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NUMERICAL MODELING OF TURBULENT TRANSPORT OF IMPURITIES IN A SPATIALLY INHOMOGENEOUS ATMOSPHERIC ENVIRONMENT

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This study presents a mathematical model for turbulent pollutant dispersion in urban airflows based on the Navier-Stokes equations and the $k-\omega$ turbulence model. The model incorporates meteorological parameters, emission sources, and urban structures. A finite difference numerical method is used to solve the equations. Computational experiments demonstrate pollutant concentration patterns in urban environments. The results indicate that wind turbulence and building geometry significantly influence dispersion. The model can aid in urban planning and environmental safety. Simulation findings highlight the importance of wind circulation in reducing pollution. The study provides practical recommendations for optimizing urban design.

Keywords: turbulent diffusion, Navier-Stokes equations, $k-\omega$ turbulence model, pollutant dispersion, urban airflows, numerical modeling, finite difference method, environmental safety.

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1 Introduction

With the development of world industry and urbanization, the amount of harmful substances released into the atmosphere is increasing. The dispersion of these substances in the air poses a serious threat to human health and the ecological environment. Especially in cities, in spatially inhomogeneous conditions, the dispersion of mixtures becomes more complicated in air flows between buildings and structures, in conditions of complex geometry and turbulence. Therefore, accurate prediction and monitoring of the dispersion of substances in such environments is of urgent scientific and practical importance. Mathematical modeling of the properties of the atmospheric surface layer and the migration processes of mixtures creates the opportunity to study and predict these processes. One of the main directions in this is the development of mathematical models based on numerical methods and their implementation in software tools.

The most widely used models for mathematical modeling of the transport processes of mixtures in the ground-air environment of the atmosphere are the Navier-Stokes equations.

The Navier-Stokes equations, as the fundamental mathematical model of fluid dynamics, have been refined through various approaches in the scientific community throughout their history. The chronological and evolutionary sequence associated with these equations is outlined below.

One of the scientists who theoretically substantiated the issue was GKBatchelor, in his work “ An Introduction to Fluid Dynamics” [1], who explained the theoretical foundations of fluid dynamics and commented on the physical nature of the Navier-Stokes equations.

ANKolmogorov In the work "The Local Structure of Turbulence in Incompressible Viscous Fluid for Very Large Reynolds Numbers" [2], turbulent flows statistic features and spectral theory presented reached J. Smagorinsky in his "General Circulation Experiments with the Primitive Equations" [3], subgrid scaled models for main principles working came out.

Turbulence models and calculation from methods using Launder and Spalding 1974 – The Numerical Computation of Turbulent Flows [4] – developed the k–ε model and provided a basic approach for calculating turbulent flows. Spalart and Allmaras 1992 – A One-Equation Turbulence Model for Aerodynamic Flows [5] - are famous for developing a one-equation turbulence model for modeling aerodynamic flows. Wilcox 2006 – Turbulence Modeling for CFD [6] - improved the method for determining turbulent kinetic energy and dissipation rate through the k-ω model.

Discretization and computational approaches in Ferziger and Peric 2002 – Computational Methods for Fluid Dynamics [7] – covered the application of finite difference and finite volume methods to the calculation of fluid flows. Patankar 1980 – Numerical Heat Transfer and Fluid Flow [8] - presented innovative methods for the calculation of advective-diffusion processes. Versteeg and Malalasekera 1995 – An Introduction to Computational Fluid Dynamics: The Finite Volume Method [9] - covered in depth the principles of the finite volume method and its application to flow problems.

Advanced modeling approaches were developed by Menter 1994 – Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications [10] – who developed the SST model, which is a combination of the K–ω and K–ε models, and made it possible to calculate turbulent flows with high accuracy. Pope 2000 – Turbulent Flows [11] - carried out fundamental research on statistical models of turbulent flows. Davidson 2004 – Turbulence: An Introduction for Scientists and Engineers [12] - covered the modeling of turbulent flows through approaches such as DNS and LES.

Simulation platforms and industrial research Moukalled et al. 2016 - The Finite Volume Method in Computational Fluid Dynamics [13] - developed algorithms for practical calculations on OpenFOAM and MATLAB platforms. Schlichting and Gersten 2016 - Boundary-Layer Theory [14] - presented mathematical models of boundary layer theory. Sharipov et al. 2019 – Numerical Modeling Method for Short-Term Air Quality Forecast in Industrial Regions [15] – developed modeling algorithms for short-term air quality forecasting using MATLAB.

Artificial intelligence and statistical modeling Duraisamy et al. 2019 – Turbulence Modeling in the Age of Data [16] – presented developments aimed at improving the stability of RANS models using artificial intelligence. Bae and Moin 2018 – Turbulence Spectra in Wall-Bounded Flows: Scaling Laws and Universality [17] – used DNS to characterize the characteristics of turbulent flows near walls learned.

High to accuracy aimed at in improvements Agresti and Veraar 2024 - Stochastic Navier–Stokes Equations for Turbulent Flows in Critical Spaces [18] - presented a statistical analysis of turbulent flows through the stochastic Navier–Stokes equations. Brun and Bertoglio 2008 - Subgrid-Scale Models for Large-Eddy Simulations Based on Energy Spectrum Considerations [19] – aims to improve LES accuracy through subgrid-scale models. Durbin 2021 - Modern Developments in Turbulence Modeling [20] – Methods for increasing accuracy using new algorithms combining RANS and LES models. Taira et al. 2017 - Modal Analysis of Fluid Flows [21] – modeling flow structural changes and predicting complex flows through modal analysis. Ishihara, Gotoh and Kaneda 2009 - Study of High-Reynolds Number Isotropic Turbulence [22] – New perspectives on the turbulent energy spectrum for high Reynolds numbers using DNS research.

2 Problem Statement

Spatially heterogeneous The mathematical model of the process of diffusion of matter in a turbulent flow of atmospheric air with complex geometry is described by the following differential equations:

The advection-diffusion equation is used to determine the spatiotemporal distribution of the concentration of a pollutant. Advection is the transport of matter or energy by a flow, that is, the process of moving matter or heat along with the liquid or gas itself. Diffusion is the process of spreading matter or heat from a high concentration to a low concentration due to the movement of molecules, or the mixing of a liquid or gas due to flow turbulence. These two processes play an important role in understanding how matter or heat moves within a liquid or gas and are used in many practical processes.

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=$$
$$=\frac{\partial}{\partial x}((\nu+\nu_t)\frac{\partial C}{\partial x})+\frac{\partial}{\partial y}((\nu+\nu_t)\frac{\partial C}{\partial y})+$$
$$+\frac{\partial}{\partial z}((\nu+\nu_t)\frac{\partial C}{\partial z})+S_C.$$

The equation above is one of the modern turbulent models for calculating wind speeds and turbulent diffusion coefficients. $k-\omega$ and Navier – Stokes from the equations we use.

Conservation of mass states that no mass is created or lost in a flow of a liquid or gas. If the flow is incompressible, that is, the density of the liquid or gas does not change over time, then the continuity equation states that at any point in the flow the sum of the velocities of the fluid flowing in different directions must be zero. This ensures that no mass is created or lost in the liquid or gas:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0.$$

The Navier–Stokes momentum equations are written as velocity projections onto the corresponding axes of a rectangular Cartesian coordinate system. These equations relate all forces acting on the fluid, including pressure gradients, shear forces, and external forces. The equations of motion for incompressible flow are introduced in the directions x, y and z. Each equation describes the time-dependent variation of the velocity component of the fluid in the corresponding direction, taking into account convection and diffusion processes, pressure gradients, and shear stresses:

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}=-\frac{1}{\rho}\frac{\partial P}{\partial x}+$$
$$+\frac{\partial}{\partial x}((\nu+\nu_t)\frac{\partial u}{\partial x})+\frac{\partial}{\partial y}((\nu+\nu_t)\frac{\partial u}{\partial y})+$$
$$+\frac{\partial}{\partial z}((\nu+\nu_t)\frac{\partial u}{\partial z})+F_u;$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}=$$
$$=-\frac{1}{\rho}\frac{\partial P}{\partial y}+\frac{\partial}{\partial x}((\nu+\nu_t)\frac{\partial v}{\partial x})+$$
$$+\frac{\partial}{\partial y}((\nu+\nu_t)\frac{\partial v}{\partial y})+\frac{\partial}{\partial z}((\nu+\nu_t)\frac{\partial v}{\partial z})+F_v;$$
$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}=$$
$$=-\frac{1}{\rho}\frac{\partial P}{\partial z}+\frac{\partial}{\partial x}((\nu+\nu_t)\frac{\partial w}{\partial x})+$$
$$+\frac{\partial}{\partial y}((\nu+\nu_t)\frac{\partial w}{\partial y})+\frac{\partial}{\partial z}((\nu+\nu_t)\frac{\partial w}{\partial z})+F_w.$$

To ensure that the flow is incompressible, the pressure distribution auxiliary equation, using the pressure correlation equation, is used in fluid dynamics, specifically the Navier-Stokes equations, to find the pressure distribution. While the Navier-Stokes equations determine the flow velocity, the pressure correlation equation allows us to find how the pressure is distributed over the entire area.

Once the temporal velocity fields are found, we write the pressure correlation equation.

To ensure that the flow complies with the incompressibility condition, the auxiliary equation for the Poisson pressure distribution is:

$$\frac{\partial^2 P}{\partial x^2}+\frac{\partial^2 P}{\partial y^2}+\frac{\partial^2 P}{\partial z^2}=$$
$$=-\rho\left(\frac{\partial u}{\partial x}\frac{\partial u}{\partial x}+2\frac{\partial u}{\partial y}\frac{\partial v}{\partial x}+\frac{\partial v}{\partial y}\frac{\partial v}{\partial y}+2\frac{\partial u}{\partial z}\frac{\partial w}{\partial x}+2\frac{\partial v}{\partial z}\frac{\partial w}{\partial y}+\frac{\partial w}{\partial z}\frac{\partial w}{\partial z}\right).$$

The turbulent kinetic energy (TKE) equation describes the change in kinetic energy in turbulent flow. In turbulent flows, kinetic energy is in the form of small vortices or eddies. The TKE equation describes how the energy of these eddies is produced, diffused, and dissipated (lost). This equation plays an important role in understanding how energy is distributed in turbulent flows and is used to calculate turbulent viscosity:

$$\frac{\partial k}{\partial t}+u\frac{\partial k}{\partial x}+v\frac{\partial k}{\partial y}+w\frac{\partial k}{\partial z}=\frac{\partial}{\partial x}\left(\left(\nu+\frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial x}\right)+$$
$$+\frac{\partial}{\partial y}\left(\left(\nu+\frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial y}\right)+\frac{\partial}{\partial z}\left(\left(\nu+\frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial z}\right)+P_k-\beta^*k\omega.$$

The turbulent kinetic energy dissipation rate equation describes the dissipation, or loss, of turbulent kinetic energy. The energy frequency changes from large eddies to small eddies, and in the process of decay, it is converted into another type of energy. This equation describes how the dissipation is separated from turbulent kinetic energy and how it is converted into heat on a small scale. The frequency equation is important in the model of turbulent flows, helping to accurately describe the loss of turbulent energy:

$$\frac{\partial \omega}{\partial t}+u\frac{\partial \omega}{\partial x}+v\frac{\partial \omega}{\partial y}+w\frac{\partial \omega}{\partial z}=$$
$$=\frac{\partial}{\partial x}\left(\left(\nu+\frac{\nu_t}{\sigma_\omega}\right)\frac{\partial \omega}{\partial x}\right)+\frac{\partial}{\partial y}\left(\left(\nu+\frac{\nu_t}{\sigma_\omega}\right)\frac{\partial \omega}{\partial y}\right)+\frac{\partial}{\partial z}\left(\left(\nu+\frac{\nu_t}{\sigma_\omega}\right)\frac{\partial \omega}{\partial z}\right)+$$
$$+\alpha\frac{\omega}{k}P_k-\beta\omega^2.$$

Usually kinematic viscosity, turbulent viscosity, resultant viscosity

$$\nu = \frac{\mu}{\rho};$$

$$\nu_t = \frac{k}{\omega}.$$

The formulas for determining turbulent kinetic energy and its frequency using pressure are as follows:

$$P_k = \nu_t\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 + \nu_t\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2 + \nu_t\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)^2.$$

The above formula means that the pressure gradients are calculated from the projections of the velocities.

The explanation of the variables and constants involved in the above system of equations, as well as their units of measurement and their space, are given in Table 1 below:

Table 1.

*	Explanation	Unity	Space
u	The velocity component of the flow in the x direction	m/s	$R^3 \to R$
v	Velocity component of the flow in the y direction	m/s	$R^3 \to R$
w	Velocity component of the flow in the z direction	m/s	$R^3 \to R$
ρ	Current density	kg/m^3	$R^3 \to R^+$
p	Pressure in a liquid or gas	Pa	$R^3 \to R$
ν	Represents internal friction (resistance)	m^2/s	R^+
ν_t	Kinematic viscosity in turbulent flow (turbulent viscosity)	m^2/s	$R^3 \to R^+$
ν_e	Effective viscosity	m^2/s	$R^3 \to R^+$
ω	Frequency of turbulent kinetic energy	m^2/s^3	$R^3 \to R^+$
k	Turbulent kinetic energy	m^2/s^2	$R^3 \to R^+$
C	Concentration of the substance being dispersed	kg/m^3	$R^3 \to R^+$
P_k	Turbulent kinetic energy generation	m^2/s^3	$R^3 \to R^+$
$C_{1\varepsilon}, C_{2\varepsilon}, C_\mu$	Empirical constants	-	R
$\sigma_k, \sigma_{\varepsilon_t}$	Diffusion coefficients of turbulent energy and frequency	-	R^+
α, β, β^*	Empirical coefficients	-	R^+
F_u, F_v, F_w	External influences on velocity fields	m/s^2	$R^3 \to R$

$R^3 \to R$ – three dimensional in space function real number value represents.
$R^3 \to R^+$ – three dimensional in space function positive real number value represents.
R^+ – positive real numbers space (parameters for permanent or functional values).
R – real numbers space (constant values).

3 Solution Algorithm

Above equations numerical research to do for every one in the equation unknown functions following to look has:

$$\Omega_{xyzt} = \left\{ \left(x_i = i\Delta x, y_j = j\Delta y, z_k = k\Delta z, t_n = \sum_{f=0}^{n} \Delta t_f \right); \right.$$
$$i = \overline{1, N_x}; j = \overline{1, N_y}; k = \overline{1, N_z}; n = \overline{0, N_t};$$
$$\left. \Delta t_f = min \begin{pmatrix} \frac{\Delta x}{max(u_f)}, \frac{\Delta y}{max(v_f)}, \frac{\Delta z}{max(w_f)}, \frac{\Delta x^2}{2(\nu + max(\nu_{tf}))}, \\ \frac{\Delta y^2}{2(\nu + max(\nu_{tf}))}, \frac{\Delta z^2}{2(\nu + max(\nu_{tf}))} \end{pmatrix} \right\}.$$

The network was considered to be defined in the field.

The initial conditions for the given equations are given below.

$$x \in \Omega^x_{x,y,z,t}, y \in \Omega^y_{x,y,z,t}, z \in \Omega^z_{x,y,z,t}, t = 0, u(x,y,z,t) = u_0,$$
$$v(x,y,z,t) = v_0, w(x,y,z,t) = w_0, k(x,y,z,t) = k_0,$$
$$\varepsilon(x,y,z,t) = \varepsilon_0, C(x,y,z,t) = C_0, p(x,y,z,t) = p_0.$$

The boundary conditions for the given equations are given below.

Initially, the function to determine whether the function is increasing or decreasing at the boundary points, that is, whether the flow is inward or outward relative to the coordinate direction, is given as follows.

$$B \in \left\{ \begin{array}{l} u, v, \\ w, u', \\ v', w', \\ k, \omega, \\ C, p', \\ P, P_k, \\ \nu_t \end{array} \right\},$$

$$Ch(x,y,z,t,B) = \begin{cases} -1, (x = 0) \wedge (B(x + 2\Delta x, y, z, t) - B(x + \Delta x, y, z, t) < 0); \\ -2, (x = L_x) \wedge (B(x - 2\Delta x, y, z, t) - B(x - \Delta x, y, z, t) < 0); \\ -3, (y = 0) \wedge (B(x, y + 2\Delta y, z, t) - B(x, y + \Delta y, z, t) < 0); \\ -4, (y = L_y) \wedge (B(x, y - 2\Delta y, z, t) - B(x, y - \Delta y, z, t) < 0); \\ -5, (z = 0) \wedge (B(x, y, z + 2\Delta z, t) - B(x, y, z + \Delta z, t) < 0); \\ -6, (z = L_z) \wedge (B(x, y, z - 2\Delta z, t) - B(x, y, z - \Delta z, t) < 0); \\ 1, (x = 0) \wedge (B(x + 2\Delta x, y, z, t) - B(x + \Delta x, y, z, t) > 0); \\ 2, (x = L_x) \wedge (B(x - 2\Delta x, y, z, t) - B(x - \Delta x, y, z, t) > 0); \\ 3, (y = 0) \wedge (B(x, y + 2\Delta y, z, t) - B(x, y + \Delta y, z, t) > 0); \\ 4, (y = L_y) \wedge (B(x, y - 2\Delta y, z, t) - B(x, y - \Delta y, z, t) > 0); \\ 5, (z = 0) \wedge (B(x, y, z + 2\Delta z, t) - B(x, y, z + \Delta z, t) > 0); \\ 6, (z = L_z) \wedge (B(x, y, z - 2\Delta z, t) - B(x, y, z - \Delta z, t) > 0); \\ 0, \text{aks holda.} \end{cases}$$

Functions borderline at the points values calculation for following from the function is used.

$$G_1(x,y,z,t,B) = \begin{cases} B_{inx}(x,y,z,t), Ch(x,y,z,t,B)=1; \\ B\left(x-\Delta x,y,z,t\right)+\left(B\left(x-\Delta x,y,z,t\right)-B\left(x-2\Delta x,y,z,t\right)\right), \\ Ch(x,y,z,t,B)=2; \\ B_{iny}(x,y,z,t), \mathrm{Ch(x,y,z,t,B)}=3; \\ B\left(x,y-\Delta \mathrm{y},z,t\right)+\left(B\left(x,y-\Delta \mathrm{y},z,t\right)-B\left(x,y-2\Delta \mathrm{y},z,t\right)\right), \\ Ch(x,y,z,t,B)=4; \\ -B\left(x,y,z+\Delta \mathrm{z},t\right)+\left(B\left(x,y,z+\Delta \mathrm{z},t\right)-B\left(x,y,z+2\Delta \mathrm{z},t\right)\right), \\ Ch(x,y,z,t,B)=5; \\ B\left(x,y,z-\Delta \mathrm{z},t\right)+\left(B\left(x,y,z-\Delta \mathrm{z},t\right)-B\left(x,y,z-2\Delta \mathrm{z},t\right)\right), \\ Ch(x,y,z,t,B)=6; \\ B\left(x-\Delta x,y,z,t\right)+ \\ +\left(B\left(x-\Delta x,y,z,t\right)-B\left(x-2\Delta x,y,z-2\Delta \mathrm{z},t\right)\right), \\ Ch(x,y,z,t,B)=-1; \\ B_{inx}(x,y,z,t), Ch(x,y,z,t,B)=-2; \\ B\left(x,y-\Delta y,z,t\right)+ \\ +\left(B\left(x,y-\Delta y,z,t\right)-B\left(x,y-2\Delta y,z-2\Delta \mathrm{z},t\right)\right), \\ Ch(x,y,z,t,B)=-3; \\ B_{iny}(x,y,z,t), Ch(x,y,z,t,B)=-4; \\ -B\left(x,y,z+\Delta \mathrm{z},t\right)+\left(B\left(x,y,z+\Delta \mathrm{z},t\right)-B\left(x,y,z+2\Delta \mathrm{z},t\right)\right), \\ Ch(x,y,z,t,B)=-5; \\ B_{iny}(x,y,z,t), Ch(x,y,z,t,B)=-6; \\ B(x,y,z,t), Ch(x,y,z,t,B)=0. \end{cases}$$

Due to the location of objects in the domain and the complexity of the domain, incoming flows enter the domain based on certain relationships. The functions listed below are used to determine the values of the incoming flow at the boundary points.

$$k_{inx} = \frac{3}{2}(Iu_{in})^2,\ k_{iny} = \frac{3}{2}(Iv_{in})^2,\ k_{inz} = \frac{3}{2}(Iw_{in})^2,\ I = \frac{\sqrt{\frac{2}{3}k}}{U}\cdot 100\%.$$
$$\omega_{inx} = \frac{\sqrt{k_{inx}}}{l},\ \omega_{iny} = \frac{\sqrt{k_{iny}}}{l},\ \omega_{inz} = \frac{\sqrt{k_{inz}}}{l},\ l \approx 0.07L_z$$
$$u = Ucos(j)cos(q),\ v = Usin(j)cos(q),\ w = Usin(q),$$
$$u_{inx} = Ucos(j)cos(q),\ v_{iny} = Usin(j)cos(q),\ w_{inz} = Usin(q),$$
$$C_{inx} = C_{kiruvchi\_x},\ C_{iny} = C_{kiruvchi\_y},\ C_{inz} = C_{kiruvchi\_z},$$

$C_{kiruvchi\_x}, C_{kiruvchi\_y}, C_{kiruvchi\_y}$ – incoming concentration with flow

U – of the wind consequential speed, φ – azimuth angle, θ – zenith angle.

In the process of solving the system of equations, since P, P_k, ν_ts are functions listed below are used to determine the values of the incoming flow at the boundary points.

$$G_2(Dx,x,Dy,y,Dz,z,t,B)=$$
$$=\begin{cases} B\left(x+Dx,y,z,t\right)+\left(B\left(x+Dx,y,z,t\right)-B\left(x+2Dx,y,z,t\right)\right), \\ Ch(x,y,z,t,B)=1; \\ B\left(x-Dx,y,z,t\right)+\left(B\left(x-Dx,y,z,t\right)-B\left(x-2Dx,y,z,t\right)\right), \\ Ch(x,y,z,t,B)=2; \\ B\left(x,y+Dy,z,t\right)+\left(B\left(x,y+Dy,z,t\right)-B\left(x,y+2Dy,z,t\right)\right), \\ Ch(x,y,z,t,B)=3; \\ B\left(x,y-Dy,z,t\right)+\left(B\left(x,y-Dy,z,t\right)-B\left(x,y-2Dy,z,t\right)\right), \\ Ch(x,y,z,t,B)=4; \\ -B\left(x,y,z+Dz,t\right)+\left(B\left(x,y,z+Dz,t\right)-B\left(x,y,z+2Dz,t\right)\right), \\ Ch(x,y,z,t,B)=5; \\ B\left(x,y,z-Dz,t\right)+\left(B\left(x,y,z-Dz,t\right)-B\left(x,y,z-2Dz,t\right)\right), \\ Ch(x,y,z,t,B)=6; \\ B\left(x+Dx,y,z,t\right)+\left(B\left(x+Dx,y,z,t\right)-B\left(x+2Dx,y,z,t\right)\right), \\ Ch(x,y,z,t,B)=-1; \\ B\left(x-Dx,y,z,t\right)+\left(B\left(x-Dx,y,z,t\right)-B\left(x-2Dx,y,z,t\right)\right), \\ Ch(x,y,z,t,B)=-2; \\ B\left(x,y+Dy,z,t\right)+\left(B\left(x,y+Dy,z,t\right)-B\left(x,y+2Dy,z,t\right)\right), \\ Ch(x,y,z,t,B)=-3; \\ B\left(x,y-Dy,z,t\right)+\left(B\left(x,y-Dy,z,t\right)-B\left(x,y-2Dy,z,t\right)\right), \\ Ch(x,y,z,t,B)=-4; \\ -B\left(x,y,z+Dz,t\right)+\left(B\left(x,y,z+Dz,t\right)-B\left(x,y,z+2Dz,t\right)\right), \\ Ch(x,y,z,t,B)=-5; \\ B\left(x,y,z-Dz,t\right)+\left(B\left(x,y,z-Dz,t\right)-B\left(x,y,z-2Dz,t\right)\right), \\ Ch(x,y,z,t,B)=-6; \\ B(x,y,z,t), Ch(x,y,z,t,B)=0. \end{cases}$$

Every one function for border at the points values to give, the following to look has:

$$\begin{gathered} u(x,y,z,t)=G_1(x,y,z,t,u), v(x,y,z,t)=G_1(x,y,z,t,v), \\ w(x,y,z,t)=G_1(x,y,z,t,w), u'(x,y,z,t)=G_1(x,y,z,t,u'), \\ v'(x,y,z,t)=G_1(x,y,z,t,v'), w'(x,y,z,t)=G_1(x,y,z,t,w'), \\ p'(x,y,z,t)=G_2(x,y,z,t,p'), P(x,y,z,t)=G_2(x,y,z,t,P), \\ P_k(x,y,z,t)=G_2(x,y,z,t,P_k), k(x,y,z,t)=G_1(x,y,z,t,k), \\ \omega(x,y,z,t)=G_1(x,y,z,t,\omega), C(x,y,z,t)=G_1(x,y,z,t,C). \end{gathered}$$

F_u, F_v, F_w components of the volumetric force vector acting in the S_c respective directions, x, y, z – source of pollutant emissions.

It should be noted that the Dirac delta function is additionally included in the advection-diffusion equation to describe the source of diffusion in space and time:

$$S_c = S\delta\left(x-x_S, y-y_S, z-z_S\right)\delta\left(t-t_S\right).$$

Here:
S – actual power of the emission source;
$\delta\left(x-x_S, y-y_S, z-z_S\right)$ – center;
(x_S, y_S, z_S) Dirac delta function in space at a point;
$\delta\left(t-t_S\right)$ - t_S Dirac delta function when the center is at the point.

Algorithm for numerical solution of models of turbulent flow and mixture transport in spatially inhomogeneous air environments of the atmosphere

To investigate the problem numerically, we discretize the search functions using a finite difference upwind-downwind scheme, divide them by time, and determine the following operations to be performed at each time step.

• We introduce initial values and initial conditions;
• the temporal velocity field;
• we set the speed boundary conditions;
• solving pressure correction (Conjugate Gradient method);
• we set the pressure boundary conditions;
• velocity field correction;
• setting speed boundary conditions;
• solving the turbulent kinetic energy equation;
• establish turbulent kinetic energy boundary conditions;
• solving the turbulent frequency level equation;
• establish turbulent frequency level boundary conditions;
• calculation of turbulent viscosity;
• solve the equation of the transport of matter;
• we establish boundary conditions for matter transport;
• recheck convergence and stop or continue iteration.

Calculation of transient velocity fields:
the x – direction.

$$u'_{i,j,k} = u^n_{i,j,k} +$$

$$+\Delta t\left(\begin{array}{l} -\left\{\begin{array}{ll} u^n_{i,j,k}\frac{u^n_{i,j,k}-u^n_{i-1,j,k}}{\Delta x} & if\ u^n_{i,j,k}>0 \\ u^n_{i,j,k}\frac{u^n_{i+1,j,k}-u^n_{i,j,k}}{\Delta x} & if\ u^n_{i,j,k}<0 \end{array}\right. - \\ -\left\{\begin{array}{ll} v^n_{i,j,k}\frac{u^n_{i,j,k}-u^n_{i,j-1,k}}{\Delta y} & if\ v^n_{i,j,k}>0 \\ v^n_{i,j,k}\frac{u^n_{i,j+1,k}-u^n_{i,j,k}}{\Delta y} & if\ v^n_{i,j,k}<0 \end{array}\right. - \left\{\begin{array}{ll} w^n_{i,j,k}\frac{u^n_{i,j,k}-u^n_{i,j,k-1}}{\Delta z} & if\ w^n_{i,j,k}>0 \\ w^n_{i,j,k}\frac{u^n_{i,j,k+1}-u^n_{i,j,k}}{\Delta z} & if\ w^n_{i,j,k}<0 \end{array}\right. \end{array}\right)+$$

$$+\Delta t\left(\begin{array}{l} +\frac{1}{\Delta x^2}\left[\nu^n_{e\ i+1/2,j,k}\left(u^n_{i+1,j,k}-u^n_{i,j,k}\right)-\nu^n_{e\ i-1/2,j,k}\left(u^n_{i,j,k}-u^n_{i-1,j,k}\right)\right]+ \\ +\frac{1}{\Delta y^2}\left[\nu^n_{e\ i,j+1/2,k}\left(u^n_{i,j+1,k}-u^n_{i,j,k}\right)-\nu^n_{e\ i,j-1/2,k}\left(u^n_{i,j,k}-u^n_{i,j-1,k}\right)\right]+ \\ +\frac{1}{\Delta z^2}\left[\nu^n_{e\ i,j,k+1/2}\left(u^n_{i,j,k+1}-u^n_{i,j,k}\right)-\nu^n_{e\ i,j,k-1/2}\left(u^n_{i,j,k}-u^n_{i,j,k-1}\right)\right] \end{array}\right).$$

y – direction.

$$v'_{i,j,k} = v^n_{i,j,k} + \Delta t\left(\begin{array}{l} -\left\{\begin{array}{ll} u^n_{i,j,k}\frac{v^n_{i,j,k}-v^n_{i-1,j,k}}{\Delta x} & if\ u^n_{i,j,k}>0 \\ u^n_{i,j,k}\frac{v^n_{i+1,j,k}-v^n_{i,j,k}}{\Delta x} & if\ u^n_{i,j,k}<0 \end{array}\right. - \\ -\left\{\begin{array}{ll} v^n_{i,j,k}\frac{v^n_{i,j,k}-v^n_{i,j-1,k}}{\Delta y} & if\ v^n_{i,j,k}>0 \\ v^n_{i,j,k}\frac{v^n_{i,j+1,k}-v^n_{i,j,k}}{\Delta y} & if\ v^n_{i,j,k}<0 \end{array}\right. - \\ -\left\{\begin{array}{ll} w^n_{i,j,k}\frac{v^n_{i,j,k}-v^n_{i,j,k-1}}{\Delta z} & if\ w^n_{i,j,k}>0 \\ w^n_{i,j,k}\frac{v^n_{i,j,k+1}-v^n_{i,j,k}}{\Delta z} & if\ w^n_{i,j,k}<0 \end{array}\right. \end{array}\right)+$$

$$+\Delta t\left(\begin{array}{l} +\frac{1}{\Delta x^2}\left[\nu^n_{e\ i+1/2,j,k}\left(v^n_{i+1,j,k}-v^n_{i,j,k}\right)-\nu^n_{e\ i-1/2,j,k}\left(v^n_{i,j,k}-v^n_{i-1,j,k}\right)\right]+ \\ +\frac{1}{\Delta y^2}\left[\nu^n_{e\ i,j+1/2,k}\left(v^n_{i,j+1,k}-v^n_{i,j,k}\right)-\nu^n_{e\ i,j-1/2,k}\left(v^n_{i,j,k}-v^n_{i,j-1,k}\right)\right]+ \\ +\frac{1}{\Delta z^2}\left[\nu^n_{e\ i,j,k+1/2}\left(v^n_{i,j,k+1}-v^n_{i,j,k}\right)-\nu^n_{e\ i,j,k-1/2}\left(v^n_{i,j,k}-v^n_{i,j,k-1}\right)\right] \end{array}\right);$$

the z – direction.

$$w'_{i,j,k}=w^n_{i,j,k}+\Delta t\left(\begin{array}{c} -\left\{\begin{array}{ll} u^n_{i,j,k}\frac{w^n_{i,j,k}-w^n_{i-1,j,k}}{\Delta x} & if\ u^n_{i,j,k}>0 \\ u^n_{i,j,k}\frac{w^n_{i+1,j,k}-w^n_{i,j,k}}{\Delta x} & if\ u^n_{i,j,k}<0 \end{array}\right. - \\ -\left\{\begin{array}{ll} v^n_{i,j,k}\frac{w^n_{i,j,k}-w^n_{i,j-1,k}}{\Delta y} & if\ v^n_{i,j,k}>0 \\ v^n_{i,j,k}\frac{w^n_{i,j+1,k}-w^n_{i,j,k}}{\Delta y} & if\ v^n_{i,j,k}<0 \end{array}\right. - \\ -\left\{\begin{array}{ll} w^n_{i,j,k}\frac{w^n_{i,j,k}-w^n_{i,j,k-1}}{\Delta z} & if\ w^n_{i,j,k}>0 \\ w^n_{i,j,k}\frac{w^n_{i,j,k+1}-w^n_{i,j,k}}{\Delta z} & if\ w^n_{i,j,k}<0 \end{array}\right. \end{array}\right)+$$

$$+\Delta t\left(\begin{array}{c} +\frac{1}{\Delta x^2}\left[\nu^n_{e\ i+1/2,j,k}\left(w^n_{i+1,j,k}-w^n_{i,j,k}\right)-\nu^n_{e\ i-1/2,j,k}\left(w^n_{i,j,k}-w^n_{i-1,j,k}\right)w\right]+ \\ +\frac{1}{\Delta y^2}\left[\nu^n_{e\ i,j+1/2,k}\left(w^n_{i,j+1,k}-w^n_{i,j,k}\right)-\nu^n_{e\ i,j-1/2,k}\left(w^n_{i,j,k}-w^n_{i,j-1,k}\right)\right]+ \\ +\frac{1}{\Delta z^2}\left[\nu^n_{e\ i,j,k+1/2}\left(w^n_{i,j,k+1}-w^n_{i,j,k}\right)-\nu^n_{e\ i,j,k-1/2}\left(w^n_{i,j,k}-w^n_{i,j,k-1}\right)\right] \end{array}\right).$$

Borderline the conditions installation.

$$u'_{0,j,k}=u'_{1,j,k},\ u'_{I,j,k}=u'_{I-1,j,k},\ u'_{i,0,k}=u'_{i,1,k},$$
$$u'_{i,J,k}=u'_{i,J-1,k},\ u'_{i,j,0}=u'_{i,j,1},\ u'_{i,j,K}=u'_{i,j,K-1},$$
$$v'_{0,j,k}=v'_{1,j,k},\ v'_{I,j,k}=v'_{I-1,j,k},\ v'_{i,0,k}=v'_{i,1,k},$$
$$v'_{i,J,k}=v'_{i,J-1,k},\ v'_{i,j,0}=v'_{i,j,1},\ v'_{i,j,K}=v'_{i,j,K-1},$$
$$w'_{0,j,k}=w'_{1,j,k},\ w'_{I,j,k}=w'_{I-1,j,k},\ w'_{i,0,k}=w'_{i,1,k},$$
$$w'_{i,J,k}=w'_{i,J-1,k},\ w'_{i,j,0}=w'_{i,j,1},\ w'_{i,j,K}=w'_{i,j,K-1}.$$

Pressure correlation equation calculation:
Poisson:

$$\nabla^2 p'_{i,j,k}\approx\frac{p'_{i+1,j,k}-2p'_{i,j,k}+p'_{i-1,j,k}}{\Delta x^2}+$$
$$+\frac{p'_{i,j+1,k}-2p'_{i,j,k}+p'_{i,j-1,k}}{\Delta y^2}+\frac{p'_{i,j,k+1}-2p'_{i,j,k}+p'_{i,j,k-1}}{\Delta z^2}.$$

Discretization of velocity divergence.

$$RHS=\left(\begin{array}{c} \left(\frac{u_{i+1,j,k}-u_{i-1,j,k}}{2\Delta x}\right)^2+2\left(\frac{u_{i,j+1,k}-u_{i,j-1,k}}{2\Delta y}\right)\left(\frac{v_{i+1,j,k}-v_{i-1,j,k}}{2\Delta x}\right)+ \\ +\left(\frac{v_{i,j+1,k}-v_{i,j-1,k}}{2\Delta y}\right)^2+ \\ +2\left(\frac{u_{i,j,k+1}-u_{i,j,k-1}}{2\Delta z}\right)\left(\frac{w_{i+1,j,k}-w_{i-1,j,k}}{2\Delta x}\right)+ \\ +2\left(\frac{v_{i,j,k+1}-v_{i,j,k-1}}{2\Delta z}\right)\left(\frac{w_{i,j+1,k}-w_{i,j-1,k}}{2\Delta y}\right)+\left(\frac{w_{i,j,k+1}-w_{i,j,k-1}}{2\Delta z}\right)^2 \end{array}\right).$$

Temporary pressure values:

$$P'_{i,j,k}=\frac{-\rho\cdot RHS-\left(\frac{P_{i+1,j,k}+P_{i-1,j,k}}{\Delta x^2}+\frac{P_{i,j+1,k}+P_{i,j-1,k}}{\Delta y^2}+\frac{P_{i,j,k+1}+P_{i,j,k-1}}{\Delta z^2}\right)}{\frac{-2}{\Delta x^2}+\frac{-2}{\Delta y^2}+\frac{-2}{\Delta z^2}}.$$

Pressure for border at points values let's count.

$$P_{0,j,k}^{n+1} = G_2(0, y_j, z_k, t_n, P^{n+1}),\ P_{I,j,k}^{n+1} = G_2(x_I, y_j, z_k, t_n, P^{n+1});$$
$$P_{i,0,k}^{n+1} = G_2(x_i, 0, z_k, t_n, P^{n+1}),\ P_{i,J,k}^{n+1} = G_2(x_i, y_J, z_k, t_n, P^{n+1});$$
$$P_{i,j,0}^{n+1} = G_2(x_i, y_j, 0, t_n, P^{n+1}),\ P_{i,j,K}^{n+1} = G_2(x_i, y_j, z_K, t_n, P^{n+1}).$$

Update pressure:

$$p_{i,j,k}^{n+1} = p_{i,j,k}^{n} + \alpha_p(p'_{i,j,k} - p_{i,j,k}^{n}).$$

Velocity field correction:

$$u_{i,j,k}^{n+1} = u'_{i,j,k} - \frac{\Delta t}{\rho}\frac{p_{i+1,j,k}^{n+1} - p_{i-1,j,k}^{n+1}}{2\Delta x};$$
$$v_{i,j,k}^{n+1} = v'_{i,j,k} - \frac{\Delta t}{\rho}\frac{p_{i,j+1,k}^{n+1} - p_{i,j-1,k}^{n+1}}{2\Delta y};$$
$$w_{i,j,k}^{n+1} = w'_{i,j,k} - \frac{\Delta t}{\rho}\frac{p_{i,j,k+1}^{n+1} - p_{i,j,k-1}^{n+1}}{2\Delta z}.$$

for speeds.

$$u_{0,j,k}^{n+1} = G_1(0, y_j, z_k, t_n, u^{n+1}),\ v_{0,j,k}^{n+1} = G_1(0, y_j, z_k, t_n, v^{n+1}),\ w_{0,j,k}^{n+1} = G_1(0, y_j, z_k, t_n, w^{n+1}),$$
$$u_{i,0,k}^{n+1} = G_1(x_i, 0, z_k, t_n, u^{n+1}),\ v_{i,0,k}^{n+1} = G_1(x_i, 0, z_k, t_n, v^{n+1}),\ w_{i,0,k}^{n+1} = G_1(x_i, 0, z_k, t_n, w^{n+1}),$$
$$u_{i,j,0}^{n+1} = G_1(x_i, y_j, 0, t_n, u^{n+1}),\ v_{i,j,0}^{n+1} = G_1(x_i, y_j, 0, t_n, v^{n+1}),\ w_{i,j,0}^{n+1} = G_1(x_i, y_j, 0, t_n, w^{n+1}),$$
$$u_{I,j,k}^{n+1} = G_1(x_I, y_j, z_k, t_n, u^{n+1}),\ v_{I,j,k}^{n+1} = G_1(x_I, y_j, z_k, t_n, v^{n+1}),\ w_{I,j,k}^{n+1} = G_1(x_I, y_j, z_k, t_n, w^{n+1}),$$
$$u_{i,J,k}^{n+1} = G_1(x_i, y_J, z_k, t_n, u^{n+1}),\ v_{i,J,k}^{n+1} = G_1(x_i, y_J, z_k, t_n, v^{n+1}),\ w_{i,J,k}^{n+1} = G_1(x_i, y_J, z_k, t_n, w^{n+1}),$$
$$u_{i,j,K}^{n+1} = G_1(x_i, y_j, z_K, t_n, u^{n+1}),\ v_{i,j,K}^{n+1} = G_1(x_i, y_j, z_K, t_n, v^{n+1}),\ w_{i,j,K}^{n+1} = G_1(x_i, y_j, z_K, t_n, w^{n+1}).$$

Turbulent kinetic energy and his/her frequency harvest doer to pressure related coefficient discretization:

$$P_{k\,i,j,k}^{n+1} = \nu_{t\,i,j,k}^{n}\left[\begin{array}{c}\left(\frac{u_{i,j+1,k}^{n+1} - u_{i,j-1,k}^{n+1}}{2\Delta y} + \frac{v_{i+1,j,k}^{n+1} - v_{i-1,j,k}^{n+1}}{2\Delta x}\right)^2 + \\ +\left(\frac{u_{i,j,k+1}^{n+1} - u_{i,j,k-1}^{n+1}}{2\Delta z} + \frac{w_{i+1,j,k}^{n+1} - w_{i-1,j,k}^{n+1}}{2\Delta x}\right)^2 + \\ +\left(\frac{v_{i,j,k+1}^{n+1} - v_{i,j,k-1}^{n+1}}{2\Delta z} + \frac{w_{i,j+1,k}^{n+1} - w_{i,j-1,k}^{n+1}}{2\Delta y}\right)^2\end{array}\right].$$

Border at the points values update:

$$P_{k\,0,j,k}^{n+1} = G_2(0, y_j, z_k, t_n, P_k^{n+1}),\ P_{k\,I,j,k}^{n+1} = G_2(x_I, y_j, z_k, t_n, P_k^{n+1});$$
$$P_{k\,i,0,k}^{n+1} = G_2(x_i, 0, z_k, t_n, P_k^{n+1}),\ P_{k\,i,J,k}^{n+1} = G_2(x_i, y_J, z_k, t_n, P_k^{n+1});$$
$$P_{k\,i,j,0}^{n+1} = G_2(x_i, y_j, 0, t_n, P_k^{n+1}),\ P_{k\,i,j,K}^{n+1} = G_2(x_i, y_j, z_K, t_n, P_k^{n+1}).$$

Turbulent kinetic energy discretization and separation by time.

$$k_{i,j,k}^{n+1} = k_{i,j,k}^{n} - \Delta t \left(\begin{array}{c} \begin{cases} u_{i,j,k}^{n+1} \frac{k_{i,j,k}^{n} - k_{i-1,j,k}^{n}}{\Delta x} & if\ u_{i,j,k}^{n+1} > 0 \\ u_{i,j,k}^{n+1} \frac{k_{i+1,j,k}^{n} - k_{i,j,k}^{n}}{\Delta x} & if\ u_{i,j,k}^{n+1} < 0 \end{cases} + \\ + \begin{cases} v_{i,j,k}^{n+1} \frac{k_{i,j,k}^{n} - k_{i,j-1,k}^{n}}{\Delta y} & if\ v_{i,j,k}^{n+1} > 0 \\ v_{i,j,k}^{n+1} \frac{k_{i,j+1,k}^{n} - k_{i,j,k}^{n}}{\Delta y} & if\ v_{i,j,k}^{n+1} < 0 \end{cases} + \\ + \begin{cases} w_{i,j,k}^{n+1} \frac{k_{i,j,k}^{n} - k_{i,j,k-1}^{n}}{\Delta z} & if\ w_{i,j,k}^{n+1} > 0 \\ w_{i,j,k}^{n+1} \frac{k_{i,j,k+1}^{n} - k_{i,j,k}^{n}}{\Delta z} & if\ w_{i,j,k}^{n+1} < 0 \end{cases} - P_{k\ i,j,k}^{n+1} + \beta^* k_{i,j,k} \omega_{i,j,k} \end{array} \right) +$$

$$+\Delta t \left(\begin{array}{c} \frac{1}{\Delta x} \left[\left(\nu + \frac{\nu_{t\ i+1/2,j,k}^{n}}{\sigma_k} \right) \frac{k_{i+1,j,k} - k_{i,j,k}}{\Delta x} - \left(\nu + \frac{\nu_{t\ i-1/2,j,k}^{n}}{\sigma_k} \right) \frac{k_{i,j,k} - k_{i-1,j,k}}{\Delta x} \right] + \\ + \frac{1}{\Delta y} \left[\left(\nu + \frac{\nu_{t\ i+1/2,j,k}^{n}}{\sigma_k} \right) \frac{k_{i,j+1,k} - k_{i,j,k}}{\Delta y} - \left(\nu + \frac{\nu_{t\ i-1/2,j,k}^{n}}{\sigma_k} \right) \frac{k_{i,j,k} - k_{i,j-1,k}}{\Delta y} \right] + \\ + \frac{1}{\Delta z} \left[\left(\nu + \frac{\nu_{t\ i,j,k+1/2}^{n}}{\sigma_k} \right) \frac{k_{i,j,k+1} - k_{i,j,k}}{\Delta z} - \left(\nu + \frac{\nu_{t\ i,j,k-1/2}^{n}}{\sigma_k} \right) \frac{k_{i,j,k} - k_{i,j,k-1}}{\Delta z} \right] \end{array} \right).$$

Turbulent frequency level discretization to do and time according to separation

$$\omega_{i,j,k}^{n+1} = \omega_{i,j,k}^{n} - $$

$$-\Delta t \left(\begin{array}{c} \begin{cases} u_{i,j,k}^{n} \frac{\omega_{i,j,k}^{n} - \omega_{i-1,j,k}^{n}}{\Delta x} & if\ u_{i,j,k}^{n} > 0 \\ u_{i,j,k}^{n} \frac{\omega_{i+1,j,k}^{n} - \omega_{i,j,k}^{n}}{\Delta x} & if\ u_{i,j,k}^{n} < 0 \end{cases} + \\ + \begin{cases} v_{i,j,k}^{n} \frac{\omega_{i,j,k}^{n} - \omega_{i,j-1,k}^{n}}{\Delta y} & if\ v_{i,j,k}^{n} > 0 \\ v_{i,j,k}^{n} \frac{\omega_{i,j+1,k}^{n} - \omega_{i,j,k}^{n}}{\Delta y} & if\ v_{i,j,k}^{n} < 0 \end{cases} \\ + \begin{cases} w_{i,j,k}^{n} \frac{\omega_{i,j,k}^{n} - \omega_{i,j,k-1}^{n}}{\Delta z} & if\ w_{i,j,k}^{n} > 0 \\ w_{i,j,k}^{n} \frac{\omega_{i,j,k+1}^{n} - \omega_{i,j,k}^{n}}{\Delta z} & if\ w_{i,j,k}^{n} < 0 \end{cases} \end{array} \right) +$$

$$+\Delta t \left(\begin{array}{c} \frac{1}{\Delta x} \left[\left(\nu + \frac{\nu_{t\ i+1/2,j,k}^{n}}{\sigma_\omega} \right) \frac{\omega_{i+1,j,k}^{n} - \omega_{i,j,k}^{n}}{\Delta x} - \left(\nu + \frac{\nu_{t\ i-1/2,j,k}^{n}}{\sigma_\omega} \right) \frac{\omega_{i,j,k}^{n} - \omega_{i-1,j,k}^{n}}{\Delta x} \right] + \\ + \frac{1}{\Delta y} \left[\left(\nu + \frac{\nu_{t\ i,j+1/2,k}^{n}}{\sigma_\omega} \right) \frac{\omega_{i,j+1,k}^{n} - \omega_{i,j,k}^{n}}{\Delta y} - \left(\nu + \frac{\nu_{t\ i,j-1/2,k}^{n}}{\sigma_\omega} \right) \frac{\omega_{i,j,k}^{n} - \omega_{i,j-1,k}^{n}}{\Delta y} \right] + \\ + \frac{1}{\Delta z} \left[\left(\nu + \frac{\nu_{t\ i,j,k+1/2}^{n}}{\sigma_\omega} \right) \frac{\omega_{i,j,k+1}^{n} - \omega_{i,j,k}^{n}}{\Delta z} - \left(\nu + \frac{\nu_{t\ i,j,k-1/2}^{n}}{\sigma_\omega} \right) \frac{\omega_{i,j,k}^{n} - \omega_{i,j,k-1}^{n}}{\Delta z} \right] + \\ + \alpha \frac{\omega_{i,j,k}}{k_{i,j,k}} P_{k\ i,j,k}^{n} - \beta \omega_{i,j,k}^{2} \end{array} \right).$$

Boundary conditions.

$$
\begin{aligned}
k_{0,j,k}^{n+1} &= G_1(0, y_j, z_k, t_n, k^n), \;\; k_{i,j,N_k}^{n+1} = G_1(x_i, y_j, z_{N_k}, t_n, k^n);\\
k_{i,0,k}^{n+1} &= G_1(x_i, 0, z_k, t_n, k^n), \;\; k_{i,N_y,k}^{n+1} = G_1(x_i, y_{N_y}, z_k, t_n, k^n);\\
k_{i,j,0}^{n+1} &= G_1(x_i, y_j, 0, t_n, k^n), \;\; k_{i,j,N_k}^{n+1} = G_1(x_i, y_j, z_{N_k}, t_n, k^n).\\
\omega_{0,j,k}^{n+1} &= G_1(0, y_j, z_k, t_n, \omega^n), \;\; \omega_{i,j,N_k}^{n+1} = G_1(x_i, y_j, z_{N_k}, t_n, \omega^n);\\
\omega_{i,0,k}^{n+1} &= G_1(x_i, 0, z_k, t_n, \omega^n), \;\; \omega_{i,N_y,k}^{n+1} = G_1(x_i, y_{N_y}, z_k, t_n, \omega^n);\\
\omega_{i,j,0}^{n+1} &= G_1(x_i, y_j, 0, t_n, \omega^n), \;\; \omega_{i,j,N_k}^{n+1} = G_1(x_i, y_j, z_{N_k}, t_n, \omega^n).
\end{aligned}
$$

Calculation of turbulent viscosity:

$$
\nu_{t\,i,j,k}^{n+1} = \frac{k_{i,j,k}^{n+1}}{\omega_{i,j,k}^{n+1}}.
$$

Material transport discretization and time separation are as follows.

$$
C_{i,j,k}^{n+1} = C_{i,j,k}^{n} - \Delta t \left(\begin{array}{c}
\begin{cases} u_{i,j,k}^{n+1} \dfrac{C_{i,j,k}^{n} - C_{i-1,j,k}^{n}}{\Delta x} & if \;\; u_{i,j,k}^{n+1} > 0 \\ u_{i,j,k}^{n+1} \dfrac{C_{i+1,j,k}^{n} - C_{i,j,k}^{n}}{\Delta x} & if \;\; u_{i,j,k}^{n+1} < 0 \end{cases} + \\
+ \begin{cases} v_{i,j,k}^{n+1} \dfrac{C_{i,j,k}^{n} - C_{i,j-1,k}^{n}}{\Delta y} & if \;\; v_{i,j,k}^{n+1} > 0 \\ v_{i,j,k}^{n+1} \dfrac{C_{i,j+1,k}^{n} - C_{i,j,k}^{n}}{\Delta y} & if \;\; v_{i,j,k}^{n+1} < 0 \end{cases} + \\
+ \begin{cases} w_{i,j,k}^{n+1} \dfrac{C_{i,j,k}^{n} - C_{i,j,k-1}^{n}}{\Delta z} & if \;\; w_{i,j,k}^{n+1} > 0 \\ w_{i,j,k}^{n+1} \dfrac{C_{i,j,k+1}^{n} - C_{i,j,k}^{n}}{\Delta z} & if \;\; w_{i,j,k}^{n+1} < 0 \end{cases}
\end{array} \right) +
$$

$$
+\Delta t \left(\begin{array}{c}
\dfrac{1}{\Delta x} \left[\left(\nu + \nu_{t\;i+1/2,j,k}^{n+1} \right) \dfrac{C_{i+1,j,k} - C_{i,j,k}}{\Delta x} - \left(\nu + \nu_{t\;i-1/2,j,k}^{n+1} \right) \dfrac{C_{i,j,k} - C_{i-1,j,k}}{\Delta x} \right] + \\
+ \dfrac{1}{\Delta y} \left[\left(\nu + \nu_{t\;i,j+1/2,k}^{n+1} \right) \dfrac{C_{i,j+1,k} - C_{i,j,k}}{\Delta y} - \left(\nu + \nu_{t\;i,j-1/2,k}^{n+1} \right) \dfrac{C_{i,j,k} - C_{i,j-1,k}}{\Delta y} \right] + \\
+ \dfrac{1}{\Delta z} \left[\left(\nu + \nu_{t\;i,j,k+1/2}^{n+1} \right) \dfrac{C_{i,j,k+1} - C_{i,j,k}}{\Delta z} - \left(\nu + \nu_{t\;i,j,k-1/2}^{n+1} \right) \dfrac{C_{i,j,k} - C_{i,j,k-1}}{\Delta z} \right] + \\
+ S_{C\;i,j,k}^{n}
\end{array} \right).
$$

Determining the values of functions at boundary points

$$
\begin{aligned}
C_{0,j,k}^{n+1} &= G_1(0, y_j, z_k, t_n, C^n), \;\; C_{i,j,N_k}^{n+1} = G_1(x_i, y_j, z_{N_k}, t_n, C^n);\\
C_{i,0,k}^{n+1} &= G_1(x_i, 0, z_k, t_n, C^n), \;\; C_{i,N_y,k}^{n+1} = G_1(x_i, y_{N_y}, z_k, t_n, C^n);\\
C_{i,j,0}^{n+1} &= G_1(x_i, y_j, 0, t_n, C^n), \;\; C_{i,j,N_k}^{n+1} = G_1(x_i, y_j, z_{N_k}, t_n, C^n);
\end{aligned}
$$

All functions descritization so that they time according to to divide, to calculate algorithm using calculation process Let's start.

Check convergence and continue iteration:

$$R_p = \left|\frac{p^{n+1}-p^n}{p^{n+1}}\right|,\ R_u = \left|\frac{u^{n+1}-u^n}{u^{n+1}}\right|,\ R_v = \left|\frac{v^{n+1}-v^n}{v^{n+1}}\right|,$$

$$R_w = \left|\frac{w^{n+1}-w^n}{w^{n+1}}\right|,\ R_k = \left|\frac{k^{n+1}-k^n}{k}\right|,$$

$$R_\varepsilon = \left|\frac{\varepsilon^{n+1}-\varepsilon^n}{\varepsilon}\right|,\ R_C = \left|\frac{C^{n+1}-C^n}{C^{n+1}}\right|.$$

If $R_p, R_u, R_v, R_w, R_k, R_\varepsilon, R_C$the residual values are less than a specified value, the iteration process is stopped.

If the residual values are greater than the specified value, we continue the iteration from step 2. Iteration Continue:

If the residual values are greater than the specified value, we continue the iteration process: This iterative process can be used to solve a general discretized system of equations. At each iteration, the pressure, velocity, turbulent kinetic energy, turbulent frequency, and mass transport are updated, and the process continues until the convergence conditions are met.

4 Results

The suitability of the developed mathematical apparatus was verified by conducting computer experiments. For this purpose, the considered mathematical model and numerical algorithm were implemented as a software tool written in the Python programming language.

To model the studied process of pollutant dispersion in the surface layer of the atmosphere, the following conditions and constraints were adopted, taking into account urban planning elements.

The pollutant is considered as a single linear source of emission. The total volume of exhaust gases emitted by the movement of vehicles along the overpass section (Figure 1) CO_2 is taken as the amount of carbon dioxide released into the atmosphere per unit of time.

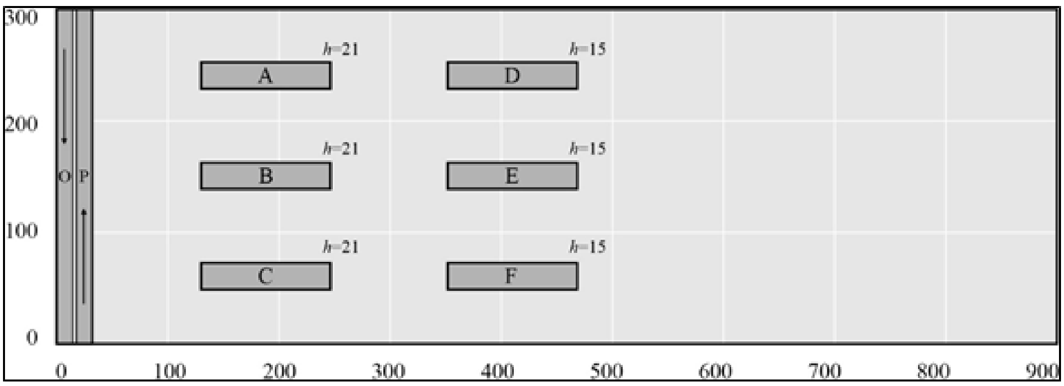

Figure 1 Calculation experience being transferred of the industry geometry

Figure 2 Within the industry, vehicles have been considered as a source of harmful gases emitted into the atmosphere

An example of a simulated section of an intercity overpass with car traffic considered as a source of air pollution.

A schematic representation of the problem solving area with a linear emission source and urban development elements is shown in Figure 2. Schematic representation of the physical region under consideration.

OP – A section of an 8-lane highway measuring 300 m by 32 m;

A, B, C, D, E, F – 7 and 5-story buildings;

h - height of buildings (m).

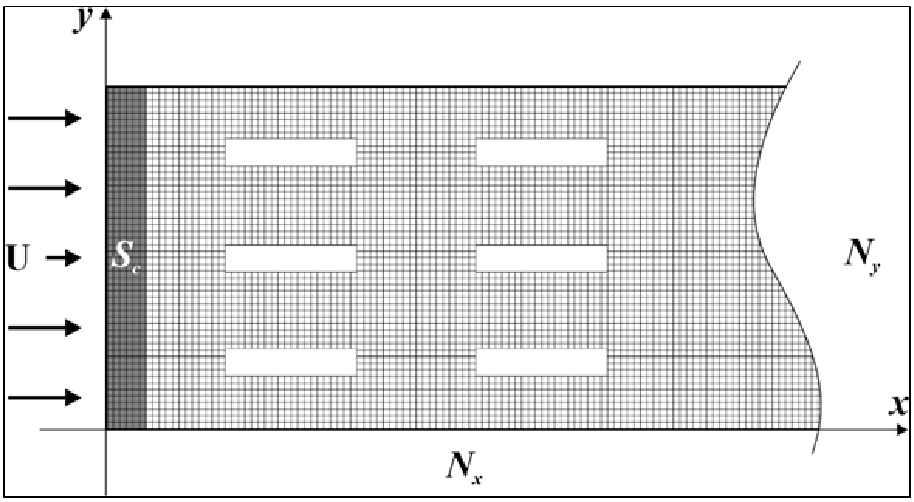

Figure 3 Node to the points separation

Networked knots number $N_x \times N_y \times N_z$ with calculation of the field schematic image. This on the groundU $= [u, v, w]$ air flow speed vector; S_c– pollutant emission linear source.

Calculation experience during in the region wind speed components following initial values determined Ω: $u_0 = 2, v_0 = 1, w_0 = 0,1$; turbulent diffusion coefficient $D = 1,0$; pollutant substances concentration CO_2: $C_0 = 0,0\ kg/m^3$.

Emission source power value see outgoing 300 meters of road part of minimum or — one of time up to 5 in the cars from being come came out without chosen. That is, light of the car average emission $180 g/km$ that into account if we get, source power $S = 10,0$ g/s what organization does.

Other process of parameters to the values as for them dry, low windy weather, average temperature $20°C$ and atmosphere pressure normal within the limits (725-730 mm Hg) into account taken without It is installed.

Initial experiments under consideration in the field of the wind stream magnitude to clarify, to that end suitable concentration spread to the suitability In this case, we obtain the following results.

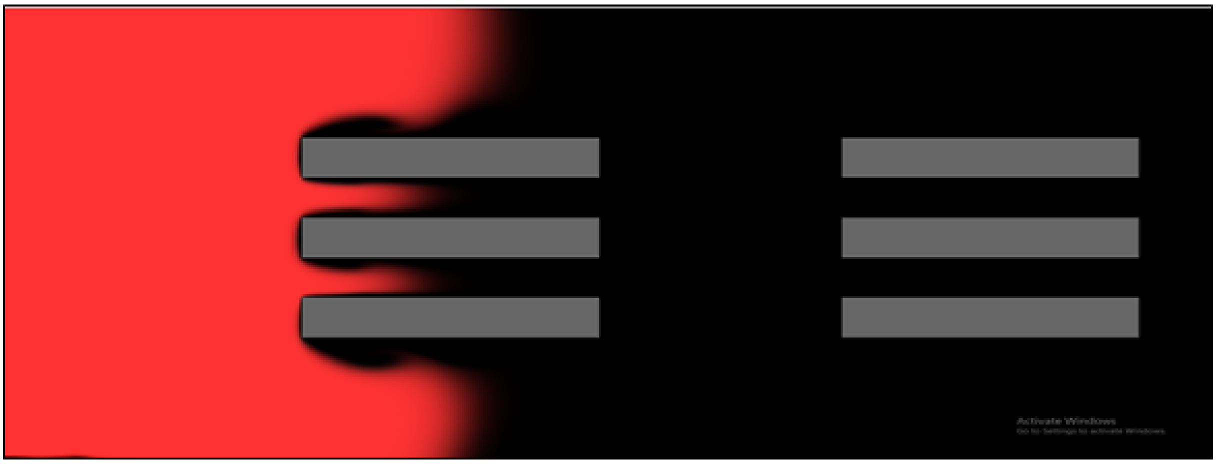

Figure 4 Velocity magnitude value at $t = 50$ [s], height $z = 2$ [m]

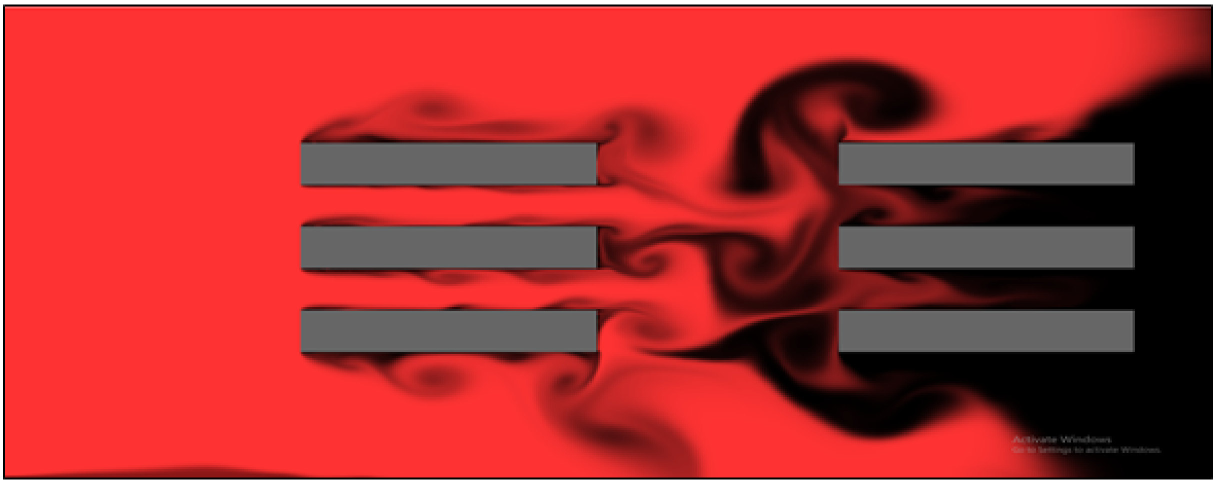

Figure 5 Velocity magnitude value at $t = 150$ [s], height $z = 2$ [m].

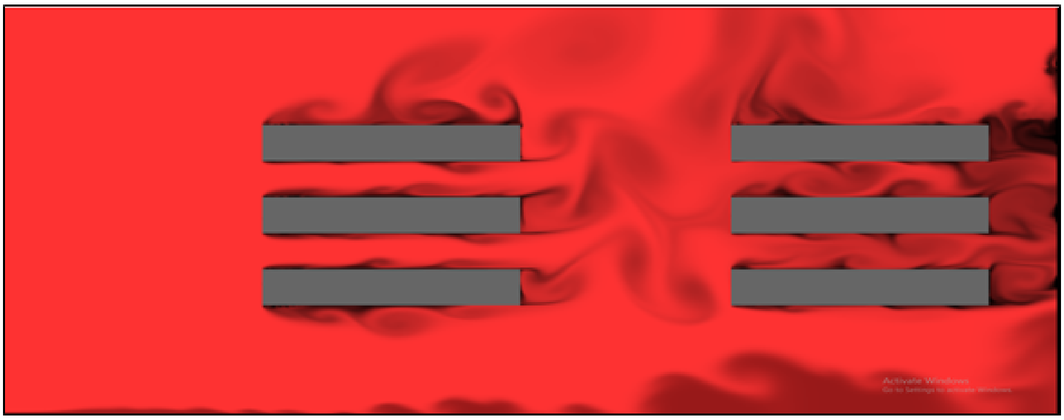

Figure 6 Velocity magnitude value at $t = 500$ [s], height $z = 2$ [m]

In the above figures 4-6, it can be observed that the external and internal boundary conditions work with sufficient accuracy in the observed wind magnitude and in a complex area. At the same time, we have achieved a significant reduction in the calculation time by dividing the boundary conditions into 4 types.

The algorithm for selecting boundary conditions depending on the direction and nature of the flow inside the object, on the object wall, on the object surface and at the external boundaries works very accurately.

The calculation experiments are shown in a graphical, visual representation of the results of the calculation of the distribution of points at different time steps, taking into account the limitations of memory and computing machines, in relation to the concentration, wind speed, pressure, flow t magnitude, turbulent kinetic energy and its frequency.

Initially, experiments were carried out by placing a building in a sphere and calculating in a small sphere. In this case, the sphere was considered as 100x100x40 meters, and the dimensions of the building were considered as 15x35x15 meters. The wind speeds within the boundaries of the sphere were considered as 2 m/s and 1 m/s, respectively.

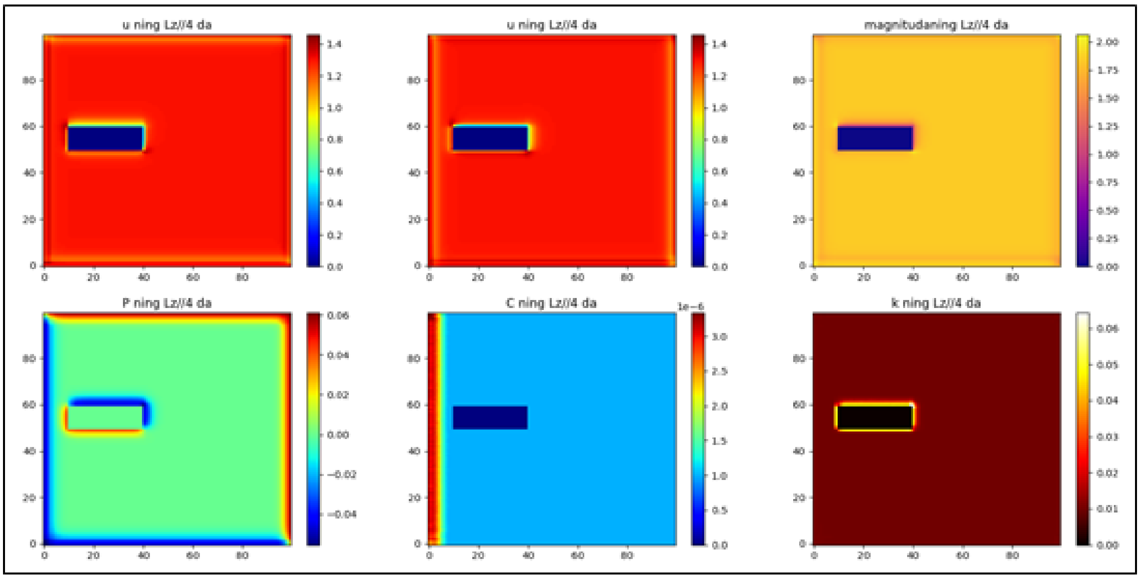

Figure 7 Values of functions at t= 5 [s], height $z = 2$ [m]

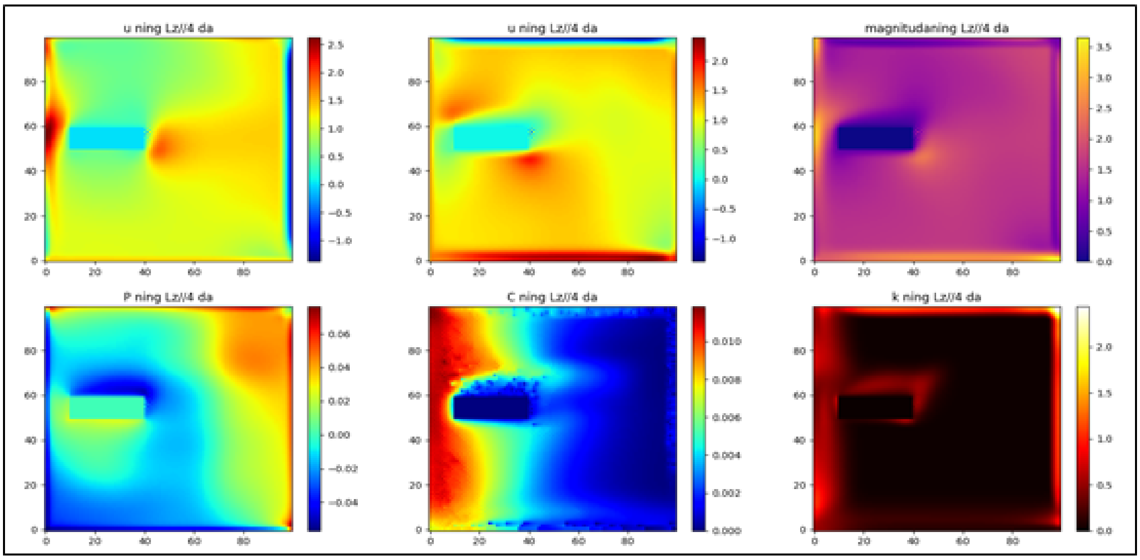

Figure 8 Values of functions at t= 100 [s], height $z = 2$ [m]

As mentioned above, $\Delta t$the algorithm selects the optimal values of at each time integration step. Note that for given process parameters, in general, the stability of the computational process is generally $\Delta t = 0,00001$ maintained.

Our above calculation experiments show that the turbulence of the wind flow is stronger near the building and it can be observed that the concentration values around the building are higher. This fully explains the faster dispersion of impurities in turbulent flows in real physical processes and the decrease in the directional values of velocities due to the change in the direction of velocity and pressure drop within the accumulation areas in the flow.

In subsequent computational experiments, we observe the dynamics of the flow and the concentration distribution in the field as a result of increasing the number of buildings to six and complicating the field by several simple geometries.

In this case, a conditional rectangular urban area with dimensions of was considered as the problem area $L_x = 100m, L_y = 100m, L_z = 30m$, and a section of an 8-lane highway 300 m long and 32 m wide, located on the left border of the area, was taken.

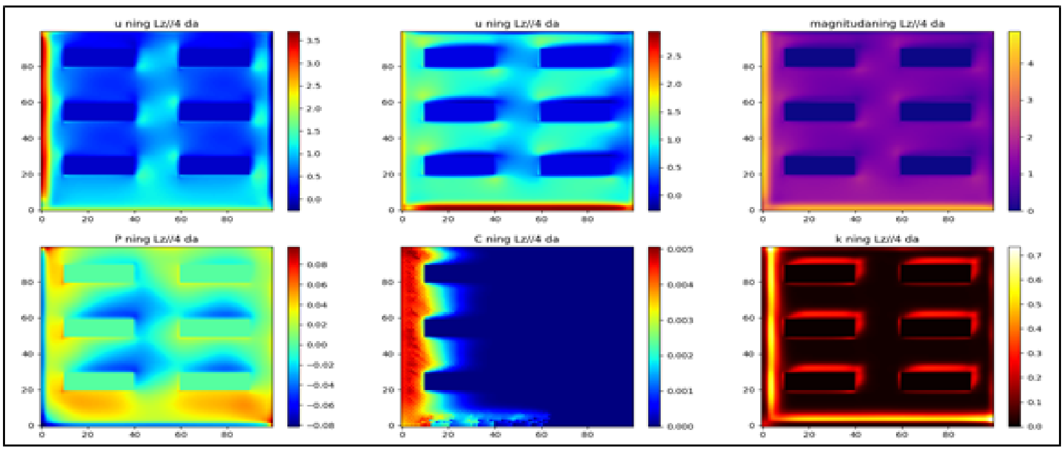

Figure 9 Calculated concentration $t = 5$s, height $z = 2$m

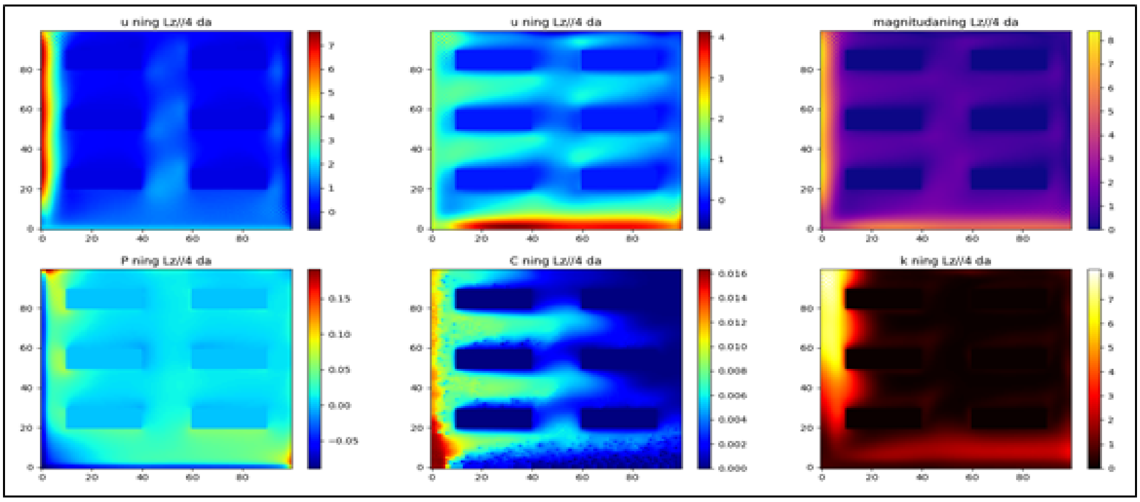

Figure 10 Calculated concentration $t = 20$s, height $z = 2$m

From the analysis of the results of the computational experiment, it can be seen that under the conditions and constraints given for the numerical modeling of the process under study in Figures 9 and 10, the steady- state emission dispersion occurs quite intensively, and its decrease, the concentration level, is linear. It should be noted that the modeling did not take into account the impact of vehicle traffic on the air flow.

In light winds (up to 2-3 m/s), high concentration indicators are observed, as expected, near the road. When moving away from the source at a distance of about 100 meters, the concentration of the harmful substance decreases sharply, and after another 100 meters, the concentration indicators approach zero.

The same process can be said about the nature of the distribution of the concentration field in height, with the difference that the scale of vertical mass transfer is much smaller. In other words, the upward movement of mixtures due to turbulent eddies and thermal convection occurs much slower and over a much smaller distance (height) than with advective transport. In addition, due to the increase in wind speed with height, the dispersion of mixtures with height also occurs more strongly. Thus, at a height of 25 meters and above, the values of pollutant concentrations decrease almost to zero (Fig. 10).

Buildings adjacent to the road and flowing around the air flow significantly block and reduce the wind speed, thereby preventing the intensive transfer of impurities in the transverse direction from the street canyon (Fig. 7-9). As can be seen from the figures, under the given conditions of the calculation experiment, the particles of the pollutant practically do not reach the second row of buildings. That is, the concentration of automobile emissions harmful to health does not spread deep into populated areas.

This is explained by several effects: in some places, for example, in a road canyon, the speed and level of turbulence of the main flow are significantly reduced, and, conversely, outside the highways between multi-storey buildings, the speed and turbulence of air flows increase significantly, intensively distributing the concentration of impurities. This effect can be considered an active point, but in order to avoid the formation of large concentrations as a result of constant pollution of the roads, it is advisable to align the direction of such street canyons with the prevailing wind directions, ensuring their good ventilation. In addition, it is also necessary to control the density of buildings along the sides of the highways to ensure a certain level of ventilation in the transverse direction.

5 Conclusion

Modeling the turbulent transport of mixtures in the atmosphere: A mathematical model was developed to study the transport of mixtures in spatially inhomogeneous atmospheric air based on the Navier-Stokes equations and the $k-\omega$ turbulent model. The model takes into account urban planning elements, meteorological parameters, and the characteristics of emission sources, as well as the physicochemical properties of pollutants.

Numerical algorithm and calculation method: The calculations were performed using the finite difference method based on the implicit difference scheme of second-order approximation. This method allows for high accuracy in time and spatial variables. The calculation algorithm is aimed at determining the optimal parameters to ensure stability.

Model description and efficiency: The results obtained showed that the model is sufficiently accurate. The calculations allowed to successfully describe the dispersion of pollutants through turbulent flows in atmospheric conditions. This model can be used as an effective tool for planning urban infrastructure and ensuring environmental safety.

Urban design elements: Urban design elements have a significant impact on the turbulent transport of mixtures. In environments such as road canyons, the reduced flow velocity and turbulence level lead to high concentrations of pollutants in places. Although the dispersion of pollutants in such areas is limited, widespread pollution is observed outside the canyon. When designing urban road canyons and other structures, it is necessary to direct them to improve wind circulation opportunities. Urban development plans should be drawn up taking into account the natural wind circulation processes of atmospheric flows. It is important to carefully determine the location and orientation of structures to minimize the accumulation of pollutants in areas of low flow velocity.

References

[1] Batchelor G.K. 1967. An Introduction to Fluid Dynamics. // Springer. https://link.springer.com/book/10.1007/978-1-4612-4682-3

[2] Kolmogorov A.N. 1941. The Local Structure of Turbulence in Incompressible Viscous Fluid for Very Large Reynolds Numbers. Springer. https://link.springer.com/article/10.1007/BF01341274

[3] Smagorinsky J. 1963. General Circulation Experiments with the Primitive Equations. // Springer. https://doi.org/10.1175/1520-0469(1963)020<0223:GCEWTP>2.0.CO;2

[4] Launder B.E., Spalding D.B. 1974. The Numerical Computation of Turbulent Flows. Springer. https://doi.org/10.1016/0021-9991(74)90029-2

[5] Spalart P.R., Allmaras S.R. 1992. A One-Equation Turbulence Model for Aerodynamic Flows. La Recherche Aérospatiale. https://arc.aiaa.org/doi/10.2514/3.48238

[6] Wilcox D.C. 2006. Turbulence Modeling for CFD. DCW Industries. https://www.dcwindustries.com/turbulence-modeling-for-cfd

[7] Patankar S.V. 1980. Numerical Heat Transfer and Fluid Flow. Hemisphere Publishing. // https://www.taylorfrancis.com/books/mono/10.1201/9781482234213/numerical-heat-transfer-fluid-flow-suhas-patankar

[8] Togrul I.T., Pehlivan D. 2004. Modelling of thin layer drying kinetics of some fruits under open-air sun drying process // J. Food Eng. – Vol. 65, – № 3. – P. 413–425.

[9] Versteeg H.K., Malalasekera W. 1995. An Introduction to Computational Fluid Dynamics: The Finite Volume Method. Pearson Education. // https://www.pearson.com/store/p/introduction-to-computational-fluid-dynamics-the-finite-volume-method/P100000150280

[10] Menter F.R. 1994. Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications. // AIAA Journal. https://doi.org/10.2514/3.12149

[11] Pope S.B. 2000. Turbulent Flows. Cambridge University Press.

[12] Davidson P.A. 2004. Turbulence: An Introduction for Scientists and Engineers. // Springer. https://doi.org/10.1093/acprof:oso/9780198722595.001.0001

[13] Moukalled F., Mangani L., Darwish M. 2016. The Finite Volume Method in Computational Fluid Dynamics. // Springer. https://link.springer.com/book/10.1007/978-3-319-16874-6

[14] Schlichting H., Gersten K. 2016. Boundary-Layer Theory. // Springer. https://link.springer.com/book/10.1007/978-3-662-52919-5

[15] Sharipov D., Muradov F., Akhmedov D. 2019. Numerical Modeling Method for Short-Term Air Quality Forecast in Industrial Regions. // Applied Mathematics E-Notes. https://doi.org/10.1051/matecconf/201818203002

[16] Duraisamy K., Iaccarino G., Xiao H. 2019. Turbulence Modeling in the Age of Data. // Annual Review of Fluid Mechanics. https://doi.org/10.1146/annurev-fluid-010518-040547

[17] Bae H.J., Lozano-Durán A., Moin P. 2018. Turbulence Spectra in Wall-Bounded Flows: Scaling Laws and Universality. // Journal of Fluid Mechanics. https://doi.org/10.1017/jfm.2018.499

[18] Agresti A., Veraar M. 2024. Stochastic Navier–Stokes Equations for Turbulent Flows in Critical Spaces. // Communications in Mathematical Physics. https://link.springer.com/article/10.1007/s00220-023-04867-7

[19] Brun C., Bertoglio J.P. 2008. Subgrid-Scale Models for Large-Eddy Simulations Based on Energy Spectrum Considerations. // Journal of Fluid Mechanics. https://doi.org/10.1017/S0022112008004396

[20] Durbin P.A. 2021. Modern Developments in Turbulence Modeling. Annual Review of Fluid Mechanics. // https://doi.org/10.1146/annurev-fluid-011020-073553

[21] Taira K., et al 2017. Modal Analysis of Fluid Flows. // AIAA Journal. https://doi.org/10.2514/1.J056060

[22] Ishihara T., Gotoh T., Kaneda Y. 2009. Study of High-Reynolds Number Isotropic Turbulence. Annual Review of Fluid Mechanics. // https://doi.org/10.1146/annurev.fluid.010908.165203P. – P. 575–584.

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ТУРБУЛЕНТНОГО ПЕРЕНОСА ПРИМЕСЕЙ В ПРОСТРАНСТВЕННО НЕОДНОРОДНОЙ СРЕДЕ АТМОСФЕРЫ

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В данном исследовании представлена математическая модель турбулентного рассеяния загрязняющих веществ в городских воздушных потоках на основе уравнений Навье-Стокса и $k{-}\omega$ модели турбулентности. В модель включены метеорологические параметры, источники выбросов и городские сооружения. Для решения уравнений используется численный метод конечных разностей. Вычислительные эксперименты демонстрируют закономерности концентрации загрязняющих веществ в городской среде. Результаты показывают, что турбулентность ветра и геометрия зданий существенно влияют на дисперсию. Модель может помочь в градостроительстве и экологической безопасности. Результаты моделирования подчеркивают важность циркуляции ветра в снижении загрязнения. В исследовании даны практические рекомендации по оптимизации градостроительства.

Ключевые слова: турбулентная диффузия, уравнения Навье-Стокса, $k-\omega$ модель турбулентности, дисперсия загрязняющих веществ, городские воздушные потоки, численное моделирование, метод конечных разностей, экологическая безопасность.

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