Investigation of the Stability and Convergence of Difference Schemes for the Three-dimensional Equations of the Atmospheric Boundary Layer

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Abstract—In this article we construct a finite-difference scheme for the three-dimensional equations of the atmospheric boundary layer. The solvability of the mathematical model is proved and quality properties of the solutions are studied. A priori estimates are derived for the solution of the differential equations. The mathematical questions of the difference schemes for the equations of the atmospheric boundary layer are studied. Nonlinear terms are approximated such that the integral term of the identity vanishes when it is scalar multiplied. This property of the difference scheme is formulated as a lemma. Main a priori estimates for the solution of the difference problem are derived. Approximation properties are investigated and the theorem of convergence of the difference solution to the solution of the differential problem is proved.

Keywords—atmospheric boundary layer equations, difference scheme, approximation error, stability, convergence algorithm, numerical solution.

I. INTRODUCTION

MATHEMATICAL models of computational fluid dynamics serves as the basis for the study of various natural phenomena, technological processes and environmental problems. In this regard, the development and study of efficient and stable numerical algorithms for solving the system of equations of the atmospheric boundary layer and their practical implementation is relevant. There are various methods for the numerical solution of differential equations, new techniques have been developing, the work on their improvement has been continuously performed, and reassessing the methods is carried out. Basic methods for solving grid equations are systematized and described in detail in [1]. When solving the Navier–Stokes equations, explicit schemes are inefficient due to hard restrictions on the ratio of temporal and spatial steps of the computational grid, especially on finding stationary establishing solutions. Therefore, the most frequently used implicit difference scheme is unconditionally stable or has weaker constraints on the stability. An overview of the most commonly used numerical algorithms is presented e.g. in papers [2]-[10].

In [11] a new symmetric method of approximation of the non-stationary Navier-Stokes equations of the Cauchy-Kovalevskaya type is proposed. The properties of the modified problem are studied. The convergence of the solution of modified problem to the solution of the original problem is proved on an infinite time interval when $\varepsilon \to 0$. In [12] the convergence of a finite-difference scheme, approximating the primitive equations with the second order in the spatial variables, to the solution of the differential problem is proved under the natural assumption of smoothness of the solution of the original problem. Paper [13] studies difference schemes by time which accuracy order can be arbitrarily high. Difference schemes by time for solving the Navier-Stokes equations are presented. The impact of the scheme order on the calculations accuracy is examined. In [14]-[16] numerical algorithms for solving the Navier-Stokes equations using the finite element method are proposed. The analysis of stability and convergence of the proposed methods is conducted.

In [17], stable and convergent difference schemes for the boundary layer equations of the atmosphere, transport and transformation of impurities of harmful substances were constructed. A package of applied programs for the numerical simulation of atmospheric air pollution taking into account photochemical transformations and visualizations of the corresponding scenarios was developed. The problem of impurities’ distribution from point sources was considered. The results of numerical modeling of the harmful impurities’ propagation and transformation on the mesometeorological processes were presented on the example of Ust-Kamenogorsk.

II. STATEMENT OF THE PROBLEM

Consider the three-dimensional equations of the atmospheric boundary layer in a domain $\Omega = \{0 < x_i < l_i, i = 1, 2, 3\}$ with a border $S$:

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x_1} + v \frac{\partial u}{\partial x_2} + w \frac{\partial u}{\partial x_3} + \frac{\partial p}{\partial x_3} = \frac{1}{De} \frac{\partial}{\partial x_3} \left( \frac{\partial u}{\partial x_3} \right) + \frac{1}{Re_l \chi_i} \left( \frac{\partial}{\partial x_i} \left( \frac{\partial u}{\partial x_i} \right) \frac{\partial}{\partial x_1} \left( \frac{\partial u}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( \frac{\partial u}{\partial x_2} \right) + f_i(x,t) \right) \]

(1)
\[
\begin{align*}
\frac{\partial \vec{v}}{\partial t} + \vec{u} \cdot \nabla \vec{v} + \frac{\partial \rho}{\partial x_i} = -\frac{1}{\text{De}} \nabla \rho + \\
+ \left[ \frac{\partial}{\partial x_j} \left( a_{ij} \frac{\partial \vec{u}}{\partial x_j} \right) + \frac{\partial}{\partial x_k} \left( a_{jk} \frac{\partial \vec{u}}{\partial x_k} \right) + \frac{\partial}{\partial x_i} \left( a_{ik} \frac{\partial \vec{u}}{\partial x_i} \right) \right] + f_s(x,t),
\end{align*}
\]

where \( \vec{v} \) is the wind velocity vector with components \( u, v, w \), \( p \) is pressure, \( \text{De} \) is a dimensionless characteristic describing deviation of the wind from the geostrophic value, \( \text{Re}_T \) is a dimensionless number of turbulent exchange, \( \Lambda \) is a dimensionless parameter of convection, \( a_{11}, a_{22} \) are horizontal coefficients of atmospheric turbulence for the amount of movement, \( a_{33} \) is a vertical coefficient of atmospheric turbulent exchange for the amount of movement.

The system of equations (1)-(4) is complemented by the following initial and boundary conditions:

\[
V(x,0) = \vec{V}^0(x), \quad x \in \Omega; \quad V(x,t) = 0, \quad x \in S.
\]

In \( \Omega \) the function \( \vec{V}^0(x) \) is set as follows:

\[
div \vec{V}^0(x) = 0.
\]

For the numerical solution of the equations of the atmospheric boundary layer (1)-(4), a mesh with distributed velocities is used. In \( \Omega \), we introduce the meshes \( \Omega_H, \Omega_I = \Omega_h \cup \Omega_k \cup \Omega_y \cup \Omega_z \), where

\[
\Omega_h = \{ \{x_1, x_2, x_3 \} \mid x_1 = \text{i}h_j, x_2 = \text{i}h_k, x_3 = \text{i}k \},
\]

\( j = 0,1, \ldots, N_j - 1, k = 0,1, \ldots, N_k - 1 \).

\[
\Omega_h = \{ \{x_1, x_2, x_3 \} \mid x_1 = \text{i}h_j, x_2 = \text{i}h_k, x_3 = \text{i}k \},
\]

\( j = 0,1, \ldots, N_j - 1, k = 0,1, \ldots, N_k - 1 \).

\[
\Omega_h = \{ \{x_1, x_2, x_3 \} \mid x_1 = \text{i}h_j, x_2 = \text{i}h_k, x_3 = \text{i}k \},
\]

\( j = 0,1, \ldots, N_j - 1, k = 0,1, \ldots, N_k - 1 \).

Thus, the following difference scheme is constructed:

\[
\begin{align*}
\frac{\partial v_i^{\text{nl}}}{\partial t} + & u_j v_i^{\text{nl}} + \frac{\partial P_i}{\partial x_j} = \frac{1}{\text{De}} \frac{\partial P_i}{\partial x_j} + \\
+ & \left[ a_{ij} u_i^{\text{nl}} + a_{ik} u_i^{\text{nl}} \right] + f_{\text{nl}}^{\text{i},j,k},
\end{align*}
\]

\[
\begin{align*}
\frac{\partial v_j^{\text{nl}}}{\partial t} + & v_k v_j^{\text{nl}} + \frac{\partial P_j}{\partial x_k} = \frac{1}{\text{De}} \frac{\partial P_j}{\partial x_k} + \\
+ & \left[ a_{jk} v_j^{\text{nl}} + a_{ik} v_j^{\text{nl}} \right] + f_{\text{nl}}^{\text{j},i,k},
\end{align*}
\]

\[
\begin{align*}
\frac{\partial v_k^{\text{nl}}}{\partial t} + & w_i v_k^{\text{nl}} + \frac{\partial P_k}{\partial x_i} = \frac{1}{\text{De}} \frac{\partial P_k}{\partial x_i} + \\
+ & \left[ a_{ki} v_k^{\text{nl}} + a_{ik} v_k^{\text{nl}} \right] + f_{\text{nl}}^{\text{k},i,j},
\end{align*}
\]

where \( t \) is time, \( x_1, x_2, x_3 \) are Cartesian coordinates, \( \vec{V} \) is the wind velocity vector with components \( u, v, w \), \( \text{De} \) is a dimensionless characteristic describing deviation of the wind from the geostrophic value, \( \text{Re}_T \) is a dimensionless number of turbulent exchange, \( \Lambda \) is a dimensionless parameter of convection, \( a_{ij}, a_{ik} \) are horizontal coefficients of atmospheric turbulence for the amount of movement, \( a_{ik} \) is a vertical coefficient of atmospheric turbulent exchange for the amount of movement.

The continuity equation in a difference form is written as follows:

\[
div \vec{V}^{\text{nl}} = u_i^{\text{nl}} + v_j^{\text{nl}} + w_k^{\text{nl}} + \omega_{i,j,k} = 0.
\]

The following initial and boundary conditions are satisfied:

\[
\begin{align*}
u_i^{\text{nl}}(x_1, x_2, x_3, 0) &= V_0(x_1, x_2, x_3), \\
\partial_{x_i} u_i^{\text{nl}}(x_1, x_2, x_3, 0) &= 0.
\end{align*}
\]

The following identities hold:

\[
\begin{align*}
u_i^{\text{nl}}(x_1, x_2, x_3, j) &= \frac{1}{\text{De}} \frac{\partial P_i}{\partial x_j}, \\
\partial_{x_j} P_i^{\text{nl}}(x_1, x_2, x_3, j) &= \frac{1}{\text{De}} \frac{\partial P_j}{\partial x_k}, \\
\partial_{x_k} P_k^{\text{nl}}(x_1, x_2, x_3, j) &= \frac{1}{\text{De}} \frac{\partial P_k}{\partial x_i}.
\end{align*}
\]

Thus, the following basic energy inequality:

\[
\begin{align*}
\int_{\Omega} (P + & 2u_i v_i + v_j v_j + w_i w_i) \, dx + \int_{\Gamma} \left\{ \partial_{n_i} u_i^{\text{nl}} + \partial_{n_j} v_j^{\text{nl}} + \partial_{n_k} w_k^{\text{nl}} \right\} \, ds \\
+ & \sum_{i,j,k} \int_{\Omega} a_{ij} u_i^{\text{nl}} v_j^{\text{nl}} + a_{ik} u_i^{\text{nl}} w_k^{\text{nl}} + a_{jk} v_j^{\text{nl}} w_k^{\text{nl}} \, dx \\
+ & \sum_{i,j,k} \int_{\Omega} \frac{\partial_{n_i} P_i^{\text{nl}} + \partial_{n_j} P_j^{\text{nl}} + \partial_{n_k} P_k^{\text{nl}}}{\text{De}} \, dx \\
+ & \sum_{i,j,k} \int_{\Gamma} \frac{\partial_{n_i} P_i^{\text{nl}} + \partial_{n_j} P_j^{\text{nl}} + \partial_{n_k} P_k^{\text{nl}}}{\text{De}} \, ds \\
= & \int_{\Omega} \int_{0}^{T} \left\{ \frac{\partial_{n_i} P_i^{\text{nl}} + \partial_{n_j} P_j^{\text{nl}} + \partial_{n_k} P_k^{\text{nl}}}{\text{De}} \right\} \, dx \, dt.
\end{align*}
\]

Let us evaluate the term in equation (14). Considering the conditions (11), it can be seen that

\[
\begin{align*}
\text{d}_e &= \frac{1}{\text{De}} \frac{\partial_{n_i} P_i^{\text{nl}} + \partial_{n_j} P_j^{\text{nl}} + \partial_{n_k} P_k^{\text{nl}}}{\text{De}} \int_{\Gamma} \int_{0}^{T} \left\{ \frac{\partial_{n_i} P_i^{\text{nl}} + \partial_{n_j} P_j^{\text{nl}} + \partial_{n_k} P_k^{\text{nl}}}{\text{De}} \right\} \, ds \, dt.
\end{align*}
\]
Using Young's inequality and the boundedness of the coefficient \( a(x_1, x_2, x_3) \) from below, we have

\[
|k| C \left[ |\nabla u|^2 + |\nabla v|^2 + |\nabla w|^2 + |\nabla \nabla u|^2 \right]
\]

where

\[
\left|\nabla v\right| = \left|\nabla u\right| + \left|\nabla w\right|
\]

and

\[
C_i = 0.5 \text{ are } C \nu.
\]

The term \( S_k \) can be written as follows:

\[
S_k = \sum_{n=0}^{\infty} \sum_{i,j,k} \bar{u}_{n,i,j,k} \bar{v}_{n,i,j,k} \bar{w}_{n,i,j,k} = \sum_{n=0}^{\infty} \sum_{i,j,k} \bar{u}_{n,i,j,k} \bar{v}_{n,i,j,k} \bar{w}_{n,i,j,k}.
\]

Further, using Young's inequality, we have

\[
\sum_{n=0}^{\infty} \sum_{i,j,k} \bar{u}_{n,i,j,k} \bar{v}_{n,i,j,k} \bar{w}_{n,i,j,k} + \sum_{n=0}^{\infty} \sum_{i,j,k} \bar{u}_{n,i,j,k} \bar{v}_{n,i,j,k} \bar{w}_{n,i,j,k}
\]

Adding non-negative summations

\[
\sum_{n=0}^{\infty} \sum_{i,j,k} \bar{u}_{n,i,j,k} \bar{v}_{n,i,j,k} \bar{w}_{n,i,j,k} + \sum_{n=0}^{\infty} \sum_{i,j,k} \bar{u}_{n,i,j,k} \bar{v}_{n,i,j,k} \bar{w}_{n,i,j,k} + \sum_{n=0}^{\infty} \sum_{i,j,k} \bar{u}_{n,i,j,k} \bar{v}_{n,i,j,k} \bar{w}_{n,i,j,k}
\]

to the right-hand side of the inequality, we obtain

\[
\left[\sum_{n=0}^{\infty} \sum_{i,j,k} \bar{u}_{n,i,j,k} \bar{v}_{n,i,j,k} \bar{w}_{n,i,j,k}\right]^2.
\]

By virtue the Lemma proved above, we have

\[
2\sigma \left( V^2 \phi^2 \right) = 2\sigma \left( V^2 \phi \right)^2.
\]

Using the Cauchy-Schwarz inequality we obtain:

\[
\left[2\sigma \left(L_{\phi^2} V^2 \phi^2\right) \leq C \sigma^2 \left( \sum_{n=0}^{\infty} \sum_{i,j,k} (u^2_{n,i,j,k} + v^2_{n,i,j,k} + \omega^2_{n,i,j,k}) \right)^{1/2} \right]^2
\]

The term \( \left[ V^2 \phi \right]^2 \) is evaluated as follows [18]:

\[
\left[ V^2 \phi \right]^2 \leq \left( \frac{4}{3} \right)^2 \left[ V^2 \phi (V^2 \phi)^2 \right]^2.
\]

Then

\[
\left[2\sigma \left(L_{\phi^2} V^2 \phi^2\right) \leq C \sigma^2 \left( \sum_{n=0}^{\infty} \sum_{i,j,k} (u^2_{n,i,j,k} + v^2_{n,i,j,k} + \omega^2_{n,i,j,k}) \right)^{1/2} \right]^2
\]

where

\[
C_\phi = C \sigma^2 \left( \frac{4}{3} \right)^2.
\]

\[
\left[ V^2 \phi \right]^2 \leq \left( \frac{4}{3} \right)^2 \left[ V^2 \phi (V^2 \phi)^2 \right]^2
\]

Hence we have

\[
V^2 \phi \leq C_\phi \sum_{n=0}^{\infty} \sum_{i,j,k} \left( u^2_{n,i,j,k} + v^2_{n,i,j,k} + \omega^2_{n,i,j,k} \right)
\]

\[
\leq 2 \left( \frac{4}{3} \right)^2 \left( \sum_{n=0}^{\infty} \sum_{i,j,k} \left( u^2_{n,i,j,k} + v^2_{n,i,j,k} + \omega^2_{n,i,j,k} \right) \right).
\]

In order to study the convergence of the solution of finite difference problem to the solution of the differential problem, we consider the finite difference equations for the equations of the atmospheric boundary layer:
\begin{equation}
\phi_{k,j}^{(1)} = \frac{1}{2} \sum_{i=0}^{N_k} \phi_{i,j}^{(1)} + \frac{1}{2} \sum_{i=0}^{N_j} \phi_{k,i}^{(1)} + \frac{1}{2} \sum_{i=0}^{N_k} \phi_{i,j}^{(1)} + \frac{1}{2} \sum_{i=0}^{N_j} \phi_{k,i}^{(1)} + \sum_{i=0}^{N_k} \sum_{i=0}^{N_j} \phi_{i,j}^{(1)}
\end{equation}

and it has the second order of approximation by \( h \) and the first order by \( \tau \) [19].

The initial and boundary conditions for the problem of errors (34)-(37) are defined as follows:

\begin{align*}
\phi_{k,j}^{(1)}(x,0) &= 0, \quad \phi_{k,j}^{(1)}(0,y) = 0, \\
\phi_{k,j}^{(1)}(I_1,0) &= \phi_{k,j}^{(1)}(0,y) = 0
\end{align*}

where \( I_1 \) is the characteristic scale of length, the wind speed and temperature are set as follows: \( L = 35000 \) m, \( U^* = 10 \) m/s, \( \theta^* = 20^\circ C \).

Multiplying the differential equation (34)-(37) by \( 2\phi_{k,j}^{(1)} h_{1/2} h_{1/2} h_{1/2}, \) and summing by grid domains \( Q_x, Q_y, Q_z, \), we obtain

\begin{equation}
\sigma^{\alpha+1} = 1 + \frac{5}{2} \frac{C_\nu}{2} \sigma^{\alpha} + \frac{2}{\tau} (1 - 2C_\nu) \sigma^{\alpha} + (1 - 2C_\nu) \sigma^{\alpha} + 2 (1 - 2C_\nu) \sigma^{\alpha}
\end{equation}

Let us denote \( \alpha = 1; \beta = 1; \) and rewrite (40) as follows:

\begin{equation}
\sigma^{\alpha+1} - \sigma^{\alpha} = \left( \frac{2}{\tau} \right) (1 - 2C_\nu) \sigma^{\alpha} + (1 - 2C_\nu) \sigma^{\alpha} + 2 (1 - 2C_\nu) \sigma^{\alpha}
\end{equation}

where \( C_\nu = 1 - 2C_\nu. \)

Considering that \( \alpha = 1 \), we have

\begin{equation}
\sigma^{\alpha+1} - \sigma^{\alpha} = \left( \frac{2}{\tau} \right) (1 - 2C_\nu) \sigma^{\alpha} + (1 - 2C_\nu) \sigma^{\alpha} + 2 (1 - 2C_\nu) \sigma^{\alpha}
\end{equation}

where \( C_\nu = 1 - 2C_\nu. \)

IV. NUMERICAL CALCULATIONS

The numerical calculations with different values of the input parameters were performed based on the model and the proposed algorithm described above. The considering area is \( 35 \times 35 \) km², and the height of the surface layer is 3500 m. The convection parameter \( \lambda = 0.16 \) \( m^2 / (kg \cdot °C) \). The stratification parameter \( S \) in terms of physical meaning determine the temperature variations with altitude; therefore the calculations were performed based on the vertical temperature gradient. Caroles force is equal to \( I = 10^{-3} \) s⁻¹.

The values of the horizontal and vertical turbulent exchange coefficients were taken as follow: \( \mu_x = \mu_y = 6 \times 10^2 m^2 / s \), \( \nu = 30 m^2 / s \).

The characteristic scale of length, the wind speed and temperature are set as follows: \( L = 35000 \) m, \( U^* = 10 \) m/s, \( \theta^* = 20^\circ C \).

The following formulas were used for determination of dimensionless values of the input parameters \( \lambda, L, S, \mu_x, \mu_y, X, Y, H \):

\begin{align*}
\lambda^* &= \frac{\lambda}{U^*}, \quad I^* = \frac{I}{U^*}, \quad S^* = \frac{S}{\theta^*}, \quad \mu_x^* = \frac{\mu_x}{L \cdot U^*}, \quad \mu_y^* = \frac{\mu_y}{L \cdot U^*}, \quad X^* = \frac{X}{L}, \quad Y^* = \frac{Y}{L}, \quad H^* = \frac{H}{L}
\end{align*}

where \( U^* \) is characteristic velocity, \( \theta^* \) is characteristic temperature, \( L \) is the length scale.

Figures 1 and 2 show the wind deflection over the water surfaces. This process is observed at moderate wind speeds and it is difficult to see it at high speeds of the fluctuations wind over water surfaces.
Fig. 2. The deviation of wind direction above the water surfaces at a wind speed equal to 2 m/s

Fig. 3. Isolines of CO (carbon monoxide) distribution under the unstable weather conditions (in the absence of wind)

Fig. 4. Isolines of CO$_2$ (carbon dioxide) distribution under the unstable weather conditions (in the absence of wind)

Fig. 5. Isolines of CO (carbon monoxide) distribution at the west wind direction at a speed equal to 1 m/s

Fig. 6. Isolines of the distribution of CO$_2$ (carbon dioxide) in the west wind direction at a speed equal to 2 m/s

Fig. 7. The isolines of CO distribution (carbon monoxide) in the north-west direction of the wind at a speed equal to 6 m/s
The source of carbon monoxide CO is the gas emission of cars. It is formed by the combustion of fuel in the internal combustion engines at insufficient temperatures [20]-[22]. Under the natural conditions, CO carbon monoxide is formed on the surface of the earth during the incomplete decomposition of organic compounds and the combustion of biomass, mainly during the forest fires. Figures 3 and 4 show the distribution isolines of this substance over the city of Ust-Kamenogorsk in the absence of wind.

Figures 5, 6 and 7 show the isolines of contaminant distribution in the west and north-west wind directions.

As a result of numerical experiments, it was established that the anthropogenic impurity produced by industrial enterprises and picked up by wind currents at different directions, moves to large distances depending on the wind speed, which leads to the imposition of pollution fields. At unfavorable meteorological conditions, anthropogenic impurity forms a cloud over an industrial city.

REFERENCES