$
P_8	$NO_2 = 10$
P_9	$NO_3 = 2$
P_{10}	$HNO_3 = 2$
P_{11}	$MgO = 5$
P_{12}	$CaO = 5$
P_{13}	$H_2SO_4 = 0$
P_{14}	$MgSO_4 = 0$
P_{15}	$CaSO_4 = 0$

The calculation was carried out with a weak wind of the easterly direction of 1 m/s (Figures 2-7).
According to the result of numerical calculations, H_2SO_4 appeared in the atmosphere in a significant amount.

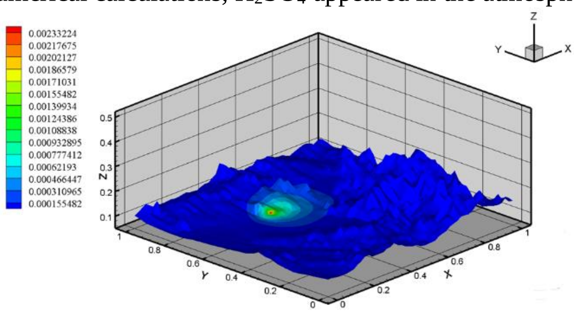

Figure 2. Spread of amount of harmful substances CH_2O

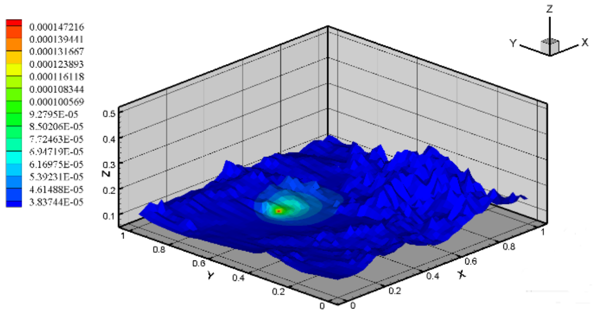

Figure 3. Spread of amount of harmful substances CO

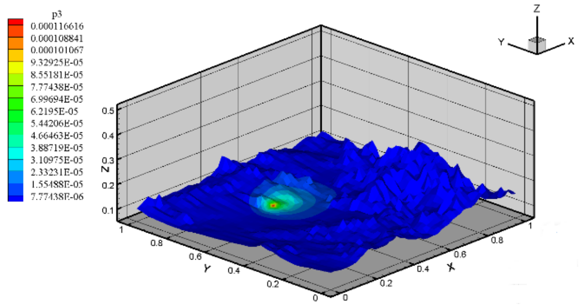

Figure 4. Spread of amount of harmful substances CO_2

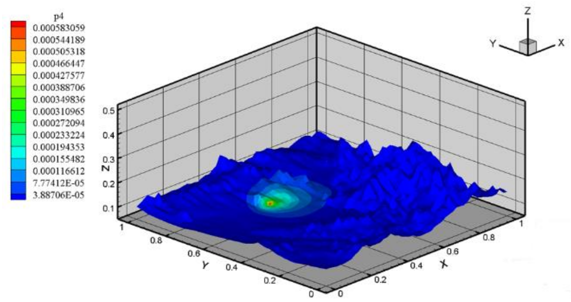

Figure 5. Spread of amount of harmful substances SO_2

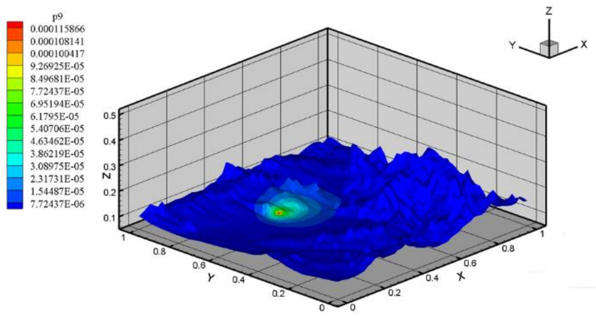

Figure 6. Spread of amount of harmful substances NO_3

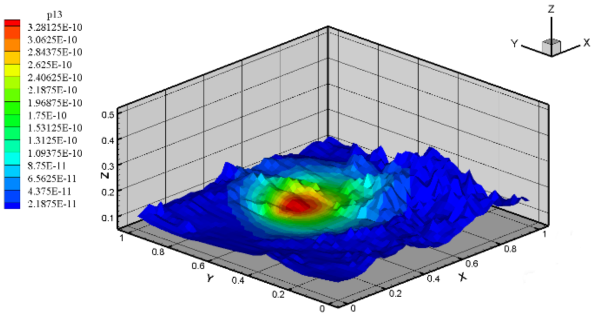

Figure 7. Spread of amount of harmful substances H_2SO_4

4. CONCLUSION

A mathematical model of mesoscale atmospheric processes in the non-hydrostatic approximation, transport and transformation of impurities, taking into account the relief, thermal inhomogeneities of the underlying surface, weather conditions and time of day, has been developed.

A new model has been constructed to describe the process of transformation of the fraction of impurity substances due to photochemical reactions in the surface layer of the atmosphere using emission data characteristic of industrial regions. The basic mathematical model describing photochemistry has been supplemented with new terms that take into account the withdrawal from the atmosphere formed in the form of droplets, small particles, dust and particles, etc.

The problem of the propagation of harmful impurities in the atmosphere from point sources, taking into account the photochemical transformations was considered.

The atmosphere is a constantly changing environment in which processes that change in time and space take place. All processes in the atmosphere take place during the irradiation of the air by the rays of the Sun, but they proceed at different speeds, in different ways, depending on the intensity of light radiation. During the day, these processes proceed in one direction, and at night they proceed in the opposite direction. The processes occurring in the atmosphere are influenced by the pressure and movement of air. Taking into account these processes, the monitoring of atmospheric pollution and the dynamics of the formation of harmful chemicals was carried out.

The analysis of the distribution of concentrations of substances is carried out, taking into account the transformation of substances that make up the harmful admixture.

Separate and total distribution were calculated for the selected harmful substances. This model takes into account the terrain and water surfaces of the city of Ust-Kamenogorsk. Calculations were carried out at different wind directions and speeds.

At moderate wind speeds, it is possible to observe the influence of water surfaces and the orography of the terrain on the spread of pollutants, and at high wind speeds these factors do not cause any special deviations.

As a result of numerical experiments, it was found that anthropogenic impurity released by industrial enterprises and picked up by wind currents in different directions moves over longer distances depending on wind speed, which leads to the imposition of pollution fields. With adverse weather conditions (AWC), anthropogenic admixture forms a cloud over an industrial city. Various scenarios of the spread of the concentration of harmful substances in the atmosphere of the city, taking into account photochemical transformations, have been obtained.

The developed software makes it possible to assess the degree of pollution of the air basin for an industrial city, taking into account the transformation of harmful substances and the orography of the area, and to obtain a complete picture of pollution at all nodal points using the pollution database and meteorological data.

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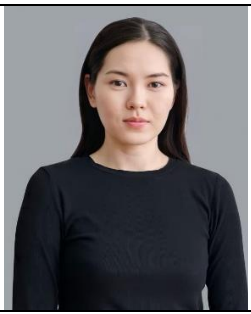	**Dinara Tamabay** is a doctoral student at Al-Farabi Kazakh National University. In 2018, she completed her bachelor's degree and defended her master's dissertation in 2020. Her research interests revolve around computational sciences, numerical analysis, computational fluid dynamics, and the investigation of atmospheric boundary layer models.

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