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MATHEMATICAL MODELING OF POLLUTANT DISPERSION IN TURBULENT AIRFLOWS OF THE ATMOSPHERIC BOUNDARY LAYER

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The paper presents a mathematical model of pollutant dispersion in turbulent airflows within the atmospheric boundary layer. The model is based on the advection–diffusion equation and the system of Navier–Stokes equations, complemented by the $k-\varepsilon$ turbulence model. In this formulation, the model provides an accurate description of the spatiotemporal dynamics of pollutant concentration. A point emission source is introduced through the Dirac delta function, which makes it possible to correctly represent localized pollutant releases. For the numerical solution of the problem, an algorithm based on a finite-difference scheme with directional (upwind) flux approximation and iterative pressure correction using the conjugate gradient method is proposed. Boundary and initial conditions are formulated for the near-surface atmospheric layer, taking into account the spatial inhomogeneity of the wind field and the vertical gradient of turbulent energy. The developed model ensures a stable solution and can be applied to analyze pollutant dispersion dynamics, forecast air quality, and optimize urban ventilation systems under various meteorological conditions.

Keywords: atmospheric modeling, turbulent diffusion, finite-difference approximation, velocity and pressure field, environmental forecasting.

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1 Introduction

Air, water, soil pollution and others such as pollution many forms available. Air pollution in the world of death main ecological reason is [1–4]. Atmosphere the air pollutant substances, including carbonate anhydride, lead, nitrogen dioxide, ozone particles and sulfur dioxide [5–10] factories, industry and from transport Transport sector car waste because of large city in the centers air pollution big part for is responsible for the population health save, how storage necessary understanding street in the canyons or other in cities acceptance to be done air quality important to the community has. Last one how many ten in years many researchers experimental and digital from models used without air quality control to do attention they focused. experimental research pollutant of substances spread right show not received because of, digital models last one how many ten in years street canyons in the environment air pollution local sources plants existence such as one how many in aspects study for main tool as used [11, 12] and dust [13], surrounding air flow and the air pollutant of substances spread [14–24]. Chan and etc. insulation done street in the canyon the air pollutant dispersion two measurable model offer [16] Dust and others. various high altitude city street in the canyons pollutant dispersion prophecy to do for wind tunnel model used [17]. Who and others. city street in the canyons stream and pollutant of substances to spread heat the impact [20]. In 2011, Liu wind area was or not been in cities car exhausts spread prophecy to do for two digital the model offer [25] His in the model building and street canyon configuration impact and pollutant substances in the spread moving vehicles by working released turbulent energy studied. One how many year later, in 2014 emission sources husband under to the level close located street in the canyons pollutant of substances spread according to digital research Madalozzo by mass storage pseudo-convulsion hypothesis, Navier-Stokes equations, energy equations and pollutant substances transportation from the equations used without done [26]. Their results this shows that the temperature and street-canyon geometry wind of the flow movement, polluting substances also affects concentration does. Aristodemou and others mesh- flexible incompressible turbulent flow big whirlwind simulation using seven building in the configuration tall buildings to turbulent flows and pollution to spread the impact learned [24]. Suebi and Pochai In Bangkok, Thailand Skytrain platform under traffic jam in the zone air pollution digital accordingly [27] Ravshanov, Sharipov and other scientists by of the atmosphere border in the layer harmful of substances spread processes mathematician models offer was done [28]. Available from models taken results mainly row buildings located street in the canyons pseudo-convulsion guess with or not been without incompressible liquid to the flow based on because of, street with transportation in the canyon related air pollution about our understanding very limited.

This in the study we wind speed street with transportation in the canyon related air pollution to dispersion the impact we learn. Atmosphere pollution only for pollutant CO_2, adiabatic in process of the problem manager Reynolds equations average Navier-Stokes (RANS) compressible turbulent flow equations and CO_2 concentration convection-diffusion equations The issue is being considered. solution for limited elements method is applied.

2 Mathematical model

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:

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

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

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:

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

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. The explanation of the variables and constants

*	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).

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

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

The network was considered to be defined in the field.

The initial conditions for the given equations are given below.

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

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.

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

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

The following function is used to calculate the values of functions at their limit points.

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

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.

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

$C_{input\_x}, C_{input\_y}, C_{input\_y}$ – incoming concentration with flow,
U – resultant flow velocity,

φ – azimuth angle,

θ – zenith angle.

In the process of solving a system of equations, P_k, ν_t since functions such as are functions of other functions, the following relations were established at their limit points.

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

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.

3 Numerical solution algorithm

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;
- calculation of the temporal velocity field;
- 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:

Descritization *in the x -direction.*

$$\frac{u'_{i,j,k}-u^n_{i,j,k}}{\Delta t} = -\begin{cases} u^n_{i,j,k}\frac{u^n_{i,j,k}-u^n_{i-1,j,k}}{\Delta x}, & u^n_{i,j,k}>0 \\ u^n_{i,j,k}\frac{u^n_{i+1,j,k}-u^n_{i,j,k}}{\Delta x}, & u^n_{i,j,k}<0 \end{cases}$$
$$-\begin{cases} v^n_{i,j,k}\frac{u^n_{i,j,k}-u^n_{i,j-1,k}}{\Delta y}, & v^n_{i,j,k}>0 \\ v^n_{i,j,k}\frac{u^n_{i,j+1,k}-u^n_{i,j,k}}{\Delta y}, & v^n_{i,j,k}<0 \end{cases} - \begin{cases} w^n_{i,j,k}\frac{u^n_{i,j,k}-u^n_{i,j,k-1}}{\Delta z}, & w^n_{i,j,k}>0 \\ w^n_{i,j,k}\frac{u^n_{i,j,k+1}-u^n_{i,j,k}}{\Delta z}, & w^n_{i,j,k}<0 \end{cases} +$$
$$+\frac{1}{\Delta x^2}\left[\nu^n_{e\ i+1/2,j,k}\left(u^n_{i+1,j,k}-u^n_{i,j,k}\right)-\nu^n_{e\ i-1/2,j,k}\left(u^n_{i,j,k}-u^n_{i-1,j,k}\right)\right]+$$
$$+\frac{1}{\Delta y^2}\left[\nu^n_{e\ i,j+1/2,k}\left(u^n_{i,j+1,k}-u^n_{i,j,k}\right)-\nu^n_{e\ i,j-1/2,k}\left(u^n_{i,j,k}-u^n_{i,j-1,k}\right)\right]+$$
$$+\frac{1}{\Delta z^2}\left[\nu^n_{e\ i,j,k+1/2}\left(u^n_{i,j,k+1}-u^n_{i,j,k}\right)-\nu^n_{e\ i,j,k-1/2}\left(u^n_{i,j,k}-u^n_{i,j,k-1}\right)\right].$$

The update equation over time is:

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

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

Descritization in the y *-direction.*

$$
\frac{v'_{i,j,k}-v^n_{i,j,k}}{\Delta t}=-\begin{cases} w^n_{i,j,k}\frac{v^n_{i,j,k}-v^n_{i,j,k-1}}{\Delta z}, & w^n_{i,j,k}>0 \\ w^n_{i,j,k}\frac{v^n_{i,j,k+1}-v^n_{i,j,k}}{\Delta z}, & w^n_{i,j,k}<0 \end{cases} -
$$

$$
-\begin{cases} u^n_{i,j,k}\frac{v^n_{i,j,k}-v^n_{i-1,j,k}}{\Delta x}, & u^n_{i,j,k}>0 \\ u^n_{i,j,k}\frac{v^n_{i+1,j,k}-v^n_{i,j,k}}{\Delta x}, & u^n_{i,j,k}<0 \end{cases} - \begin{cases} v^n_{i,j,k}\frac{v^n_{i,j,k}-v^n_{i,j-1,k}}{\Delta y}, & v^n_{i,j,k}>0 \\ v^n_{i,j,k}\frac{v^n_{i,j+1,k}-v^n_{i,j,k}}{\Delta y}, & v^n_{i,j,k}<0 \end{cases} +
$$

$$
+\frac{1}{\Delta x^2}\left[\nu^n_{e\ i+1/2,j,k}\left(v^n_{i+1,j,k}-v^n_{i,j,k}\right)-\nu^n_{e\ i-1/2,j,k}\left(v^n_{i,j,k}-v^n_{i-1,j,k}\right)\right]+
$$

$$
+\frac{1}{\Delta y^2}\left[\nu^n_{e\ i,j+1/2,k}\left(v^n_{i,j+1,k}-v^n_{i,j,k}\right)-\nu^n_{e\ i,j-1/2,k}\left(v^n_{i,j,k}-v^n_{i,j-1,k}\right)\right]+
$$

$$
+\frac{1}{\Delta z^2}\left[\nu^n_{e\ i,j,k+1/2}\left(v^n_{i,j,k+1}-v^n_{i,j,k}\right)-\nu^n_{e\ i,j,k-1/2}\left(v^n_{i,j,k}-v^n_{i,j,k-1}\right)\right].
$$

The update equation over time is: y – direction.

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

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

Descritization in the z *-direction.*

$$
\frac{w'_{i,j,k}-w^n_{i,j,k}}{\Delta t}=-\begin{cases} u^n_{i,j,k}\frac{w^n_{i,j,k}-w^n_{i-1,j,k}}{\Delta x}, & u^n_{i,j,k}>0 \\ u^n_{i,j,k}\frac{w^n_{i+1,j,k}-w^n_{i,j,k}}{\Delta x}, & u^n_{i,j,k}<0 \end{cases} -
$$

$$
-\begin{cases} v^n_{i,j,k}\frac{w^n_{i,j,k}-w^n_{i,j-1,k}}{\Delta y}, & v^n_{i,j,k}>0 \\ v^n_{i,j,k}\frac{w^n_{i,j+1,k}-w^n_{i,j,k}}{\Delta y}, & v^n_{i,j,k}<0 \end{cases} -
$$

$$
-\begin{cases} w^n_{i,j,k}\frac{w^n_{i,j,k}-w^n_{i,j,k-1}}{\Delta z}, & w^n_{i,j,k}>0 \\ w^n_{i,j,k}\frac{w^n_{i,j,k+1}-w^n_{i,j,k}}{\Delta z}, & w^n_{i,j,k}<0 \end{cases} +
$$

$$
+\frac{1}{\Delta x^2}\left[\nu^n_{e\ i+1/2,j,k}\left(w^n_{i+1,j,k}-w^n_{i,j,k}\right)-\nu^n_{e\ i-1/2,j,k}\left(w^n_{i,j,k}-w^n_{i-1,j,k}\right)w\right]+
$$

$$
+\frac{1}{\Delta y^2}\left[\nu^n_{e\ i,j+1/2,k}\left(w^n_{i,j+1,k}-w^n_{i,j,k}\right)-\nu^n_{e\ i,j-1/2,k}\left(w^n_{i,j,k}-w^n_{i,j-1,k}\right)\right]+
$$

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

The update equation over time is:

$$w'_{i,j,k} = w^n_{i,j,k} + \Delta t \begin{pmatrix} -\begin{cases} u^n_{i,j,k} \frac{w^n_{i,j,k} - w^n_{i-1,j,k}}{\Delta x} & if\ u^n_{i,j,k} > 0 \\ u^n_{i,j,k} \frac{w^n_{i+1,j,k} - w^n_{i,j,k}}{\Delta x} & if\ u^n_{i,j,k} < 0 \end{cases} - \\ -\begin{cases} v^n_{i,j,k} \frac{w^n_{i,j,k} - w^n_{i,j-1,k}}{\Delta y} & if\ v^n_{i,j,k} > 0 \\ v^n_{i,j,k} \frac{w^n_{i,j+1,k} - w^n_{i,j,k}}{\Delta y} & if\ v^n_{i,j,k} < 0 \end{cases} - \\ -\begin{cases} w^n_{i,j,k} \frac{w^n_{i,j,k} - w^n_{i,j,k-1}}{\Delta z} & if\ w^n_{i,j,k} > 0 \\ w^n_{i,j,k} \frac{w^n_{i,j,k+1} - w^n_{i,j,k}}{\Delta z} & if\ w^n_{i,j,k} < 0 \end{cases} \end{pmatrix} +$$

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

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.

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

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:

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

Linear conditions 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:

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

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.

$$\frac{k_{i,j,k}^{n+1}-k_{i,j,k}^{n}}{\Delta t} + \begin{cases} u_{i,j,k}^{n+1}\frac{k_{i,j,k}^{n}-k_{i-1,j,k}^{n}}{\Delta x}, & u_{i,j,k}^{n+1} > 0 \\ u_{i,j,k}^{n+1}\frac{k_{i+1,j,k}^{n}-k_{i,j,k}^{n}}{\Delta x}, & u_{i,j,k}^{n+1} < 0 \end{cases} + $$
$$+ \begin{cases} v_{i,j,k}^{n+1}\frac{k_{i,j,k}^{n}-k_{i,j-1,k}^{n}}{\Delta y}, & v_{i,j,k}^{n+1} > 0 \\ v_{i,j,k}^{n+1}\frac{k_{i,j+1,k}^{n}-k_{i,j,k}^{n}}{\Delta y}, & v_{i,j,k}^{n+1} < 0 \end{cases} +$$

$$+ \begin{cases} w_{i,j,k}^{n+1}\frac{k_{i,j,k}^{n}-k_{i,j,k-1}^{n}}{\Delta z}, & w_{i,j,k}^{n+1} > 0 \\ w_{i,j,k}^{n+1}\frac{k_{i,j,k+1}^{n}-k_{i,j,k}^{n}}{\Delta z}, & w_{i,j,k}^{n+1} < 0 \end{cases} = +P_{k\ i,j,k}^{n+1} - \beta^* k_{i,j,k}\omega_{i,j,k} +$$
$$+\frac{1}{\Delta x}\left[\left(\nu + \frac{\nu_{t\ i+1/2,j,k}^{n}}{\sigma_k}\right)\frac{k_{i+1,j,k}-k_{i,j,k}}{\Delta x} - \left(\nu + \frac{\nu_{t\ i-1/2,j,k}^{n}}{\sigma_k}\right)\frac{k_{i,j,k}-k_{i-1,j,k}}{\Delta x}\right] +$$
$$+\frac{1}{\Delta y}\left[\left(\nu + \frac{\nu_{t\ i+1/2,j,k}^{n}}{\sigma_k}\right)\frac{k_{i,j+1,k}-k_{i,j,k}}{\Delta y} - \left(\nu + \frac{\nu_{t\ i-1/2,j,k}^{n}}{\sigma_k}\right)\frac{k_{i,j,k}-k_{i,j-1,k}}{\Delta y}\right] +$$
$$+\frac{1}{\Delta z}\left[\left(\nu + \frac{\nu_{t\ i,j,k+1/2}^{n}}{\sigma_k}\right)\frac{k_{i,j,k+1}-k_{i,j,k}}{\Delta z} - \left(\nu + \frac{\nu_{t\ i,j,k-1/2}^{n}}{\sigma_k}\right)\frac{k_{i,j,k}-k_{i,j,k-1}}{\Delta z}\right].$$

The update equation over time is:

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

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

Turbulent frequency level discretization to do:

$$\frac{\omega_{i,j,k}^{n+1} - \omega_{i,j,k}^{n}}{\Delta t} + \begin{cases} u_{i,j,k}^{n+1}\frac{\omega_{i,j,k}^{n}-\omega_{i-1,j,k}^{n}}{\Delta x}, & u_{i,j,k}^{n+1} > 0 \\ u_{i,j,k}^{n+1}\frac{\omega_{i+1,j,k}^{n}-\omega_{i,j,k}^{n}}{\Delta x}, & u_{i,j,k}^{n+1} < 0 \end{cases} +$$

$$+ \begin{cases} v_{i,j,k}^{n+1}\frac{\omega_{i,j,k}^{n}-\omega_{i,j-1,k}^{n}}{\Delta y}, & v_{i,j,k}^{n+1} > 0 \\ v_{i,j,k}^{n+1}\frac{\omega_{i,j+1,k}^{n}-\omega_{i,j,k}^{n}}{\Delta y}, & v_{i,j,k}^{n+1} < 0 \end{cases} + \begin{cases} w_{i,j,k}^{n+1}\frac{\omega_{i,j,k}^{n}-\omega_{i,j,k-1}^{n}}{\Delta z}, & w_{i,j,k}^{n+1} > 0 \\ w_{i,j,k}^{n+1}\frac{\omega_{i,j,k+1}^{n}-\omega_{i,j,k}^{n}}{\Delta z}, & w_{i,j,k}^{n+1} < 0 \end{cases} =$$

$$
\begin{gathered}
= +\alpha\frac{\omega_{i,j,k}}{k_{i,j,k}}P^{n+1}_{k\,i,j,k} - \beta\omega^2_{i,j,k} + \\
+\frac{1}{\Delta x}\left[\left(\nu + \frac{\nu^n_{t\;i+1/2,j,k}}{\sigma_\omega}\right)\frac{\omega^n_{i+1,j,k}-\omega^n_{i,j,k}}{\Delta x} - \left(\nu + \frac{\nu^n_{t\;i-1/2,j,k}}{\sigma_\omega}\right)\frac{\omega^n_{i,j,k}-\omega^n_{i-1,j,k}}{\Delta x}\right] + \\
+\frac{1}{\Delta y}\left[\left(\nu + \frac{\nu^n_{t\;i,j+1/2,k}}{\sigma_\omega}\right)\frac{\omega^n_{i,j+1,k}-\omega^n_{i,j,k}}{\Delta y} - \left(\nu + \frac{\nu^n_{t\;i,j-1/2,k}}{\sigma_\omega}\right)\frac{\omega^n_{i,j,k}-\omega^n_{i,j-1,k}}{\Delta y}\right] + \\
+\frac{1}{\Delta z}\left[\left(\nu + \frac{\nu^n_{t\;i,j,k+1/2}}{\sigma_\omega}\right)\frac{\omega^n_{i,j,k+1}-\omega^n_{i,j,k}}{\Delta z} - \left(\nu + \frac{\nu^n_{t\;i,j,k-1/2}}{\sigma_\omega}\right)\frac{\omega^n_{i,j,k}-\omega^n_{i,j,k-1}}{\Delta z}\right].
\end{gathered}
$$

The update equation over time is:

$$
\begin{gathered}
\omega^{n+1}_{i,j,k} = \omega^n_{i,j,k} - \\
-\Delta t\left(\begin{gathered}
\begin{cases} u^n_{i,j,k}\dfrac{\omega^n_{i,j,k}-\omega^n_{i-1,j,k}}{\Delta x} & if\ u^n_{i,j,k} > 0 \\ u^n_{i,j,k}\dfrac{\omega^n_{i+1,j,k}-\omega^n_{i,j,k}}{\Delta x} & if\ u^n_{i,j,k} < 0 \end{cases} + \\
+\begin{cases} v^n_{i,j,k}\dfrac{\omega^n_{i,j,k}-\omega^n_{i,j-1,k}}{\Delta y} & if\ v^n_{i,j,k} > 0 \\ v^n_{i,j,k}\dfrac{\omega^n_{i,j+1,k}-\omega^n_{i,j,k}}{\Delta y} & if\ v^n_{i,j,k} < 0 \end{cases} + \\
+\begin{cases} w^n_{i,j,k}\dfrac{\omega^n_{i,j,k}-\omega^n_{i,j,k-1}}{\Delta z} & if\ w^n_{i,j,k} > 0 \\ w^n_{i,j,k}\dfrac{\omega^n_{i,j,k+1}-\omega^n_{i,j,k}}{\Delta z} & if\ w^n_{i,j,k} < 0 \end{cases}
\end{gathered}\right)
\end{gathered}
$$

$$
+\Delta t\left(\begin{gathered}
\frac{1}{\Delta x}\left[\left(\nu + \frac{\nu^n_{t\;i+1/2,j,k}}{\sigma_\omega}\right)\frac{\omega^n_{i+1,j,k}-\omega^n_{i,j,k}}{\Delta x} - \left(\nu + \frac{\nu^n_{t\;i-1/2,j,k}}{\sigma_\omega}\right)\frac{\omega^n_{i,j,k}-\omega^n_{i-1,j,k}}{\Delta x}\right] + \\
+\frac{1}{\Delta y}\left[\left(\nu + \frac{\nu^n_{t\;i,j+1/2,k}}{\sigma_\omega}\right)\frac{\omega^n_{i,j+1,k}-\omega^n_{i,j,k}}{\Delta y} - \left(\nu + \frac{\nu^n_{t\;i,j-1/2,k}}{\sigma_\omega}\right)\frac{\omega^n_{i,j,k}-\omega^n_{i,j-1,k}}{\Delta y}\right] + \\
+\frac{1}{\Delta z}\left[\left(\nu + \frac{\nu^n_{t\;i,j,k+1/2}}{\sigma_\omega}\right)\frac{\omega^n_{i,j,k+1}-\omega^n_{i,j,k}}{\Delta z} - \left(\nu + \frac{\nu^n_{t\;i,j,k-1/2}}{\sigma_\omega}\right)\frac{\omega^n_{i,j,k}-\omega^n_{i,j,k-1}}{\Delta z}\right] + \\
+\alpha\frac{\omega_{i,j,k}}{k_{i,j,k}}P^n_{k\;i,j,k} - \beta\omega^2_{i,j,k}.
\end{gathered}\right)
$$

Boundary conditions.

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

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

Calculation of turbulent viscosity:

$$
\nu^{n+1}_{t\,i,j,k} = \frac{k^{n+1}_{i,j,k}}{\omega^{n+1}_{i,j,k}}.
$$

Material transport discretization:

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

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

The update equation over time is:

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

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

Borderline at points of functions values determination

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

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 Conclusion

study the transport of pollutants 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 emission source characteristics, as well as the physicochemical properties of pollutants.

The results obtained showed that the model is sufficiently suitable. 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.

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УДК 519.6

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ РАСПРОСТРАНЕНИЯ ПРИМЕСЕЙ В ТУРБУЛЕНТНЫХ ВОЗДУШНЫХ ПОТОКАХ ПОГРАНИЧНОГО СЛОЯ АТМОСФЕРЫ

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В работе представлена математическая модель распространения примесей в турбулентных воздушных потоках пограничного слоя атмосферы, основанная на уравнении адвекции–диффузии, системе уравнений Навье–Стокса и дополненная моделью турбулентности $k-\varepsilon$. В такой постановке модель позволяет получить достаточно точное описание пространственно-временной динамики концентрации загрязняющих веществ. Точечный источник выброса задан через дельта-функцию Дирака, что позволяет корректно описывать локализованные эмиссии примеси. Для численного решения поставленной задачи предложен алгоритм на основе конечно-разностной схеме с направленной аппроксимацией потоков и итерационной коррекцией давления методом сопряжённых градиентов. Граничные и начальные условия сформулированы для приземного слоя атмосферы с учетом пространственной неоднородности ветрового поля и вертикального градиента турбулентной энергии. Разработанная модель обеспечивает устойчивое решение задачи и может быть использована для анализа динамики распространения загрязняющих веществ, прогноза качества воздуха и оптимизации систем вентиляции городской среды при различных метеорологических условиях.

Ключевые слова: атмосферное моделирование, турбулентная диффузия, конечно-разностная аппроксимация, поле скоростей и давления, экологическое прогнозирование.

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