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Two–Parameter Model and Method for Computations of Turbulent Mixing in 2D Compressible Flows*

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1 Introduction

There is a wide class of 2D problems where gravitational and tangent mixing both separately and in the aggregate must be accounted. The use of direct numerical simulation using 2D gas-dynamic codes for solving such problems is possible but not always yield acceptable results. Therefore, currently a most real way is to use within 2D gas-dynamic methods the codes implementing semi- empirical models of turbulent mixing. Nowadays there are many papers devoted to numerical simulation of turbulent mixing (the review of these papers can be found, for example, in [1]). Here the greatest application was found by the two-parameter $k - \varepsilon$ — models owing to their fair simplicity. Only a few papers consider the gravitational and tangent turbulent mixing in combination (see, for example, [2]). This paper suggests the two-parameter $k - \varepsilon$ model describing turbulent mixing in the general case of 2D compressible flows. The model is implemented in the EGAK program complex [3] basing on the Lagrangian-Eulerian gas-dynamic method [4]. The initial version of the model is described in paper [5].

2 Turbulent mixing model

The model relies upon the following assumptions: a) the Reynolds number is great; b) each mixture component (fluid, gas) is described by the complete set of thermodynamic

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parameters : mass ($\alpha_i = M_i/M$) and volume ($b_i = V_i/V$) fractions as well as by specific energies (per mass unit) $e_i = E_i/M_i$; c) the mixture is isotropic.

The equations for averaged values in Lagrangian-Eulerian coordinates have the following form for the above assumptions: equation of motion

$$\frac{d}{dt}(\rho\vec{u}) = -\nabla P + \mathrm{div}\sigma_T, \tag{1}$$

continuity equation for components

$$\frac{d}{dt}(\alpha_i\rho) = c_\alpha \mathrm{div}(\rho D\nabla\alpha_i), \tag{2}$$

volume conservation law for components

$$\frac{d}{dt}(\beta_i) = \mathrm{DIF}(\beta_i), \tag{3}$$

energy equation for components

$$\frac{d}{dt}(\alpha_i\rho e_i) = c_\alpha \mathrm{div}(\rho D\nabla\alpha_i e_i) - (P + P_T)\mathrm{div}\vec{u} + \alpha_i\rho e. \tag{4}$$

The above notation is as follow: P_T — turbulent pressure, σ_T — Reynolds stress tensor, ε — turbulent energy k dissipation rate, $\rho = 1/\sum\limits_{i=1}^{N}\frac{\alpha_i}{\rho_i}$ — average density, $\vec{u}$ — velocity, $\vec{w}$ — turbulent mass flow, i — component number, $i = 1, 2, \ldots, N$, the term $DIF(\beta_i)$ in equation (3) is responsible for relative change of component volumes due to the mass diffusion.

The differential equations for turbulent quantities have the form: turbulent energy equation

$$\frac{\partial k}{\partial t} = G_1 + G_2 - \frac{1}{\rho}\mathrm{div}\rho k(\vec{u} - \vec{w}) - \varepsilon - \frac{2}{3}k\ \mathrm{div}(\vec{u} - \vec{w}) + c_k\frac{1}{\rho}\mathrm{div}\rho D\nabla k, \tag{5}$$

dissipation rate equation

$$\begin{aligned}\frac{\partial\varepsilon}{\partial t} &= \frac{\varepsilon}{k}(c_{\varepsilon 1}G_1 + c_{\varepsilon 2}G_2 - c_{\varepsilon 3}\varepsilon) - \frac{1}{\rho}\mathrm{div}\rho\varepsilon(\vec{u} - \vec{w}) - \frac{4}{3}\varepsilon\mathrm{div}(\vec{u} - \vec{w}) \\ &\quad + c_\varepsilon\frac{1}{\rho}\mathrm{div}\rho D\nabla\varepsilon - \frac{2}{3}c_{\varepsilon 4}\varepsilon(\vec{w}\vec{A}),\end{aligned} \tag{6}$$

where $G_1 = D\frac{\partial u_j}{\partial x_k}(\frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j}), G_2 = \vec{w}\frac{\nabla P}{\rho}$ — generation term of turbulence.

To close the system (1)–(6) the following relations are used: for Reynolds stress tensor and turbulent pressure

$$\sigma_T = \rho D \left(\frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j} \right) - \frac{2}{3} \rho k \delta_{jk}, \qquad P_T = \frac{2}{3} \rho k, \tag{7}$$

for turbulent diffusion coefficient

$$D = c_D \frac{k^2}{\varepsilon}, \tag{8}$$

for turbulent flow $\vec{w}$

$$\vec{w} = D\vec{A}, \tag{9}$$

where

$$\vec{A} = \frac{\nabla P}{\left(\rho\lambda_1 + \frac{T}{\rho C_V} \lambda_2^2 \right)} - \frac{\nabla \rho}{\rho}, \quad \lambda_1 = \left. \frac{\partial P}{\partial \rho} \right|_T, \lambda_2 = \left. \frac{\partial P}{\partial T} \right|_S, C_v = \left. \frac{\partial k}{\partial T} \right|_\rho,$$

in the case of perfect gas

$$\vec{A} = \frac{\nabla P}{\gamma P} - \frac{\nabla \rho}{\rho}, \tag{10}$$

where γ is the adiabatic gas index.

The above equation system contains several coefficients: c_e, c_k, c_α, c_D, $c_{\varepsilon 1}$, $c_{\varepsilon 2}$, $c_{\varepsilon 3}$, $c_{\varepsilon 4}$, which can be evaluated either from some theoretic considerations or basing on test computations. These coefficients are selected basing on known experimental data on evolution of gravitational and tangent mixing. However, owing to the wide scatter of the experimental data selection of the coefficients depends on intuition and predilections of authors of the models. We make use off two sets of coefficients with one being selected at gas tests of Vasilenko et al. [6] on gravitational mixing and the other at the tests of Kucherenko et al. [7] with immiscible fluids (see Table 1). In addition, at selection of the coefficients it was also necessary to secure an acceptable result for tangent mixing.

Note that the coefficient $c_{\varepsilon 3}$ is selected from theoretic consideration based on the experimental data on uniform isotropic turbulence decay.

	c_e	c_k	c_α	c_D	c_ε	$c_{\varepsilon 1}$	$c_{\varepsilon 2}$	$c_{\varepsilon 3}$	$c_{\varepsilon 4}$
at tests [6]	3	3	3	0.75	2	1.55	1.25	2	1
at tests [7]	3	3	3	0.12	2	1.3	0.9	2	1

Table 1: Values of the coefficients for the turbulence model

3 Equation approximation

Eqs. (1)–(10) are approximated in Lagrangian-Eulerian variables on a moving arbitrary quadrangular computational grid in several stages with the method of fractional steps being involved. At the first stage changes in velocities due to deviator terms of the stress tensor, the values of the diffusion coefficient D, as wells the values $\vec{w}$, A are defined.

At the second stage the gas dynamics equations are solved in Lagrangian variables with account of turbulent pressure $\widetilde{P} = P + P_T$. The implicit method from paper [5] with appropriate modifications is used for this purpose.

At the third stage the equations for turbulent energy and rates of dissipation without diffusion terms, as well as terms of energy equations for components related with turbulent flow and turbulent energy dissipation are approximated. At the approximation the schemes are used which secure solution positivity.

At the fourth stage the convective terms of Eqs. (1)–(5) are approximated. For this purpose the modified code [5] is used. The modification is related both to the need to update additional values and to the need to change computation of component mass flows from mixed cells containing a mixture of several components. For the problems under consideration it is assumed that from a mixed cell to a mixed cell mixture with thermodynamic parameters of the donor cell always flows.

At the fifth stage the diffusion terms of Eqs. (1)–(5) are approximated. The difference scheme used is described in paper [5]. After computation of diffusion component asses their volume fractions are updated to smooth component pressures using the algorithm close to that given in paper [8]. On the whole the scheme is of the first order of approximation in time and space. The number of the components is not limited both on the whole over the computational domain and in a separate mixed cell.

4 Choice of initial conditions

When the computations used the $k - \varepsilon$ model, the problem is to set initial data for initial values of turbulent energy dissipation rate ε and turbulent energy k. The computation results are usually assumed to depend slightly on "reasonably" selected initial values. We propose a specific "reasonable" restriction on the choice of initial data. The evaluation of initial data for k and ε in some cases can restrict to consideration of flow with uniform deformation and turbulence. The asymptotic properties of solutions were studied for the above conditions. It was found that in most cases the solutions have the asymptote in (k, ε)-plane so that initial conditions may be chosen at this asymptote.

Assumption 1. First, we assume that the main gas- dynamic flow is the flow with the uniform deformation that is all characteristics of gas- dynamic flow influencing the turbulent energy k and the dissipation rate of turbulent energy ε, do not depended on the space point. Second, we neglect potential time and space dependence of thermo-

dynamic gas parameters (density, pressure, temperature etc.). Third, we assume that the turbulence generation rates G_1 and G_2 are fixed and do not depend on space and time. Fourth, we assume that the turbulent energy and the dissipation rate of turbulent energy do not greatly influence the gas-dynamic (averaged parameters) of the flow considered.

The above assumption permit to consider only the equation for turbulent energy k and dissipation rate ε where the variability of all parameters is determined only by the variability of k and ε, so that we may not involve the gas- dynamic equations.

Assumption 2. For further simplification, we suppose that we deal with the uniform turbulence, that is k and ε may depend only on time and are independent on spatial coordinates.

In this case, equation (5) and (6) yield the system of ordinary differential equations for k and ε.

$$\frac{dk}{dt} = (G_1 + G_2)\frac{k^2}{\varepsilon} - \varepsilon + \sigma k; \tag{11}$$

$$\frac{d\varepsilon}{dt} = \frac{\varepsilon}{k}(c_{\varepsilon 1}G_1 + c_{\varepsilon 2}G_2)k - c_{\varepsilon 3}\frac{\varepsilon^2}{k} + 2\sigma\varepsilon - c_0 k^2. \tag{12}$$

where the following notation is used for constants:

$c_0 = \frac{2}{3}c_{\varepsilon 4}c_D\left\langle \vec{A}; \vec{A}\right\rangle; \quad \sigma = \frac{2}{3}\mathrm{div}\vec{u};$

In most cases, the system for the variables k and $\psi = e/k$ has a special (stationary) point with the coordinate

$$\psi_S \equiv \frac{\sigma + \sqrt{\sigma^2 + 4G_3(c_{\varepsilon 3} - 1)}}{2(c_{\varepsilon 3} - 1)} \geq 0. G_3 = (c_{\varepsilon 1} - 1)G_1 + (c_{\varepsilon 2} - 1)G_2$$

in the first quadrant.

This stationary point, if unique, is repulsive. If there are some stationary points then the given point is the only attracting one. Therefore the recommendation is to select initial conditions as close to the stationary point (ψ_s, k_s) as possible, namely from the formula

$$\frac{\varepsilon(0)}{k(0)} = \psi_2 \equiv \frac{\sigma + \sqrt{\sigma^2 + 4g_3(c_{\varepsilon 3} - 1)}}{2(c_{\varepsilon 3} - 1)}. \tag{13}$$

Then we will have more time to achieve computational consistency of gas-dynamic processes with diffusion and turbulence generation.

Formula (13) determines initial values for the relations ε/k. At this point we do not propose the formula for the selection of the initial "amplitude" for the turbulent energy k and dissipation rate of the turbulent energy e. Formula (13) may be useful for some elementary flows allowing to automate the specification of initial data; however we can not expect it to be a universal solution for this problem.

5 Some computations

The above features of the turbulent mixing model and the gas-dynamic method on whose basis it is implemented allow to use it to model a wide spectrum of gas-(and hydro-) dynamics problems. The method was used to perform numerous test and methodological computations which were used as the basis for selection of the two sets of coefficients given in Table 1. Some computed results are given below. Unless stated otherwise, the computations were performed with the first set of the coefficients. In some cases for comparison the computed results for the second set of the coefficients are also given.

Problem 1. Rayleigh-Taylor instability. The described method was used for computations for $\delta = 1.66, 3, 7, 20$.

The computed results are in good agreement with those using the TOGA method [9]. Figure 1 shows the dependencies of TMZ width L on deceleration path value $S = 0.5\,gt^2$. The zone width was estimated as a distance where volume fraction of one of the fluids varied from 0.01 to 0.99. From the figure it is seen that the dependencies, as they showed be, are linear. They can be represented in the $L = F(A)S$, where $A = (\delta - 1)/(\delta + 1)$ — the Atwood number, $S = gt^2/2$. The graph of the function F obtained in the computations by the TOGA method is given in Figure 2; the same figure gives the results of our computations and those of direct 2D numerical simulation from paper [10].

The self-similar nature of flow is also confirmed by the profile $\tilde{\rho}(\tilde{x})$, where $\tilde{\rho} = (\rho - \rho_1)/(\rho_2 - \rho_1)$, $\tilde{x} = x/(x_{0.9} - x_{0.1})$. For the length unity the distance is taken between points $x_{0.1}$ and $x_{0.9}$, where $\tilde{\rho}$ is $\tilde{\rho} = 0.1$ and $\tilde{\rho} = 0.9$ respectively. Note that in these variables the profiles do not practically depend on the value δ which is illustrated by Figure 3 which gives dependencies $\tilde{\rho}(\tilde{x})$ for $\delta = 3$ and $\delta = 20$.

Problem 2. Tangent mixing. At the plane interface is a tangent velocity discontinuity $\Delta u = 6$. The normal velocity component is taken to equal zero. The computations are performed for $\rho_2 = \rho_1$ and $\rho_2 = 3\rho_1$.

Figure 4 gives TMZ width as function of time. The zone width L was estimated as the distance where volume fraction of one of the fluids varied from 0.01 to 0.99. It is seen that in some time this dependence for the case of $\delta = 1$ transfers to the self-similar mode, in doing to the value $\partial L/\partial t/\Delta u$ is located between the results of the phenomenological models [11] and paper [12]. As δ increases, zone growth rate decreases.

The given figures show rather good agreement between our computed results and the semi- empirical theory predictions which, as it is mentioned in paper [11], in their turn, are in good agreement with the experimental data.

Problem 3. Tangent-gravitational mixing. Two incompressible fluids with a plane interface have a discontinuity of the velocity tangent component Δu_0 and move

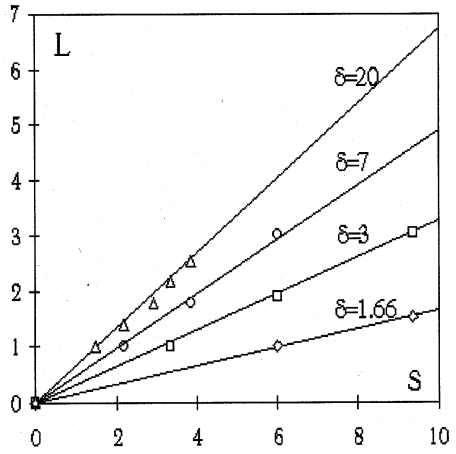

Figure 1: TMZ width L vs. deceleration path S in the gravitational mixing problem.

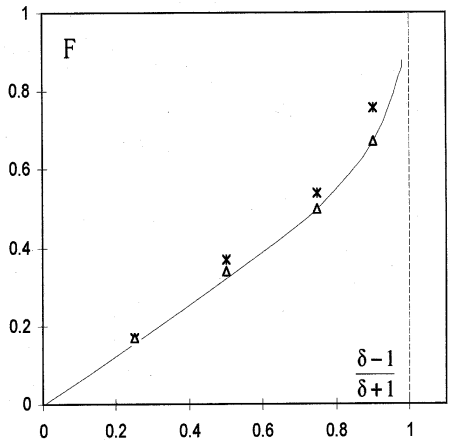

Figure 2: Function F vs. the Atwood number in the gravitational mixing problem, —— the TOGA method; $\triangle$ — $k-\varepsilon$ model; $*$ — direct simulation [10].

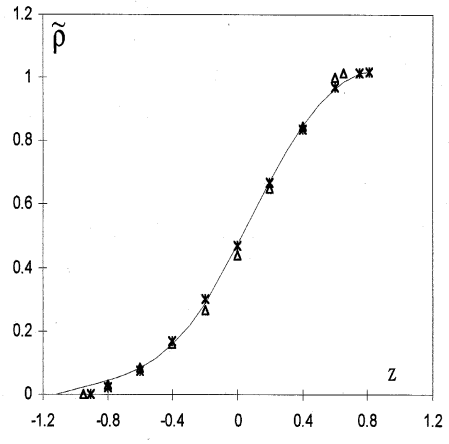

Figure 3: Self-similar profile of density $\tilde{\rho}$ vs. y in the gravitational mixing problem, —— TOGA method; $*$ — $k-\varepsilon$ model($\delta = 3$); $\triangle$ — $k-\varepsilon$ model ($\delta = 10$).

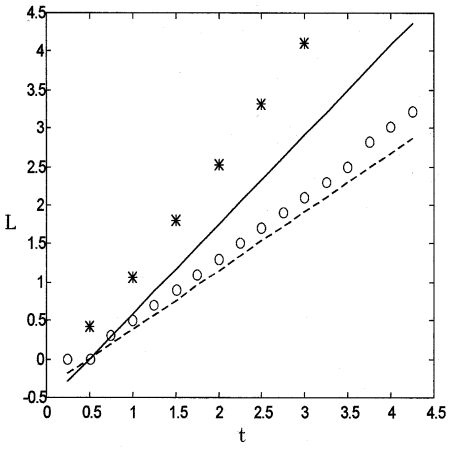

Figure 4: TMZ width vs. time, numerical computation using the $k-\varepsilon$ model: $\circ$ — first set of coefficients, $*$ — second set of coefficients; semi-empirical models: —— [11], - - - [12].

at acceleration g in the normal direction (Figure 5). By its setting-up the problem combines the two first problems. It can be show that at $g > 0$ the mixing zone growth should be faster than in each individual case, while at $g < 0$ the zone growth should stop with time. In the latter case the zone width should be proportional to $\Delta u_0^2/g$, i.e. $L = A\Delta u_0^2/g$. The proportionality coefficient A can be determined from computations.

Five computations were performed. The initial data for the computations are given in Table 2.

The computations entirely confirm the theoretic conclusions regarding TMZ (see Figure 6). For all three computations with $g < 0$ the coefficient A was practically constant, $A = 5/6$, i.e. it is universal. For $g > 0$ the TMZ width growth much faster than in each individual case considered above.

Problem 4. Turbulent mixing at acceleration at an angle to the interface. The EGAK method with the $k - \varepsilon$ model of turbulence was used in computations of experiment [13] on turbulent mixing development on an inclined interface. The problem is formulated as follows. In an ampule of rectangular cross section (64×120 mm) moving at a constant acceleration there are two fluids separated with a plane. The plane is directed at a angle to the acceleration vector. In the experiments the angles of interface inclination, ampule acceleration, as well as a fluids being accelerated were varied.

In the computations the interface inclination angles were varied. Ampule acceleration was $730\,g$, the fluid density ratio was $1 : 3$, the incompressibility condition was satisfied approximately by appropriate section of sound speed.

Among other results in the experiments it was found that with time the TMZ width stabilized and then begins to decrease. The stabilization time is therewith dependent on the discontinuity plane inclination problem angle. Note that earlier a similar problem was numerically modeled by Youngs [14], and, though the TMZ width is also stabilized in his computations, however, he did not find decrease in the zone.

The result [13] on stabilization and reduction of the TMZ width was confirmed in all performed computations. A characteristic flow pattern in the form of volume fraction isolines is given in Figure 7 for several times obtained by calculating with the interface angle $\varphi = 5°46'$. Figure 10 shows the function $L(S*)$ for the TMZ width

Computation N_0	g	Δ_{u_0}
1	0	6
2	+10	6
3	−10	6
4	−20	6
5	−10	4.24

Table 2: Initial data of the computations.

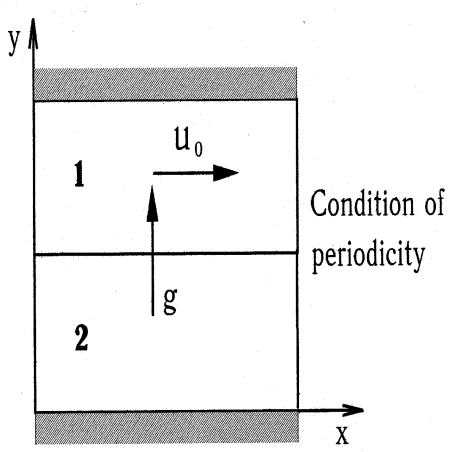

Figure 5: Initial computational geometry in the tangent-gravitational mixing problem.

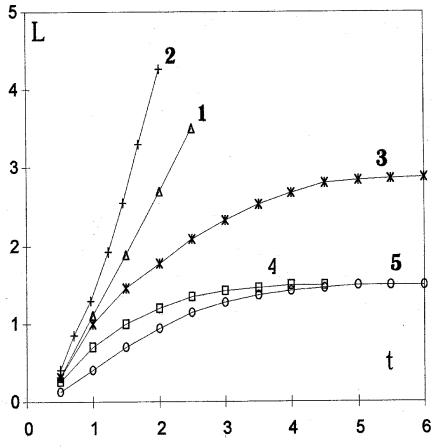

Figure 6: Mixing Zone width dependence in the tangent-gravitational mixing problem,1 — $g = 0$, $u_0 = 6$; 2 — $g = +10$, $u_0 = 6$; 3 — $g = -10$, $u_0 = 6$; 4 — $g = -20$, $u_0 = 6$; 5 — $g = -10$, $u_0 = 4.24$.

were $S* = 0.5\,gt^2 \cos\varphi$. As is seen from the figure the theoretical and experimental curves agree qualitatively though they greatly differ quantitatively. The some pattern is observed in all computations.

Problem 5. A jet from a reservoir. For various applications, it is interesting to consider the jet flowing from a reservoirs and the mixing with environment. In this connection a computation was performed where a nitrogen jet with the Mach number $M = 3 (u = 1020\,\text{m/s})$ effused. This problem was experimentally studied in paper [15]. The initial system geometry is given in Figure 8, input diameter was $d = 1.25\,\text{cm}$. The equation of state of gases are $P = (\gamma - 1)\rho E$ with $\gamma_1 = \gamma_2 = 1.4$.

Figure 10b shows nitrogen volume fraction isolines obtained in the computation for three times. It is seen that rather severe jet washing-out takes place, the apex angle being close to the experimental value ($tg\alpha \approx 0.09$). The length of the initial jet portion $L/d \cong 14$ is also close to the experimental value. In the computation L defined as the length of the portion where nitrogen fraction on the symmetry axis $\beta > 0.95$.

Figure 9 gives the profile of the nitrogen volume fraction in the cross section $x/d = 21.6$ at the latest time ($t = 2.8$) when the flow in this cross section is already close to steady. The same figure also gives the experimental data for the cross section $x/d = 19.2$.

On the whole it can be noted that the computed results at the steady flow portion

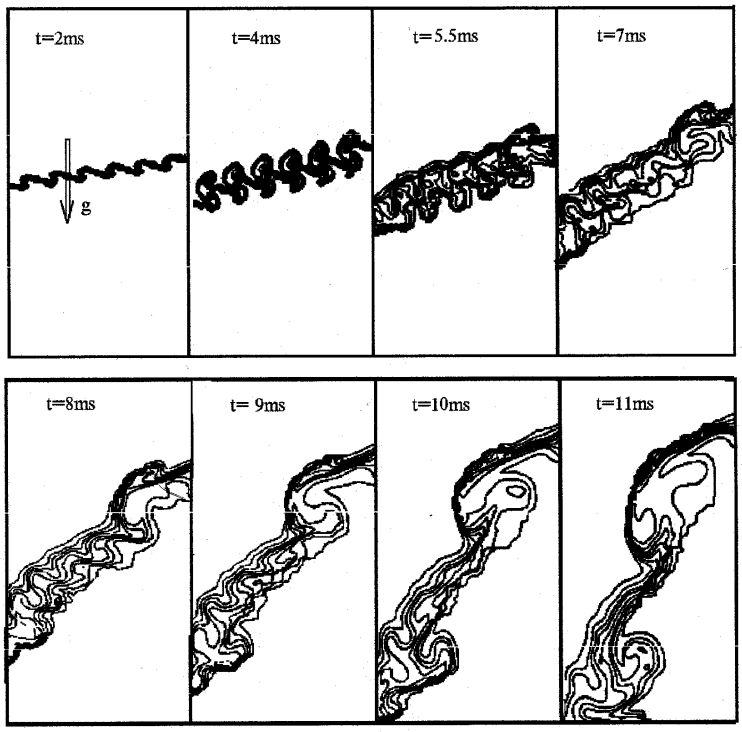

Figure 7: Isolines of volume fraction $\beta = 0.01, \ldots, 0.99$.

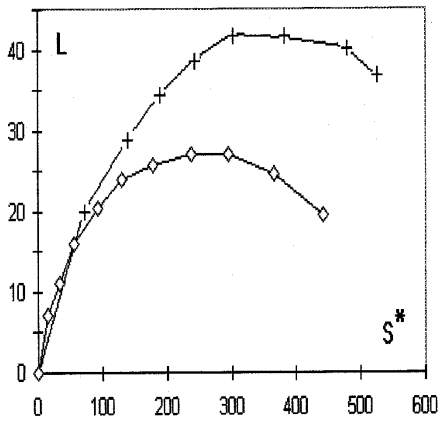

Figure 8: TMZ width vs. S^*, + — experiment [13], $\diamond$ — computation.

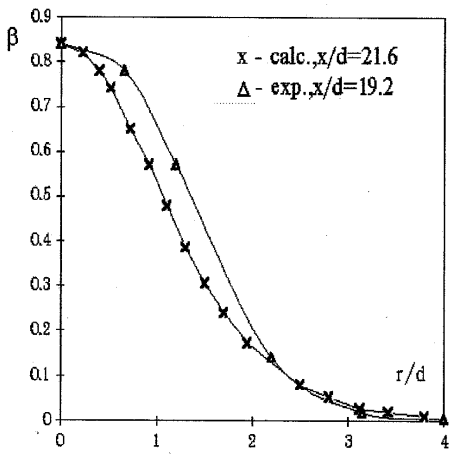

Figure 9: Nitrogen volume fraction profile in jet cross section.

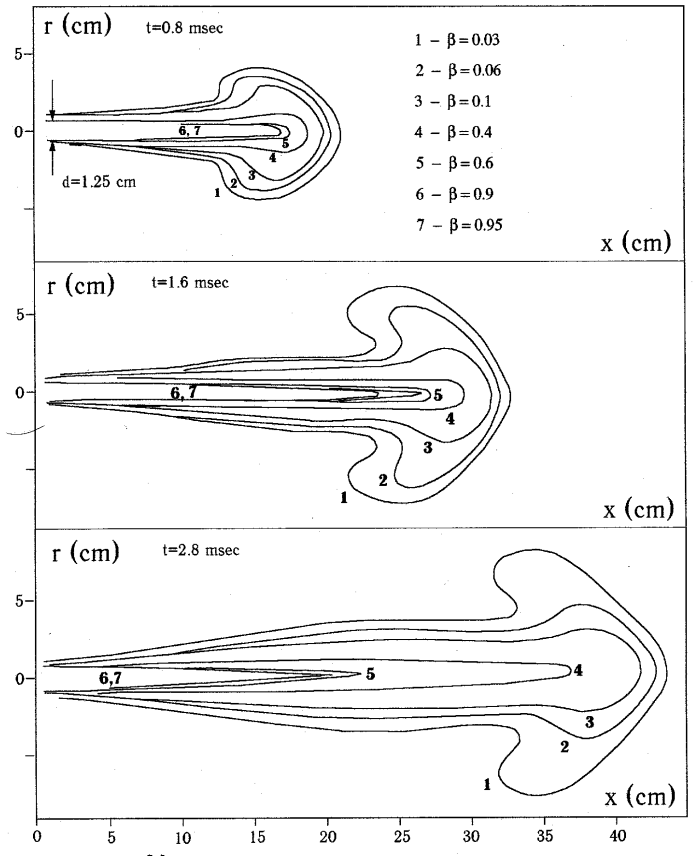

Figure 10: Isolines of volume fraction β of nitrogen jet into air.

are in good agreement with the experimental data.

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