Mathematical simulation of the Kelvin—Helmholtz instability using the method of large particles

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Abstract. The simplest shear flow – a two-dimensional (plane) nonstationary mixing layer – is considered. Results obtained from the direct numerical simulation of mixing at the boundary between two compressible gases (of different densities) moving with a tangential velocity shear in the field of strong external acceleration are described. The simulation was performed using the well-known method of large particles for a two-dimensional case. The reliability of calculation results is supported by their comparison with analytical calculations, results obtained from the numerical solution of a similar problem, and experimental data.

1. Introduction

The Kelvin—Helmholtz instability (KHI) – is one of the first discovered hydrodynamic instabilities, which occurs at the boundary between two fluids or gases moving with different velocities. The formation of billow clouds in the atmosphere (Fig. 1), wind-generated waves in seas and oceans, the rings of Saturn, the great red spot on Jupiter, instability of the solar corona, and others are the examples of such an instability in nature [1, 2]. Much attention is given to the study of the KHI because it is a frequently occurring phenomenon.

The dispersion equation to describe the KHI at the early stages in the development of disturbances has the form [2]:

\[ C = \frac{\omega}{k} = \frac{\rho_1 u_1 + \rho_2 u_2}{\rho_1 + \rho_2} \pm \sqrt{\frac{g}{k} \left( \frac{\rho_2 - \rho_1}{\rho_2 + \rho_1} \right) - \frac{\rho_1 \rho_2}{(\rho_1 + \rho_2)^2} (u_1 - u_2)^2} \]

where \( C \) is the phase propagation velocity of disturbances with frequency \( \omega \) and wavenumber \( k = 2\pi/\lambda, \lambda \)
is the disturbance wavelength, \( \rho_1 \) and \( \rho_2 \) are the densities of media (in regions 1 and 2) moving with velocities \( u_1 \) and \( u_2 \), and \( g \) is acceleration due to external mass force. Figure 2 shows the scheme of the classical problem of the development of a nonstationary plane mixing layer between two semi-infinite regions.

The first term in Eq. (1) is the weighted mean velocity of both medium (fluid or gas) regions, with respect to which the disturbances move with a phase velocity depending on a shear at the boundary. The KHI develops, if the radical expression in (1) is negative.

In this case, if the phase velocity of the disturbances is expressed in the complex form

\[
C = C_0 \pm \omega
\]

the imaginary part of the frequency of disturbances \( kC_0 \) is the measure of the rate of their increase. In other words, the amplitude of disturbed motion \( u_{1,2} \sim \exp(kCt) \) gains the opportunity for an unlimited increase with time. The dependence of the time constant \( \tau_* \) of an exponential increase in the amplitudes of disturbances in incompressible fluid or gas has the form

\[
\tau_* = \frac{1}{kC_0} = \frac{1}{\sqrt{\frac{(u_1-u_2)^2}{\rho_1\rho_2}\left(\frac{2\pi}{\lambda}ight)^2 - \frac{g(\rho_2-\rho_1)}{(\rho_1+\rho_2)}\frac{2\pi}{\lambda}}.
\]

2. Numerical scheme

Let us consider results obtained from the solution of the two-dimensional problem of the KHI development at the plane boundary between two air layers (of different densities) moving with a tangential velocity discontinuity and in the field of external constant acceleration. Plane approximation is chosen in order to obtain a more accurate solution when the number of calculation cells in the finite-difference grid is limited. Moreover, according to the results obtained in [3, 4], the KHI evolution observed in calculations for a three-dimensional case is, on the whole, similar to that in two-dimensional calculations. Thus, the three-dimensional flow region under consideration (Fig. 2) for the case of plane motion is transformed into the MNPQ square with side \( \Delta x \) (Fig. 3).

The problem for performing calculations was considered similarly to that in [3, 4]. The MNPQ calculation region of size \( \Delta x = 2.5 \cdot 10^{-3} \) m is divided in two by the BD plane (Fig. 2). Two half-spaces Nos. 1 (BNPD) and 2 (MBDQ) formed in such a way are filled with air (adiabatic index \( \chi = 1.4 \)) with initial pressure \( p_0 = 100 \text{kPa} \) and densities \( \rho_1 = 1.293 \text{kg/m}^3 \) and \( \rho_2 = (1.5\ldots30) \cdot \rho_1 \), the Atwood number \( A = (\rho_2 - \rho_1)/(\rho_2 + \rho_1) = 0.2\ldots0.935 \). External acceleration \( g = (10^3 \pm 10^5) \cdot g_0 \) is directed perpendicularly to the BD plane from less to more dense air.

At the initial time \( t = 0 \) in the MBDQ region, the air moves with velocities \( u_{20} = 8.3\ldots41.4 \text{ m/s,} \) and, in the BNPD region, the air is still – \( u_{10} = 0 \text{ m/s.} \) The velocity disturbances \( u'_0 \) and \( v'_0 \), whose development is the objective of the direct numerical simulation of the KHI development, are specified at the boundary. The initial disturbances themselves are determined from the formulas.
\[ u'_0 = A_u \cdot \sin \left( \frac{2\pi y}{\lambda} \right) \cdot e^{-\mu x}, \]
\[ v'_0 = A_v \cdot \sin \left( \frac{2\pi y}{\lambda} \right) \cdot e^{-\mu y}, \]

where \( A_u = (0.01 + 0.1) \cdot u_{20} \) is the disturbance amplitude, \( \lambda = 6.25 \cdot 10^{-4} \) m is the disturbance wavelength, and \( \mu^* = 3.2 \cdot 10^3 \) m is the parameter regulating the effective width \( h \) (Fig. 3) of the disturbed region.

![Figure 3. Geometry of calculation region.](image)

Sliding conditions are used at the MQ and NP boundaries and penetration conditions are used at the MN and PQ boundaries. The number of cells \( N_y = 400 \) and \( N_z = 400 \) in the spatial finite-difference grid along the coordinates \( y \) and \( z \) (Fig. 3), respectively, is specified from the condition that 100 calculation cells are along the wavelength \( \lambda \) of one disturbance.

The KHI was mathematically simulated through the integration of the Euler system of nonstationary differential equations, which includes the mass, momentum, and energy conservation laws

\[
\begin{align*}
\frac{d\rho}{dt} + \frac{\partial}{\partial x}(\rho u^i) &= 0, \\
\frac{d}{dt}(\rho u^i) + \frac{\partial}{\partial x}(\rho u^i u^j - \delta^i_j \cdot p) &= g^i, \\
\frac{d}{dt}(\rho E) + \frac{\partial}{\partial x}(\rho u^i \cdot E - \rho u^i) &= 0.
\end{align*}
\]

Here, \( p \) and \( \rho \) are the air pressure and density, \( u^i \) is the velocity vector component, \( E \) is the specific total energy, \( t \) is time, and \( \delta^i_j \) is the Kronecker symbol. The equation for the state of an ideal gas closes this system

\[ p = (\gamma - 1) \cdot \rho \cdot \left( E - \frac{(u^i)^2}{2} \right) \]

Using numerical schemes based on the Lagrangian method of describing medium motions for the integration of Eqs. (3) – (5) is wholly unacceptable because of significant cell deformations in the KHI gasdynamic flow under consideration. In the combined Eulerian—Lagrangian schemes ([5] for example), the above-indicated drawback implies difficulties in calculations using rearrangeable grids, and the problem of their adaptation arises in order to minimize parasitic oscillations of grid functions due to lost monotonicity of the difference scheme.

In this connection, the large-particle method based on the Eulerian method of describing medium motions was chosen to integrate Eqs. (3) – (5). This is a sufficiently general algorithm, which makes it possible to calculate both compound spatially nonstationary subsonic and supersonic flows using average-capacity computers [6, 7, 8]. In particular, this algorithm has proved to be efficient in studying the development of hydrodynamic instabilities [6, 7, 9].

The main idea of the method of large particles is in the splitting of Eqs. (4) and (5) (written in the form of the conservation laws) into physical processes [6].
fluid (gas) particles coinciding with the Eulerian grid cells at a given time point. The calculation of each time step is divided into three stages. At stage I (Eulerian stage), only the effects of accelerating medium due to pressure gradient are taken into account, and intermediate values for the flow parameters \( \tilde{u}^n \) and \( \tilde{E}^n \) are determined for a large particle. At stage II (Lagrangian stage), the mass fluxes \( \Delta M^n \) through the boundaries of the Eulerian cells during the motion of medium are calculated. And, at stage III, the final gas-dynamic flow parameters \( \rho^n, u^n, E^n \), and \( p^n \) are calculated for each cell of the calculation grid.

In this work, one of the versions of the difference scheme of the method of large particles is used \[8\]. As in the initial method \[6\], the integration domain is covered by the space-fixed calculation grid of size \( N_x \times N_z \). The cell centers are denoted by integers \( i,j \). At time \( t = n \Delta t \), in each cell, density \( \rho^i_j \), velocity \( u^i_j \), specific total energy \( E^i_j \), and pressure \( p^i_j \) are known. The calculation cycle to determine these parameters for the next time point \( t = (n+1) \Delta t \) is divided into two stages.

At the first stage, only the effects of accelerating medium due to pressure forces are taken into account. The convective terms of the form \( d(\Psi \rho u)/dt \), where \( \Psi = \{1, u, E\} \), in system (4) are considered missing. For the plane case under consideration (Fig. 3), in the Cartesian coordinate system \( (y, z) \), the finite-difference equations of stage I have the form of explicit relations

\[
\tilde{u}^n_{i,j} = u^i_j - \frac{\Delta t}{\rho^i_j} \left[ p^n_{i+1/2,j} - p^n_{i-1/2,j} + \frac{\Delta t}{\rho^i_j} \left( q^n_{i+1/2,j} - q^n_{i-1/2,j} \right) \right],
\]

\[
\tilde{v}^n_{i,j} = v^i_j - \frac{\Delta t}{\rho^i_j} \left[ p^n_{i,j+1/2} - p^n_{i,j-1/2} + \frac{\Delta t}{\rho^i_j} \left( q^n_{i,j+1/2} - q^n_{i,j-1/2} - g \right) \right],
\]

\[
\tilde{E}^n_{i,j} = E^i_j - \frac{\Delta t}{\rho^i_j} \left[ p^n_{i+1/2,j} \tilde{u}^n_{i+1/2,j} - p^n_{i-1/2,j} \tilde{u}^n_{i-1/2,j} + p^n_{i,j+1/2} \tilde{v}^n_{i,j+1/2} - p^n_{i,j-1/2} \tilde{v}^n_{i,j-1/2} \right].
\]

Here, the intermediate values of \( \tilde{u}^n_{i,j} \) and \( \tilde{v}^n_{i,j} \) are found using central differences. Then, the values with fractional indices \( \Psi^n_{i+1/2,j} \), \( \Psi^n_{i-1/2,j} \) and \( \Psi^n_{i,j+1/2} \), \( \Psi^n_{i,j-1/2} \), where \( \Psi = \{\rho, u, E, p\} \), which relate to the cell boundaries, are determined from the relations

\[
\Psi^n_{i+1/2,j} = \frac{1}{2} \left( \Psi^n_{i,j+1} + \Psi^n_{i,j} \right) \quad \text{and} \quad \Psi^n_{i-1/2,j} = \frac{1}{2} \left( \Psi^n_{i-1,j} + \Psi^n_{i,j} \right),
\]

\[
\Psi^n_{i,j+1/2} = \frac{1}{2} \left( \Psi^n_{i+1,j} + \Psi^n_{i,j} \right) \quad \text{and} \quad \Psi^n_{i,j-1/2} = \frac{1}{2} \left( \Psi^n_{i,j-1} + \Psi^n_{i,j} \right).
\]

It is suggested that the intermediate values of the specific total energy \( \tilde{E}^n_{i,j} \) be calculated using differences against the second-type flow \[10\] (instead of central differences as in \[6\]). This implies that the corresponding values of \( \Psi^n_{Y^+}, \Psi^n_{Y^-}, \Psi^n_{Z^+}, \Psi^n_{Z^-} \) are determined by the flow direction:

\[
\Psi^n_{Y^+} = \begin{cases} 
\Psi^n_{i,j}^+, & \text{as } \tilde{u}^n_{i+1/2,j} > 0, \\
\Psi^n_{i+1,j}^+, & \text{as } \tilde{u}^n_{i+1/2,j} < 0,
\end{cases}
\]

\[
\Psi^n_{Y^-} = \begin{cases} 
\Psi^n_{i,j}^-, & \text{as } \tilde{u}^n_{i-1/2,j} > 0, \\
\Psi^n_{i-1,j}^-, & \text{as } \tilde{u}^n_{i-1/2,j} < 0,
\end{cases}
\]

\[
\Psi^n_{Z^+} = \begin{cases} 
\Psi^n_{i,j}^+, & \text{as } \tilde{v}^n_{i,j+1/2} > 0, \\
\Psi^n_{i,j+1}^+, & \text{as } \tilde{v}^n_{i,j+1/2} < 0,
\end{cases}
\]

\[
\Psi^n_{Z^-} = \begin{cases} 
\Psi^n_{i,j}^-, & \text{as } \tilde{v}^n_{i,j-1/2} > 0, \\
\Psi^n_{i,j-1}^-, & \text{as } \tilde{v}^n_{i,j-1/2} < 0.
\end{cases}
\]

The one-sided differences used are conservative and transportable \[10\]. In order to improve the monotonicity of the scheme, it is suggested that intermediate velocities \( \tilde{u}^n_{i,j} \) (but not \( \tilde{u}^n \)) obtained at the same calculation step be used in the finite-difference equation for energy.

Artificial viscosity \( q \) is introduced into the finite-difference equations for \( \tilde{u}^n_{i,j} \) and \( \tilde{v}^n_{i,j} \) to provide the monotonicity of the difference scheme. This viscosity is calculated from the relations of the form
mined by the convective terms of the form is the sound speed. Artificial viscosity is pronounced only in compression waves and compression shocks.

may be considered as mass, momentum, and energy fluxes formed at the boundary from the initial periodic disturbance is easily seen. Then, their development ac-

Fig. 3, and the increase in time patterns of the isolines of equal density). Here, the coordinate system

the mixing layer, and the KHI suppression are easily seen in Fig. 5. The comparison of Fig. 4 with Figs.

1 and 5 suggests that the calculated flow pattern qualitatively corresponds to experimental data.

The characteristic KHI development obtained in calculations using the method of large particles under the

method \[7, 11\]. The finite-difference equations of stage II have the form

\[
q_{i+1/2,j} = \begin{cases}
Q\rho_{i+1/2,j}c_{i+1/2,j} \Delta y \left( \frac{u_{i+1,j}^n - u_{i,j}^n}{\Delta y} \right), & \text{as } \frac{u_{i+1,j}^n - u_{i,j}^n}{\Delta y} < 0, \\
0, & \text{as } \frac{u_{i+1,j}^n - u_{i,j}^n}{\Delta y} \geq 0.
\end{cases}
\]

Here, \(Q = 0.7\) is the dimensionless coefficient of artificial viscosity and \(c_{i+1/2,j} = \left( \frac{\rho_{i+1/2,j}}{\rho_{i+1/2,j}} \right)^{1/2}\)
is the sound speed. Artificial viscosity is pronounced only in compression waves and compression shocks.

In the used version of the difference scheme of the method of large particles, the second stage, in fact, combines both the Lagrangian and final stages of the initial method [6]. Here, the transport effects determined by the convective terms of the form \(d(\Psi \rho u)/dr\) (where \(\Psi = \{1, u, E\}\)) are taken into account. Since \(\rho u \sim \Delta M\), the product \(\Psi \rho u\) is similar to \(\Psi \Delta M\). In this interpretation, the convective terms \(d(\Psi \rho u)/dr\) in (4) may be considered as mass, momentum, and energy fluxes \(d(\Psi \Delta M)/dr\) through the boundaries of Eulerian cells (large particles), and the difference scheme may be interpreted within the framework of the flux method [7, 11]. The finite-difference equations of stage II have the form

\[
\rho_{i,j}^{n+1} = \rho_{i,j}^n - \Delta t \left[ \rho_{Y}^n \frac{\overline{u}_{i,j}^{n+1} - \overline{u}_{i,j}^n}{\Delta y} + \rho_{Z}^n \frac{\overline{v}_{i,j}^{n+1} - \overline{v}_{i,j}^n}{\Delta z} \right],
\]

\[
u_{i,j}^{n+1} = \overline{v}_{i,j}^{n+1} - \overline{v}_{i,j}^n - \Delta t \left[ \rho_{Y}^n \frac{\overline{v}_{i,j}^{n+1} - \overline{v}_{i,j}^n}{\Delta y} + \rho_{Z}^n \frac{\overline{v}_{i,j}^{n+1} - \overline{v}_{i,j}^n}{\Delta z} \right],
\]

\[
E_{i,j}^{n+1} = \overline{E}_{i,j}^{n+1} - \overline{E}_{i,j}^n - \Delta t \left[ \rho_{Y}^n \frac{\overline{E}_{i,j}^{n+1} - \overline{E}_{i,j}^n}{\Delta y} + \rho_{Z}^n \frac{\overline{E}_{i,j}^{n+1} - \overline{E}_{i,j}^n}{\Delta z} \right].
\]

At the end of the second stage, new values of pressure \(p_{i,j}^{n+1}\) are determined from state equation (5) for each cell, and the calculation cycle is completed.

As in the initial method [6], the boundary conditions are fulfilled with the aid of fictitious cells, which makes it possible not to use special formulas for boundary cells and, thus, not to violate the homogeneity of the numerical algorithm.

3. Calculation results

The characteristic KHI development obtained in calculations using the method of large particles under the initial conditions \(\rho_2 = 5 \cdot \rho_1\), \(u_{20} = 41.4\) m/s, \(g = 10^4\cdot g_0\) and \(A_0 = 0.1 \cdot u_{20}\) is shown in Fig. 4 (nine patterns of the isolines of equal density). Here, the coordinate system \((\xi, \zeta)\) is oriented similarly to that in Fig. 3, and the increase in time \(t\) corresponds to the increase in the pattern number. The effect of vortices formed at the boundary from the initial periodic disturbance is easily seen. Then, their development accompanied by the corresponding extension of the mixing zone is observed. Finally, the vortices reach equilibrium and collapse.

The calculation results in Fig. 4 are in satisfactory agreement with experimental data obtained by different authors and given, for example, in [2] and in Figs. 1 and 5. Figure 5 shows the sequence of the shadow photos of the density interface affected by a stationary velocity shear. Here, the increase in time \(t\) also corresponds to the increase in the photo number. The increase in KHI disturbances, the thickening of the mixing layer, and the KHI suppression are easily seen in Fig. 5. The comparison of Fig. 4 with Figs. 1 and 5 suggests that the calculated flow pattern qualitatively corresponds to experimental data.
In Fig. 4, the last photo shows the penetration of distortions (associated with inaccuracies in the finite-difference approximation of Eqs. (4) and (5) by the boundary conditions) into the central flow region. These distortions in the form of the isoline of equal density are denoted by the arrows. However, it should be noted that the distortions start to affect calculation results only by the time of vortex collapsing and do not affect the results of numerical calculations of the KHI at the times when vortices are formed and reach equilibrium. All this suggests that the number of cells in the spatial finite-difference calculation grid \( \frac{Z \cdot Y}{N_{N1}} \), which is specified from the condition that 100 calculation cells are along the wavelength of one disturbance, and the accuracy of the finite-difference approximation of Eqs. (4) and (5) and their numerical solution using the method of large particles provide an adequate spatial resolution of the KHI development pattern and a slight effect of the boundary conditions on it.

Under the KHI, a developing vortex motion results in the penetration of disturbances deep into the BNPD and MBDQ layers from the boundary BD (Fig. 3), which, in turn, is accompanied by the deviation \( \Delta u \) of horizontal velocity from its initial values. Since, within the MBDQ layer, at first, the medium moves with constant velocity \( u_{20} \), the deviation is calculated as \( \Delta u \bigg|_{MBDQ} = |u - u_{20}| \); within the BNPD layer, at first, the medium rests, therefore, \( \Delta u \bigg|_{BNPD} = |u| \). Figure 6 shows the increase in the sum of these parameters

\[
\Delta u = \Delta u \bigg|_{MBDQ} + \Delta u \bigg|_{BNPD}
\]

with time at \( \rho_2 = 5 \cdot \rho_1 \), \( u_{20} = 41.4 \text{ m/s} \) and \( A_u = 0.05 \cdot u_{20} \) and at different external accelerations:

- \( g = 10^3 \cdot g_0 \) (1);
- \( 3 \cdot 10^3 \cdot g_0 \) (2);
- \( 10^4 \cdot g_0 \) (3);
- \( 3 \cdot 10^4 \cdot g_0 \) (4);
- \( 10^5 \cdot g_0 \) (5).
Figure 6. Increase in the amplitudes of the KHI disturbances

The comparison of calculation data in Figs. 4 and 6 shows that, with developing vortices that occur at the boundary and with extending mixing zone, the parameter $\Delta u$ also increases and by some time $t_{\text{max}}$ reaches its maximum $\Delta u_{\text{max}}$. This maximum value characterizes the increase in the amplitudes of vortex KHI disturbances in a shear flow and makes it possible to quantitatively estimate the time constant $\tau_*$ of their exponential increase from the simple relation $\Delta u_{\text{max}} = \Delta u_{20} \exp(t_{\text{max}}/\tau_*)$.

In [4], the qualitative dependence of variations in the mixing-layer width $h$ (Fig. 3) on time $t$, which results from the corresponding increase in the size of vortices

$$h = 67.88 \cdot \alpha^2 \cdot \sqrt{\zeta} \cdot u_{20} \cdot t,$$

where $u_{20}$ is the relative velocity of layers, $\alpha$ and $\zeta$ are constants. The indicated linear dependence is also reproduced in integrating Eqs. (3) – (5) with the method of large particles (the calculation results are shown in Fig. 7, gray broken lines). In Fig. 7, the results obtained under different initial conditions are denoted by figures. In the calculations, the mixing-zone width $h(t)$ was defined as the distance between the extreme points in the MNPQ region, at which KHI disturbances accompanied by gas-density deviations from initial values $\rho_1$ and $\rho_2$ penetrate at time $t$. In other words, $h$ is the distance, at which the condition $\rho_1 < \rho < \rho_2$ is fulfilled.

Figure 7a shows the $h(t)$ graphs for the invariable initial conditions $\rho_1 = 5 \cdot \rho_2$ kg/m$^3$ and $g = 10^4 \cdot g_0$ m/s$^2$. The initial discontinuity velocity varied for different calculation versions: $u_{20} = 8.3$ (1); 10.4 (2); 20.7 (3); 31.1 (4), and 41.4 (5) m/s. Figure 7b shows the results of $h(t)$ calculations, in which the initial acceleration varied: $g = 10^3 \cdot g_0$ (1); $3 \cdot 10^3 \cdot g_0$ (2); $10^4 \cdot g_0$ (3); $3 \cdot 10^4 \cdot g_0$ (4); $10^5 \cdot g_0$ (5) and $3 \cdot 10^5 \cdot g_0$ (6) m/s$^2$. The initial conditions $\rho_2 = 5 \cdot \rho_1$ kg/m$^3$ and $u_{20} = 41.4$ m/s were held fixed. Finally, Fig. 7c shows the $h(t)$ graphs obtained under the fixed conditions
\[ u_{20} = 41.4 \text{ m/s} \] and \[ g = 10^4 \cdot g_0 \text{ m/s}^2 \], and the initial air density varied \( \rho_2 = n \cdot \rho_1 - n = 1.5 \rho_2 = n \cdot \rho_1 - n = 1.5 \) (1), 5 (2); 10 (3); 20 (4) and 30 (5). In all calculation versions, the amplitude of initial periodic velocity disturbances in formulas (3) was \( A_0 = 0.1 \cdot u_{20} \text{ m/s} \).

The data in Fig 7 show that the increase in the mixing-zone width is of linear character and depends on external acceleration (Fig. 7b) and difference between gas-layer densities (Fig. 7c) to a greater extent than on difference between discontinuity velocities \( u_{20} \) (Fig. 7a). The following dependence makes it possible to estimate the effect of each of the indicated factors

\[
h \approx 4 \cdot 10^{-4} \cdot \left( \frac{u_{20} + 29}{u_{20} + 3} \right)^2 \cdot \frac{g \cdot (\rho_2 - \rho_1)}{\rho_2 + \rho_1} \cdot u_{20} \cdot t. \tag{7}
\]

New formula (7) and its numerical coefficients \( 4 \cdot 10^{-4}, 29 \) and 3 were obtained in this work from the approximation of calculation data (---), which is denoted by the black solid lines (---) in Fig. 7.

It is easily seen that, throughout the whole structure, dependence (7) is similar to formula (6) from [4].

In [4], numerical calculations were performed at two values of the Atwood number \( A = (\rho_2 - \rho_1)/(\rho_2 + \rho_1) = 0 \) and 0.82 and one value of the initial velocity difference \( u_{20} \). Therefore, the authors of (6) from [4] had to introduce the constants \( \alpha \) and \( \zeta \) into this formula. In our work, due to multiple calculations with different initial data, we have managed to specify the form of these constants:

\[
\alpha = \frac{u_{20} + 29}{u_{20} + 3} \quad \text{and} \quad \zeta = \frac{g \cdot (\rho_2 - \rho_1)}{\rho_2 + \rho_1}.
\]

The qualitative agreement between the results of KHI simulation with the method of large particles using Eqs. (3) – (5) and the general KHI development pattern, which is shown in Figs. 1, 4, and 5, is also quantitatively supported. Figure 8 shows the time constant \( (\tau_0) \) values estimated from the formula

\[
\tau_0 = t_{\text{max}} \cdot \left( \ln \left( \frac{\Delta u_{\text{max}}}{\Delta u_{20}} \right) \right)^{-1}
\]

the numerical-calculation results obtained under different initial conditions are denoted by the figures.

Thus, Fig. 8a shows the behavior of the time constant \( \tau_0 \) under variations in the initial discontinuity velocity \( u_{20} \) and for the two initial air densities \( \rho_2 = 5 \cdot \rho_1 \) (1) and \( \rho_2 = 30 \cdot \rho_1 \) (2). The initial external acceleration did not change and was \( g = 10^4 \cdot g_0 \). Figure 8b gives the results for \( \tau_0 = f(\rho_2 - \rho_1) \) under the conditions \( u_{20} = 20.7 \) (1) and 41.4 (2) m/s. The initial external acceleration was \( g = 10^4 \cdot g_0 \). Finally, Fig. 8c shows the behavior of \( \tau_0 \) under variations in the initial acceleration. The rest of the initial conditions were held fixed: \( u_{20} = 41.4 \text{ m/s} \) and \( \rho_2 = 5 \cdot \rho_1 \) (1); \( u_{20} = 20.7 \text{ m/s} \) and \( \rho_2 = 10 \cdot \rho_1 \) (2); \( u_{20} = 20.7 \text{ m/s} \) and \( u_{20} = 30 \text{ m/s} \) (3). In all the calculation versions, the amplitude of the initial periodic velocity disturbances in (3) was \( A_0 = 0.1 \cdot u_{20} \text{ m/s} \).

The comparison of the data given in Fig. 8 shows a satisfactory agreement between the \( \tau_0 \) values obtained from numerical calculations using Eqs (3) – (5) and estimated from Eq. (2). In this case, the increase in the amplitude \( \Delta u \) of initial disturbances at the BD boundary (Fig. 3) results in the improvement of this agreement – deviations in the values of \( \tau_0 \), obtained in the numerical calculations from its estimates obtained using Eq. (2) decrease. This is supported by the data given in Fig. 9, in which the symbols (●) and (○) denote the estimates of the time constant \( \tau_0 \) of the exponential disturbance increase at \( A_0 = 0.1 \cdot u_{20} \) and \( A_0 = 0.01 \cdot u_{20} \), respectively.

Figure 9a shows the behavior of \( \tau_0 \) for the initial air density \( \rho_2 = 5 \cdot \rho_1 \) and the initial external acceleration \( g = 10^4 \cdot g_0 \). The results obtained for the initial conditions \( u_{20} = 41.4 \text{ m/s} \) and \( g = 10^4 \cdot g_0 \) are shown in Fig. 9b and for the conditions \( \rho_2 = 5 \cdot \rho_1 \) and \( u_{20} = 41.4 \text{ m/s} \) shown in Fig. 9c. The continuous lines in Fig. 9 (as in Fig. 8) denote \( \tau_0 \) variations in a linear approximation of incompressible fluid.
In Fig. 9, the calculation data may also be interpreted as a support of the fact that dispersion equation (1) describes the development of the classical KHI from extremely slight initial disturbances. Therefore, there is such a good agreement between the results of numerical calculations (○) using Eqs. (3) – (5) at $A_u = 0.01 \cdot u_{20}$ and the estimates of $\tau_*$ from Eq. (2). However, with the amplitude of initial disturbances increased up to $A_u = 0.1 \cdot u_{20}$, the numerical estimates (●) for $\tau_*$ become less accurate.

4. Conclusions
Both qualitative and quantitative comparisons (shown in Figs. 1, 4 – 9) of the results of calculations of the KHI from Eqs. (3) – (5) using the method of large particles with experimental [1, 2] and theoretical [3, 4] data (obtained by other authors) on the KHI development and with the analytical solution of (2) make it possible to draw the following conclusions:

1. The results of direct (with no semiempirical models) numerical simulation of the KHI development in compressible gas (Figs. 8 and 9) are in satisfactory agreement with the estimates (2) for the case of incompressible fluid.

2. Equations (3) – (5), their finite-difference approximation and numerical solution using the method of large particles satisfactorily reproduce the KHI development at the boundary between two compressible gases (with different densities) moving with the tangential constant velocity discontinuity and in the field of external constant acceleration. The number of cells in the calculation grid $N_Y \times N_Z$, which is specified from the condition that 100 calculation cells are along the wavelength $\lambda$ of one disturbance, results only in slight effect of the boundary conditions on the spatial resolution of the KHI development pattern.

3. The results of calculations of the KHI development, which are shown in Figs. 7 – 9 and in the form of Eq. (7) obtained by us, may be used in predicting the extension of mixing zones in different flows with
tangential velocity discontinuity, which frequently occur in technology and in the atmosphere (for example, within the initial zone of airflow, at the initial stage of mixing in a cylindrical vortex, during the development of billow clouds or instability of a clear sky in the atmosphere [2]).

4. The results obtained in this work may be useful in substantiating the hypothesis on the transformation of shock waves into acoustic disturbances (during their propagation throughout the atmosphere) under the influence of irreversible diffusion-convection matter exchange in their front regions. In this case, diffusion must be implemented at the meso (but not molecular) level [12].

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References

[1] Evstigneev N M and Magnitskii N A 2013 Nonlinear dynamics of the initial laminar-turbulent transition in the problem of the Kelvin—Helmholtz instability Numerical Methods and Programming 64(3) 45–52

[2] Turner J S 1977 Buoyancy Effects in Fluids (Moscow) ed by S A Kitaigorodskii and A S Monin p 432

[3] Zhmailo V A et al 1996 Direct numerical simulation of gravitational turbulent mixing Problems of Atomic Science and Technology Ser. Theoretical and Allied Physics 1-2 29–37

[4] Zhmailo V A et al 1996 Direct numerical simulation of turbulent mixing in shear flows Problems of Atomic Science and Technology Ser. Theoretical and Allied Physics 1-2 38–47

[5] Golovizin V M, Ryazanov M A, Samarskii A A et al 1986 Difference schemes of gas dynamics with balanced convective streams (Moscow State University Press) Numerical Methods in Mathematical Physics 5–41

[6] Belotserkovskii O M and Davydov Yu M 1982 Method of Large Particles in Gas Dynamics (Nauka Moscow) p 392

[7] Belotserkovskii O M and Oparin A M 2001 Numerical Experiment in Turbulence: From Order to Chaos 2nd edition, revised and supplemented (Nauka Moscow) p 223

[8] Kosyakov S I, Samovarov A N and Vasil’ev N N 2017 Mathematical simulation of air shock waves as a tool for analyzing results obtained from blast resistance tests Problems of Defense Technology Ser. 16 Anti-Terrorism Technologies 7-8 40–46

[9] Davydov Yu M, Dem’yanov A Yu and Tsvetkov G A 1987 Numerical Simulation of the Stabilization and Integration of Harmonics under the Rayleigh—Taylor Instability Using the Method of Large Particles (Moscow: Academy of Sciences Computing Center of the USSR) p 52

[10] P J Roache 1980 Computational Fluid Dynamics (Moscow Mir) ed by P I Chushkin p 616

[11] Belotserkovskii O M and Severinov L I 1973 Conservative method for flows and calculation of viscous heat-conducting gas flow over a finite-size body J Computational Mathematics and Mathematical Physics 13(2) 285–397

[12] Evterev L S and Kosykov S I 2008 Mechanism and mathematical model of the transformation of a strong shock wave in the air into a continuous disturbance Dokl Akad Nauk 419(3) 334–337