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AN EXPERIENCE OF USING THE METHOD OF DIRECT NUMERICAL SIMULATION OF LARGE-SCALE TURBULENCE TO THE COMPUTATION OF SUPERSONIC TURBULENT SHEAR LAYER

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Abstract

One of the modification of Large Eddy Simulation method is developed. It is applied to the problem of mixing of two supersonic flows. Kelvin-Helmholtz instability is obtained. Instantaneous data are averaged and the shear layer thickness is calculated. It is compared with the experimental one. The conclusion about the sensitivity of the method to the change in model constants is made.

Introduction

CFD group, in which an author works on the diploma, deals with viscous and turbulent flows. Numerical method in use is based on time-averaging of Navier-Stokes equation system. This method was tested thoroughly, one of test problems was considered by the author. (1) Some good results are obtained with this method. But we are looking for the further improvements.

Now there are three ways of numerical calculation of complex turbulent flows. The first approach is the use of semiempirical turbulence models for the closure of time-averaged Navier-Stokes equation system. Its advantage consists in the possibility of using relatively large grid cells and therefore the time of calculation is acceptable. But there is an obvious drawback of this method. However, it is well-known that all methods based on semiempirical turbulence models have one essential and *unavoidable* defect: they use *the averaging over all range of turbulent motions*. But among these motions there are scales that are determined by concrete flow geometry and therefore *principally* cannot be described in universal way.

The second way – Direct numerical Simulation (DNS)- could solve the problem of universality. It doesn't use any averaging and therefore - any empirical constants. But in high Reynolds number flows the largest scales (eddies) can be 10^3 times as big as the smallest ones. It requires an enormous number of mesh points to reproduce directly all scales appeared and it takes a lot of processor time. So, a significant disadvantage of this method is the limitations to relatively law Reynolds numbers and simple geometry.

The third way – Large Eddy Simulation – seems to be very attractive. Its idea is to simulate the large scales only, accepting that the influence of the small ones is taken into account through subgrid scale (SGS) model. It is the large eddies which determine the characteristics of the individual flow, vary from one flow to another and are hard to be modeled in any universal way. In contrast, the smallest eddies are fairly universal and isotropic provided that they are in the equilibrium range. Models for them are expected to be more universal in comparison with those for time average method.

It was proposed to the author to develop a numerical method based on LES: our CFD group is going to use this perspective approach in various problems.

In this work the application of this method to the problem of mixing of two supersonic flows is presented. Various configurations of computational grid are examined in order to find the dependence of the solution on the grid. Some constants included in the subgrid scale model are varied and the conclusion is made about the sensitivity of the model to their variaton. Kelvin-Helmholtz instability characteristic for the tangential discontinuities is obtained in computation. Averaged pattern of the flow is also obtained. Shear layer growth rate is calculated using averaged data and compared with the experimental one.

1. Description of LES method

1.1. The separation process and basic equations.

The mathematical separation of eddies into large and small ones is accomplished through the filtering procedure

$$\bar{f}(\vec{x}) = \int G(\vec{x},\vec{x}')\, f(\vec{x}')\, d\,\vec{x}$$

$G(\vec{x},\vec{x}')$ -filter function with the characteristic width Δ.

Various filters are possible: Gaussian filter, filter of finite Fourier method, box filter. The latter is used at the present work. It has the form

$$G(\vec{x},\vec{x}') = \begin{cases} \dfrac{1}{V}, \left| x_i - x_i' \right| < \dfrac{h_i}{2} \\ 0 \quad \text{in the rest of space} \end{cases}$$

It corresponds to the averaging through the cell's volume (here V is the cell's volume).

This averaging procedure is applied to the Navier-Stokes equation system: Favre approach to averaging is used for all parameters except P and ρ:

$\tilde{f} = \dfrac{\overline{\rho f}}{\overline{\rho}}$. Then the system of equations to be solved has the following form:

$$\frac{\partial \vec{\mathbf{u}}}{\partial t} + \frac{\partial (\vec{\mathbf{F}}_k^{conv} + \vec{\mathbf{F}}_k^{diff})}{\partial x_k} = \vec{0}, \qquad (1),$$

where

$$\vec{\mathbf{u}} = [\overline{\rho};\ \overline{\rho}\,\tilde{u}_i;\ \overline{\varepsilon}]^T;$$

$$\vec{\mathbf{F}}_k^{conv} = \begin{bmatrix} \overline{\rho}\,\tilde{u}_k \\ \overline{\rho}\,\tilde{u}_i\,\tilde{u}_k + \overline{p}\,\delta_{ik} \\ (\overline{\varepsilon} + \overline{p})\,\tilde{u}_k \end{bmatrix} \qquad (2)$$

$$\vec{\mathbf{F}}_k^{diff} = \begin{bmatrix} 0 \\ \overline{\rho}\,\tilde{R}_{ik} - \overline{\tau}_{ik} \\ (\overline{\rho}\,\tilde{R}_{ik} - \overline{\tau}_{ik})\,\tilde{u}_i + (\overline{\rho}\,\tilde{\sigma}_k - \tilde{q}_k) + K_k \end{bmatrix} \qquad (3)$$

Well-known expressions for the full gas energy, internal gas energy per unit mass, components of the tensor of viscous stresses, heat fluxes, Satherland formula for molecular and viscous coefficients and state equation of the gas are used for the closure of the system (1). Subgrid turbulence is taken into account through the following SGS model.

1.2. Subgrid modeling. The simplest subgrid model due to Smagorinsky-Lilly is used in this method. It is based on the gradient transport hypothesis. [2-4]

$$\overline{\rho}\,(\tilde{R}_{ik} - \frac{1}{3}\tilde{R}_{kk}\,\delta_{ik}) = 2\mu_T\left[\tilde{S}_{ik} - \frac{1}{3}\tilde{d}\,\delta_{ik}\right],$$

where

$$\tilde{S}_{ik} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_k} + \frac{\partial \tilde{u}_k}{\partial x_i}\right).$$

$$\tilde{d} = \tilde{S}_{ii} = div\,\tilde{u}$$

$\tilde{R}_{ik} = \tilde{u_i''u_k''}$ - subgrid stresses.

Smagorinsky had also proposed:

$\mu_T = \overline{\rho}\cdot C_\mu \Delta^2 \tilde{\tilde{S}}$, where $\tilde{\tilde{S}} = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$,

Δ is the characteristic filter width or the mesh spacing. It could be either equal to

$$\Delta = \left(h_x h_y h_z\right)^{1/3}, \qquad (4)$$

$$\text{or } \Delta = \left(h_x^2 + h_y^2 + h_z^2\right)^{1/2}, \qquad (5)$$

$$\text{or } \Delta = min\left(h_x, h_y, h_z\right) \qquad (6)$$

depending on the structure of the problem. Lilly justified the model in terms of turbulence theory and evaluated the constant C_μ as 0.0162. [2] But in general authors vary it from ≈0.005 up to ≈0.025. [2-4]

1.3 Modeling the kinetic energy of the subgrid turbulence. Kinetic energy is directly related to the trace of the tensor of subgrid stresses

$$\tilde{k} = \frac{\tilde{u_k''u_k''}}{2} = \frac{1}{2}\tilde{R}_{kk},$$

so it is included in the formula for them:

$$\overline{\rho}\,\tilde{R}_{ik} = \frac{2}{3}\overline{\rho}\tilde{k}\,\delta_{ik} - 2\mu_T\left[\tilde{S}_{ik} - \frac{1}{3}\tilde{d}\,\delta_{ik}\right] \qquad (7).$$

Certainly, we can add the term $\frac{1}{3}\tilde{R}_{kk}$ to the pressure, i.e. replace $\overline{p} + \frac{1}{3}\tilde{R}_{kk} \to \overline{p}$ and don't distinguish "molecular" pressure from the "turbulent". [4-5] But we can also model the value of $\tilde{k}$ on the base of the following considerations.

Subgrid stresses are proportional to $\tilde{k}$:

$$\tilde{R}_{ik} = c_{ik}\cdot\tilde{k} \qquad (8)$$

After comparison with (7) we obtain

$$\mu_T\frac{\partial \tilde{u}_i}{\partial x_k} = \alpha_{ik}\overline{\rho}\tilde{k} \qquad (9)$$

Small eddies are expected to be in the range of universal equilibrium (it is the condition of the success of LES). Then the total dissipation rate of turbulent energy $\overline{\rho}\tilde{\varepsilon}$ is equal to the rate of energy transfer trough the cascade of eddies C from resolved to unresolved scales (that is, the rate of production of SGS turbulent energy).

The energy cascade is

$$C = -\overline{\rho}\,\tilde{R}_{ik}\frac{\partial \tilde{u}_i}{\partial x_k}.$$

Substituting (8) and (9) we have

$$P = -c_{ik}\alpha_{ik}\frac{\overline{\rho}^2\tilde{k}^2}{\mu_T} = c\cdot\frac{\overline{\rho}^2\tilde{k}^2}{\mu_T}, c > 0$$

From the considerations of dimensionality

$$\tilde{\varepsilon} = c_\varepsilon\frac{\tilde{k}^{3/2}}{\Delta}.$$

Then the condition $P - \overline{\rho}\tilde{\varepsilon} = 0$ gives:

$$\tilde{k} = c_k\left(\frac{\mu_T}{\overline{\rho}\,\Delta}\right)^2$$

Value of the constant c_k given in literature is 45,8. [6]

The knowledge of the value of $\tilde{k}$ enables us to simulate its diffusive and turbulent fluxes:

$$\overline{\rho}\,\widetilde{k}u_i'' - \sum_{j=1}^{3}\overline{\tau_{ij}\,u_j''} = -\left(\mu_T + \mu\right)\left(c_{ij} + \delta_{ij}\right)\frac{\partial \widetilde{k}}{\partial x_j}$$

2. Numerical method

Our numerical method and explicit and has the 2nd order of accuracy. [11,12] Approximation of basic equations is accomplished using finite-volume computational method. [7] The general form of the numerical scheme is:

$$u_{i\,jk}^{n+1} = u_{i\,jk}^{n} + \frac{\tau}{V_{i\,jk}}\left[\vec{\mathbf{Q}}^{conv} + \vec{\mathbf{Q}}^{diff}\right]$$

Godunov-Kolgan-Rodionov scheme [7-10] is chosen for the approximation of convective fluxes (2). It is the explicit monotone second order scheme. Exact solution of the Riemann problem about the decay of an arbitrary discontinuity is used for the calculation of parameters on the cell's borders by iterative method. This scheme is proved to be an optimal for the calculation of inviscid laminar flows. The modification of central-difference approximation of derivatives is used for the calculation of diffusive and turbulent fluxes (3). Predictor-corrector method is used to get the second order of approximation in time.

3. Testing of the method

3.1. Formulation of the test problem. The method described above was applied to the problem of mixing of two supersonic air streams with the following parameters:

	Upper stream	Lower stream
M	2	1.4
T, K	163	214
P, kPa	50	50

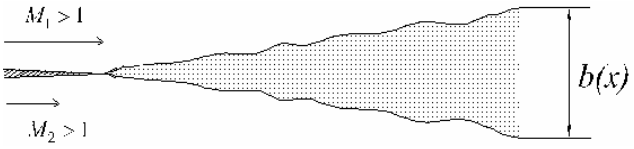


FIG.1. Flat supersonic mixing layer

Tangential discontinuity is known to be unstable with the so-called Kelvin-Helmholtz instability arising. This instability results in the transition to turbulence and formation of the turbulent shear layer. Such layer is self-similar with the growth rate *db/dx* being constant and independent on *x*.

A lot of experiments were carried out for various shear layers and the generalization of experimental data gives the following formula:

$$db/dx = \left(db/dx\right)_i \cdot K, \qquad (10)$$

where $\left(db/dx\right)_i = 0.165\dfrac{|1-r|\left(1+\sqrt{s}\right)}{2\left(1+r\sqrt{s}\right)}$,

$$r = \frac{u_2}{u_1}, \quad s = \frac{\rho_2}{\rho_1}, \quad M_{conv} = 2\frac{|u_1 - u_2|}{a_1 + a_2},$$

$$K = \begin{cases} 1 & M_{conv} \le 0.4 \\ 0.4 & M_{conv} \ge 2.0 \\ 1.15 - 0.375\,M_{conv} & 0.4 < M_{conv} < 2.0 \end{cases}$$

This value for our flows is $db/dx \sim 0.018$.

3.2. Structure of the computational grid. Both flows are supposed to have an initial velocity directed along the *x* –axis. *y*-axis is perpendicular to the surface of discontinuity. Planar shear layer is modeled, but the program used for the calculations is three-dimensional, so one cell is given in *z*-direction with the size $h_z = min\left(h_x, h_y\right)$

Characteristic filter width is chosen as (6). With any other formula for Δ (4,5) the largest aspect of the cell will define turbulent viscosity for non-square grid basically. It will result in smoothing small disturbances (they are proportional to *y*-size of the cell) by this large value of turbulent viscosity.

The primary configuration of the computational grid was the following:

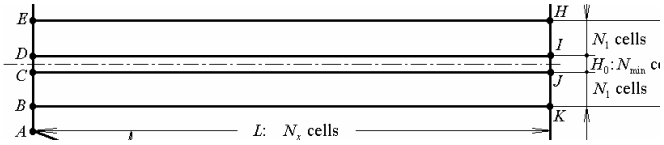


FIG.2. Configuration of the grid

The length of the computational domain in *x*-direction is 1 *m*; (so the length of each cell is 0.00167 *m*). Fine grid in *y* –direction (N_{min}=8 with H_0=0.0008 *m*) is made in order to describe more precisely the origin of the turbulence – rectangle *CDIJ* at the Fig.2. Out from this layer with fine cells the grid becomes coarser by the power-law (N_1=*16* on rectangles *DEHI* and *BCJK*). Large-scale turbulence must not theoretically go out beyond the thickness of the shear layer but we have wanted to secure ourselves from such deviations. That's why we have made the total height of the computational domain equal $KH \approx 2L \cdot \left(db/dx\right)_{theory}$, where $\left(db/dx\right)_{theory}$ is given by the formula (10).

3.1. Formulation of boundary conditions. Two eddies with random fluctuations of the velocity, density and pressure are considered to be initial disturbances to cause the turbulence. They are given at each time step at the left boundary near the surface of the discontinuity, i.e. in the layer with fine grid. In our early computations we have used the random

disturbances along the whole left boundary regarding their correlation in space, so that there was an eddy in each grid cell. It was rather difficult procedure. But it turned out to be unnecessary and two eddies are sufficient for initializing the turbulent mixing.

For each large-scale parameter of such eddy we can write $\tilde{f} = \bar{\tilde{f}} + \tilde{f}'$. $\bar{\tilde{f}}$ is the mean large-scale value of the parameter in time. We accept it equal to appropriate value of the undisturbed coming flow. Its pulsation $\tilde{f}'$ is taken to have a Gaussian distribution in time and modeled with the help of random number generator. The question is to find the value of the mean-square fluctuation for each parameter.

The dispersion of each component of the velocity can be calculated from the following considerations. Turbulent Mach number is $M_T = \dfrac{\sqrt{\overline{\tilde{u}_i'\tilde{u}_i'}}}{a}$ (summation with the repeated indexes is supposed). We consider that $\overline{\tilde{u}_x'^2} = \overline{\tilde{u}_y'^2} = \overline{\tilde{u}_z'^2}$, therefore $D_x = D_y = D_z = \dfrac{1}{3}\overline{\tilde{u}_i'\tilde{u}_i'} = \dfrac{1}{3}\left(M_T \cdot a\right)^2$.

M_T is usually considered as 0.1÷0.5, *a* is the speed of sound. We take M_T equal to 0.3 for both flows. It leads to the following value of the mean-square fluctuation for the velocity components: $\sqrt{D}$ = 44.76 *m/s* for the upper stream and $\sqrt{D}$ = 51.16 *m/s* for the lower stream; mean longitudinal velocities are 517 *m/s* and 414 *m/s,* respectively. So, the disturbances of the parameters are approximately 10% from their mean values.

If we know the value of the velocity pulsation we can also find the value of those for pressure and density from the following considerations.

Let us consider the pulsation of the full gas energy (sings of averaging are omitted).

$$e' = \left(\frac{\gamma}{\gamma-1}\frac{p}{\rho} + \frac{u^2+v^2+w^2}{2}\right)' = 0.$$

From here $p' = -\dfrac{\gamma-1}{\gamma}\rho\left(\dfrac{u^2+v^2+w^2}{2}\right)'$ (density is taken to be constant)

$\left(u^2\right)' = u^2 - \overline{u^2} = \left(\bar{u}+u'\right)^2 - \overline{\left(\bar{u}+u'\right)^2} = 2\bar{u}u' + u'^2 - \overline{u'^2}$.

Analogous expressions can be written for $\left(v^2\right)'$ and $\left(w^2\right)'$. Pulsation for density is calculated then as $\rho' = \dfrac{\gamma}{a^2}p'$.

Boundary condition at the exit is the linear extrapolation of parameters. It is correct, as both flows are supersonic. Mirror reflection of parameters is accomplished at the upper and lower surfaces of the domain. Parameters of undisturbed coming flow are taken to be an initial field. Global time step is used in the calculations since the development of the large-scale turbulence is essentially non-stationary process. Constant C_μ is taken to be 0.02.

3.4. Computation results. Such rather strong disturbances of the discontinuity surface must result in Kelvin-Helmholtz instability. Indeed, after 3-4 thousands time steps the surface begins to oscillate; fully developed structure of mixing can be observed after 15 thousands steps (see Fig.3).

FIG. 3. Instantaneous field of Mach number.

It can be seen that mirror condition slightly distorts the picture. Buffer subregions were added above and below the computational domain to avoid the reflection of eddies from the boundary. External boundaries of these subregions constitute Mach lines coming from upper and lower points of the left boundary, respectively. With such buffer subregions the solution doesn't suffer from the drawback cited above (see Fig.4)

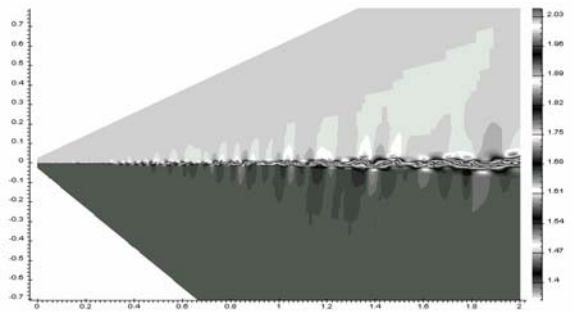
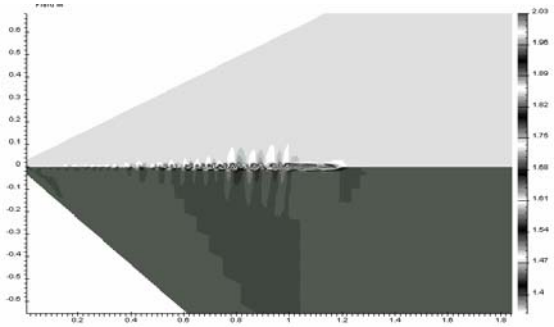


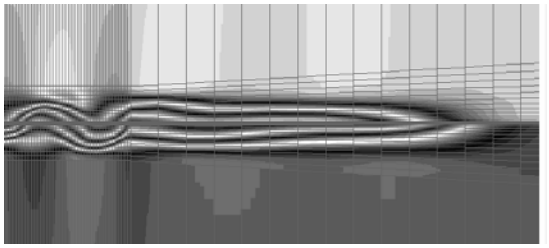
FIG. 4. Calculation with buffer subregions.

Some variants of grid modification were investigated in order to find the sensitivity of our computation to the structure of grid:

1. Grid is enlarged in *x*-direction (the length of grid cells is increased by 10 times). Smoothing of eddies occurs (see Fig.5 a,b).



a)



b)

FIG. 5. Damping of Kelvin-Helmholtz instability in the case of coarse grid in *x* direction
a) The whole computational region;
b) Fragment: the beginning of smoothing.

2. Grid is enlarged in y-direction (12 cells instead 32). The height of non-buffer subregions is diminished by 2 times. We can see only oscillations of discontinuity surface, any eddy structure isn't observed. Moreover, the shear layer goes out from the region of fine grid into coarser buffer subregions (Fig.6).

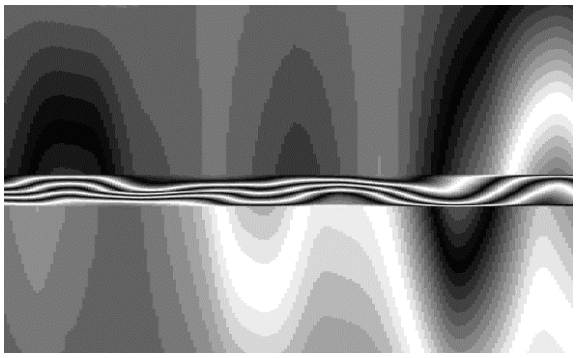
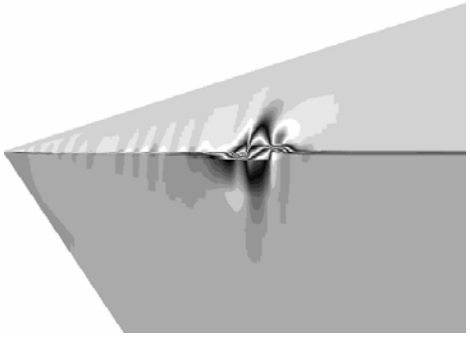


FIG. 6. The height of the region with fine grid is $KH \approx L \cdot (db/dx)_{theory}$.

It justifies our decision to make the region of fine grid larger then the theoretical value for shear layer thickness.

3. The best grid for the computation of this task by time-averaging method is the self-similar one. [12] But for LES method such grid proved to be

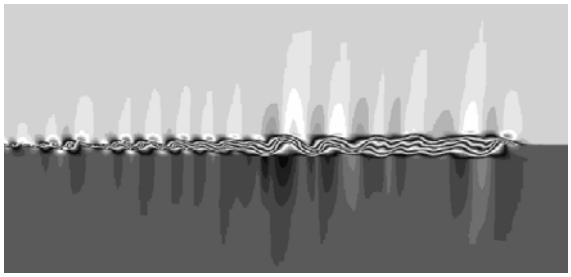


inadequate. It describes the flow very badly (Fig.7).

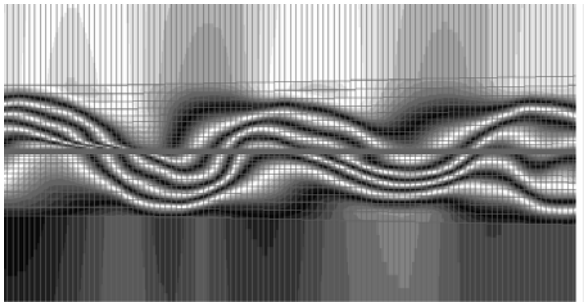
FIG. 7. Grid is self-similar from the beginning of mixing.

It is explained by the fact that the turbulent viscosity is proportional to the size of the cell and increases with the increase in it. Turbulent structures are still week at the beginning of mixing and increasing turbulent viscosity suppresses them, doesn't give them to develop. So, the origin of the turbulence seems to be better described with the uniform grid (even if one direction). But once the turbulence has been developed, self-similar grid can be used for the computation rather successfully.

4). Fig.8 (a,b) confirms this statement. Here another domain with the same length (1 *m*) is appointed to the developed shear layer pattern. The added part has the self-similar grid in the region of intensive mixing, 4 finest cells in both streams are uniform as before.



a)



b)

FIG. 8. Grid is self-similar beginning from the point *x*=1 *m* a) General view;
b) Fragment near the point *x*=1 *m*

The averaged picture of the flow is also obtained in addition to the instantaneous one (see Fig.9). All parameters of the flow are averaged over the interval of 10 thousands time steps. Such length of the interval is more than sufficient to obtain averaged data not including random fluctuations of parameters.

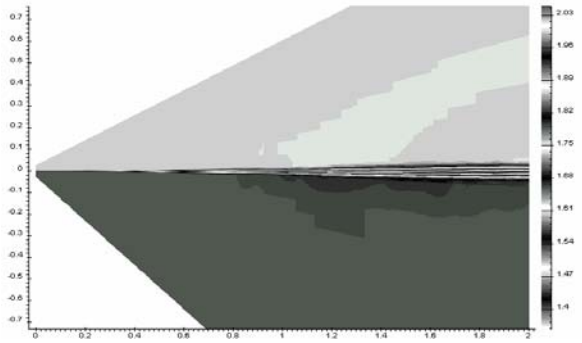


FIG. 9. Time-averaged field of Mach number

Thickness of the shear layer is calculated on the basis of averaged data. Its value for the doubled

domain is shown at Fig.10. Graphics present results for the first, third and fifth averaging respectively. After the first 10 thousands time steps there is a part of the flow that is still not involved in mixing at all. For the third interval of averaging the distant cells still experience only small fluctuations and contribute to the averaged thickness less then they must. At the fifth 10 thousands time steps the flow is fully developed, so further calculation hardly can give some new results. Thickness of the shear layer corresponding to the theoretical formula (9) is also shown at this figure. We must notice that our computed layer approximately 1,5 times exceeds the experimental one.

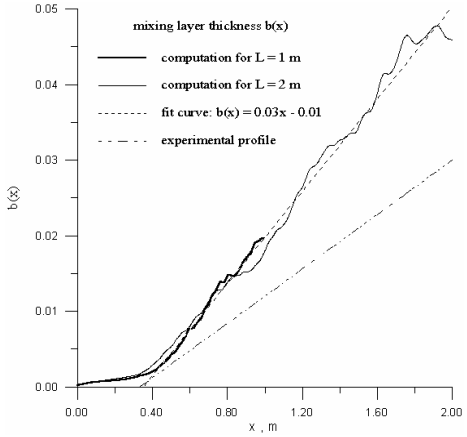


FIG.10. Distributions of mixing layer thickness

If one describe time-averaged flow with shear layer by semiempirical model of turbulence, than turbulent viscosity is proportional to the growth rate of the shear. That's why we have tried to decrease the constant C_μ by 1,5 times hoping the thickness of the shear layer to be diminished too. But this value remains the same as in the previous calculation (see Fig.11, where results for the first and the third averaging are shown). Considerable change in c_k - from 45,8 to 1 - also doesn't influence the results. To all appearance, the method in use is insensitive to the value of constants inserting in SGS model.

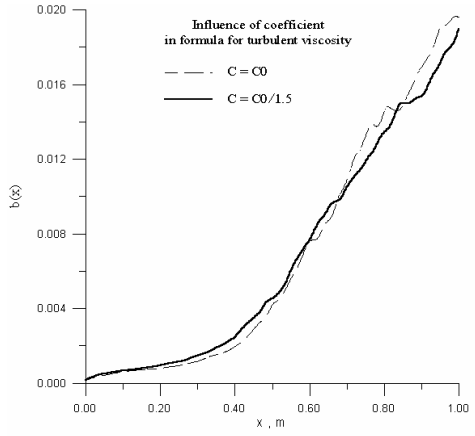


FIG.11. Computations for various values of C_μ

This conclusion is not extraordinary. It is known that in LES a change in SGS model has the relatively small effect on the statistical properties of the large-scale flow. This feature is termed as "model-independence" of LES. [4] Leslie [2] believes one of the essential drawbacks of the LES is that one cannot improve the results of an unsatisfactory simulation by adjusting constants. It is due to the fact that LES is attempting to reproduce the flow rather then to model it: there is therefore almost nothing to adjust.

I think this simulation shouldn't be named as very unsatisfactory. Certainly, there is a great field for further improvements, but these improvements can be done. Although Smagorinsky model isn't the best, potential of this calculation doesn't lie in improvement SGS model due to the relative insensitivity of LES to SGS models. There are two possibilities for getting more plausible results.

1. Transition to three-dimensional computation. It is necessary because the properties of turbulence in 2D and 3D flows are essentially different. [13]
2. Using more detailed grid. Indeed, for the simulation to have some chance of success, it is necessary for subgrid scales (unresolved wavenumbers) to be entirely in the equilibrium range where the structure of the small scale turbulence depends only on local conditions. Once it is satisfied further diminishing in sizes of cells shouldn't influence the solution. It is not so in our case. We observe strong dependence of the solution on the grid. Consequently, we don't ensure yet that our small-scale structures belong to the equilibrium range.

Indeed, true inertial subrange will appear for wavenumbers $k>10^2$, where $k = 2\pi / l$, l is the character length of motions. k of the order of unity characterizes the largest eddies, i.e. those with sizes of about the thickness of the shear layer. It implies we must have minimum 100 cells across the shear layer with the size $\sim 10^{-4}$ *m* and they are to be square. But we have only 20.

It was observed that turbulent structures develop only in the region of finest grid (8 cells near the discontinuity surface). When they goes beyond this region they begins to spread with a flow only growing in size, without any developing. The finest grid actually has necessary size ($2 \cdot 10^{-4}$ *m*), while the rest of the grid being much more largely. This observation also confirms the conclusion about the inadequacy of such coarse grid.

But while recognizing the need for these measures (using more detailed grid and transition to 3D computation) we don't have an opportunity to realize them in the nearest future. Our limitation is power of available computers. These calculations were performed at Alpha XL 266 workstation (DEC). They occupy approximately 50 Mb of virtual memory for the computational domain of the length 1 *m* with buffer subreigons, each time step takes 30 sec. So it takes about 5 days to obtain the developed picture of the flow even for such coarse mesh.

The smaller cell size, the stronger time step limitation, so refinement of the grid by 5 times will increase the time of calculation to month or more. Transition to 3D simulation even for the old grid will require approximately 2,5 months of calculation. These numbers seem to be unrealistic, as not one computation is required to obtain really good results (we should try various configurations of grid, various constants in the model, various models etc.) So, it's hardly possible to perform computations by LES method on modern Personal Computer.

Conclusions

1. The modification of Large Eddy Simulation method is developed for the calculation of flows with viscosity and turbulence. This method allows obtaining Kelvin-Helmholtz instability characteristic for tangential discontinuities.
2. In calculations the qualitatively correct picture of both non-stationary and time-averaged flows is obtained. However, growth rate of mixing layer is 1.5 times overestimated in calculation in comparison with the experimental data.
3. The solution of this problem reveals strong dependence on grid. On the contrary, constants including in subgrid scale model doesn't influence it. The improvement of the quality of calculations, therefore, lies in the transition to more detailed grid and 3D simulations. It's worthless to change constants in SGS model and the model itself.
4. Expense in computer memory and time are too large even for relatively coarse grid if calculate this problem on PC. Therefore, it seems unreasonable yet to use PC for computations by LES method.

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