Indonesian Journal of Electrical Engineering and Computer Science
Vol. 32, No. 3, December 2023, pp. 1405~1416
ISSN: 2502-4752, DOI: 10.11591/ijeecs.v32.i3.pp1405-1416

Mathematical and computer modeling of atmospheric air pollutants transformation with input data refinement

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Article Info

Article history:

Received Aug 16, 2023
Revised Sep 27, 2023
Accepted Oct 3, 2023

Keywords:

Atmospheric boundary layer equation
Computational algorithm
Difference scheme
Mathematical modeling
Numerical experiment
Transformation of harmful substances

ABSTRACT

This article addresses the critical issue of harmful impurity dispersion in industrial facility atmospheres, considering point sources and factoring in photochemical changes. Conjugate equations are employed to assimilate pollutant data into the transfer equations' right side. Boundary conditions derive from global models like weather research and forecasting (WRF) and system for integrated modeling of atmospheric composition (SILAM), customized for the unique characteristics of an industrial city's pollutants. To encompass anthropogenic heat sources and surface heterogeneity, the model incorporates differential schemes for the atmospheric boundary layer, transport equations, and impurity transformation equations. Parameters for photochemical transformations, varying with weather and time of day, are derived from Ust-Kamenogorsk. A cloud-based geoinformation system (GIS) is developed for monitoring and forecasting air pollution. It assimilates data sources and accounts for photochemical transformations, enabling visualization of diverse weather and environmental scenarios. The article presents numerical modeling results of impurity spread and transformation influenced by mesometeorological processes, topography, and water resources within a specific city.

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1. INTRODUCTION

Air pollution remains a significant concern in many cities throughout the Republic of Kazakhstan due to inadequate implementation of environmental protection measures. This issue primarily stems from outdated technologies in various sectors, including thermal power generation, metallurgy, oil and coal extraction, construction, as well as road and rail transportation. In 2015, $PM_{2.5}$ was identified as the fifth leading cause of global mortality, contributing to 7.6% of worldwide deaths [1]. In 2019, it was estimated that air pollution led to premature deaths of 4.2 million people globally [2]. Kazakhstan ranked as the 23rd most polluted country in 2021 [3]. Unfortunately, most Kazakh cities lack monitoring data in global databases, a common issue in post-Soviet cities.

Both domestic and foreign research highlights the lack of information on air pollution and underscores the need for comprehensive studies [4], [5]. Studies [6], [7] emphasize the high risk of chronic exposure to heavy metals in cities like Ust-Kamenogorsk, Almaty, and Balkhash, where residents have shown elevated

levels of heavy metals in their blood, possibly linked to metallurgical activities. Kerimray *et al*. [5] assessed the impact of COVID-19 quarantine measures on air quality in Almaty, revealing a significant reduction in pollution during the quarantine period.

According to the WHO regional office for Europe, well-designed measures to combat air pollution can mitigate disease and climate change risks, substantially improving quality of life [8]. While some countries have made progress in reducing emissions, Kazakhstan still grapples with air pollution [9]. Human activities significantly contribute to lower atmospheric environmental issues. Industrial enterprises release substantial quantities of chemicals, leading to environmental contamination and health hazards. Impurities play a critical role in chemical reactions, affecting thermal radiation transparency and water vapor condensation [10].

The East Kazakhstan region, with its diverse industrial sectors, faces severe pollution exacerbated by adverse meteorological conditions due to its geographical location. Specific pollutants in Ust-Kamenogorsk include sulfur dioxide, nitrogen dioxide, carbon monoxide, phenol, formaldehyde, chlorine, inorganic arsenic compounds, and various heavy metals like lead, zinc, copper, cadmium, beryllium, and mercury [10].

Worldwide, including in Kazakhstan, numerous scientific publications address various methods for modeling pollutant dispersion in the atmosphere, as works of [11]–[28]. Recent advancements in computer technology have also led to the utilization of deep machine learning and artificial neural networks for atmospheric air quality monitoring and forecasting [29]–[33]. Deep learning techniques have demonstrated their effectiveness in the detection and prediction of atmospheric air pollution and the evaluation of the environmental impact caused by various industries [29]. For example, Li *et al*. [30], machine learning and remote sensing were employed to investigate the influence of $PM_{2.5}$ on the environments of Iraq and Kuwait between 2001 and 2018, identifying abnormal $PM_{2.5}$ levels. Another successful application was presented in [31], which introduced an internet of things (IoT)-based air pollution monitoring system utilizing the Malaysian air pollution index. Furthermore, Talib and Jasim [32] proposed a mobile and cost-effective air pollution monitoring system using Arduino microcontrollers and gas sensors. Tan *et al*. [33], machine learning methods and a time series regression model were utilized to predict PM_{10} concentrations in a dusty region of the Tibetan plateau.

Machine learning methods offer distinct advantages in scenarios lacking precise mathematical models, allowing systems to replicate intricate patterns based on complex expert assessments that are challenging to formalize. According to [34]–[36], the study determined the approximation error, stability, and convergence of the difference scheme for the atmospheric boundary layer model and impurity transport and transformation equations. An implementation scheme for the studied difference scheme was developed.

This article expands on the dispersion of impurities originating from specific point sources, accounting for the influence of weather conditions and time of day on the photochemical transformation of these impurities. An automated geoinformation system has been developed, amalgamating data from air pollution monitoring stations and global hydrometeorological models. This input data is processed in real-time with a 48-hour forecast using cloud computing on a server situated in a data center.

Two challenges are addressed when utilizing input data for numerical modeling of atmospheric processes with pollutant transport. The first pertains to the volume of pollutants emitted into the atmosphere from sources. To clarify this, data from automated monitoring stations (AMS) installed by Ecoservice-S LLP in the city are assimilated as shown in Figure 1, as only gross emissions from industrial enterprises are available in the bulletins of the Republican State Enterprise.

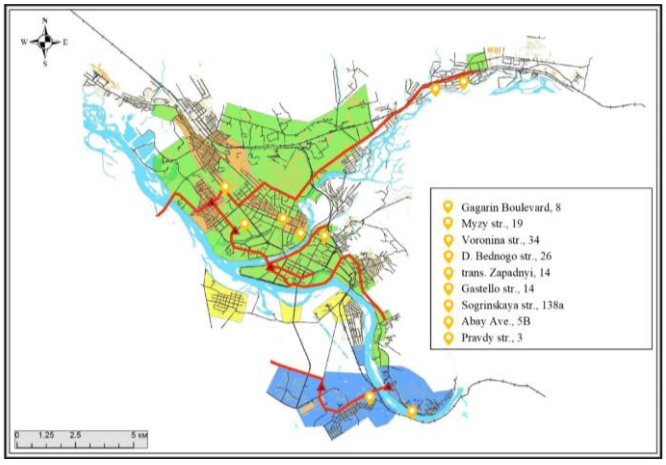

Figure 1. Map of the location of AMS with aderesses in city Ust-Kamenogorsk, Kazakhstan

The second challenge relates to setting boundary conditions for the industrial city's atmospheric boundary layer model. for boundary conditions data from RSE "Kazhydromet" obtained through weather research and forecasting (WRF) and system for integrated modeling of atmospheric composition (SILAM) packages are used. This real-time data, including a 48-hour forecast, is received at a server located in the data center of Akademset LLP.

Our research delves into the dynamics of impurity dispersion and transformation, considering prevailing mesometeorological processes in Ust-Kamenogorsk. This has led to the development of a geoinformation system for monitoring the city's atmospheric air quality. The results are relayed to the situation center for use by local authorities and the public.

2. METHOD

2.1. Mathematical model of the boundary layer of the atmosphere

To assess the influence of anthropogenic heat sources, harmful substances, and surface variations on the atmosphere within an industrial urban setting, we employ a three-dimensional domain denoted as Ω. This domain adheres to a model of the atmospheric boundary layer, which is constructed based on prior investigations [10]–[15]. Motion equations and continuity equation:

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

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

$$\frac{\partial \theta}{\partial t}+\frac{\partial u_i\theta}{\partial x_i}+Su_3=\frac{\partial}{\partial x_3}\left(\nu\frac{\partial \theta}{\partial x_3}\right)+\Delta\theta, i=1,2,3, \quad (2)$$

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:

$$\frac{\partial \varphi_q}{\partial t}+u_j\frac{\partial \varphi_q}{\partial x_j}=\Delta\varphi_q+\frac{\partial}{\partial x_3}\left(\nu\frac{\partial \varphi_q}{\partial x_3}\right)+\alpha_q\varphi_q+\beta_q+f_q,\sum_q\varphi_q=1,\ f_q=\sum_{j=1}^{m}\delta\left(\vec{r}-\vec{r}_j\right)Q_i, \quad (3)$$

here $\Delta=\frac{\partial}{\partial x_1}\mu_{x_1}\frac{\partial}{\partial x_1}+\frac{\partial}{\partial x_2}\mu_{x_2}\frac{\partial}{\partial x_2}$ is the differential operator of horizontal turbulent diffusion, m is the number of sources, $\vec{r}_j$ is the radius vector of the source coordinate, $Q_i$is the power of the source, $\lambda=\frac{g}{T}$- convection parameter, $S=\frac{\partial\theta}{\partial x_3}$ is a stratification parameter, g - gravity acceleration, T - air temperature, μ_{x_1}, μ_{x_2}- 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. φ_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.

As shown in (2) and (3) as in (1), summation in the second term is performed by the index j. For the system of (1) to (3) the following initial and boundary conditions are given:

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

$$u_i=u_{130}^{(i)}(x_2,x_3,t),\ \theta=\theta_{130}(x_1,x_3,t),\ \varphi_q=0 \text{ when } x_2=0,\ 0\le x_1\le X,$$

$$u_i=u_{13Y}^{(i)}(x_1,x_3,t),\ \theta=\theta_{13Y}(x_1,x_3,t),\ \varphi_q=0 \text{ when } x_2=Y,\ 0\le x_1\le X,$$

$$u_i=u_{230}^{(i)}(x_2,x_3,t),\ \theta=\theta_{230}(x_2,x_3,t),\ \varphi_q=0 \text{ when } x_1=0,\ 0\le x_2\le Y,$$

$$u_i=u_{23X}^{(i)}(x_2,x_3,t),\ \theta=\theta_{23x}(x_2,x_3,t),\ \varphi_q=0 \text{ when } x_1=X,\ 0\le x_2\le Y,$$

$$u_i=0,\ \theta=0,\ p=0\ ,\varphi_q=0 \text{ when } x_3=H,\ 0\le x_1\le X,\ 0\le x_2\le Y, \quad (4)$$

$$u_3 = 0,\ h\frac{\partial u_1}{\partial x_3} = a_{u_1}u_1,\ h\frac{\partial u_2}{\partial x_3} = a_{u_1}u_2,\ h\frac{\partial \theta}{\partial x_3} = a_\theta(\theta - \theta_0),\ \varphi_{q,0} = \frac{f_q + a_\theta \varphi_{q,h} v_h}{\beta + a_\theta v_d} \text{ when } x_3 = h.$$

here H is the atmospheric boundary layer height, X, Y - lateral boundaries of the region, $\varphi_{q,0},\ \varphi_{q,h}$ - 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, v_h, v_d - turbulence coefficients at altitude $x_3 = h$ and $x_3 = d$, respectively, i=1,2,3, 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 [24]–[26]. In our task, we utilized interpolation functions with (5).

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

$$\eta_{u_1}(\varsigma, \varsigma_{u_1}) = \int_{\varsigma_{u_1}}^{\varsigma} \frac{\psi_{u_1}(\varsigma)}{\varsigma} d\varsigma, \quad \eta_\theta(\varsigma,\ \varsigma_0) = \int_{\varsigma_0}^{\varsigma} \frac{\psi_\theta(\varsigma)}{\varsigma} d\varsigma \tag{5}$$

Based on meteorological conditions, the boundary conditions for wind speed and temperature are determined from the data of the global SILAM model. The similarity theory of Monin-Obukhov and empirical functions from [11] were chosen for modeling the surface layer of the atmosphere at $x_3 = h$. The terrain equation $x_3 = \delta(x, y)$ is taken into account when setting boundary conditions for θ, φ_q in the surface layer at $x_3 = h$. The remaining boundary conditions ensure the perturbations remain smooth, while also maintaining the continuity equation's validity at the border of the integrable domain.

2.2. The algorithm of numerical implementation

After completing the preceding mathematical inquiries, we delve into the practical aspect, focusing on the issue of how harmful pollutants spread in the atmosphere from specific sources while considering photochemical transformations. To address the problems outlined earlier (1) to (4), we employ the finite difference method and execute numerical computations using the splitting method for handling physical processes. This approach has a proven track record in numerical solutions for equations related to aerohydrodynamics in natural variables. In the area $\Omega = \{0 \le x_1 \le l_1, 0 \le x_2 \le l_2, 0 \le x_3 \le l_3\}$, we introduce the following uniform grids:

$$\Omega_h = \left\{(x_{1_i}, x_{2_j}, x_{3_k}) = (ih_1, jh_2, kh_3),\ i = 0, \rightleftarrows 1, \dots,\ N_1,\ j = 0,1, \dots,\ N_2,\ k = 0,1, \dots, N_3\right\},$$

$$\Omega_{x,h} = \left\{(x_{i-1/2}, x_{2_j}, x_{3_k}) = ((i-1/2)h_1, jh_2, kh_3), i = 1,2, \dots, N_1, j = 0,1, \dots, N_2, k = 0,1, \dots, N_3\right\},$$

$$\Omega_{y,h} = \left\{\left(x_{1_i}, y_{j-1/2}, x_{3_k}\right) = (ih_1, (j-1/2)h_2, kh_3), i = 0,1, \dots, N_1, j = 1,2, \dots, N_2, k = 0,1, \dots, N_3\right\},$$

$$\Omega_{z,h} = \left\{\left(x_{1_i}, x_{2_j}, z_{k-1/2}\right) = (ih_1, jh_2, (k-1/2)h_3), i = 0,1, \dots, N_1, j = 0,1 \dots, N_2, k = 1,2, \dots, N_3\right\},$$

here $h_1 = l_1/N_1, \quad h_2 = l_2/N_2, \quad h_3 = l_3/N_3$.

When the method of splitting by physical processes is considered, the wind speed u_1 component is determined in the nodes of the grid $\Omega_{x_1,h}$, the component u_2 in the nodes of the grid $\Omega_{x_2,h}$, the component u_3 in the nodes of the grid $\Omega_{x_3,h}$, a pressure p, temperature θ, the proportion of concentrations of harmful substances φ_q in the nodes of the grid Ω_h.

Let the velocity field $\vec{U}_h = (u_{1h}, u_{2h}, u_{3h})$, pressure field p_h^n, for concentrations of harmful substances $\varphi_{q,h}^n$, temperature ${\theta_h}^n$ be known at the nodal points of the grid regions $\Omega_{x_1,h}$, $\Omega_{x_2,h}$, $\Omega_{x_3,h}$, 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: 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:

$$\frac{\vec{U}_h^{n+1/2}-\vec{U}_h^n}{\tau} = -L_h\vec{U}_h^n + \Lambda_h\vec{U}_h^n + \vec{G}_h^n \quad (6)$$

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. 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 (7).

$$\Lambda_h p_h{}^{n+1} = \frac{div_h\vec{U}_h^{n+1/2}}{\tau} \quad (7)$$

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:

$$\frac{\vec{U}_h^{n+1}-\vec{U}_h^{n+1/2}}{\tau} = -\nabla_h p_h{}^{n+1}, \quad (8)$$

where ∇_h is the difference analog of the nabla operator $\nabla = (\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3})$.

The calculation of temperature transfer and diffusion is carried out according to the following difference scheme according to the velocity fields found (9).

$$\frac{\theta_h^{n+1}-\theta_h^n}{\tau} = -L_h\theta_h^n + \Lambda_h\theta_h{}^n \quad (9)$$

Further, the transfer and transformation of the fractions of concentrations of harmful substances $\varphi_{q,h}^{n+1}$ into impurities is determined. 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 (10).

$$\frac{\varphi_{q,h}^{n+1/2}-\varphi_{q,h}^n}{\tau} = -L_h\varphi_{q,h}^n + \Lambda_h\varphi_{q,h}^n; \quad (10)$$

Influence of external sources the transformation of the concentration fractions of harmful substances into impurities is calculated as:

$$\frac{\varphi_{q,h}^{n+1}-\varphi_{q,h}^{n+1/2}}{\tau} = \alpha_q\varphi_{q,h}^{n+1} + \beta_q + f_q. \quad (11)$$

where $\varphi_{q,h}^{n+1}$ 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 (1) to (3). For example, for the fraction of concentrations of the substance HSO_3 we have:

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

where

- $\alpha_{HSO_3} = -\gamma_{154}(p)k_{154}\varphi_{HSO_3}$,
- $\beta_{HSO_3} = \gamma_{149}(p)k_{149}\varphi_{SO_2}$,
- $\gamma_i(p)$ is a parameter, that is determined depending on weather conditions and time of day.

2.3. Exploring the transformation 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. For each harmful substances there will be considered transformation, that 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 SO2 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 becomes prevalent in Ust-Kamenogorsk during adverse weather conditions (AWC). In the realm of smog, two distinct categories exist: the reducing London type and the photochemical oxidative Los Angeles type. Industrial cities commonly experience a restorative smog, characterized by a mixture of smoke, soot, and sulfur dioxide (SO_2). Typically, the highest smog levels are observed in the early morning when temperatures hover around 0°C.

Let's explore the key types of smog: one originating from atmospheric pollution by soot or smoke, which includes sulfur dioxide (SO_2), and the other stemming from vehicle exhaust emissions that contain nitrogen oxides. The second type, known as photochemical smog, necessitates the occurrence of photochemical reactions leading to the formation of ozone (O_3). This reaction is initiated by the presence of hydrocarbons and nitrogen oxides. The concentration of O_3 in air samples begins to rise when the ratio of NO_2 to NO concentrations reaches its maximum. The generation of O_3, in the presence of nitrogen oxides, is initiated by solar radiation with a wavelength less than 580 nm, and it becomes more pronounced in air with higher levels of NO_2. Solar radiation with wavelengths ranging from 285 nm to 580 nm can penetrate 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_2:

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

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.

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

The chemical transformations are described by a system of fifteen differential equations [10]. Some equations, for example, for CH_2O, CO, CO_2 the equations have the following form:

$$\frac{d\varphi_{CH_2O}}{dt} = -k_{60}\varphi_{CH_2O} - k_{62}\varphi_{CH_2O} + f_{CH_2O}$$

$$\frac{d\varphi_{CO}}{dt} = k_{60}\varphi_{CH_2O} - k_{65}\varphi_{CO} - k_{141}\varphi_{CO} + f_{CO}$$

$$\frac{d\varphi_{CO_2}}{dt} = k_{65}\varphi_{CO} - k_{141}\varphi_{CO} + f_{CO_2}$$

in contrast to the approach in [10], this study considers the parameter $\gamma_i(p)$, where the value of γ_i varies based on prevailing weather conditions and the time of day, with i representing the specific reaction number. To ensure the preservation of the mass conservation principle, differential equations were developed as part of the methodology. These equations encompass the process of subtracting a fraction from its original substance and adding it to the volume of the newly formed substance during a chemical reaction. In the equations of chemical kinetics, the coefficients k_{60}, k_{62} and others, called the rate constants of chemical reactions, are known in advance [11].

2.4. Mathematical model of assimilation of data on pollution of the air basin of an industrial city or facility

Currently, IT technologies are very convenient for using DBMS, allowing you to efficiently store, extract information and manage large amounts of data. To interpolate and extrapolate the missing data, a mathematical model of the transfer of impurities of harmful substances in the atmospheric air of the city of Ust-Kamenogorsk is used by assimilation of data obtained from automated monitoring stations as shown in Figure 1. Simple interpolation using the available data is insufficient to obtain a real picture of pollution in all

points of the city. This is obvious, because the points where the AMS are located are not sources of emissions. Therefore, it is not possible to determine values in other points of the city only from these data. On the other hand, such a simple approach does not take into account meteorological data and the nature of the underlying surface.

To obtain a more realistic picture of pollution, the following algorithm is used in this work to assimilate the data of the effective use of the pollutant transfer model and monitoring data obtained from automated monitoring stations. The enlarged algorithm of the method looks like this:

- The direct problem (1) to (3) with boundary conditions (4) is solved.
- Then the problem conjugate to (3) with homogeneous boundary conditions is solved.

$$\frac{\partial \varphi_q^*}{\partial t} + u_j \frac{\partial \varphi_q^*}{\partial x_j} = \Delta \varphi_q^* + \frac{\partial}{\partial x_3}\left(\nu \frac{\partial \varphi_q}{\partial x_3}\right) + \alpha_q \varphi_q^* + \beta_q + F, \quad (12)$$

Where $F = \sum_{i=1}^{n} \delta_i(\vec{r} - \vec{r}_i) \cdot (\psi - \varphi_q)\, \alpha_i, (x_i)$–coordinates of the AMS location, ψ_i −pollution values in ACM, φ_q −solution of (3), α_1- is the preference coefficient, n is the number AMS, $\vec{r}_i$ is the radius vector of AMS coordinates. Next, an amendment is introduced to the mathematical model based on monitoring data, i.e. the error is found:

$$r = \alpha_2 \varphi^* \cdot \delta(\vec{r} - \vec{r}_j), \quad (13)$$

where φ^* − solution the conjugate problem (12), α_2 − is the preference coefficient, (x_j) − coordinates of point sources of atmospheric pollution.

Then we correct the right side of (3) and solve the direct problem:

$$f_q' = f_q + r \quad (14)$$

thus, with the help of this algorithm, we can get a more accurate picture of the content of pollutants in the city's atmospheric air, since the mathematical model takes into account all mesometeorological data and all sources of pollution, and an amendment is introduced into the model taking into account the measured AMS data.

3. RESULTS AND DISCUSSION

3.1. Numerical results and discussion

The numerical implementation procedure can be found in [10]. We employed the aforementioned model and the devised algorithm to simulate atmospheric air pollution, incorporating photochemical transformations, with varying input parameter values as detailed in Table 1. The numerical computations were carried out over a 35×35 kilometers area, with a constant surface layer height of 3,500 meters. The stratification parameter S, signifying temperature variations with altitude, was calculated based on the vertical temperature gradient during the computation process.

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	$35{,}000m$
Wind	U^*	$10\ m\ s^{-1}$
Speed temperature	θ^*	20^0C

Calculations were carried out on grids 100×100×50, 200×200×100, and 400×400×200. 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. Information regarding meteorological characteristics and harmful substances in the atmosphere of the industrial city was acquired from the AMS of LLP Ecoservice-S that are located in Ust-Kamenogorsk. Data on point sources of pollution were obtained from the Bureau of National Statistics of the Republic of Kazakhstan [37]. When modeling the chemical transformation of harmful substances in the atmosphere, the following input data of the composition of harmful substances were taken by

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

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

Corresponding reaction number	Amount of harmful substances in μg/hour
φ_1	CH_2O=40
φ_2	CO=2
φ_3	CO_2=2
φ_4	SO_2=10
φ_5	SO_3=10
φ_6	HSO_3=2
φ_7	NO=10
φ_8	NO_2=10
φ_9	NO_3=2
φ_{10}	HNO_3=2
φ_{11}	MgO=5
φ_{12}	CaO=5
φ_{13}	H_2SO_4=0
φ_{14}	$MgSO_4$=0
φ_{15}	$CaSO_4$=0

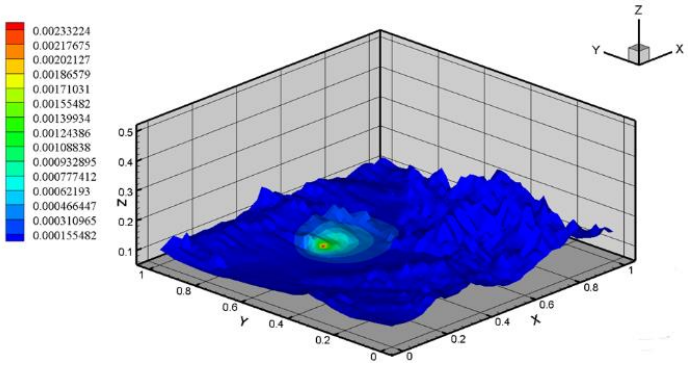

Figure 2. Spread of amount of harmful substances CH_2O

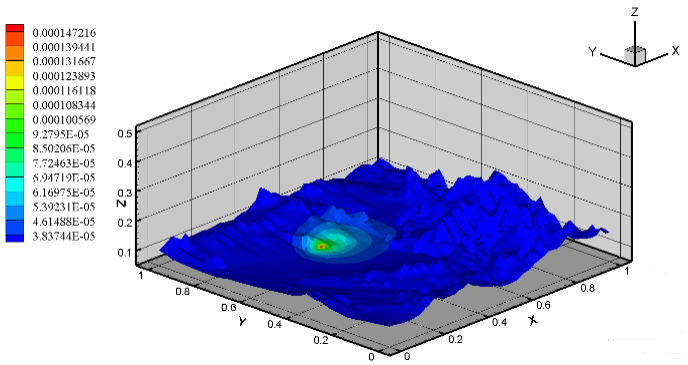

Figure 3. Spread of amount of harmful substances CO

Taking into account the transformation of impurities and photochemistry of pollutants with the presented initial indicators and with data from point sources of pollution, including emissions from point sources, an amendment is being implemented. This amendment takes into account the measured data of AMS in order to clarify the pollution parameters from the specified point sources [37] using the data assimilation algorithm. We base the boundary conditions for this model on calculations carried out using the WRF and SILAM application programs for the East Kazakhstan region. All this apparatus of numerical modeling is performed at the regional level and applied to the city of Ust-Kamenogorsk.

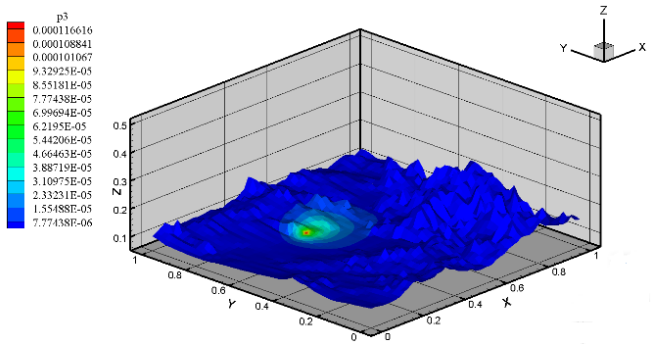

Figure 4. Spread of amount of harmful substances CO_2

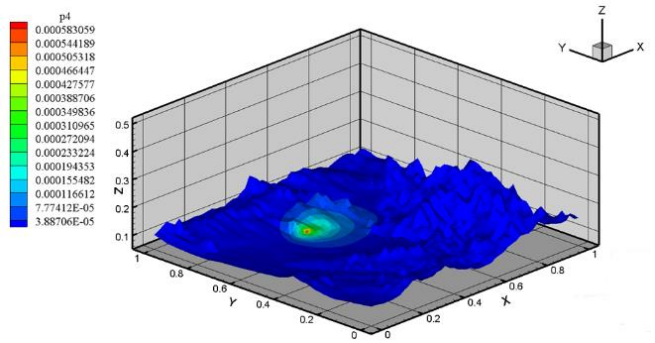

Figure 5. Spread of amount of harmful substances SO_2

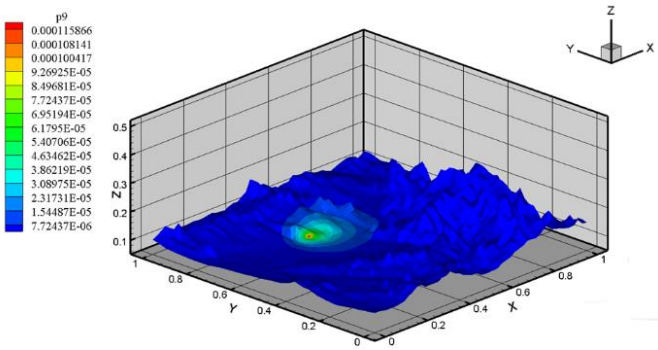

Figure 6. Spread of amount of harmful substances NO_3

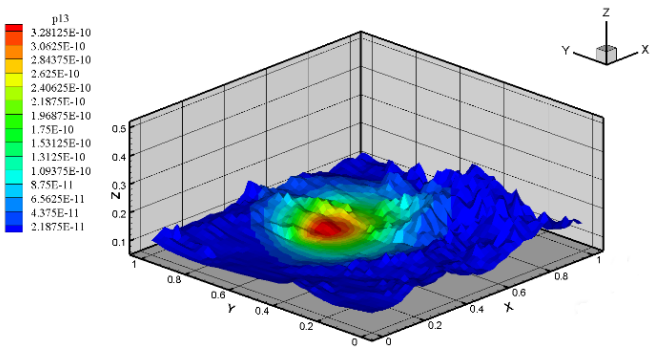

Figure 7. Spread of amount of harmful substances H_2SO_4

4. CONCLUSION

A comprehensive mathematical model has been formulated to capture mesoscale atmospheric processes in the non-hydrostatic approximation, encompassing the transport and transformation of impurities. This model considers various factors, including the local terrain, thermal variations in the underlying surface, weather conditions, and the time of day. A novel model has been developed to describe the transformation of impurity fractions due to photochemical reactions within the atmospheric surface layer, utilizing emission data characteristic of industrial regions. Additional terms have been incorporated into the fundamental mathematical model governing photochemistry, accounting for the removal of substances from the atmosphere in the form of droplets, fine particles, dust, and other particles. The article delves into the issue of harmful impurity dispersion in the atmosphere originating from point sources, factoring in photochemical transformations. The atmosphere is a dynamic environment where processes evolve both spatially and temporally. All these processes occur under the influence of solar radiation, albeit at varying rates and directions, contingent on the intensity of sunlight. The diurnal cycle influences the progression of these processes. Furthermore, atmospheric processes are subject to the effects of air pressure and movement.

The study conducts atmospheric pollution monitoring and analyzes the dynamics of harmful chemical compound formation, taking into account these multifaceted atmospheric processes. The analysis includes the assessment of substance concentration distributions, considering the transformation of the constituent elements of harmful mixtures. Concentration distributions are computed both individually for specific harmful substances and collectively. The model incorporates the terrain and water surfaces of Ust-Kamenogorsk, and calculations are conducted under different wind conditions, including varying wind directions and speeds. In order to obtain a more accurate picture of the atmospheric air content of the city, all mesometrological data and all point sources of pollution are taken into account. Also, an amendment is introduced into the model taking into account the measured AMS data to clarify the pollution indicators from point sources using the data assimilation algorithm. The resulting complex model allows a comprehensive study of pollution, taking into account the characteristic pollutants and impurities and their transformation, as well as the geographical features of the city. Boundary conditions were taken from calculations of WRF and SILAM packages. The results of numerical experiments reveal that under moderate wind speeds, water surfaces and terrain features have a noticeable impact on pollutant dispersion, whereas at high wind speeds, these factors have less pronounced effects. In adverse weather conditions, anthropogenic impurities released by industrial facilities and carried by wind currents can accumulate, leading to pollution fields. Under such circumstances, an industrial city may experience the formation of pollutant clouds. The study provides various scenarios illustrating the dispersion of harmful substance concentrations in the city's atmosphere, accounting for photochemical transformations. The developed software offers a means to evaluate the extent of air pollution in an industrial city, taking into consideration the transformation of harmful substances and the local topography. It provides a comprehensive overview of pollution levels across all critical points, utilizing a pollution database and meteorological data.

ACKNOWLEDGEMENTS

This research is funded by the Science Committee of the Ministry of Higher Education and Science of the Republic of Kazakhstan, grant number BR18574148 "Development of geoinformation systems and monitoring of environmental objects".

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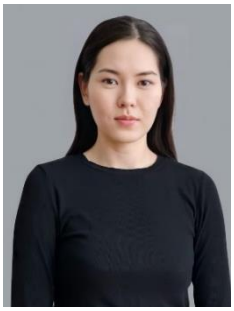

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