

## Development of the Turbulent Diffusion Model of Fine Suspended Substances in the Lower Atmosphere Layer

Ivan KOZII<sup>1\*</sup>, Leonid PLYATSUK<sup>1</sup>, Tetyana ZHYLENKO<sup>2</sup>, Larysa HURETS<sup>1</sup>, Yevhen BATALTSEV<sup>1</sup>, Dmytro SAYENKOV<sup>1</sup>

<sup>1</sup> Sumy State University, Department of Ecology and Environmental Protection Technologies, Sumy, 2 Rymkogo-Korsakova str., 40007, Ukraine

<sup>2</sup> Sumy State University, Department of Mathematical Analysis and Optimization Methods, Sumy, 2 Rymkogo-Korsakova str., 40007, Ukraine

**crossref** <http://dx.doi.org/10.5755/j02.ms.30223>

Received 05 December 2021; accepted 14 February 2022

A promising direction for solving the problem of air pollution by fine substances is the use of numerical modeling in the development of mathematical models of the transport of pollutants in the atmosphere. An urgent problem in applying mathematical models with numerical algorithms and software is constructing a qualitative model that would meet both the physical parameters and fulfill all the optimal conditions of numerical analysis. The main objective of this study was to develop an algorithm of a mathematical model based on the equation of distribution of impurities in a turbulent medium. That allows considering the simultaneous influence of wind speed, turbulence of atmospheric air, pollution parameters, direction, and wind force on the size of scattering zones. The unique feature of the study is the use of the coordinate splitting equation of impurities distribution in a turbulent environment with subsequent normalization and parameterization of conditions. Finding integrands functions in the calculation algorithm allows obtaining a stable computational algorithm of the proposed propagation model of fine suspended particles. The solution of the function implemented in the Mathcad Prime 7 software. Distributions of concentrations and their levels for various values of turbulence of atmospheric air and dangerous wind speed are received. The most significant number of fine particles is at a distance of up to 4 km from the emission source. Still, there is also the transfer of contaminants at more than 5 km (up to 57 % of the initial emission concentration). The model has convenient software and algorithmic software, the time of calculation of graphic visualizations up to 20 minutes on medium-power computers. The obtained mathematical model can use in systems of forecasting man-caused load on the environment for the prompt solution of environmental problems.

**Keywords:** atmospheric pollution, fine substances, surface layer, numerical model, air turbulence.

### 1. INTRODUCTION

In the general system of monitoring environmental pollution, the study of atmospheric pollution plays a vital role because the atmosphere pollutes all-natural environment components. Processes in the atmosphere are the most difficult to control, predict, and manage, significantly complicate environmental measures. In urban areas, the most dangerous sources of air pollution are emissions from energy and industrial enterprises, emissions from vehicles.

Statistical databases [1, 2] have shown that environmental factors associated with air pollution provoke about 1/3 of diseases. The problematic environmental situation of most cities in the world requires implementing some ecological measures. The feasibility and effectiveness of such estimates depend on the quality of information about the environmental state, which must be considered during the simulation and forecasting of the spread of pollutants from potentially dangerous objects.

The modeling of the process of air pollution is devoted to works [3, 4], which combine the use of modern satellite equipment and powerful computers to predict and assess the level of environmental pollution. In [3] considered the

model of fine dust distribution at the regional level with a minimum step of the calculated grid of 10 km. In [4], the algorithm of the model working with satellite images considers the parameters of emission sources. Still, with deviations of wind speed, the error of aerosol propagation in height is up to 500 m. Models of pollutant distribution in [3, 4] require significant material resources for their use at the local level (estimated density not less than 1 km).

In works [5–7] the growth of scientific and practical interest in mathematical modeling of transfer and diffusion of aerosol particles in the atmosphere due to technogenic and anthropogenic impact on the environment is noted.

In [5] presented a mathematical model of propagation and diffusion of fine aerosols and carbon dioxide entering the atmosphere from industrial facilities. The paper presents the main parameters that affect the propagation and distribution of fine particles in the air: wind speed, direction, terrain, the turbulence of air masses. But the issue of considering the parameters of emission sources remains unresolved. It's maybe due to objective difficulties associated with versatility, non-stationary problems, and initial data uncertainty.

In [6] they were considered spreading pollutants from a planar source of pollution (peat fires). During fires, a

\* Corresponding author. Tel.: 380 (542) 33-12-05.

E-mail address: [i.kozii@ecolog.sumdu.edu.ua](mailto:i.kozii@ecolog.sumdu.edu.ua) (I. Kozii)

significant amount of fine aerosols and other polydisperse substances are released, which obtained a two-dimensional model of pollutant distribution in the surface layer of the atmosphere, taking into account the thermal inhomogeneity of the underlying surface. The model is based on a system of equations of diffusion distribution of pollutants, allowing us to further consider the three-dimensional numerical simulation problem.

In [7] obtained a predictive numerical model of the distribution of fine suspended solids over oil sands in Canada. The model considers the particle size distribution and four propagation algorithms. The disadvantage is the duration of data processing and the complexity of the forecast process.

In [8] performed numerical modeling of the turbulent fluctuations of air masses in the surface layer that affects the distribution of pollutants. The disadvantage is the lack of a consistent relationship with suspended solids.

In particular, in [9] it was shown that the numerical mathematical model should consider the chemistry of the pollutant reactions in the air, the turbulence of the atmospheric layer to consider the distribution of pollutants. Noted that it is important to consider the relationship between the concentration of impurities and environmental parameters:

- wind speed and its direction;
- the turbulence of air masses;
- absorption of pollutants by air masses;
- changes in air temperature.

The use of the proposed model involves understanding the chemistry of reactions in the surface layer and the complexity of the formation of the initial data formation.

Due to the versatility, non-stationary problem, and uncertainty in the initial data, creating a model corresponding to natural processes [10, 11]. OND-86 method implemented analytical and numerical solutions of the diffusion equation, which has many advantages (normalization of pollutant emissions) and disadvantages (forecasting and analysis of pollutant concentrations for specific meteorological parameters). Some methods for calculating the area of contamination (software packages ANSYS CFX, FLOTRAN, or PHAST DNV) have the difficulty of choosing the initial and boundary conditions, long calculation time, the need for specially certified personnel. All this suggests that it is appropriate to conduct a study on developing a mathematical model of the transport of pollutants in the atmosphere based on numerical modeling [12, 13].

The development and application of special mathematical software [14] are necessary for reliable forecasting of the ecological state of the environment (surface layer of the atmosphere) of industrial zones of settlements. It is important to develop a model that would consider the parameters of emission sources, wind speed, and turbulence of air masses that was comprehensive and ensure the efficiency and reliability of the obtained values.

To achieve this goal, set the following tasks:

1. To investigate the uncertainty of initial data of mathematical model of the parameterized equation of transfer of pollutants in the atmosphere;
2. To obtain simple analytical solutions and to build appropriate algorithms for numerical modeling of the

process of scattering pollutants (appropriate iterative and recursive computational algorithms);

3. To build a high-quality computer model of pollutant scattering, which fulfills all the optimal conditions of numerical analysis with algorithmic software for forecasting the levels of pollution of the surface layer of the atmosphere with fine impurities.

## 2. METHODOLOGY

### 2.1. Research algorithm

The system of equations of diffusion propagation of fine substances in the turbulent surface layer of the atmosphere is based on [15 – 18]:

– Navier-Stokes equation:

$$\partial v_j / \partial t = -1/\rho \cdot \partial p / \partial x_j + \text{div}(\mu \text{grad}(v_j)) - g; \quad (1)$$

– equation of mass transfer of pollutants:

$$\partial \varphi_i / \partial t = \text{div}(\mu \text{grad}(\varphi_i)) + I_\varphi; \quad (2)$$

– heat transfer equation:

$$\partial Q / \partial t = \text{div}(\mu \text{grad}(Q)) + \text{div}(\lambda \text{grad}(T)) + I_Q; \quad (3)$$

– the condition of continuity:

$$\partial \rho / \partial t = -\text{div}(\rho \bar{v}) + \text{div}(\mu \text{grad}(\rho)) + I_\rho; \quad (4)$$

– and equation of state:

$$p = \sum_i (\rho_i / M_i) \cdot RT, \quad (5)$$

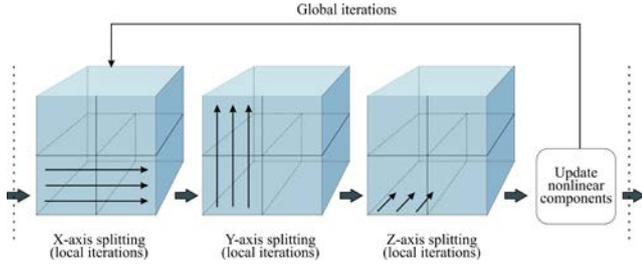
where  $v_j$  is the projection of velocity components on the axis  $Ox_j$ ;  $t$  is the time;  $\rho$  is the pollutants density;  $p$  is the atmospheric pressure;  $x_j$  is the distance from the source;  $\mu$  is the dynamic viscosity of air;  $\varphi_i$  is the volume fractions of the  $i$ -th phase ( $i = 0$  – air,  $i = 1$  – water in the gaseous state,  $i = 2$  – gas at the emission source,  $i = 3$  – water in the liquid state,  $i = 4$  – soot);  $g$  – free fall acceleration;  $I_\varphi$  is the fluctuation volume component;  $Q$  is the quantity of heat;  $T$  is the gas phase temperature;  $\lambda$  is the coefficient of thermal conductivity;  $I_Q$  is the fluctuation heat component;  $v$  is the flow velocity;  $I_\rho$  is the fluctuation component of pollutants density;  $M$  is the molar mass;  $R$  is the universal gas constant.

We consider the numerical method for solving Eq. 1 – Eq. 5. The calculation algorithm is as follows:

1. Numerical determination of the limits of existence of initial and boundary conditions based on data on fine dust emissions into the atmosphere;
2. Calculation of distribution values based on the Navier-Stokes vector equation, continuity equation, and Clapeyron equation;
3. Estimation of turbulence field values;
4. Calculation of impurity concentrations propagating from emission sources in the surface layer of the atmosphere based on the transfer equation.

Using the method of coordinate splitting, we perform the tasks (Fig. 1). This method uses to solve parabolic or elliptic partial differential equations. The idea of the method is to split the equations into several simpler ones – by the equation along each coordinate axis. This procedure is performed so that the derivatives along the corresponding

direction are determined implicitly, and the remaining coordinates are considered constant.



**Fig. 1.** The structure of the algorithm for the three-dimensional transfer problem within the recursive-iterative approach

## 2.2. Software and physical parameters of modeling

PTC Mathcad Prime 7 (© PTC Inc. (PTC), 2021) was used to perform numerical calculations of the mathematical model.

The range from 5 to 10 m/s took the value of wind speed in the model, which is a dangerous wind speed (reach the highest surface concentration of harmful substances) [19]. Air temperatures in the calculations were taken based on the average values of warm (+20 °C) and cold (0 °C) periods of the year. The height of the source of pollution is 65 m, the diameter of the pipe is 1.2 m, the emission temperature is 70 °C, the concentration of the pollutant is  $0.25 \cdot 10^{-6}$  kg/m<sup>3</sup>. The dispersed composition of the calculated particles of the contaminant is  $0.3 \cdot 10^{-6}$  m, the particle density is  $3 \cdot 10^3$  kg/m<sup>3</sup>. Atmospheric air turbulence is in the range of 10 – 155 m<sup>2</sup>/s. The size of the settlement area is 10 · 10 km.

## 3. RESULTS AND DISCUSSION

### 3.1. Determination of the impurities' distribution conditions in the atmosphere

The three-dimensional equation of impurities' distribution in a turbulent medium can be written as follows [20]:

$$\begin{aligned} & \partial n(M, t) / \partial t + \eta(t) n(M, t) + \left( \partial / \partial t (\vartheta_x(M, t) n(p, t)) + \right. \\ & \left. + \partial / \partial t (\vartheta_y(M, t) n(p, t)) + \partial / \partial t (\vartheta_z(M, t) n(M, t)) \right) - \\ & - \left( \partial / \partial x (\tau_x(M, t) \cdot \partial n(M, t) / \partial x) + \partial / \partial y (\tau_y(M, t) \cdot \right. \\ & \left. \cdot \partial n(M, t) / \partial y) + \partial / \partial z (\tau_z(M, t) \cdot \partial n(M, t) / \partial z) \right) = \\ & = \omega(M, t), \end{aligned} \quad (6)$$

where  $n(M, t)$  is the concentration of the pollutant at a given point  $M$  from emissions source at a certain point in time  $t$ , kg/m<sup>3</sup>;  $\eta(t)$  is the coefficient characterizing the degree of removal or introduction of impurities into a given volume due to chemical or other processes occurring in the surface layer of the atmosphere;  $\vartheta_x, \vartheta_y, \vartheta_z$  is the vector components wind speed, m/s;  $\tau$  is the turbulence, characterized by the coefficient of turbulent diffusion, m<sup>2</sup>/s, the transfer is carried out along the coordinate axes  $Ox, Oy, Oz$ ;  $\omega$  is the emissions source of pollutants, kg/m<sup>3</sup>s.

For the surface layer of the air, we use the conservation law, and then Eq. 6 will take such form:

$$\begin{aligned} & \partial n(M, t) / \partial t + \eta(t) n(M, t) + \left( \vartheta_x \partial / \partial t (n(M, t)) + \right. \\ & \left. + \vartheta_y \partial / \partial t (n(M, t)) + \vartheta_z \partial / \partial t (n(M, t)) \right) - \\ & - \left( \partial / \partial x (\tau_x(M, t) \cdot \partial n(M, t) / \partial x) + \partial / \partial y (\tau_y(M, t) \cdot \right. \\ & \left. \cdot \partial n(M, t) / \partial y) + \partial / \partial z (\tau_z(M, t) \cdot \partial n(M, t) / \partial z) \right) = \\ & = \omega(M, t). \end{aligned} \quad (7)$$

Under the theory of the method of coordinate splitting, we formulate the following statement: the process of problem-solving Eq. 7 can have a solution under the following conditions:

1.  $M=M(x, y, z)$  is the point of the studied area of space,  $n(x|t)$ , where  $M \in \Omega \subset R_3, t \in [0; T]$ ;
2. under initial conditions  $n(M, t)|_{t=0} = n(M, 0) = n_0(M)$ ;
3. under extreme conditions  $n(M, t) = (M, t), p \in \bar{\Omega}$ ,

where  $n_0(M), (M, t)$  are the predefined functions;  $\bar{\Omega}$  is the boundary of the space zone  $\Omega$ ;  $n(M, t)$  is the concentration of impurities at a point in space at a certain point in time  $t$ . The turbulence field has the form of a diagonal matrix:

$$\tau(M, t) = \begin{pmatrix} \tau_{xx} & 0 & 0 \\ 0 & \tau_{yy} & 0 \\ 0 & 0 & \tau_{zz} \end{pmatrix}, \quad (8)$$

where  $\tau_{xx} = \tau_x(M, t); \tau_{yy} = \tau_y(M, t); \tau_{zz} = \tau_z(M, t); \tau(M, t)$  is the tensor.

Eq. 7 and Eq. 8 are the initial conditions for constructing the algorithm and model of the distribution of pollutants in the surface layer of air.

### 3.2. Algorithm of pollutant distribution model

According to the method of coordinate splitting, we divide the solution of problem (Eq. 7) into three parts ( $t_j \leq t \leq t_{j+1}$ ):

$$\begin{aligned} & \tilde{n}_1 + \eta n_1 + \partial / \partial z (\vartheta_z n_1) - \partial / \partial z (\tau_z \partial n_1 / \partial z) = \delta_1 \omega(M, t); \\ & M_1 = M(z|x, y); M_4 = M(0|x, y); \\ & M_5 = M(z|x, y); n_1(M_1, t = 0) = n_0(M_1), \text{ при } t = 0; \quad (9) \\ & n_1(M, t_j) = n_3(M, t_{j+1}), \text{ при } t > 0; \\ & n_1(M_4, t) = \bar{n}_4(x, y, t), n_1(M_5, t) = \bar{n}_5(x, y, t). \end{aligned}$$

$$\begin{aligned} & \tilde{n}_2 + \partial / \partial x (\vartheta_x n_2) - \partial / \partial x (\tau_x \partial n_2 / \partial x) = \delta_2 \omega(M, t); \\ & M_2 = M(x|y, z); M_6 = M(0|y, z); \quad (10) \\ & M_7 = M(x|y, z); n_2(M, t_j) = n_1(M, t_{j+1}); \\ & n_2(M_6, t) = \bar{n}_6(y, z, t); n_2(M_7, t) = \bar{n}_6(y, z, t). \end{aligned}$$

$$\begin{aligned} & \tilde{n}_3 + \partial / \partial y (\vartheta_y n_3) - \partial / \partial y (\tau_y \partial n_3 / \partial y) = \delta_3 \omega(p, t); \\ & M_3 = M(y|x, z); M_8 = M(0|x, z); M_9 = M(Y|x, z); \quad (11) \\ & n_3(M, t_j) = n_2(M, t_{j+1}); n_3(M_8, t) = \bar{n}_8(x, z, t); \\ & n_3(M_9, t) = \bar{n}_9(x, z, t); \delta_1 + \delta_2 + \delta_3 = 1. \end{aligned}$$

To solve Eq. 7, we assume that  $n(M, t) = n_3(M, t)$ . Then, we fulfill the condition of parameterization: normalization

of parameters and functions, initial and boundary conditions, coefficients of the parameterized system.

To calculate the integrals included in the basic calculation formulas of the iterative-recursive computational method, the values of the subintegral functions corresponding to the initial distribution are required. This leads to the inclusion in the general scheme of algorithms for approximation procedures at a given interval of initial functions. In generalized form, the algorithm takes the record for Eq. 7:

$$\begin{aligned} & \partial \langle n \rangle (\langle x \rangle, \langle t \rangle) / \partial \langle t \rangle + \langle n \rangle (\langle x \rangle, \langle t \rangle) (\eta + \sigma \partial \langle \vartheta \rangle (\langle x \rangle, \langle t \rangle) / \\ & / \partial \langle x \rangle) + \partial \langle n \rangle (\langle x \rangle, \langle t \rangle) / \partial \langle x \rangle \cdot (\sigma \langle \vartheta \rangle (\langle x \rangle, \langle t \rangle) - \\ & - \epsilon \partial \langle \tau \rangle (\langle x \rangle, \langle t \rangle) / \partial \langle x \rangle) - \partial^2 \langle n \rangle (\langle x \rangle, \langle t \rangle) / \partial \langle x \rangle^2 \cdot \\ & \cdot (\epsilon \langle \tau \rangle (\langle x \rangle, \langle t \rangle)) = \zeta \langle \omega \rangle (\langle x \rangle, \langle t \rangle). \end{aligned} \quad (12)$$

We perform normalization of initial and boundary conditions, normalized parameters from [0; 1], and simplify Eq. 12:

$$\dot{n}(\langle x \rangle, \langle t \rangle) + B(\langle x \rangle, \langle t \rangle)n(\langle x \rangle, \langle t \rangle) + C(\langle x \rangle, \langle t \rangle) = 0. \quad (13)$$

Eq. 13 is solved as a homogeneous first order differential equation concerning the parameter  $t$ , for  $x = \text{const}$  [21]. Then

$$\begin{aligned} n(x, t) = & e^{-\int_{t_0}^t (\eta(t') + \sigma(t') \frac{\partial \vartheta(x, t')}{\partial x}) dt'} \cdot \left( n(x, t_0) - \right. \\ & \left. - \int_{t_0}^t \left( f(x, t') - \right. \right. \\ & \left. \left. - \zeta \omega(x, t') e^{\int_{t_0}^{t'} (\eta(t'') + \sigma(t'') \frac{\partial \vartheta(x, t'')}{\partial x}) dt''} \right) dt' \right); \end{aligned} \quad (14)$$

which in turn results in a function:

$$n(x, t) = k(x, t) - \int_{t_0}^t \tilde{\omega}(x, t, t') f(x, t') dt'. \quad (15)$$

Thus, Eq. 15 is a function of the distribution of impurities in the surface layer of the atmosphere based on Eq. 6 of the distribution impurities in a turbulent medium.

### 3.3. Computer simulation

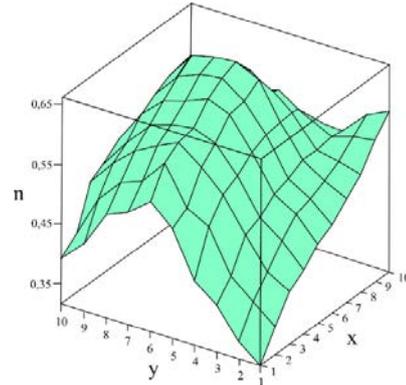
Finding function (Eq. 15) is reduced to numerical simulation. Introduction of the function  $n(x|t)$ , where  $x \in [0; 1]$ , plays the role of a parameter. Then the integral equation for  $n(x|t)$  is an integral Voltaire equation of the second order for each fixed value of  $x$ . Its numerical solution is carried out by the gradual approximations' method.

Since, according to the study, it is possible to consider the input and output variables with a sufficient degree of accuracy, it was rational to construct a regression equation. Based on it, a complete central orthogonal composition plan of the second order was implemented. The input variables were normalized according to the formulas of the sample mean value to further compare the concentrations, velocity, and temperature.

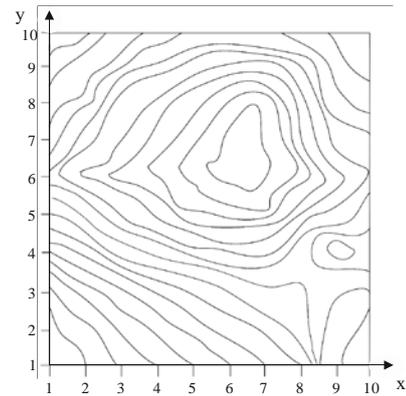
The squares sum of the deviation's experimental values of original variables from the calculated ones were calculated to assess the accuracy of obtained model.

The adequacy of the model was checked by Fisher's test, and the significance of the coefficients of the model was assessed based on the Student's distribution. Then, ensuring the adequacy of the normalized data, the process of scattering the emission concentration near the source was numerically modeled using an iterative-recursive method.

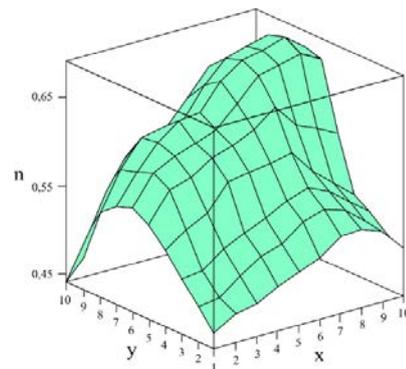
The visual results of numerical simulations in three-dimensional and two-dimensional visualizations in the mathematical environment Mathcad Prime 7 are shown in Fig. 2 – Fig. 7.



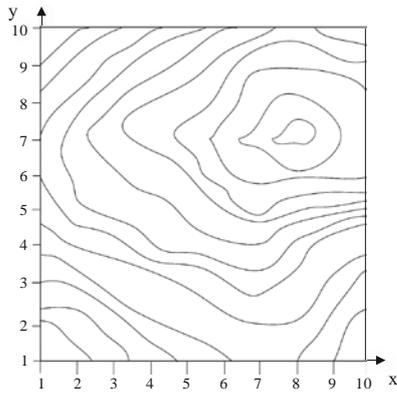
**Fig. 2.** Distribution surface  $n(M, t)$  for  $v = 5$  m/s,  $\tau_{1,0} = 155$  m<sup>2</sup>/s,  $\tau_{2,0} = 55$  m<sup>2</sup>/s;  $\tau_{3,0} = 15$  m<sup>2</sup>/s



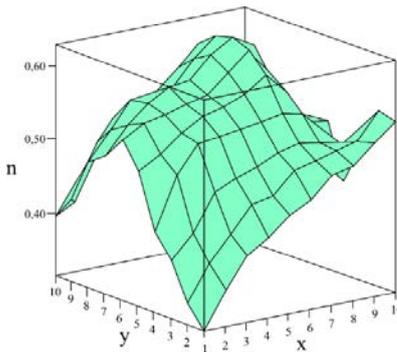
**Fig. 3.** Concentration lines for  $n = 0.5$  kg/m<sup>3</sup> ( $v = 5$  m/s,  $\tau_{1,0} = 155$  m<sup>2</sup>/s,  $\tau_{2,0} = 55$  m<sup>2</sup>/s,  $\tau_{3,0} = 15$  m<sup>2</sup>/s)



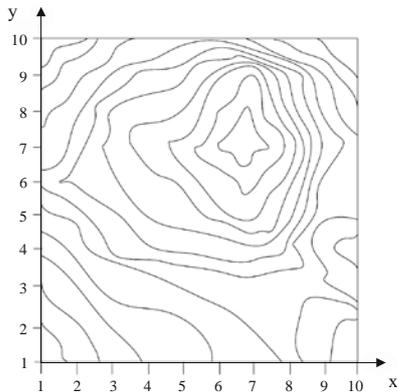
**Fig. 4.** Distribution surface  $n(M, t)$  for  $v = 10$  m/s,  $\tau_{1,0} = 100$  m<sup>2</sup>/s,  $\tau_{2,0} = 100$  m<sup>2</sup>/s,  $\tau_{3,0} = 10$  m<sup>2</sup>/s



**Fig. 5.** Concentration lines for  $n = 0.5 \text{ kg/m}^3$  ( $v = 10 \text{ m/s}$ ,  $\tau_{1,0} = 100 \text{ m}^2/\text{s}$ ,  $\tau_{2,0} = 100 \text{ m}^2/\text{s}$ ,  $\tau_{3,0} = 10 \text{ m}^2/\text{s}$ )



**Fig. 6.** Distribution surface  $n(M, t)$  for  $v = 7.5 \text{ m/s}$ ,  $\tau_{1,0} = 65 \text{ m}^2/\text{s}$ ,  $\tau_{2,0} = 65 \text{ m}^2/\text{s}$ ,  $\tau_{3,0} = 10 \text{ m}^2/\text{s}$



**Fig. 7.** Concentration lines for  $n = 0.5 \text{ kg/m}^3$  ( $v = 7.5 \text{ m/s}$ ,  $\tau_{1,0} = 65 \text{ m}^2/\text{s}$ ,  $\tau_{2,0} = 65 \text{ m}^2/\text{s}$ ,  $\tau_{3,0} = 10 \text{ m}^2/\text{s}$ )

The indicators of the equations system of distribution substances in a turbulent atmosphere are different at different seasons, so the simulation results shown in Fig. 2–Fig. 7 meet different conditions depending on the season.

For each source of emissions, the value of the dangerous wind speed zone is different. The larger the volume of gases coming out of the pipe, the more wind force is required to press the smoke plume. Gradual increase of wind speed over dangerous (5 m/s and more) in combination with change of turbulence (unstable stratification) of air and constant conditions of parameters of sources of pollutants emissions allows to receive the following results:

– At a wind speed of 5 m/s (the smallest value of the dangerous wind speed based on the conditions of the problem) and values of turbulence surface layer of air

15–155 m<sup>2</sup>/s (Fig. 2, Fig. 3), impurities concentration  $n$  (graph surface) at a distance of 5 km varies in the range of 0.3–0.57 concentration from the emission source;

– At a wind speed of 10 m/s (the highest value of the dangerous wind speed) and values of turbulence surface layer of air 10–100 m<sup>2</sup>/s (Fig. 4, Fig 5), impurities concentration  $n$  at a distance of 5 km varies in the range of 0.4–0.57 concentration from the emission source. This combination of conditions gives the most harmful result for the environment from the dispersion of finely dispersed pollutant.

– At a wind speed of 7.5 m/s (as the average value of dangerous wind speed) and values of turbulence surface layer of air 10–65 m<sup>2</sup>/s (Fig. 6, Fig. 7), impurities concentration  $n$  at a distance of 5 km varies in the range of 0.3–0.54 concentration from the emission source.

Surface oscillations are caused by turbulent diffusion and wind speed. Fig. 2–Fig. 7 allow us to speak of a significant dispersion distance of fine particles from the source of emissions, considering different initial parameters of emission sources and conditions of impurity distribution.

The software algorithm for calculating the distribution of fine pollutants model requires modern computer software available to most users. The calculation takes 30–40 minutes for each new initial condition, which is an advantage of the proposed model. The model has a wide range of input data for wind speed and atmospheric turbulence, within which the results are adequate.

The adequacy of the results was checked at a real object of the chemical industry – PJSC «SUMYKHIMPROM» (coordinates 50.88632, 34.87668), which has similar initial conditions of the mathematical model, fine dust TiO<sub>2</sub> has a size of  $0.305 \cdot 10^{-6} \text{ m}$ . Full-scale measurements allowed to set the content of TiO<sub>2</sub> dust in the air at a distance of 4 km (subject to the wind conditions 5 m/s) from the emission source at 26–32 % of the initial emission concentration.

All this allowed obtaining an integrated equation of distribution of pollutants for any stationary source. The accepted mathematical model can be used in forecasting man-caused load on the environment for the prompt solution of environmental problems.

#### 4. CONCLUSIONS

1. In the comparative analysis, the main advantages and disadvantages of existing mathematical models with a numerical algorithm and software for predicting the distribution of pollutants in the atmosphere are identified. The necessary initial parameters for constructing reliable models are established: air temperature, wind speed and direction, air turbulence, and parameters of pollutant emissions and sources of their emissions.
2. As a result of modeling, the simplified analytical decision is received, and the algorithm of numerous modeling of the distribution of fine pollutants in a ground layer is constructed. The algorithm of numerical modeling is developed using the method of coordinate splitting of the equation of impurities distribution in a turbulent environment with the subsequent normalization and parameterization of conditions. Finding subintegral functions in the calculation

algorithm allows obtaining a stable computational algorithm of the proposed model to distribute fine suspended particles.

- An integral equation for the distribution of pollutants is obtained, which can find practical application in predicting and modeling the diffusion of impurities from emission sources.
- The authors have got a simplified numerical model of the fine pollutants' distribution into the air which is based on the three-dimensional equation of distribution of impurities in a turbulent environment considering the parameters of emission sources, wind strength and direction, the turbulence of air masses. The constructed model of scattering of fine suspended solids showed that the maximum concentration of pollutants is observed at a distance of 4 km from the source of pollution. It was obtained the distribution of impurity concentrations for different values of atmospheric air turbulence ( $10 - 155 \text{ m}^2/\text{s}$ ) and dangerous wind speed ( $5 - 10 \text{ m/s}$ ). The analysis of the visualization of the calculations shows the effectiveness of the adopted model at pollution distances of 5 km, considering the different initial parameters of emission sources and conditions of impurity distribution. The resulting model has a wide range of input data for wind speed and atmospheric turbulence. The simulation results are adequate and can be used to solve environmental problems quickly.

### Acknowledgments

The research project was carried out as planned research projects of the Department of Applied Ecology, Sumy State University, connected with subjects "Reduction of technogenic loading on the environment of enterprises of chemical, machine-building industry and heat and power engineering" according to the scientific and technical program of the Ministry of Education and Science of Ukraine (state registration No 0116U006606).

### REFERENCES

- The Organisation for Economic Co-operation and Development (OECD).** Statistic base 2021. Accessed on October 20, 2021. <https://stats.oecd.org/Index.aspx?DataSetCode=CPL>.
- State Statistics Service of Ukraine.** Vykydy zabrudnyuyuchykh rehovyn i parnykovykh haziv u atmosferne povitrya vid stacionarnykh dzherel zabrudnennya za 2004–2020 roky *Statystychni dani 2020*. Accessed on October 12, 2021. (In Ukrainian) [http://www.ukrstat.gov.ua/operativ/operativ2018/ns/vzap/arc\\_h\\_vzrap\\_u.htm](http://www.ukrstat.gov.ua/operativ/operativ2018/ns/vzap/arc_h_vzrap_u.htm).
- Daisuke, G., Kayo, U., Chris, F. S., Akinori, T., Toshinori, A., Keisuke, M., Teruyuki, N.** Estimation of Excess Mortality Due to Long-Term Exposure to PM<sub>2.5</sub> in Japan Using A High-Resolution Model for Present and Future Scenarios *Atmospheric Environment* 140 2016: pp. 320–332. <https://doi.org/10.1016/j.atmosenv.2016.06.015>
- Yang, T., Gbaguidi, A., Zhang, W., Wang, X., Wang, Z., Yan, P.** Model-Integration of Anthropogenic Heat for Improving Air Quality Forecasts over the Beijing Megacity *Aerosol Air Quality Research* 18 2018: pp. 790–802. <https://doi.org/10.4209/aaqr.2017.04.0155>
- Ravshanov, N., Tashtemirova, N.** Advanced Model of Transfer Process and Diffusion of Harmful Substances in the Atmospheric Boundary Layer *Theoretical & Applied Science* 46 2017: pp. 129–138. <https://doi.org/10.15863/TAS.2017.02.46.24>
- Shvarts, K. G., Shklyayev, V. A.** Chislennoye Modelirovaniye Atmosferykh Mezomasshtabnykh Protsesov Perenosa Mnogokomponentnoy Primesi Pri Torfyanom Pozhare *Vychislitel'naya Mekhanika Sploshnykh Sred* 5 (3) 2012: pp. 274–283. (In Russian)
- Ayodeji, A., Paul, A. M., Junhua, Z., Darlington, A., Shao-Meng, L., Gordon, M., Michael D. M., Qiong, Z.** A Chemical Transport Model Study of Plume-Rise and Particle Size Distribution for the Athabasca Oil Sands *Atmosphere Chemistry and Physics* 18 2018: pp. 8667–8688. <https://doi.org/10.5194/acp-18-8667-2018>
- Daniel, L., Alexander, G., Mathias, W. R.** Quantifying Horizontal and Vertical Tracer Mass Fluxes in an Idealized Valley During Daytime *Atmosphere Chemistry and Physics* 16 2016: pp. 13049–13066. <https://doi.org/10.5194/acp-16-13049-2016>
- Cathy, W. Y., Guy, P. B., Hauke, S., Juan, P. M.** Error Induced by Neglecting Subgrid Chemical Segregation Due to Inefficient Turbulent Mixing in Regional Chemical-Transport Models in Urban Environments *Atmosphere Chemistry and Physics* 21 2021: pp. 483–503. <https://doi.org/10.5194/acp-21-483-2021>
- Zhylenko, T., Koziy, I., Bozhenko, V., Shuda, I.** Using a Web Application to Realize the Effect of AR in Assessing the Environmental Impact of Emissions Source *CEUR Workshop Proceedings* 2731 2020: pp. 193–204. <http://ceur-ws.org/Vol-2731/paper10.pdf>
- Ramli, H. M., Esler, J. G.** Quantitative Evaluation of Numerical Integration Schemes for Lagrangian Particle Dispersion Models *Geoscientific Model Development* 9 (7) 2016: pp. 2441–2457. <https://doi.org/10.5194/gmd-9-2441-2016>
- Bellasio, R., Bianconi, R., Mosca, S., Zannetti, P.** Incorporation of Numerical Plume Rise Algorithms in the Lagrangian Particle Model LAPMOD and Validation against the Indianapolis and Kincaid Datasets *Atmosphere* 9 (10) 2018: p. 404. <https://doi.org/10.3390/atmos9100404>
- Ferrero, E., Maccarini, F.** Concentration Fluctuations of Single Particle Stochastic Lagrangian Model Assessment with Experimental Field Data *Atmosphere* 12 (5) 2021: p. 589. <https://doi.org/10.3390/atmos12050589>
- Zhu, J., Wang, H., Li, J., Xu, Z.** Research and Optimization of Meteo-Particle Model for Wind Retrieval *Atmosphere* 12 (9) 2021: p. 1114. <https://doi.org/10.3390/atmos12091114>
- Stohl, A.** Computation, Accuracy and Applications of Trajectories – A Review and Bibliography *Atmosphere Environment* 32 (6) 1998: pp. 947–966. [https://doi.org/10.1016/S1352-2310\(97\)00457-3](https://doi.org/10.1016/S1352-2310(97)00457-3)
- Schwetlick, H., Zimmer, J.** The Computation of Long Time Hamiltonian Trajectories for Molecular Systems via Global Geodesics *Numerical Mathematics and Advanced Applications* 2011 2012: pp. 227–234. [https://doi.org/10.1007/978-3-642-33134-3\\_25](https://doi.org/10.1007/978-3-642-33134-3_25)
- Khorsand, Z.** Particle Trajectories in the Serre Equations *Applied Mathematics and Computation* 230 2014: pp. 35–42. <https://doi.org/10.1016/j.amc.2013.12.018>

18. **Anderson, R. S.** Particle Trajectories on Hillslopes: Implications for Particle Age and  $^{10}\text{Be}$  Structure *Journal of Geophysical Research: Earth Surface* 120 (9) 2015: pp. 1626–1644.  
<https://doi.org/10.1002/2015jf003479>
19. **Antonova, A. M., Vorobev, A. V., Vorobev, V. A., Dutova, Ye. M., Pokrovskiy, V. D.** Modelling Distribution of Contaminating Substances of Electric Power Emissions in the Atmosphere on the Basis of the Skat Programming Complex *Bulletin of the Tomsk Polytechnic University. Geo Assets Engineering* 330 (6) 2019: pp. 174–186.
20. **Naats, V. I., Naats, I. E., Ryskalenko, R. A., Yartseva, Ye. P.** Matematicheskiye Modeli i Vychislitelnyy Eksperiment v Probleme Kontrolya i Prognoza Ekologicheskogo Sostoyaniya Atmosfery *Monografiya, Stavropol: SKFU* 2016: 376 p. (In Russian)
21. **Viorel, B.** Differential Equations *Springer International Publishing* 2016: p. 224  
<https://doi.org/10.1007/978-3-319-45261-6>.



© Kozii et al. 2022 Open Access This article is distributed under the terms of the Creative Commons Attribution 4.0 International License (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made.