

Numerical Modeling Method For Short-Term Air Quality Forecast In Industrial Regions*

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Abstract

The actual practice shows that in order to sufficiently accurately predict the process of air pollution dispersion it is necessary to take into account within the models such factors as: the change in the velocity of aerosol emissions in the atmosphere in three directions; the change in the diffusion coefficient and the turbulent mixing coefficient for a stable and unstable stratification; wind rose characteristic and terrain orography; the phase transition of substances arising due to changes in temperature in the layers of the atmosphere. In this work, a mathematical model that takes into account these factors and focused on short-term prediction of pollutants concentration in the atmosphere boundary layer in industrial regions is considered. The developed mathematical model is based on the law of conservation of mass and momentum and described by the transport and diffusion equation. A numerical algorithm and software were developed as well for conducting computational experiments. Model verification was performed on short-term prediction of the concentration of solid fine particles emitted from an existing cement plant in the Samarkand region of Uzbekistan.

1 Introduction

Ecology of the atmosphere is one of the most important indicators of the state of the environment. This circumstance makes it necessary to make predictions of the harmful substances concentration in the surface layer of the atmosphere for different time frames. In particular, short-term forecasts associated with the determination of the maximum permissible concentration level of harmful substances in the course of designing and construction of new production facilities are of practical interest.

Transfer and diffusion of pollutants in the surface layer of the atmosphere as well as pollutants precipitation on the underlying surface are very complex processes influenced by many factors, including geographic and climatic characteristic of any considered region. Moreover, it should be mentioned that meteorological conditions change during the day and in the seasons.

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Soil erosion caused by turbulent movement of air mass in the surface layer of the atmosphere is another source of harmful particles emission apart from industrial facilities. This problem is particularly relevant for the Aral region in Uzbekistan. The shoaling of the Aral Sea has led to an exposure of more than 35,000 square kilometers of sea-bed. Over 75 million tons of dust and toxic salts (sulphate and chloride salts) annually rise from the exposed sea bottom.

One of the effective means of monitoring and forecasting the process of transfer and diffusion of harmful substances in the atmosphere is computer simulation, which results can provide support for appropriate decisions making. A lot of theoretical and applied studies have been carried out in recent years in the field of computer simulation of atmospheric transport and dispersion of air pollutants.

Barton, Zarzecki and Russell [1] assessed the usefulness of AERMOD model for predicting air concentrations and deposition of perfluorooctanoate near a manufacturing facility. Measured field data were compared with modeling predictions. AERMOD had adequately located the maximum air concentration in the study area. Errors in predictions of air concentrations were explained by meteorological input uncertainty and conservatism in the PRIME algorithm used to account for building downwash. Overall, AERMOD was found to be a useful screening tool for modeling the dispersion and deposition of perfluorinated compounds in air near a manufacturing facility.

Dresser and Huizer [2] described a near-field validation study involving the steady-state AERMOD and the nonsteadystate CALPUFF models. Relative model performance was compared with field measurements collected near Martins Creek-a rural, hilly area along the Pennsylvania-New Jersey border. The emission sources in the study were two coal-fired power plants with tall stacks and buoyant plumes. The ability of the two models to predict monitored sulfur dioxide concentrations was assessed in a four-part model validation. The performance of CALPUFF was judged to be superior to that of AERMOD.

Liu J. et al. [3] proposed a method for studying the concentration of solid suspension in the atmosphere based on AERMOD model. The authors established the relationship between pollutant emission intensity and the measured concentration of atmospheric environment. The harbor cement production was simulated with AERMOD to calculate the influence degree of harbor cement production on the suspended solids concentration in the atmosphere surrounding. Experiments show that when the discharge diameter is $2.458 \mu\text{m}$, the mass concentration of particulate matter is the maximum of 2.353 mg/m . The obtained results can be used for gasping the distribution of pollutants in the harbor cement production enterprises.

Dey, Gupta, Sibanda and Chakraborty [4] focused on the spatio-temporal variation of nitrogen dioxide (NO_2) during June 2013 to May 2015 and its futuristic emission scenario over an Durgapur urban area of eastern India. Coupled AERMOD and WRF model was used for predicting the concentration of NO_2 . Comparison of the observed and simulated data showed that the model overestimates the concentration of NO_2 in all the seasons (except winter). The results showed that coupled AERMOD+WRF model can overcome the unavailability of hourly surface as well as upper air meteorological data required for predicting the pollutant concentration, but improvement of emission inventory along with better understanding of the sinks and sources of ambient NO_2 is essential for capturing the more realistic scenario.

Szintai, Kaufmann and Rotach [5] investigated a new scaling approach, based on the convective velocity obtained from the sun-exposed eastern slopes and thus suited for steep and narrow Alpine valleys with respect to pollutant dispersion. The capability of the new method was demonstrated with the operational emergency response system of MeteoSwiss, which consists of the COSMO numerical weather prediction model coupled with a Lagrangian particle dispersion model. The new scaling approach was compared to results of a classical similarity theory approach and to the operational coupling type, which uses the turbulent kinetic energy from the COSMO model directly. The ability of the COSMO model to simulate the valley wind system was assessed with several meteorological surface stations, and the dispersion simulation was evaluated with the measurements from 25 surface samplers. The sensitivity of the modelling system towards the soil moisture, horizontal grid resolution, and boundary-layer height determination was investigated, and it was shown that, if the flow field was correctly reproduced, the new scaling approach improves the tracer concentration simulation when compared to classical coupling methods.

Actual practice, showed that in order to sufficiently accurately predict the process of distribution of harmful substances in the atmosphere it is necessary to take into account within the models such factors as: the change in the velocity of aerosol emissions in the atmosphere in three directions; the change in the diffusion coefficient and the turbulent mixing coefficient for a stable and unstable stratification; wind rose characteristic and terrain orography; the phase transition of substances arising due to changes in temperature in the layers of the atmosphere.

2 Problem Statement

Thus, in this paper, we propose a mathematical model that takes into account these factors and focused on short-term prediction of pollutants concentration in the atmosphere boundary layer in industrial regions. A numerical algorithm and software were developed as well for conducting computational experiments. The developed mathematical model is described by the transport and diffusion equation, and it is based on the law of conservation of mass and momentum. The model has the following form

$$\begin{aligned}
 & \frac{\partial \theta(x, y, z, t)}{\partial t} + u \frac{\partial \theta(x, y, z, t)}{\partial x} + v \frac{\partial \theta(x, y, z, t)}{\partial y} \\
 & + (w - w_g) \frac{\partial \theta(x, y, z, t)}{\partial z} + \sigma \theta(x, y, z, t) \\
 = & \mu \frac{\partial^2 \theta(x, y, z, t)}{\partial x^2} + \mu \frac{\partial^2 \theta(x, y, z, t)}{\partial y^2} \\
 & + \frac{\partial}{\partial z} \left(\kappa \frac{\partial \theta(x, y, z, t)}{\partial z} \right) + \delta(x, y, z) Q
 \end{aligned} \tag{1}$$

with appropriate initial and boundary conditions

$$\theta(x, y, z, t) |_{t=0} = \theta_0(x, y, z), \tag{2}$$

$$\left. \begin{aligned} -\mu \frac{\partial \theta}{\partial x} \Big|_{x=0} &= \xi (\theta_n - \theta); \quad \mu \frac{\partial \theta}{\partial x} \Big|_{x=L_x} = \xi (\theta_n - \theta); \\ -\mu \frac{\partial \theta}{\partial y} \Big|_{y=0} &= \xi (\theta_n - \theta); \quad \mu \frac{\partial \theta}{\partial y} \Big|_{y=L_y} = \xi (\theta_n - \theta); \\ -\kappa \frac{\partial \theta}{\partial z} \Big|_{z=0} &= (\beta \theta_n - f(x, y)); \quad \kappa \frac{\partial \theta}{\partial z} \Big|_{z=H} = \xi (\theta_n - \theta). \end{aligned} \right\} \quad (3)$$

Here θ , θ_n -concentration of harmful substances in the atmosphere in the considered and near-boundary area of the problem solution; θ_0 -the primary concentration of harmful substances in the atmosphere; x, y, z -coordinate system; u, v, w -wind speed in three directions; w_g -particles precipitation rate; σ -coefficient of absorption of harmful substances in the atmosphere; μ, κ -diffusion and turbulence coefficients; $\delta(x, y, z)$ -Dirac function; $f(x, y)$ -source of emission of harmful substances into the atmosphere from the underlying earth surface; ξ -the parameter for reduction to the same dimension; L -area length; H -absolute altitude; β -the coefficient of interaction of aerosol particles with underlying surface; Q -pollution source intensity.

3 Solving Method

For the numerical solution of the problem in order to increase the approximation accuracy, we introduce the following notation

$$\bar{w} = w - w_g,$$

$$\theta(x, y, z, t) = e^{\frac{ux+vy}{2\mu} + \frac{\bar{w}z}{2\kappa}} \bar{\theta}(x, y, z, t).$$

Omitting the score above $\theta(x, y, z, t)$ variable, instead of equation (1) we get:

$$\begin{aligned} & \frac{\partial \theta(x, y, z, t)}{\partial t} + \sigma_1 \theta(x, y, z, t) \\ &= \mu \frac{\partial^2 \theta(x, y, z, t)}{\partial x^2} + \mu \frac{\partial^2 \theta(x, y, z, t)}{\partial y^2} \\ & \quad + \frac{\partial}{\partial z} \left(\kappa \frac{\partial \theta(x, y, z, t)}{\partial z} \right) + e_1 \delta(x, y, z) Q, \end{aligned} \quad (4)$$

where

$$\sigma_1 = \frac{\kappa u^2 + \kappa v^2 + \mu \bar{w}^2 + 4\sigma \mu \kappa}{4\mu \kappa} \quad \text{and} \quad e_1 = e^{-\left(\frac{ux+vy}{2\mu} + \frac{\bar{w}z}{2\kappa}\right)}.$$

As we can see, it is difficult to obtain an analytical solution of the equation (4) with boundary conditions (2)–(3). For numerical integration, we used an implicit scheme based on the finite difference method. Replacing the discontinuous region by grid, we obtain a system of algebraic equations [6, 7].

For the straight line OX :

$$\left. \begin{aligned} a_{1,j,k} \theta_{0,j,k}^{n+\frac{1}{3}} - b_{1,j,k} \theta_{1,j,k}^{n+\frac{1}{3}} + c_{1,j,k} \theta_{2,j,k}^{n+\frac{1}{3}} &= -d_{1,j,k}, \\ a_{i,j,k} \theta_{i-1,j,k}^{n+\frac{1}{3}} - b_{i,j,k} \theta_{i,j,k}^{n+\frac{1}{3}} + c_{i,j,k} \theta_{i+1,j,k}^{n+\frac{1}{3}} &= -d_{i,j,k}, \\ a_{N,j,k} \theta_{N-2,j,k}^{n+\frac{1}{3}} - b_{N,j,k} \theta_{N-1,j,k}^{n+\frac{1}{3}} + c_{N,j,k} \theta_{N,j,k}^{n+\frac{1}{3}} &= -d_{N,j,k}, \end{aligned} \right\} \quad (5)$$

where

$$\begin{aligned}
 a_{1,j,k} &= 3\mu + 2\Delta x\xi; \quad b_{1,j,k} = 4\mu, \\
 c_{1,j,k} &= \mu; \quad d_{1,j,k} = -2\Delta x e_1 \xi \theta_n, \\
 a_{i,j,k} &= \frac{\mu}{\Delta x^2}, \quad b_{i,j,k} = \frac{3}{\Delta t} + \sigma_1 + \frac{2\mu}{\Delta x^2}, \quad c_{i,j,k} = \frac{\mu}{\Delta x^2}, \\
 a_{N,j,k} &= \mu, \quad b_{N,j,k} = 4\mu, \quad c_{N,j,k} = 3\mu + 2\Delta x\xi, \\
 d_{i,j,k} &= \left(\frac{3}{\Delta t} - \frac{2\mu}{\Delta y^2} - \frac{\kappa_{k-0,5} + \kappa_{k+0,5}}{\Delta z^2} \right) \theta_{i,j,k}^n \\
 &\quad + \frac{\mu}{\Delta y^2} \theta_{i,j-1,k}^n + \frac{\mu}{\Delta y^2} \theta_{i,j+1,k}^n + \frac{\kappa_{k-0,5}}{\Delta z^2} \theta_{i,j,k-1}^n \\
 &\quad + \frac{\kappa_{k+0,5}}{\Delta z^2} \theta_{i,j,k+1}^n + \frac{1}{3} e_1 \delta_{i,j,k} Q; \quad d_{N,j,k} = -2\Delta x e_1 \xi \theta_n.
 \end{aligned}$$

For the straight line OY :

$$\left. \begin{aligned}
 \bar{a}_{i,1,k} \theta_{i,0,k}^{n+\frac{2}{3}} - \bar{b}_{i,1,k} \theta_{i,1,k}^{n+\frac{2}{3}} + \bar{c}_{i,1,k} \theta_{i,2,k}^{n+\frac{2}{3}} &= -\bar{d}_{i,1,k}, \\
 \bar{a}_{i,j,k} \theta_{i,j-1,k}^{n+\frac{2}{3}} - \bar{b}_{i,j,k} \theta_{i,j,k}^{n+\frac{2}{3}} + \bar{c}_{i,j,k} \theta_{i,j+1,k}^{n+\frac{2}{3}} &= -\bar{d}_{i,j,k}, \\
 \bar{a}_{i,M,k} \theta_{i,M-2,k}^{n+\frac{2}{3}} - \bar{b}_{i,M,k} \theta_{i,M-1,k}^{n+\frac{2}{3}} + \bar{c}_{i,M,k} \theta_{i,M,k}^{n+\frac{2}{3}} &= -\bar{d}_{i,M,k},
 \end{aligned} \right\} \quad (6)$$

where

$$\begin{aligned}
 \bar{a}_{i,1,k} &= 3\mu + 2\Delta y\xi, \quad \bar{b}_{i,1,k} = 4\mu, \quad \bar{c}_{i,1,k} = \mu, \\
 \bar{a}_{i,j,k} &= \frac{\mu}{\Delta y^2}, \quad \bar{b}_{i,j,k} = \frac{3}{\Delta t} + \sigma_1 + \frac{2\mu}{\Delta y^2}, \quad \bar{c}_{i,j,k} = \frac{\mu}{\Delta y^2}, \\
 \bar{a}_{i,M,k} &= \mu, \quad \bar{b}_{i,M,k} = 4\mu, \quad \bar{c}_{i,M,k} = 3\mu + 2\Delta y\xi, \\
 \bar{d}_{i,1,k} &= -2\Delta y e_1 \xi \theta_n, \\
 \bar{d}_{i,j,k} &= \left(\frac{3}{\Delta t} - \frac{2\mu}{\Delta x^2} - \frac{\kappa_{k-0,5} + \kappa_{k+0,5}}{\Delta z^2} \right) \theta_{i,j,k}^{n+\frac{1}{3}} \\
 &\quad + \frac{\mu}{\Delta x^2} \theta_{i-1,j,k}^{n+\frac{1}{3}} + \frac{\mu}{\Delta x^2} \theta_{i+1,j,k}^{n+\frac{1}{3}} + \frac{\kappa_{k-0,5}}{\Delta z^2} \theta_{i,j,k-1}^{n+\frac{1}{3}} \\
 &\quad + \frac{\kappa_{k+0,5}}{\Delta z^2} \theta_{i,j,k+1}^{n+\frac{1}{3}} + \frac{1}{3} e_1 \delta_{i,j,k} Q, \\
 \bar{d}_{i,M,k} &= -2\Delta y e_1 \xi \theta_n.
 \end{aligned}$$

For the straight line OZ :

$$\left. \begin{aligned}
 \bar{a}_{i,j,1} \theta_{i,j,0}^{n+1} - \bar{b}_{i,j,1} \theta_{i,j,1}^{n+1} + \bar{c}_{i,j,1} \theta_{i,j,2}^{n+1} &= -\bar{d}_{i,j,1}, \\
 \bar{a}_{i,j,k} \theta_{i,j,k-1}^{n+1} - \bar{b}_{i,j,k} \theta_{i,j,k}^{n+1} + \bar{c}_{i,j,k} \theta_{i,j,k+1}^{n+1} &= -\bar{d}_{i,j,k}, \\
 \bar{a}_{i,j,L} \theta_{i,j,L-2}^{n+1} - \bar{b}_{i,j,L} \theta_{i,j,L-1}^{n+1} + \bar{c}_{i,j,L} \theta_{i,j,L}^{n+1} &= -\bar{d}_{i,j,L},
 \end{aligned} \right\} \quad (7)$$

where

$$\begin{aligned}\bar{a}_{i,j,0} &= 3\kappa_1 - 2\Delta z\beta, \quad \bar{b}_{i,j,0} = 4\kappa_1, \quad \bar{c}_{i,j,0} = \kappa_1, \quad \bar{a}_{i,j,k} = \frac{\kappa_{k-0,5}}{\Delta z^2}, \\ \bar{b}_{i,j,k} &= \frac{3}{\Delta t} + \sigma_1 + \frac{\kappa_{k-0,5} + \kappa_{k+0,5}}{\Delta z^2}, \quad \bar{c}_{i,j,k} = \frac{\kappa_{k+0,5}}{\Delta z^2}, \\ \bar{a}_{i,j,L} &= \kappa_L, \quad \bar{b}_{i,j,L} = 4\kappa_L, \quad \bar{c}_{i,j,L} = 3\kappa_L + 2\Delta z\xi, \\ \bar{d}_{i,j,0} &= 2e_1\Delta z f(x, y), \\ \bar{d}_{i,j,k} &= \left(\frac{3}{\Delta t} - \frac{2\mu}{\Delta x^2} - \frac{2\mu}{\Delta y^2} \right) \theta_{i,j,k}^{n+\frac{2}{3}} + \frac{\mu}{\Delta x^2} \theta_{i-1,j,k}^{n+\frac{2}{3}} \\ &\quad + \frac{\mu}{\Delta x^2} \theta_{i+1,j,k}^{n+\frac{2}{3}} + \frac{\mu}{\Delta y^2} \theta_{i,j-1,k}^{n+\frac{2}{3}} + \frac{\mu}{\Delta y^2} \theta_{i,j+1,k}^{n+\frac{2}{3}} + \frac{1}{3} e_1 \delta_{i,j,k} Q, \\ \bar{d}_{i,j,L} &= -2\Delta z e_1 \xi \theta_n.\end{aligned}$$

Thus, finally, the systems of algebraic equations was obtained for the decision variables in the direction of straight lines OX , OY , OZ . To solve these systems of algebraic equations (5)–(7), the sweep method was used [6, 7].

4 GIS Integration

On the basis of given mathematical apparatus, there was developed web application for carrying out computational experiments. The developed software consists of several modules: input data preprocessing, numerical calculations, data post-processing and results visualization.

Integration of atmospheric diffusion models with GIS can be carried out through several scenarios [8]. The basic variant of integration can be represented by a standalone application for modeling the process of air pollution advection and diffusion. Wherein all necessary data can be used independently by other software (GIS, DBMS, web applications, etc.), and the heterogeneous structures of this data need to be converted into the appropriate formats. This integration approach is quite common [9]. This is due to the fact that the development of a universal air quality modeling system, combining all the necessary functionality is quite difficult and, moreover, not always a justified objective. Scientific research is most often aimed to determine the patterns and average trends with minimal calculation time costs.

The developed web application is based on Google Maps and OpenWeatherMap data sets and APIs (Fig.1). The capabilities of the developed application include: map loading and positioning; spatial data import; interactive input of emission sources properties on the map; automatic search of meteorological information by geographic coordinates; calculation of the concentration of harmful substances in the atmosphere of given region; visualization of calculation results as semitransparent layers on the map; store the history of computational experiments into database.

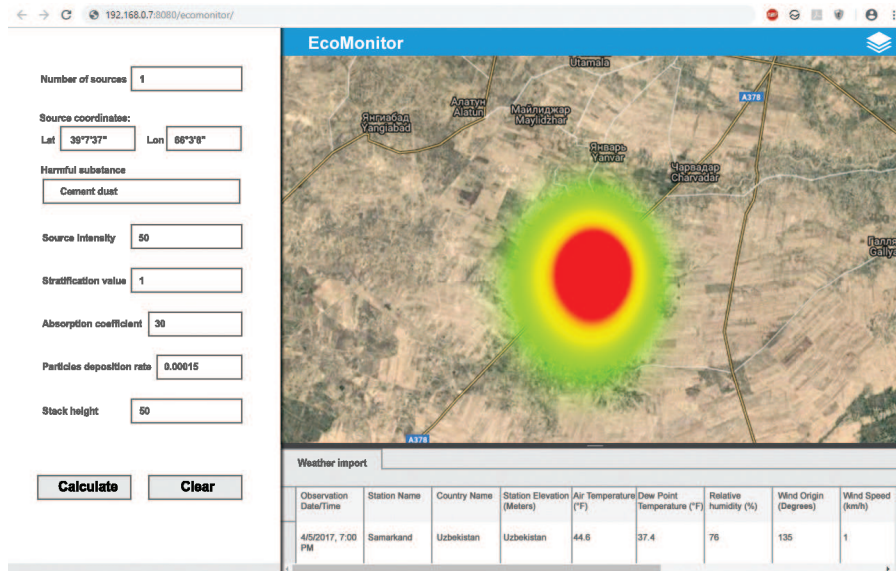


Figure 1: Web application.

5 Results

As an experiment, there was solved the problem of short-term prediction of the concentration of solid fine particles emitted from an existing cement plant in the Samarkand region of Uzbekistan. The industrial site is located south of the Charvardar, Kuru-sai, Mailaljar townships.

The considered region is a flat territory at the foot of the Zerafshan Range. The soil cover here is represented by adyrs formed mainly by sands and grey desert soil. This territory encompasses a subtropical intracontinental climate with hot dry summers and cold winters. The average annual temperature is $+16.5^{\circ}$, average annual precipitation is 310-330 mm. The weak winds up to 4-5 m/s, blowing mainly from the north-west prevail on the territory.

The source emission rate is 50 mg/m³ per second. Note that according to hygiene standards SanPiN RUz N0293-11, the value of maximum permissible concentration for cement dust is 0.3 mg/m³ - the maximum single concentration and 0.1 mg/m³ - the average daily concentration.

Examples of obtained calculation results are shown in figures 2 and 3. The forecast time for each computational experiment was set to 2 hours. The wind speed parameter was considered as nonvarying during every computation.

From the carried out numerical calculations, it follows that with moderate wind or calm the concentration of harmful fine particles in the atmosphere is accumulated directly around the emission source (Fig.2).

It can be seen from Fig.3 that as the component of the wind speed increases horizontally, the cement dust transfer process takes place and the concentration of harmful

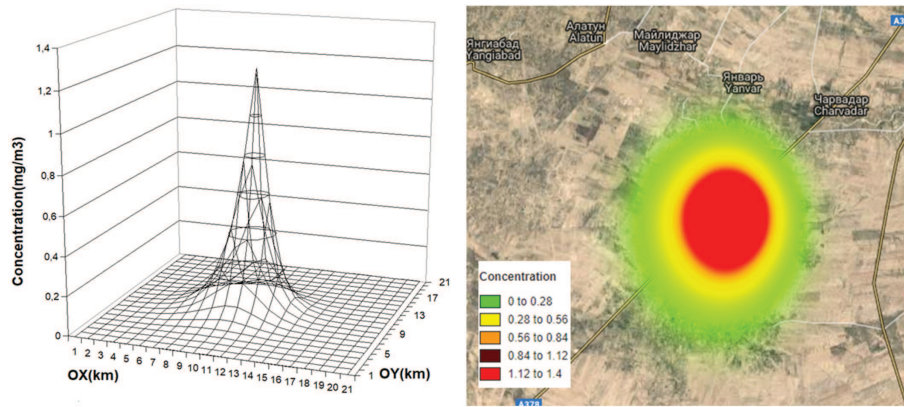


Figure 2: Distribution of cement dust concentration at a height of $z = 200$ m, wind speed and direction $U = 1$ m/s, $\alpha = 135^\circ$, coefficient of absorption $\sigma = 0.0014$ /s, time $t = 2$ h.

substances around the emission source decreases proportionally, and the area of their transportation expands with time.

An analysis of the numerical calculations showed that the maximum values of fine particles concentration in the atmosphere are accumulated near the earth surface when z changes within the interval from 200 to 350 m. The concentration of cement dust particles decreases exponentially with distance from the emission source. Numerical calculations showed that the maximum particles concentration is in the axial part of the transport plume. It was found that the maximum concentration corresponds to a level of 400–425 m with calm and moderate wind.

Computational experiments were carried out assuming the fact that the emitted cement dust particles have different diameters. This circumstance plays an important role in the transport process and in the rate of particle deposition. The vertical transport of particles is mainly dependent on the turbulence coefficient, vertical component of wind speed, particle size and density.

6 Conclusion

Thus, it has been ascertained that the process of transport and diffusion of solid dust particles in the atmosphere is mainly affected by: the horizontal component of wind speed, when its increasing the area of harmful particles propagation proportionally grows to wind direction; the absorption coefficient, as it increases, the concentration of harmful substances in the atmosphere decreases, in turn this parameter depends on the humidity of the air mass. The vertical transport of fine particles is mainly influenced by the turbulence coefficient. We found that this parameter grows fast particularly in the surface layer of the atmosphere at an altitude of 10 up to 250 m. It has also been found that the deposition rate mainly depends on the turbulence coefficient, vertical component of wind speed, particle size and density.

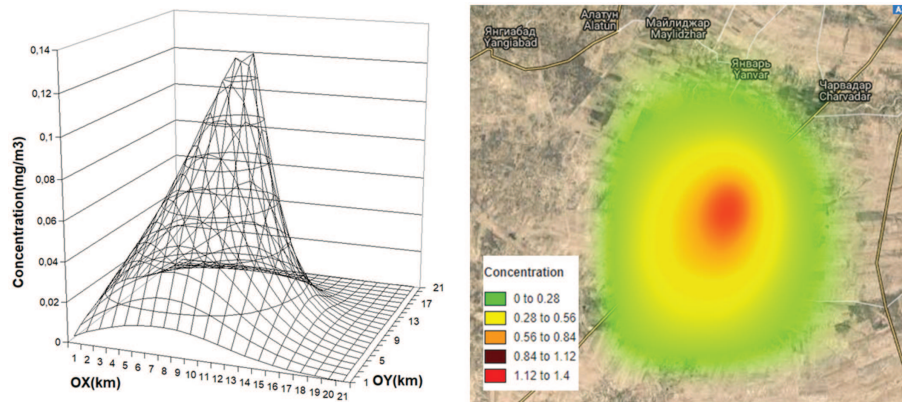


Figure 3: Distribution of cement dust concentration at a height of $z = 200$ m, wind speed and direction $U = 7$ m/s, $\alpha = 135^\circ$, coefficient of absorption $\sigma = 0.0014/s$, time $t = 2$ h.

The maximum accumulation of the concentration of harmful substances in the atmosphere of considered region can be seen during the summer season when the absorption coefficient tends to zero.

The integration of mathematical apparatus with GIS makes possible to visually monitor and forecast the considered processes, assess the environmental impact of an unfavorable ecological situation, and evaluate the effectiveness of conservation measures. That allows us to estimate quite accurately the socio-economic aspects of various ecological processes: the pollution spread in the atmosphere, soils erosion, desertification etc.

Based on the obtained results, there were formulated recommendations that were submitted to the Samarkand regional branch of the State Committee of the Republic of Uzbekistan for Ecology and Environmental Protection for the adoption of appropriate decisions.

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