Modeling of the Turbulent Mixing on Basis of the Large Eddy Simulation by Using Parallel Computing

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Abstract

In the research the numerical simulation of the room’s ventilation was performed on the basis of the large eddy simulation. The numerical algorithm was developed by using the physical parameters splitting scheme. Poisson equation for pressure field is solved by Fourier method in combination with tridiagonal matrix method for determination of Fourier coefficients. The parallel programming technique MPI in combination with directives of OpenMP was applied to solve the assign task, as the most relevant for today and the most efficient a view of the productivity improvement of complex calculations. Simulation data are represented as three-dimensional graphs.

Mathematics Subject Classification: 68M14, 76D05, 76F65

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1 Introduction

Nowadays one of the most actual problems of the continuum mechanics and the plasma physics is the simulation of complex transitional and turbulent motions by the modern computer science, algorithms and approaches of the applied mathematics. Abundant in practice turbulent flows are characterized by the pronounced nonstationarity and nonlinearity of occurring processes, by presence of large shifts of medium, by diversified and complex mechanism of interaction, by energy dissipation. These include, for instance, such gas-dynamic problems as problems on flow in the wake of the moving body, on interaction of injection stream with the main flow, etc. Among known methods of numerical simulation of three-dimensional turbulent flows, it is necessary to mark a direct numerical simulation of turbulence and the solution of averaged Navier-Stokes equations. To use the direct numerical simulation there is a need of really powerful computational resources. On the other hand, the use of averaged Navier-Stokes equations requires much less computational resources however turbulence models used for closing equations do not have acceptable universalism and may not be applied for a wide range of applied problems. The large eddy simulation method is a compromise between the direct numerical simulation and averaged Navier-Stokes equations. In the large eddy method, the solution filtered by space Navier-Stokes equations is implemented and movement of large eddy is permitted only. In this paper the problem of non-stationary turbulent three-dimensional flow on the example of the room’s ventilation was investigated. An aperture was made in a ceiling through which air flow is injected in. Apertures for air outlet from the room are made in the walls near the floor. The rectangular source of concentration was given on the bottom of the region under consideration. Actually, the algorithm property not distorting of obtained by counting process grid solutions by circuit oscillations is of great importance in case of flows with heavy gradients. If this condition is not satisfied, the computation process may be really complicated or impossible at all. The order of approximation of convective members in equations describing flow with the viscosity must exceed the first order, otherwise there will be a risk of distorting the solutions due to circuit viscosity, or spatial grid pitches shall be selected irrationally little.

2 Mathematical model

The problem of flow concentration distribution indoors was considered in this research. The mathematical model of this process is based on Navier-Stokes equations describing three-dimensional non-stationary turbulent flows and looking as follows [1]:
\[
\frac{\partial \bar{\pi}_i}{\partial t} + \frac{\partial \bar{\pi}_i u_i}{\partial x_j} = - \frac{\partial \bar{\tau}}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left( \frac{\partial \bar{\pi}_i}{\partial x_j} \right) - \frac{\partial \tau_{ij}}{\partial x_j} \tag{1}
\]

where

\[
\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j
\tag{3}
\]

Equations [1] and [3] are averaged by space and Navier-Stokes equations are obtained with additional member \( \tau_{ij} \).

Moreover three-dimensional model of active impurity indoor transportation is used for simulating of the concentration distribution.

\[
\frac{\partial C}{\partial t} + \frac{\partial u_j C}{\partial x_j} = \frac{\partial}{\partial x_j} \left( (D + \alpha T) \frac{\partial C}{\partial x_j} \right) \tag{4}
\]

\( u_i \) – velocity components, \( D \) – diffusion coefficient, \( \alpha T = \nu / \text{Pr} \).

Furthermore, initial and boundary conditions satisfying the equation were set (2) for non-stationary flow [3].

And Smagorinsky dynamic model is used as a turbulence model [2] and [7]. To apply the dynamic model, double averaging is performed with filter length \( \Delta = 2\Delta \), then

\[
\frac{\partial \bar{\pi}_i}{\partial t} + \frac{\partial \bar{\pi}_i u_i}{\partial x_j} = - \frac{\partial \bar{\tau}}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left( \frac{\partial \bar{\pi}_i}{\partial x_j} \right) - \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial (\bar{u}_j u_i - \bar{u}_j \bar{u}_i)}{\partial x_j} \tag{5}
\]

Subjected to averaging with two filters with the length \( \bar{\Delta} \) and \( \Delta \) respectively equation (1) looks as follows:

\[
\frac{\partial \bar{\pi}_i}{\partial t} + \frac{\partial \bar{\pi}_i u_i}{\partial x_j} = - \frac{\partial \bar{\tau}}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left( \frac{\partial \bar{\pi}_i}{\partial x_j} \right) - \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial T_{ij}}{\partial x_j}, \tag{6}
\]

where \( T_{ij} = \bar{u}_j \bar{u}_i - \bar{u}_j \bar{u}_i \),

from (5) and (6) it follows \( T_{ij} = \tau_{ij} + \bar{u}_j \bar{u}_i - \bar{u}_j \bar{u}_i \), then \( T_{ij} \) looks as follows:

\[
T_{ij} = - \frac{1}{3} \delta_{ij} T_{kk} = - 2(C_s \Delta)^2 (2s_{ij} s_{ij})^{1/2} s_{ij},
\]

and Leonard stresses are:

\[
L_{ij} = - \frac{1}{3} \delta_{ij} L_{kk} = - 2(C_s)^2 \left( (\bar{\Delta})^2 (2s_{ij} s_{ij})^{1/2} \bar{s}_{ij} - (\Delta)^2 (2s_{ij} s_{ij})^{1/2} \bar{s}_{ij} \right). \tag{7}
\]

Value of \( C_s \) is found in the form

\[
C_s^2 = - \frac{1}{2} \frac{L_{ij} M_{ij}}{M_{kk} M_{kk}} \text{ from (6) with the application of least-squares method.}
\]
where $M_{ij} = \left[ \Delta^2 \left( \frac{1}{2} \sigma_{ij} \sigma_{ij} \right)^{1/2} - \left( \Delta^2 \frac{1}{2} \sigma_{ij} \sigma_{ij} \right)^{1/2} \right]$.

The numerical solution of system (1) - (2) is carried out on staggered grid with the use of scheme against the flow of the second type:

$$\frac{\partial u_\zeta}{\partial x} = \frac{u_R \xi_R - u_L \xi_L}{\Delta x},$$

where $\zeta$ can be $u,v,w$

$$u_L = \frac{u_i + u_{i-1}}{2}, \quad u_R = \frac{u_{i+1} + u_i}{2},$$

$$\xi_L = \left\{ \begin{array}{ll}
\xi_{i-1}, & u_L > 0 \\
\xi_i, & u_L < 0
\end{array} \right., \quad \xi_R = \left\{ \begin{array}{ll}
\xi_i, & u_R > 0 \\
\xi_{i+1}, & u_R < 0
\end{array} \right.,$$

and compact approximation for a convective [6]

$$f(x) = \frac{du}{dx},$$

$$\alpha f_{i-1} + \beta f_i + \gamma f_{i+1} = \frac{u_j - u_{j-1}}{h}.$$

Expanding functions $f(x)$ and $u(x)$ in Taylor series we can identify $\alpha, \beta, \gamma$.

3 Numerical algorithm

The scheme of physical parameters splitting was used in order to solve the problem in view of the above proposed model of turbulence [8].

We propose the following physical interpretation of the splitting scheme. At the first stage, it is suggested that the momentum transfer is performed only at the expense of the convection and the diffusion. The intermediate velocity field is found by the fractional step method by using of the tridiagonal matrix method. At the second stage, the pressure field is determined by the found intermediate velocity field. Poisson equation for the pressure field is solved by Fourier method in combination with the tridiagonal matrix method (Thomas algorithm) used for determination of Fourier coefficients [4]. At the third stage, it is suggested that the transfer is performed only at the expense of the pressure gradient. The problem algorithm is parallelized on the high-performance system [5] and [9].

$$I \frac{\bar{u}^n - \bar{u}^m}{\tau} = - \left( \nabla \bar{u}^m \bar{u}^* - \nu \Delta \bar{u}^* \right)$$
Modeling of the turbulent mixing on basis of the

\[ II) \Delta p = \frac{\nabla \vec{u}^*}{\tau} \]

\[ III) \frac{\vec{u}^{i+1} - \vec{u}^*}{\tau} = -\nabla p. \]

Poisson equation for the pressure field is found in the following form:

\[ \frac{p_{i+1,j,k} - p_{i,j,k} + p_{i-1,j,k} + p_{i,j+1,k} - 2p_{i,j,k} + p_{i,j-1,k} + p_{i,j,k+1} - 2p_{i,j,k} + p_{i,j,k-1}}{\Delta x^2 + \Delta y^2 + \Delta z^2} = F_{i,j,k}. \]  

(8)

We apply Fourier method to Poisson equation by which for any grid function \( f(i) \) the following expansion takes place

\[ f(i) = 2 \sum_{k=0}^{N} \rho_k \phi_k \cos \frac{\pi ki}{N}, i = 0,1 \ldots N, \]

As per these relations, we have:

\[ p_{i,j,k} = 2 \sum_{l=0}^{N_3} \rho_l a_{i,j,l} \cos \frac{\pi kl}{N_3}, F_{i,j,k} = 2 \sum_{l=0}^{N_3} \rho_l b_{i,j,l} \cos \frac{\pi kl}{N_3}, \]  

(9)

where

\[ a_{i,j,l} = \sum_{k=0}^{N_3} \rho_k p_{i,j,k} \cos \frac{\pi kl}{N_3}, b_{i,j,l} = \sum_{k=0}^{N_3} \rho_k F_{i,j,k} \cos \frac{\pi kl}{N_3}. \]  

(10)

Substituting expressions (9) into equation (8) and using formula

\[ \cos \frac{\pi(k+1)l}{N_3} + \cos \frac{\pi(k-1)l}{N_3} = 2 \cos \frac{\pi kl}{N_3} \cos \frac{\pi l}{N_3}, \]

and after simplifying the expression, we write the obtained expression at fixed value =1 and divide it by the value \( \frac{2}{N_3} \rho_l a_{i,j,l} \cos \frac{\pi kl}{N_3} = b_{i,j} \):

\[ \frac{a_{i+1,j} - 2a_{i,j} + a_{i-1,j}}{\Delta x^2} + \frac{a_{i,j+1} - 2a_{i,j} + a_{i,j-1}}{\Delta y^2} + \frac{a_{i,j} (2 \cos \frac{\pi l}{N_3} - 2) + 10a_{i,j} = b_{i,j}}{\Delta z^2} \]  

(11)

This equation is re-arranged to this form:

\[ -\frac{a_{i,j-1}}{\Delta y^2} + \left[ \frac{2}{\Delta x^2} + \frac{2}{\Delta y^2} - \frac{1}{\Delta z^2} \left( 2 \cos \frac{\pi l}{N_3} - 2 \right) - 10 \right] a_{i,j} - \frac{a_{i+1,j} + a_{i-1,j}}{\Delta x^2} \frac{a_{i,j+1} + a_{i,j-1}}{\Delta y^2} = -b_{i,j}. \]
It is known that tridiagonal matrix method belongs to direct methods for solving differential equations and applied to the equations, which can be written as a system of vector equations:

$$-A_j \overrightarrow{a}_{j-1} + B_j \overrightarrow{a}_j - C_j \overrightarrow{a}_{j+1} = \overrightarrow{F}_j, i = 1,2 \ldots N_2 - 1, \quad (12)$$

The algorithm of the tridiagonal matrix method for solving equation (12) can be written as follows:

$$\alpha_{j+1} = (B_j - A_j \alpha_j)^{-1} C_j, j = 1,2 \ldots N_2 - 1, \alpha_1 = B_0^{-1} C_0 \quad (13)$$

$$\overrightarrow{\beta}_{j+1} = (C_j - A_j \alpha_j)^{-1} (\overrightarrow{F}_j + A_j \overrightarrow{\beta}_j), j = 1,2 \ldots N_2 - 1, \overrightarrow{\beta}_1 = B_0^{-1} \overrightarrow{F}_0 \quad (14)$$

$$-A_j \overrightarrow{a}_{j-1} + B_j \overrightarrow{a}_j - C_j \overrightarrow{a}_{j+1} = \overrightarrow{F}_j, j = 1,2 \ldots N_2 - 1, \overrightarrow{a}_{N_2} = \overrightarrow{\beta}_{N_2+1} \quad (15)$$

We solve the tridiagonal matrix method to find $p_{i,j,k}$ and find $A_j$ which in its turn is parallelized for each $k$ and is collected in the master node later.

<table>
<thead>
<tr>
<th>$k=1$</th>
<th>$k=2$</th>
<th>$k=3$</th>
<th>$k=N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Processor 1</td>
<td>Processor 2</td>
<td>Processor 3</td>
<td>Processor N</td>
</tr>
</tbody>
</table>

After finding $a_{i,j,k}$ coefficients the values of the pressure field are found from formula (9). To calculate total (9) and (10) we apply fast Fourier transform method allowing us to calculate these totals for $(N \ln N)$ operations. It is considerably reduces the calculation time. The productivity improvement is displayed in the form of diagrams in figure 1. Different lines in figure 1 point out to dimensionality of subareas $N$ of the computational domain.

### 4 Results

The results of the calculation obtained on the grid 100 x 100 x 100 are presented in figures. Figures 2-4 show comparison of experimental and computational data of dynamic fields of the stream impinging the lower area and causing circulation flow by the walls. Figure 5 shows the isosurface of air outlet stream.
concentration in the lower boundary of the area. Figure 6 shows the velocity vector and the impurity concentration in the plane (X,Z). The distribution of concentration in the lower part of the room is shown in figure 7. Figure 8 shows the distribution of concentration of shifted diagonally from the center in the plane (X,Z).

5 Conclusions

Simulated results of impurity transfer into a room show that the impurity transfer and the degree of its distribution depends on the direction and the force of the stream, while the impurity concentration is distributed to major part of the room. With the time, the dynamic field attenuates, and the concentration field transforms into the state of the passive impurity and migrates in the air for pretty long. In the conclusion it is noticeable that the given mathematical model can be used for the simulation of non-stationary turbulent flows of the incompressible liquid in three-dimensional areas. Thus, the constructed model adequately describes turbulent motions of non-stationary flows in three-dimensional areas, and can be used for resolving problems of the ventilation in various premises. It is also necessary to note that within frameworks of this research we developed the parallelized algorithm of solving of
Figure 2: Comparison of experimental and computational data of dynamic fields in XZ plane in the center area

Figure 3: Comparison of experimental and computational data of dynamic fields in XZ plane in the area of air outlets
Figure 4: Comparison of experimental and computation data of dynamic fields in XY plane in the area of air outlets

Figure 5: Isosurface of air output stream concentration in the lower boundary of the area
Figure 6: Velocity vector field and impurity concentration in the plane (X,Z)

Figure 7: Distribution of concentration in the lower part of the room
Modeling of the turbulent mixing on basis of the three-dimensional Poisson equations, which allows obtaining of the more accurate result, applied techniques of parallel programming OpenMP, MPI, which considerably reduces the computational time and increases the efficiency of calculations.

References


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