

Research Article

A New Approach to Solving the Problem of Atmospheric Air Pollution in the Industrial City

Zhanar Oralbekova,¹ Tamara Zhukabayeva ^{1,3} Kazizat Iskakov,^{1,2}
Makpal Zhartybayeva,¹ Nargiz Yessimova,⁴ Alma Zakirova,¹ and Ainur Kussainova¹

¹N. Gumilyov Eurasian National University, Faculty of Information Technology, Nur-Sultan 010008, Kazakhstan

²National Research Nuclear University, MEPhI (Moscow Engineering Physics Institute), Moscow 115409, Russia

³Astana International University, High School of Information Technology and Engineering, Nur-Sultan 010000, Kazakhstan

⁴E.A. Buketov Karaganda State University, Faculty of Mathematics and Information Technology, Karaganda 100026, Kazakhstan

Correspondence should be addressed to Tamara Zhukabayeva; tamara_kokenovna@mail.ru

Received 4 May 2021; Revised 18 November 2021; Accepted 23 November 2021; Published 24 December 2021

Academic Editor: Zhu Xiao

Copyright © 2021 Zhanar Oralbekova et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

In order to ensure optimal operation of the existing environmental monitoring information system, it has become essential to use mathematical modeling based on the data assimilation algorithm. In this paper, a data assimilation algorithm has been designed and implemented. An algorithmic approach was tested for the assimilation of city atmosphere monitoring data from an industrial area. An industrial district of Karaganda city was selected for the investigation of the algorithm. The industrial district of Karaganda was taken as a research object due to the high level of atmospheric air pollution in industrial cities in the Republic of Kazakhstan. The result of our research and testing of the algorithm showed the effectiveness of the data assimilation algorithm for monitoring the atmosphere of the selected city. The practical value of the work lies on the fact that the presented results can be used to assess the state of atmospheric air in real time, to model the state of atmospheric air at each point of the city, and to determine the zone of increased environmental risk in an industrial city.

1. Introduction

Nowadays, the environmental monitoring problems have received considerable attention due to the high level of atmospheric air pollution in industrial cities of many countries [1–6]. For the effective operation of the existing information system for monitoring the atmosphere for pollution by heavy metals, it has become essential to use mathematical modeling based on the data assimilation algorithm.

Data assimilation technology is used to improve forecasts of air quality in atmospheric chemistry, as well as to perform a reanalysis of three-dimensional chemical (including aerosol) concentrations and determine the values of input variables (parameters) of the inverse simulation model (for example, emissions). The concept of “data assimilation”

combines a sequence of operations starting with observations of the system and ending with the assessment of its state based on additional statistical and dynamic information. Currently, data assimilation technology is widely used in the fields of modeling the atmosphere, climate, ocean, and environment under any conditions, particularly if it is necessary to assess the state of a large dynamic system based on limited information. The purpose of data assimilation for atmospheric modeling is to obtain a better understanding of the atmosphere in terms of its meteorological and chemical parameters.

Several decades ago, I. Sasaki developed the variational method of data assimilation, and his approach is currently widely used for modern-day analysis and for prediction in meteorology [7]. R.E. Kalman also demonstrated an optimization method for linear filtering, and this filter is named

after him. The data assimilation model based on the Kalman filter has allowed the generalization of assimilation systems, such as the cycle of forecast analysis [8, 9]. The main problems of using the Kalman filter are the high order of the covariance matrix in forecasting errors and the nonlinearity of the system equations describing meteorological processes. In order to solve these problems, a method was adopted based on the Lagrange variational principle using conjugate equations for estimating and predicting natural processes. V.V. Penenko expanded this method to the assimilation of variational data using the methods of sensitivity theory and related problems [10, 11]. In dynamic meteorology, data assimilation technology has been applied for many decades to improve weather forecasting and reanalysis results. To date, research in this field has been actively conducted by many scientists [12–14].

Chemical analysis has been utilized to predict air quality since the mid-1990s with the creation of primitive databases regarding pollution, such as an air pollution index for five pollutants for each year without analytical processing and forecasts. Despite the fact that, as Zhang et al. [15–17] showed in their research, it is preferable to make air quality forecasts based on statistical approaches, data assimilation techniques have been used since the 1990s in air quality modeling to understand air pollutants, such as in concentration maps [18]. Furthermore, inverse modeling has been used to improve (or detect errors) the radiation rate [19–23], boundary conditions [24], and model parameters [25–27]. S. Rakhmetullina et al. used variational data assimilation algorithms to detect atmospheric pollution sources [28]. The 3D-Var algorithm was first implemented in 1992 by the National Center for Environmental Forecasts (NCEP) [29]. Later, in 1996, it was urgently implemented at the European Center for Medium-Term Weather Forecasts (ECMWF); then, in 1997, the 4D-Var algorithm was first applied in the ECMWF forecasting system [30]. Various models are also used to simulate atmospheric ventilation processes and, accordingly, methods for modeling the temporal and spatial dispersion of various pollutants in the atmosphere of industrial cities such as MLDP0 (Modèle Lagrangien de Dispersion de Particules d'ordre 0), HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory Model), NAME (Numerical Atmospheric-dispersion Modelling Environment), RATM (Regional Atmospheric Transport Model), FLEXPART (Lagrangian Particle Dispersion Model), a Local Scale Atmospheric Circulation Complex-Field Model (LACCM) and others. Methods and algorithms to modeling, processing, and assimilation of the industrial city atmosphere monitoring data were considered in the works [31–40].

According to previous studies, in this work, algorithm for the assimilation of atmospheric monitoring data was designed and tested for the highly air-polluted city of Karaganda, the Republic of Kazakhstan (RK). A “data assimilation” module has been developed for the information system of monitoring atmospheric air pollution.

2. Materials and Methods

The government of the RK approved a state program, “Digital Kazakhstan,” and considered the creation of a “unified state system for monitoring the environment and natural resources” [41]. Based on the current environmental code of the RK, this system monitors the means of controlling, forecasting, and evaluating pollution and is also a comprehensive system for observing the state of the environment and natural resources [42]. Currently, 146 posts and 14 mobile laboratories located in the largest cities and national industrial centers of Kazakhstan are engaged in the analysis of the state of atmospheric air pollution. According to the reports of national environmental authorities, the highest levels of air pollution are observed over industrial centers. Generally, national environmental authorities allow a maximum permissible concentration (MPC) of pollutants; this indicator also includes heavy metals (HM). For example, for the specified period of March 10–16, 2020, the following measurements were registered:

In Karaganda city, in the district of observation post 6 for atmospheric air pollution, 141 cases exceeding the maximum permissible concentration (MPC) for suspended particles $PM_{2.5}$ were found.

In Nur-Sultan city, 430 cases of excess in the range of 1.0–3.8 of the MPC for sulfur dioxide were found, along with 997 cases of excess in the range of 1.1–3.0 of the MPC for hydrogen sulfide, etc. In Ust-Kamenogorsk city, 371 cases of excess in the range of 1.0–1.9 of the MPC for hydrogen sulfide were found [43].

According to the newsletters of the Republican State Enterprise “Kazhydromet,” Karaganda occupies a leading position in terms of the cities with high air pollution in the RK [43]. Therefore, the object of our research was to investigate the atmospheric air pollution of the industrial city of Karaganda, which is characterized by a sharply continental and arid climate due to its great distance from the seas, free access in summer to warm dry winds of the deserts of Central Asia, and cold, moisture-poor arctic air in the cold season. In this city, the monitoring process is carried out by eight posts: four automatic and four manual sampling posts. The northern industrial zone of the territory in Karaganda was selected to solve the problem of data assimilation; the third regional thermal power plant (TPP-3) is located in this area. A location map of the thermal power plant in Karaganda is shown in Figure 1.

Generally speaking, the scope of our research consists of two stages (Figure 2): the first stage is the process of forming an observation plan, the selection of areas for air sampling, the analysis of meteorological data, and the determination of the content of heavy metals in air samples of Karaganda city.

Technical details and explanations of the air sampling process to assess the content of heavy metals in this selected area are shown in Table 1.

Figure 3 illustrates the main characteristics of atmospheric air pollution in Karaganda city, in which

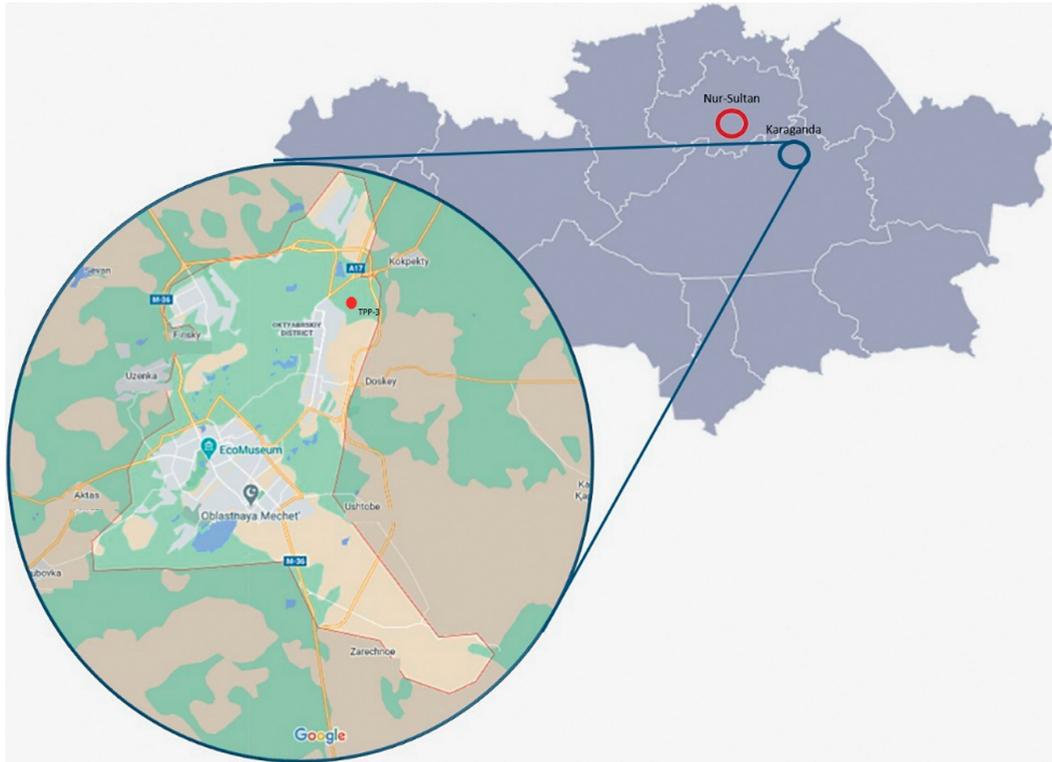


FIGURE 1: Map of the industrial area in Karaganda city.

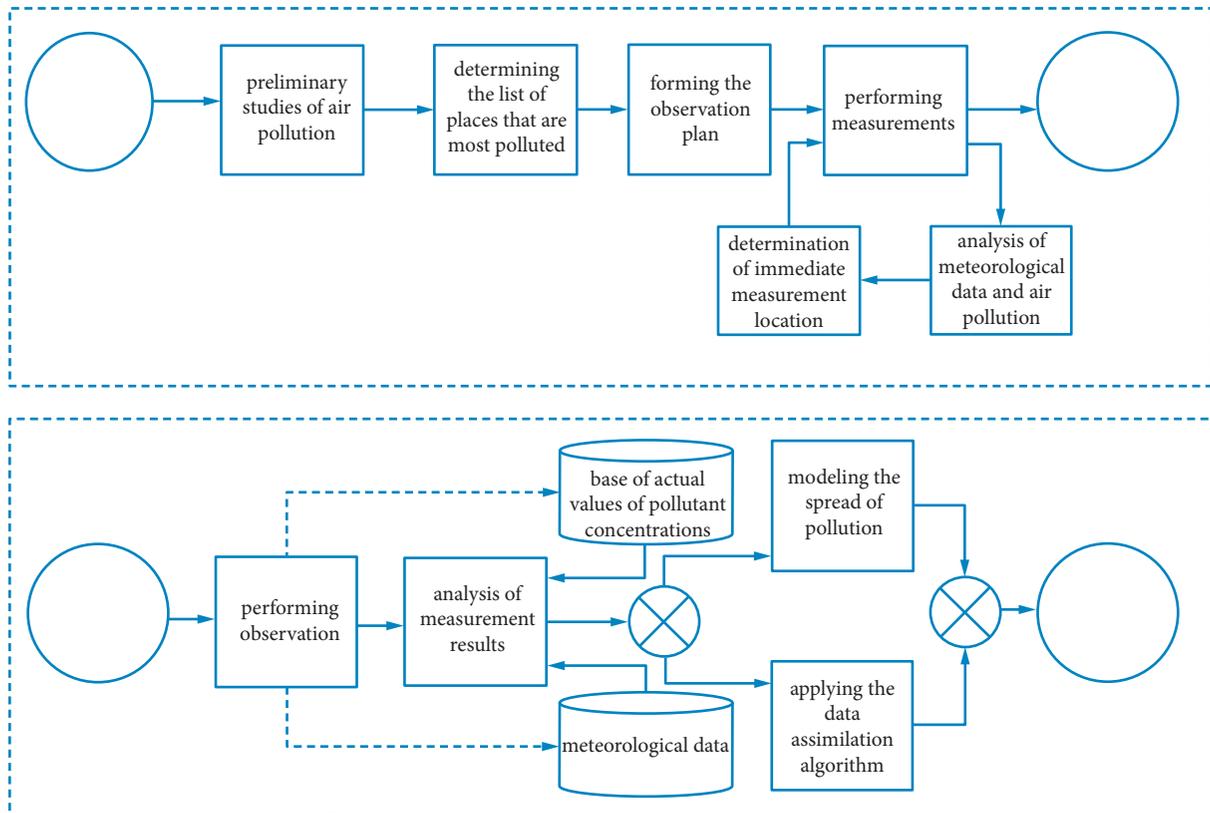


FIGURE 2: Flow chart of research framework.

TABLE 1: General characteristics of measurement.

Post Number	Address of concerns	Frequency and time of sampling	Protocol for conducting observations and pollutant contents, including heavy metals	
1	Aerological station	4 times per day 1 a.m., 7 a.m., 13 p.m., 7 p.m.	(i) Daily manual sampling (discrete methods)	Lead, copper, chromium; suspended particles (dust), sulfur dioxide, sulfates, carbon monoxide, nitrogen dioxide, phenol
4	15 biryuzova street	4 times per day 1 a.m., 7 a.m., 13 p.m., 7 p.m.	(ii) Daily manual sampling (discrete methods)	Lead, copper, chromium; suspended particles (dust), sulfur dioxide, carbon monoxide, nitrogen dioxide, phenol, formaldehyde

phenols—1.8 of the MPC—and formaldehyde—1.5 of the MPC—show the greatest excess values.

The chemical analysis of the HM content was determined as follows. First, air at a volume of 18 m³ was passed through the “ABX” filter, meaning that the HM contained in the atmospheric air was collected on this filter. Then, the filter was burned by the method of “wet salinity” in 4 mL of 5 M HNO₃. The resulting mixture of HNO₃ with a filter was slightly evaporated in a water bath under a hood until wet. Then, 0.3 mL of concentrated H₂O₂ was added to the mixture, and the mixture was settled for 0.5 h. The mixture was then evaporated to dryness; then, 0.2 mL of HNO₃ was added to the dry residue and brought to a volume of 25 mL in the cylinder with distilled water. In the obtained sample, the HM content was determined using an atomic adsorption spectrophotometer “Shimadzu” with AA-6650 electrothermal atomization [44, 45]. The chemical analysis of air samples from Karaganda city showed their HM content.

To implement algorithms for data assimilation, the results of monitoring the content of heavy metals in the air of Karaganda in the amount of 4380 measurements were used.

The obtained data regarding atmospheric pollution with HM were verified using correlation-regression analysis. According to the calculations, the value of the correlation coefficient $r=0.9$ shows a strong relationship between the content of Cu and Pb in the air of Karaganda city, which is reflected in the regression equation $y=0.7866x+0.0134$ and shown in Figure 4.

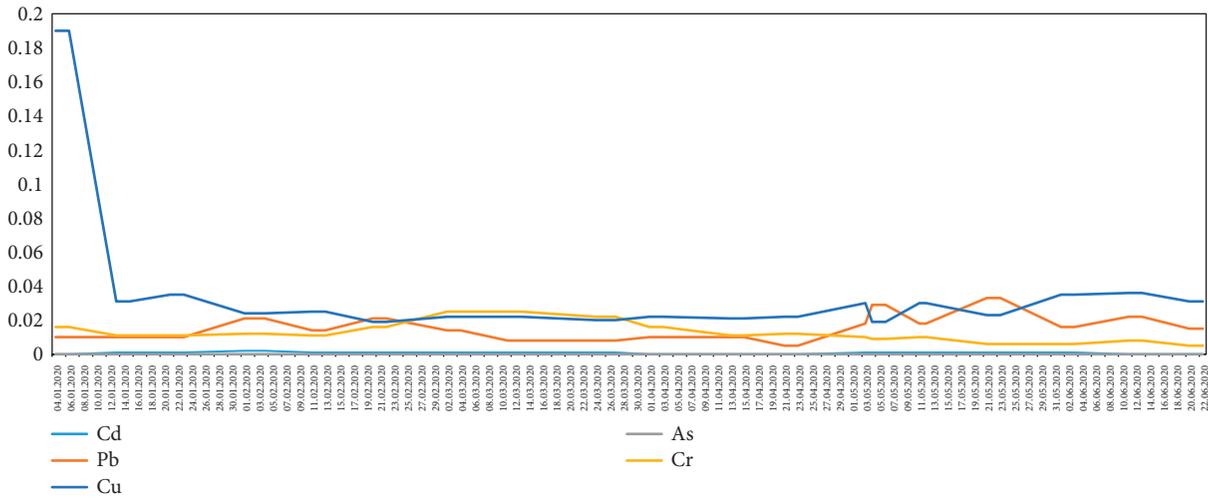
The validation of air pollution in Karaganda with HM was carried out from 1 March 2020 to 31 March 2020. Table 2 shows the values of the mean average deviation (MAD) and errors (mean square error (MSE), root mean square error (RMSE)) for this operation. Since the actual values of HM concentration are close to zero, it would be incorrect to use the mean average percentage error (MAPE).

The impurity content of the atmosphere is also affected by the wind direction. Moreover, seasonal changes in atmospheric pollution are important in this research, as they may influence the volume of atmospheric pollution. Atmospheric pollution is not only characterized by daily changes but also by the seasons of the year and by meteorological conditions. In order to achieve a comprehensive monitoring solution, information on wind, air temperature, and humidity in Karaganda was analyzed for the period of 1–31 March 2020. Weather information of the city was collected from the weather station in Karaganda (the geographic coordinates of the station are as follows: latitude 49.80, longitude 73.15, and altitude 553 m.).

The second stage of this research was applying the data assimilation algorithm to predict the spread of air pollution. Variational algorithms play an important role in modeling the distribution of pollutants and working in real time, especially when solving environmental pollution problems in the development of ecosystems. Data assimilation is the most used technique in variation algorithms. The term data assimilation covers the entire sequence of operations that begins with observations of the system with additional statistical and dynamic information that gives an assessment of its state. Data assimilation technology is a standard practice in numerical weather forecasting, and its application is becoming widespread in any circumstances in which it is intended to assess the state of a large dynamic system based on limited information. In data assimilation problems, it is necessary to predict the value of the model state function in accordance with the available observational data. Therefore, the approach is used to restore the “real” state of the system as accurately as possible, using a mathematical model, a priori information, and measurement data. The problem statement with the nonstationary transfer equation and diffusion was considered for this study [46, 47]. After multiplying the original equation by a sufficiently smooth conjugate function, the integral identity was obtained to construct discrete approximations. To evaluate and predict natural processes, the Lagrange variational principle was chosen using conjugate equations. Variational data assimilation was developed by V.V. Penenko based on the methods of sensitivity theory and conjugate problems [10, 11]. The sequential variational assimilation of observational data in real time was performed, and it was assumed that the values of the concentration field could be measured in a finite set of points in space and time. The grid function is 1 at points in the space-time grid where measurement data are available, and 0 otherwise. The approach of modeling using functions includes observational data that express the degree of proximity of the measured values and their images calculated from the models of processes and measurements. The values of the concentration field are measured in a finite set of points in space and time.

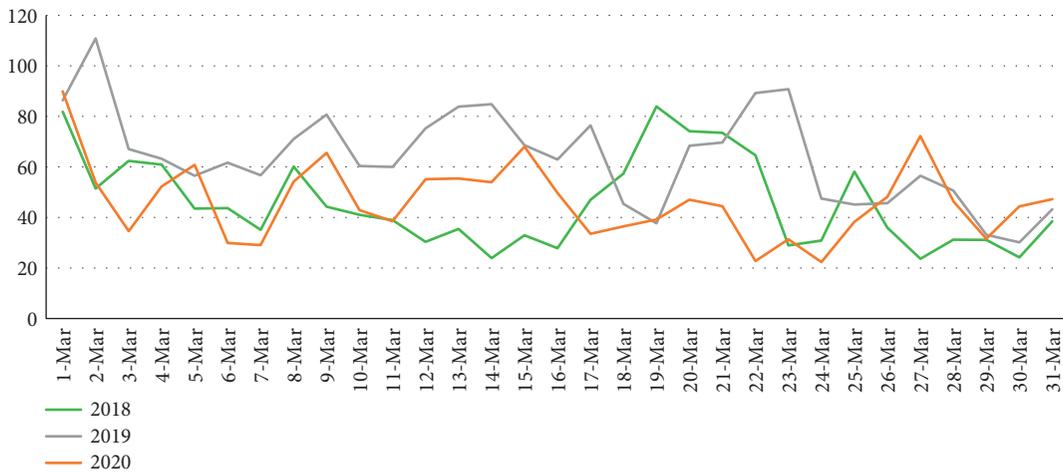
3. Results and Discussion

The existing information system for monitoring atmospheric pollution in the RK has a number of disadvantages, as its main function is to store and collect data. In this regard, for the effective operation of an atmospheric monitoring information system, it has become necessary to use mathematical modeling based on a data assimilation



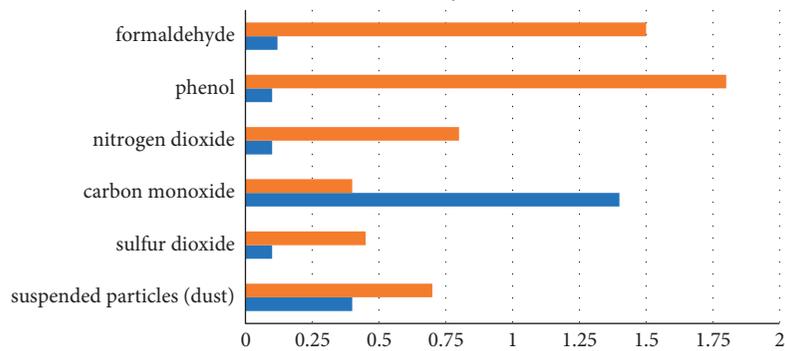
(a)

PM_{2.5} concentration, March



(b)

Characteristics of atmospheric air pollution in Karaganda city: other elements



(c)

FIGURE 3: Characteristics of atmospheric air pollution in Karaganda city: heavy metals (HM) (a), particulate matter (PM_{2.5}) (b) and other elements (c).

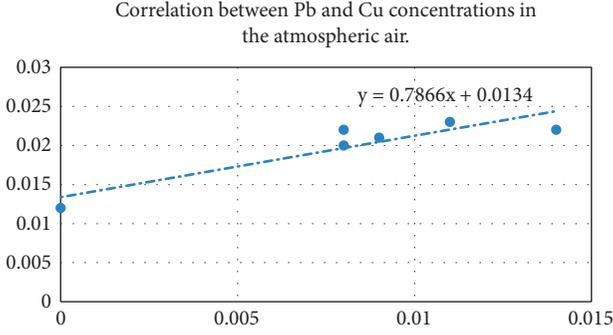


FIGURE 4: Correlation between Pb and Cu concentrations in the atmospheric air.

TABLE 2: Values of mean average deviation (MAD), mean square error (MSE), and root mean square error (RMSE) for HM.

Heavy metals	MAD	MSE	RMSE
Pb	0.009	0.001	0.023
Cu	0.026	0.003	0.055
Cr	0.004	0.001	0.004

algorithm and to develop an appropriate module for this [48–51].

3.1. Mathematical Support of the Environmental Monitoring System Based on the Data Assimilation Algorithm. As a model of impurity transfer for the nonstationary transfer equation with diffusion, we consider the following problem statement [11, 46]:

$$\begin{aligned}
 L\phi &\equiv \frac{\partial}{\partial x} \mu \frac{\partial \phi}{\partial x} - u \frac{\partial \phi}{\partial x} \\
 &= \frac{\partial \phi}{\partial x} + c\phi - f(x, t).
 \end{aligned} \tag{1}$$

We set the boundary conditions as the third kind:

$$\begin{aligned}
 -\mu \frac{\partial \phi}{\partial x} + a\phi &= q_L, \quad x = 0, \\
 \mu \frac{\partial \phi}{\partial x} + a\phi &= q_R, \quad x = L.
 \end{aligned} \tag{2}$$

We take as the initial condition

$$\begin{aligned}
 \phi &= \phi_0, \\
 t_0 &= 0,
 \end{aligned} \tag{3}$$

where ϕ —impurity concentration function, ϕ_0 —initial concentration distribution, $\mu > 0$ —turbulent exchange coefficient, u —impurity transfer rate, c —decay rate, $f(x, t)$ —source function, $x \in (0, N)$ —spacing interval, $t \in (0, M)$ —time interval, a —given coefficients, and q_L, q_R —given functions.

We assume that the function ϕ and flow $\mu(\partial\phi/\partial x)$ are continuous in space.

Let us introduce a grid region into consideration: uniform grids with steps of Δt and Δx , and the numbers of partition nodes are M and N , respectively.

For the numerical solution of the problem under consideration, we use the discrete method described in [46, 52, 53], in which a two-layer second-order approximation was used to approximate the time derivative:

$$\begin{aligned}
 &\frac{(3/2)\phi^{j+1} - 2\phi^j + (1/2)\phi^{j-1}}{\Delta t} \\
 &= \frac{\partial \phi^{j+1}}{\partial t} + \frac{1}{3}(\Delta t)^2 \left(\frac{\partial^3 \phi}{\partial t^3}(\tau_1) + \frac{\partial^3 \phi}{\partial t^3}(\tau_2) \right),
 \end{aligned} \tag{4}$$

$$\tau_1 \in (t_j, t_{j+1}),$$

$$\tau_2 \in (t_j, t_{j+1}).$$

As an approximation of the original differential equation, we use the discrete-analytic method proposed in [46, 52, 53] and obtain

$$\begin{aligned}
 &-\Delta t u \frac{\partial \phi^{j+1}}{\partial x} + \frac{\partial}{\partial x} \Delta t \mu \frac{\partial \phi^{j+1}}{\partial x} - \left(\frac{3}{2} + \Delta t c \right) \phi^{j+1} \\
 &= -\Delta t f^{j+1}(x, t) + \left(-2\phi^j + \frac{1}{2}\phi^{j-1} \right),
 \end{aligned} \tag{5}$$

where Δt is the time step and j is the step number.

Next, after writing down the integral identity and multiplying all the terms of the equation under consideration by a smooth function ϕ^* , which we call the conjugate, in the standard way, i.e., as a result of two integrations by parts, we obtain the discrete-analytical scheme:

$$\begin{aligned}
 &\int_{x_{i-1}}^{x_i} \left(\frac{\partial(\Delta t u)\phi^*}{\partial x} + \frac{\partial}{\partial x} \Delta t \mu \frac{\partial \phi^*}{\partial x} \right) \phi^{j+1} dx + \Delta t u \phi \phi^* \Big|_{x_{i-1}}^{x_i} + \Delta t \mu \frac{\partial \phi}{\partial x} \phi^* \Big|_{x_{i-1}}^{x_i} - \Delta t \mu \frac{\partial \phi^*}{\partial x} \phi \Big|_{x_{i-1}}^{x_i} \\
 &- \int_{x_{i-1}}^{x_i} \left(\left(\frac{3}{2} + \Delta t c \right) \phi^{j+1} + \Delta t f^{j+1}(x, t) - \left(-2\phi^j + \frac{1}{2}\phi^{j-1} \right) \right) \phi^* dx = 0.
 \end{aligned} \tag{6}$$

On the intervals (x_{i-1}, x_i) and (x_i, x_{i+1}) , we place the boundary conditions

$$\begin{cases} \phi^*(x_{i-1}) = 0, \\ \phi^*(x_i) = 1, \\ \begin{cases} \phi^*(x_i) = 1, \\ \phi^*(x_{i+1}) = 0. \end{cases} \end{cases} \quad (7)$$

Using the summated identity method [53], let us build a three-point diagram of the general form

$$\begin{aligned} B_i \phi_i - C_i \phi_{i+1} &= F_i, & i = 0, \\ -A_i \phi_{i-1} + B_i \phi_i - C_i \phi_{i+1} &= F_i, & 1 \leq i \leq N-2, \\ -A_i \phi_{i-1} + B_i \phi_i &= F_i, & i = N-1, \end{aligned} \quad (8)$$

where $\phi_i = \phi^{j+1}(x_i)$ and

$$\begin{aligned} A_i &= \frac{\left(e^{(\Delta x (u_L \Delta t + \sqrt{p_L^2 \Delta t^2}) / 2 \Delta t \mu_L)} \sqrt{p_L^2 \Delta t^2} \right)}{\left(-1 + e^{(\Delta x \sqrt{p_L^2 \Delta t^2} / \Delta t \mu_L)} \right)}, \\ B_i &= u_L \Delta t - u_R \Delta t + \frac{1}{2} \left(-u_L \Delta t + \sqrt{p_L^2 \Delta t^2} \operatorname{Coth} \left(\frac{\Delta x \sqrt{p_L^2}}{2 \mu_L} \right) \right) + \frac{1}{2} \left(u_R \Delta t + \sqrt{p_R^2 \Delta t^2} \operatorname{Coth} \left(\frac{\Delta x \sqrt{p_R^2}}{2 \mu_R} \right) \right), \\ C_i &= - \frac{e^{-(\Delta x (u_R \Delta t + \sqrt{p_R^2 \Delta t^2}) / 2 \Delta t \mu_R)} \sqrt{p_R^2 \Delta t^2}}{-1 + e^{(-\Delta x \sqrt{p_R^2 \Delta t^2} / \Delta t \mu_R)}}, \\ F_i &= \int_{x_{i-1}}^{x_i} S(x) \phi_R^*(x) dx + \int_{x_i}^{x_{i+1}} S(x) \phi_R^*(x) dx, \quad i = 2, \dots, N-2. \end{aligned} \quad (9)$$

The resulting three-point scheme with the found coefficients is solved using the matrix sweeping method.

3.2. Sequential Variational Assimilation of Observational Data in Real Time. Let the concentration field values be measured at a finite set of points in space and time. Let us denote by I_i^{j+1} the result of measurements at the j -th moment of time at the grid point with index i and through the

I_i^{j+1} mask of the measurement system. To apply the method of summation identities, we assume that the grid function is equal to 1 at the points of the space-time grid where measurement data are available and 0 otherwise. The algorithm used to solve the problem of the sequential variational assimilation of data is presented in matrix notation form [46, 54] as follows:

For $i = 0$,

$$\begin{pmatrix} A_i & 0 \\ 0 & C_{i+1} \end{pmatrix} \begin{pmatrix} \phi_{i+1}^{j+1} \\ \psi_{i+1} \end{pmatrix} + \begin{pmatrix} B_i - \frac{\Delta t}{2} \\ 2M_i^{j+1} \Delta t B_i \end{pmatrix} \begin{pmatrix} \phi_i^{j+1} \\ \psi_i \end{pmatrix} = \begin{pmatrix} \phi_i^j \\ 2M_i^{j+1} \Delta t I_i^{j+1} \end{pmatrix}. \quad (10)$$

For $i = 1, \dots, N-2$,

$$- \begin{pmatrix} A_i \\ 0 \\ 0 \\ C_{i+1} \end{pmatrix} \begin{pmatrix} \phi_{i+1}^{j+1} \\ \psi_{i+1} \end{pmatrix} + \begin{pmatrix} B_i \\ 2M_i^{j+1} \Delta t \\ -\frac{\Delta t}{2} \\ B_i \end{pmatrix} \begin{pmatrix} \phi_i^{j+1} \\ \psi_i \end{pmatrix} - \begin{pmatrix} C_i \\ 0 \\ 0 \\ A_{i-1} \end{pmatrix} \begin{pmatrix} \phi_{i-1}^{j+1} \\ \psi_{i-1} \end{pmatrix} = \begin{pmatrix} \phi_i^j \\ 2M_i^{j+1} \Delta t I_i^{j+1} \end{pmatrix}. \quad (11)$$

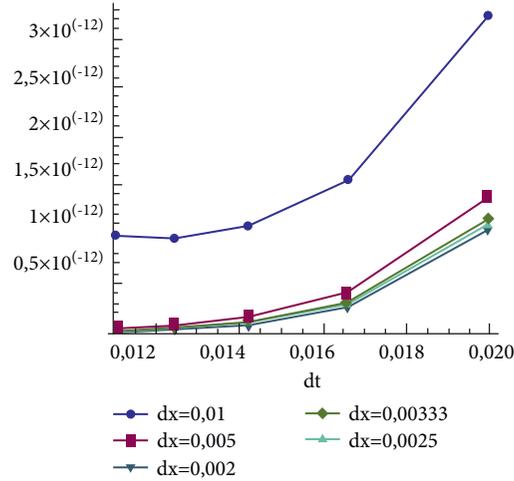


FIGURE 5: Relative errors of the numerical solution.

For $i = N - 1$,

$$\begin{pmatrix} B_i \\ 2M_i^{j+1} \Delta t \\ \frac{\Delta t}{2} \\ B_i \end{pmatrix} \begin{pmatrix} \phi_i^{j+1} \\ \psi_i \end{pmatrix} - \begin{pmatrix} C_i \\ 0 \\ 0 \\ A_{i-1} \end{pmatrix} \begin{pmatrix} \phi_{i-1}^{j+1} \\ \psi_{i-1} \end{pmatrix} = \begin{pmatrix} \phi_i^j \\ 2M_i^{j+1} \Delta t I_i^{j+1} \end{pmatrix}. \quad (12)$$

To minimize this, we considered a quadratic functional of the form

$$\Phi(\phi^{j+1}, \xi^{j+1}) = \sum_{i=0}^{N-1} (\phi_i^{j+1} - I_i^{j+1})^2 M_i^{j+1} \Delta t + \sum_{i=0}^{N-1} (\xi_i^{j+1})^2 \Delta t. \quad (13)$$

The following Figure 5 shows relative errors of the numerical solution in comparison with the exact analytical solution for different values of the time step and for different steps in space.

According to the above-described mathematical modeling, a software module has been created for the information monitoring system. Figure 6 describes the class diagram of the developed software module for data assimilation.

With the help of the data assimilation software module, a dat-file is created in which the input and output data of the observation data assimilation algorithm are recorded. These data are required to interact with the data visualization module. The dat-file has a structure that is partially shown in Figure 7.

3.3. Testing the Implemented Algorithm. In order to test the generated algorithms, 3D graphical functions from Wolfram Mathematica 10.4 were applied. Figure 8 shows the model of the industrial area which was used to test the data

assimilation algorithm. A two-dimensional version of the data assimilation was selected.

In parallel, nX (the number of points in space along the X axis = 100) * mY (the number of points in space along the Y axis = 100) of the one-dimensional data assimilation problem for each time layer was solved. Data were selected from the industrial city of Karaganda. The turbulent exchange coefficient μ (nCoefficient) was $0.1 \text{ m}^2/\text{s}$, and the transfer speed (nSpeed) was 0.1 m/s .

Figures 8(b) and 8(c) shows the solution to the data assimilation problem at different points in time and the "real" state of the system. When solving the data assimilation problems, in contrast to direct problems of modeling the propagation of pollutants, process models were complemented by observation models that describe the observed quantities in terms of state functions and the parameters of process models. This makes the procedures of applying the data assimilation algorithm correct from a mathematical point of view and increases the information content of observations. An effective algorithm for predicting the propagation of impurities in the atmosphere that simultaneously involves the parallelization of problems reduces the time required for numerical calculations, which contributes to immediate decision-making in real time when monitoring atmospheric air pollution.

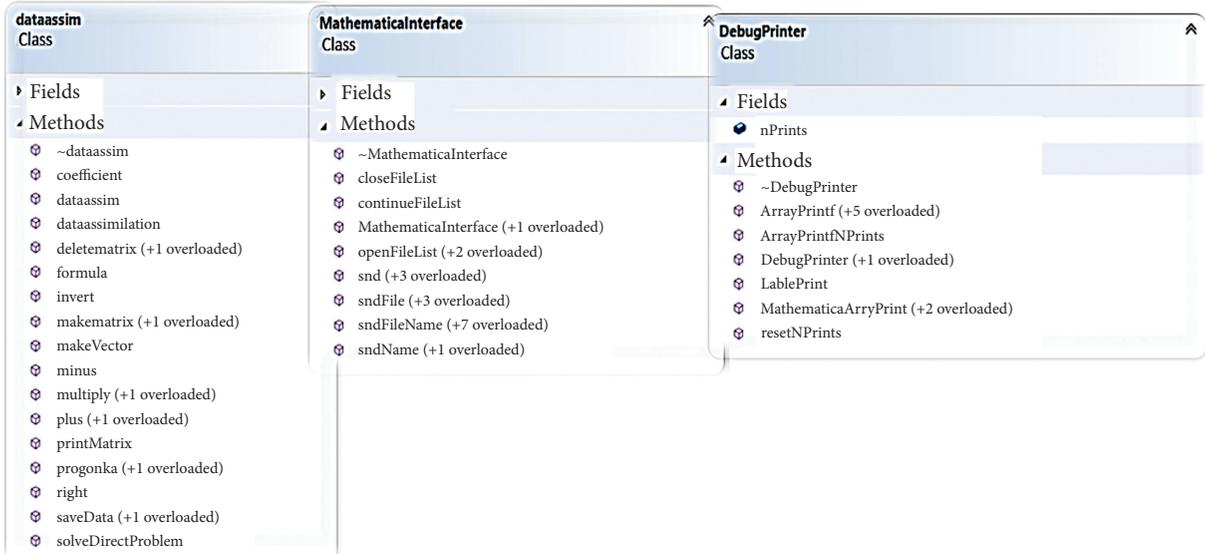


FIGURE 6: Class diagram of the concentration calculation module.

```

res = {{convExp0 -> {directPrb -> {nTimeIntervals -> 400,
    nSpaceIntervals -> 400, nCoefficient -> 0.05,
nSpeed -> 0.,
    fExact -> {{0., 0., -6.2774385622041925`
76.79778247093076*^66},
    {0., 0.0025, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.005, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.0075, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.01, -6.2774385622041925`76.79778247093076*^
66},
    {0., 0.0125, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.015, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.0175, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.02, -6.2774385622041925`76.79778247093076*^
66},
    {0., 0.0225, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.025, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.0275, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.03, -6.2774385622041925`76.79778247093076*^
66},
    {0., 0.0325, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.035, -6.2774385622041925`76.79778247093076
*^66},
    {0., 0.0375, -6.2774385622041925`76.79778247093076

```

FIGURE 7: An example dat-file containing the input and output data of the observational data assimilation algorithm.

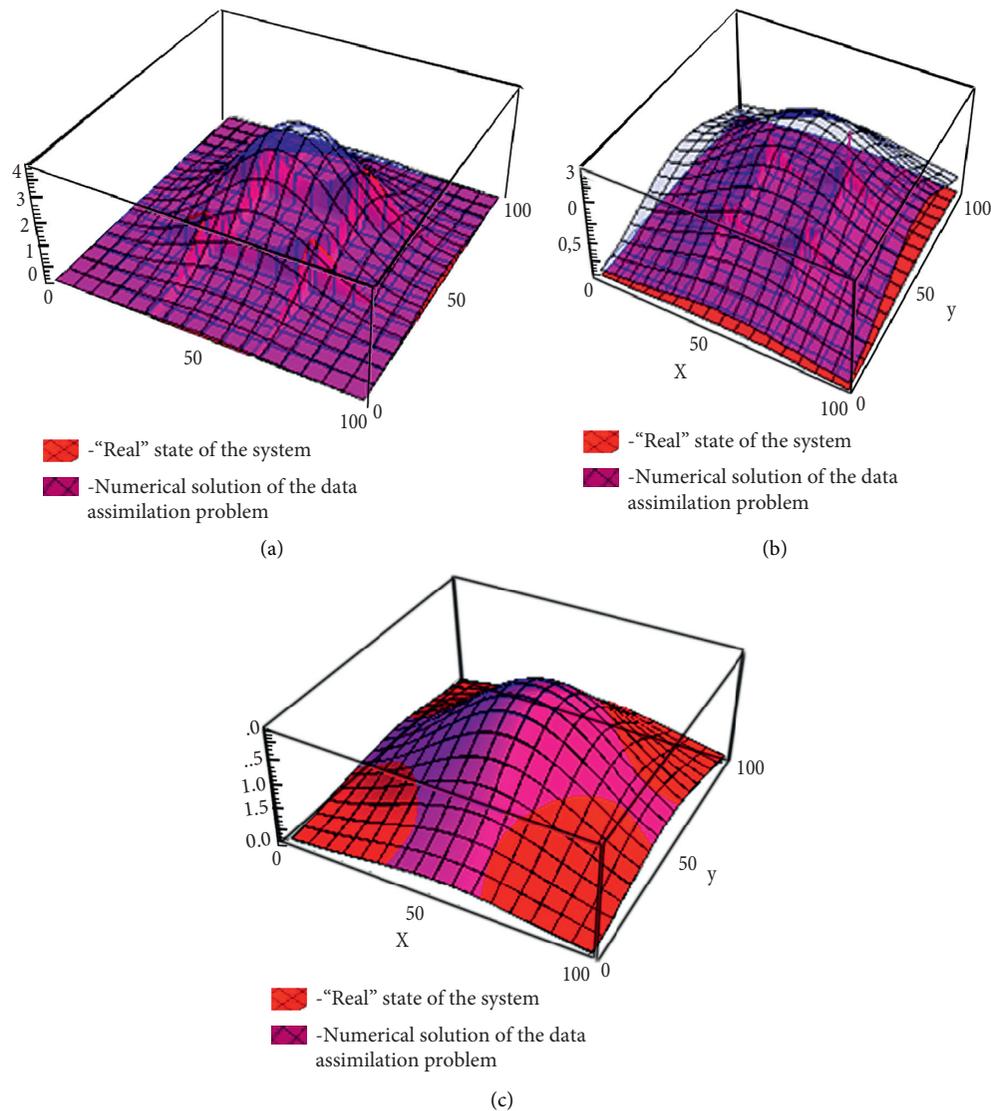


FIGURE 8: Algorithm testing model for an industrial area (a). The solution of the data assimilation problem and the "real" state of the system where $t = 20$ (b) and $t = 40$ (c).

4. Conclusions and Further Work

A data assimilation algorithm for monitoring the atmosphere of an industrial area was investigated. To study the algorithm, the industrial district of Karaganda city was selected as a research object. As a result of the research, an algorithm was implemented that combines two-layer discrete-analytical numerical schemes for convection-diffusion equations and algorithms for sequential data assimilation in real time. A two-dimensional version of a two-layer time-based numerical scheme based on splitting was implemented. An additional module for data assimilation was developed in order to expand the functions of the environmental monitoring information system.

In future, we plan to adapt the model to the conditions of Karaganda city, taking into account the terrain relief and trends of seasonal changes.

Abbreviations

HM:	Heavy metals
MPC:	Maximum permissible concentration
ECMWF:	European Center for Medium-Term Weather Forecasts
RK:	Republic of Kazakhstan
MAD:	Mean absolute deviation
MSE:	Mean square error
RMSE:	Root mean square error
MAPE:	Mean absolute percentage error.

Data Availability

Data on atmospheric air pollution are taken from information bulletins on the environmental situation of the Republic of Kazakhstan, which are publicly available (<https://kazhydromet.kz/en/ecology/ezhemesyachnyy-informacionnyy-byulleten-o-sostoyanii-okruzhayuschey-sredy/2020>).

Conflicts of Interest

The authors declare no conflicts of interest.

Acknowledgments

This research was been funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant no. AP0513599) and a grant titled “The Best Teacher.”

References

- [1] K. Biswas, A. Chatterjee, and J. Chakraborty, “Comparison of air pollutants between Kolkata and siliguri, India, and its relationship to temperature change,” *Journal of Geovisualization and Spatial Analysis*, vol. 4, no. 2, p. 25, 2020.
- [2] M. Filonchik, H. Yan, S. Yang, and V. Hurynovich, “A study of PM_{2.5} and PM₁₀ concentrations in the atmosphere of large cities in Gansu Province, China, in summer period,” *Journal of Earth System Science*, vol. 125, no. 6, pp. 1175–1187, 2016.
- [3] A. S. Akinwumiju, T. Ajisafe, and A. A. Adelodun, “Airborne particulate matter pollution in akure metro city, southwestern Nigeria, west africa: attribution and meteorological influence,” *Journal of Geovisualization and Spatial Analysis*, vol. 5, no. 1, p. 11, 2021.
- [4] N. Aiman, S. Gulnaz, and M. Alena, “The characteristics of pollution in the big industrial cities of Kazakhstan by the example of Almaty,” *Journal of Environmental Health Science and Engineering*, vol. 16, no. 1, pp. 81–88, 2018.
- [5] B. T. Zhakatayeva, “Natural and anthropogenic determinants of environmental air pollution in central Kazakhstan,” in *Bulletin of the Karaganda University; Geography Series*:Buketov Karaganda State University, Karaganda, Kazakhstan, 2009.
- [6] A. Russell, M. Ghalaieny, B. Gazdiyeva et al., “A spatial survey of environmental indicators for Kazakhstan: an examination of current conditions and future needs,” *International Journal of Environmental Research*, vol. 12, no. 5, pp. 735–748, 2018.
- [7] I. Sasaki, “An objective analysis based on variational method,” *Journal of Meteorological Society of Japan*, vol. 36, pp. 29–30, 1958.
- [8] R. E. Kalman, “A new approach to linear filtering and prediction problems,” *Journal of Basic Engineering to be Discontinued*, vol. 82, pp. 34–35, 1960.
- [9] R. E. Kalman and R. S. Bucy, “New results in linear filtering and prediction theory,” *Journal of Basic Engineering*, vol. 83, no. 1, pp. 95–108, 1961.
- [10] V. V. Penenko, *Optimization Models in Hydrodynamic Problems of the Environment*, pp. 78–80, Bulletin of Moscow State University; Alerton Press, New York, NY, USA, 1996.
- [11] V. V. Penenko, “Variational methods of data assimilation and inverse problems for studying the atmosphere, ocean, and environment,” *Numerical Analysis and Applications*, vol. 2, no. 4, pp. 341–351, 2009.
- [12] E. Kalnay, *Atmospheric Modeling, Data Assimilation and Predictability*, Cambridge University Press, Cambridge, UK, 2003.
- [13] I. M. Navon, “Data assimilation for numerical weather prediction: a review,” in *Data Assimilation for Atmospheric, Oceanic and Hydrologic Applications*, S. K. Park and L. Xu, Eds., Springer, Berlin/Heidelberg, Germany, 2009.
- [14] W. Lahoz, B. Khattatov, and R. Ménard, *Data Assimilation Making Sense of Observations*, p. 718p, Springer, Berlin/Heidelberg, Germany, 2010.
- [15] Y. Zhang, “Online-coupled meteorology and chemistry models: history, current status, and outlook,” *Atmospheric Chemistry and Physics*, vol. 8, no. 11, pp. 2895–2932, 2008.
- [16] Y. Zhang, M. Bocquet, V. Mallet, C. Seigneur, and A. Baklanov, “Real-time air quality forecasting, part I: h,” *Atmospheric Environment*, vol. 60, pp. 632–655, 2012.
- [17] Y. Zhang, M. Bocquet, V. Mallet, C. Seigneur, and A. Baklanov, “Real-time air quality forecasting, part II: state of the science, current research needs, and future prospects,” *Atmospheric Environment*, vol. 60, pp. 656–676, 2012.
- [18] H. Elbern and H. Schmidt, “Ozone episode analysis by four-dimensional variational chemistry data assimilation,” *Journal of Geophysical Research: Atmospheres*, vol. 106, no. D4, pp. 3569–3590, 2001.
- [19] H. Elbern, A. Strunk, H. Schmidt, and O. Talagrand, “Emission rate and chemical state estimation by 4-dimensional variational inversion,” *Atmospheric Chemistry and Physics*, vol. 7, no. 14, pp. 3749–3769, 2007.
- [20] J. Vira and M. Sofiev, “On variational data assimilation for estimating the model initial conditions and emission fluxes for short-term forecasting of SO_x concentrations,” *Atmospheric Environment*, vol. 46, pp. 318–328, 2012.
- [21] J. Vira and M. Sofiev, “Assimilation of surface NO₂ and O₃ observations into the SILAM chemistry transport model,” *Geoscientific Model Development*, vol. 8, no. 2, pp. 191–203, 2015.
- [22] K. Yumimoto and T. Takemura, “The SPRINTARS version 3.80/4D-Var data assimilation system: development and inversion experiments based on the observing system simulation experiment framework,” *Geoscientific Model Development*, vol. 6, no. 6, pp. 2005–2022, 2013.
- [23] K. Yumimoto, I. Uno, N. Sugimoto, A. Shimizu, Y. Hara, and T. Takemura, “Size-resolved adjoint inversion of Asian dust,” *Geophysical Research Letters*, vol. 39, Article ID L24808, 2012.
- [24] Y. Roustan and M. Bocquet, “Inverse modelling for mercury over Europe,” *Atmospheric Chemistry and Physics*, vol. 6, no. 10, pp. 3085–3098, 2006.
- [25] A. L. Barbu, A. J. Segers, M. Schaap, A. W. Heemink, and P. J. H. Builtjes, “A multi-component data assimilation experiment directed to sulphur dioxide and sulphate over Europe,” *Atmospheric Environment*, vol. 43, no. 9, pp. 1622–1631, 2009.
- [26] M. Bocquet, “Parameter-field estimation for atmospheric dispersion: application to the Chernobyl accident using 4D-Var,” *Quarterly Journal of the Royal Meteorological Society*, vol. 138, no. 664, pp. 664–681, 2012.
- [27] M. Bocquet and P. Sakov, “Joint state and parameter estimation with an iterative ensemble Kalman smoother,” *Nonlinear Processes in Geophysics*, vol. 20, no. 5, pp. 803–818, 2013.
- [28] S. Rakhmetullina, Y. Turganbayev, and K. Gromaszek, “Application of variational data assimilation algorithms in the

- ecological monitoring system,” *IAPGOS*, vol. 4a, pp. 33–35, 2012.
- [29] D. F. Parrish and J. C. Derber, “The national meteorological spectral statistical-interpolation analysis system,” *Monthly Weather Review*, vol. 120, no. 8, pp. 1747–1763, 1992.
- [30] F. Rabier, H. Järvinen, E. Klinker, J. -F. Mahfouf, and A. Simmons, “The ECMWF operational implementation of four dimensional variational assimilation. Part I: experimental results with simplified physics,” *Quarterly Journal of the Royal Meteorological Society*, vol. 126, pp. 1143–1170, 2000.
- [31] R. Voss and U. Mikolajewicz, “Long-term climate changes due to increased CO₂ concentration in the coupled atmosphere-ocean general circulation model ECHAM3/LSG,” *Climate Dynamics*, vol. 17, no. 1, pp. 45–60, 2001.
- [32] A. J. Cimorelli, S. G. Perry, A. Venkatram et al., “AERMOD: a dispersion model for industrial source applications. Part I: general model formulation and boundary layer characterization,” *Journal of Applied Meteorology*, vol. 44, no. 5, pp. 682–693, 2005.
- [33] S. G. Perry, A. J. Cimorelli, R. J. Paine et al., “AERMOD: a dispersion model for industrial source applications. Part II: model performance against 17 field study databases,” *Journal of Applied Meteorology*, vol. 44, no. 5, pp. 694–708, 2005.
- [34] A. V. Glushkov, O. Y. Khetselius, E. V. Agayar, V. V. Buyadzhi, A. V. Romanova, and V. F. Mansarliysky, “Modelling dynamics of atmosphere ventilation and industrial city’s air pollution analysis: new approach,” *IOP Conference Series: Earth and Environmental Science*, vol. 92, Article ID 012014, 2017.
- [35] C. D. Argyropoulos, G. M. Sideris, M. N. Christolis, Z. Nivolianitou, and N. C. Markatos, “Modelling pollutants dispersion and plume rise from large hydrocarbon tank fires in neutrally stratified atmosphere,” *Atmospheric Environment*, vol. 44, no. 6, pp. 803–813, 2010.
- [36] O. Yu. Khetselius, A. V. Glushkov, S. N. Stepanenko, A. N. Sofronkov, A. A. Svinarenko, and A. V. Ignatenko, “New theoretical approach to dynamics of heat-mass-transfer, thermal turbulence and air ventilation in atmosphere of an industrial city,” *Physics of Aerodispersed Systems*, vol. 58, pp. 93–101, 2020.
- [37] R. D’Amours, A. Malo, T. Flesch, J. Wilson, J.-P. Gauthier, and R. Servranckx, “The Canadian meteorological centre’s atmospheric transport and dispersion modelling suite,” *Atmosphere-Ocean*, vol. 53, no. 2, pp. 1–24, 2013.
- [38] I. Korsakissok, A. Mathieu, and D. Didier, “Atmospheric dispersion and ground deposition induced by the Fukushima Nuclear Power Plant accident: a local-scale simulation and sensitivity study,” *Atmospheric Environment*, vol. 70, pp. 267–279, 2013.
- [39] M. Bocquet, H. Elbern, H. Eskes et al., “Data assimilation in atmospheric chemistry models: current status and future prospects for coupled chemistry meteorology models,” *Atmospheric Chemistry and Physics*, vol. 15, no. 10, pp. 5325–5358, 2015.
- [40] S. Mahajan, H.-M. Liu, T.-C. Tsai, and L.-J. Chen, “Improving the accuracy and efficiency of PM_{2.5} forecast service using cluster-based hybrid neural network model,” *IEEE Access*, vol. 6, Article ID 19193, 2018.
- [41] Resolution of the Government Republic of Kazakhstan, “No.827 on approval of the state program Digital Kazakhstan (with amendments and additions as at December 20, 2019),” 2020, <http://adilet.zan.kz/rus/docs/P1900000949> (in Russian).
- [42] Code of the Republic of Kazakhstan, “N. 212-III Environmental code of the Republic of Kazakhstan (with amendments and additions as at July 25, 2020),” 2020, https://online.zakon.kz/Document/?doc_id=30085593#pos=4 (in Russian).
- [43] kazhydromet, “Internet resource of republican state Enterprise kazhydromet Ministry of ecology, geology and natural resources of the republic of Kazakhstan,” 2020, <https://kazhydromet.kz/ru/ecology/ezhemesyachnyy-informacionnyy-byulleten-o-sostoyanii-okruzhayushey-sredy/2020> (in Russian).
- [44] M. E. Berlyand, *Method for Calculating the Concentrations of Harmful Substances in the Atmospheric Air Contained in the Emissions of Enterprises. OND-86*, Gidrometeoizdat, Saint Petersburg, Russia, (In Russian), 1987.
- [45] B. N. Mynbayeva, Z. O. Oralbekova, D. N. Issabayeva, K. T. Iskakov, and Z. T. Khassenova, “An employment of mathematical toolkit for ecological information processing during heavy metals pollution monitoring in particular reference to Almaty city’s atmosphere,” in *Proceedings of the 18th International Multidisciplinary Scientific Geoconference (SGEM)*, Varna, Bulgaria, July 2018.
- [46] A. V. Penenko and A. T. Kussainova, “Development of a data assimilation algorithm for the model of convection-diffusion of an impurity in the atmosphere based on a non-stationary two-layer discrete-analytical numerical scheme,” *Vestnik of D.Serikbaev EKTU*, vol. 2, pp. 84–97, 2013, (in Russian).
- [47] Z. T. Khassenova and A. T. Kussainova, “Applying data assimilation on the urban environment,” in *Communications in Computer and Information Science* Springer Nature, Berlin, Germany, 2019.
- [48] Ncste, “Development of a new information system and database for optimizing monitoring of air pollution by heavy metals (report on research work),” 2018, https://is.ncste.kz/object/view/50507?reg_card_id=1102&info_card_id=854 (In Russian).
- [49] Z. Oralbekova, Z. Khassenova, B. Mynbayeva, M. Zhartybayeva, and K. Iskakov, “Information system for monitoring of urban air pollution by heavy metals,” *Indonesian Journal of Electrical Engineering and Computer Science*, vol. 22, no. 3, pp. 1590–1600, 2021.
- [50] Z. O. Oralbekova, Z. T. Khassenova, and M. G. Zhartybayeva, “Collection and processing of data to optimize the monitoring of atmospheric air pollution,” in *Communications in Computer and Information Science* Springer Nature, Berlin, Germany, 2019.
- [51] A. V. Penenko, Z. T. Khassenova, V. V. Penenko, and E. A. Pyanova, “Numerical study of a direct variational data assimilation algorithm in Almaty city conditions,” *European Journal of Mathematics Computational Application*, vol. 7, pp. 53–64, 2019.
- [52] V. Penenko and E. Tsvetova, “Discrete-analytical methods for the implementation of variational principles in environmental applications,” *Journal of Computational and Applied Mathematics*, vol. 226, no. 2, pp. 319–330, 2009.
- [53] G. I. Marchuk, *Numerical Methods and Applications*, p. 272, CRC Press, Boca Raton, FL, USA, 2017.
- [54] A. V. Penenko, V. V. Penenko, and E. A. Tsvetova, “Sequential data assimilation algorithms for air quality monitoring models based on a weak-constraint variational principle,” *Numerical Analysis and Applications*, vol. 9, no. 4, pp. 312–325, 2016.