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Simulation of Multi-Gas Jet Flows by Use of Quasi Gas Dynamic Equation System

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Abstract. In the present paper, we use the quasi gas dynamic (QGD) model together with a finite volume method for the simulation of a gas jet inflowing region filled with another gas in the presence of gravity forces. A flow picture for such flow strongly depends on the gases density ratio. Numerical simulations are held for a region filled with air under atmospheric pressure. Three variants of inflowing gas are considered: methane (light gas), butane (heavy gas) and helium (extremely light gas). A difference between flow pictures for these test cases is demonstrated. Results obtained with the presence of wind in the air are also compared. Grid convergence is established by use of different spatial meshes. Here, the the QGD model demonstrated good efficiency in modeling multi-gas jet flows. The calculations were also used for the adjustment of the numerical method parameters.

Introduction

There are many engineering and ecological problems including simulation of fluid flows of various compositions and natures. Examples are the mixing of gas streams in reactors, gas outflow in pipeline accidents, mixing of gases for their effective combustion, and numerous others. Accordingly, the simulation of multicomponent gas flows is undoubtedly of practical importance.

The quasi gas dynamic, or regularized, equations for describing gas flows of various natures were derived more than thirty years ago and were successfully used to construct numerical algorithms for both traditional computer systems and massively parallel ones. A detailed description can be found in e.g. [1, 2]. Estimates show that the QGD approach is especially efficient for the simulation of unsteady or transient gas flows. At present, the use of this approach is additionally supported by the fact that QGD algorithms are included in the free open-source OpenFOAM toolbox and is available to the user community all over the world [3]. It was natural to extend the family of QGD algorithms to unsteady multicomponent gas flows.

The first attempts to write QGD system of equations for gas mixtures was intended for rarefied gas flows [4]. This system used a two-fluid model with its own continuity, momentum, and total energy equations written for each species of the mixture. The equations were related via exchange terms that appeared in the right-hand sides of the momentum and energy equations and ensured momentum and energy exchange between the species of the mixture. Significant improvements to this system of equations were made in [5]. The equation system was written in the form of conservation laws, an entropy transport equation with a nonnegative dissipative function was derived for it, and the exchange terms were generalized to polyatomic gases. However, these exchange terms lead to the necessity of integrating a generally stiff ODE system at every time step, which significantly complicates the algorithm. As a result, the experience of numerical modeling has shown that the two-liquid model is ineffective in modeling the flows of dense gases. For the case of such non-rarefied gases, the QGD system required modification.

In [6], a new QGD system of equations is proposed for binary mixtures of viscous compressible gases (in the absence of chemical reactions). It is based on a well-known single-fluid model. This model is used very often to describe multicomponent gas flows [7, 8]. In this model, the density of each species of the mixture satisfies its own continuity equation. It is assumed that molecules of different species interact quickly as compared to hydrodynamic times, so the velocity and temperature in the flow are identical for the species of the mixture. Accordingly, the momentum and total energy

equations are written for the mixture as a whole without considering equations for each species separately. Viscosity and heat conduction are treated for the mixture as a whole and are determined by the viscosity coefficient and thermal conductivity for the mixture. The equation for the density of the mixture is split into equations for the densities of individual components without explicit description of phase boundaries. Accordingly, the model did not involve a separate equation for determining phase boundaries between the species. They are formed automatically in domains with high gradients of species concentrations. The mutual diffusion between the species of the mixture is not taken into account.

QGD Equation System for a Gas Mixture

Regularized or QGD equations for flows of mixture of ideal polytropic gases have the following form (for brevity, we consider a mixture of two gases, a and b):

$$\frac{\partial \rho_a}{\partial t} + div(\rho_a(\mathbf{u}-\mathbf{w})) = 0, \tag{1}$$

$$\frac{\partial \rho_b}{\partial t} + div(\rho_b(\mathbf{u}-\mathbf{w})) = 0, \tag{2}$$

$$\frac{\partial \rho\mathbf{u}}{\partial t} + div(\rho(\mathbf{u}-\mathbf{w})\otimes\mathbf{u}) + \nabla p = div\Pi + (\rho - \tau div(\rho\mathbf{u}))\mathbf{F}, \tag{3}$$

$$\frac{\partial E}{\partial t} + div((E+p)(\mathbf{u}-\mathbf{w})) = -div\mathbf{q} + div(\Pi\cdot\mathbf{u}) + \rho(\mathbf{u}-\mathbf{w})\cdot\mathbf{F} + Q \tag{4}$$

The standard notations for gas dynamic quantities are used in this system. Additionally, the vector **F** and the scalar Q denote a specific external force and an external energy source respectively. Here $E = \rho\left(\mathbf{u}^2/2 + \varepsilon\right)$ is the total energy per unit volume. Density, pressure, gas constant R and specific internal energy ε of the mixture are defined as weighted values of gas component values and depend of the fractions of mixture components in each time-space point:

$$\rho = \rho_a + \rho_b, \quad p = p_a + p_b, \tag{5}$$

$$R = \frac{R_a\rho_a + R_b\rho_b}{\rho}, \quad \varepsilon = \frac{\varepsilon_a\rho_a + \varepsilon_b\rho_b}{\rho} = c_{\mathrm{V}}T, \quad c_{\mathrm{V}} = \frac{c_{\mathrm{V}a}\rho_a + c_{\mathrm{V}b}\rho_b}{\rho}. \tag{6}$$

The gas mixture obeys the usual relations for ideal polytropic gas:

$$p = \rho RT = \rho\varepsilon(\gamma-1), \quad \gamma = \frac{c_{\mathrm{p}}}{c_{\mathrm{v}}}, \quad R = c_{\mathrm{p}} - c_{\mathrm{v}}. \tag{7}$$

$\gamma = c_{\mathrm{p}}/c_{\mathrm{v}}$ is the adiabatic index. The viscous stress tensor Π and heat flux vector **q** are given by the following equations:

$$\Pi = \Pi_{\mathrm{NS}} + \rho\mathbf{u}\otimes\hat{\mathbf{w}} + \tau(\mathbf{u}\nabla p + \gamma p\,\mathrm{div}\,\mathbf{u} - (\gamma-1)Q),$$

$$\mathbf{q} = \mathbf{q}_{NS} - \tau\rho\mathbf{u}\left(\mathbf{u}\nabla\varepsilon + p(\mathbf{u}\nabla)\left(\frac{1}{\rho}\right) - \frac{Q}{\rho}\right),$$

with Navier-Stokes expressions for viscous stress tensor and heat flux vector in the form:

$$\Pi_{\mathrm{NS}} = \mu\left((\nabla \otimes \mathbf{u}) + (\nabla \otimes \mathbf{u})^T - \frac{2}{3}\mathrm{I}\,\mathrm{div}\,\mathbf{u} \right), \quad \mathbf{q}_{\mathrm{NS}} = -\kappa \nabla T .$$

Note, that the QGD system differs from Navier-Stokes equations in additional dissipative terms containing the multiplier τ (some relaxation parameter having a dimension of time). These additives are introduced to the viscous stress tensor, heat flux as well as to the velocity vector **u**, using the relations:

$$\mathbf{w} = \frac{\tau}{\rho}\left(\mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p - \rho \mathbf{F}\right), \tag{8}$$

$$\hat{\mathbf{w}} = \frac{\tau}{\rho}\left(\rho(\mathbf{u}\nabla)\mathbf{u} + \nabla p - \rho \mathbf{F}\right). \tag{9}$$

These terms can be interpreted as efficient numerical stabilizers, which provide smoothness of the solution and act as an adaptive to solution "built in" regularization that contributes to the stability of the numerical algorithm. The relaxation parameter τ appearing here we define as follows:

$$\tau = \alpha h / c_{\mathrm{s}}, \tag{10}$$

where c_{s} is the sound speed estimated locally, h is the grid resolution. The value of τ defines the time required for a perturbation to travel across a grid cell and the coefficient α is a tuning parameter that defines the level of subgrid dissipation. According to numerical practice it ranges in the interval between 0 and 1. This coefficient is the only tuning parameter of the QGD computational model. A sound speed for the gas mixture c used here to calculate the coefficient τ in (10) can be calculated from the following formula: $\rho c_{\mathrm{s}}^2 = \gamma_a p_a + \gamma_b p_b$.

Five basic hydrodynamic laws are satisfied for the QGD system as for NS equations: mass, momentum, total energy, angular momentum conservation laws and the second law of thermodynamics.

Obviously, it is not difficult to generalize the model described here to the case of a mixture with a large number of components. Despite of more complicated form compared to NS equations QGD system is simple for numerical realization including parallel implementation for modern supercomputer systems with different architectures.

Test Problem Simulation

The above system of equations was used to model different gas mixture flows. For example, the extremely slow process of the Rayleigh-Taylor instability in two-component gas mixtures in a wide range of Atwood numbers [9] and the transonic flow resulting from the interaction of a plane shock wave, propagating in air, with a cylindrical bubble of another gas [10]. The results showed nice properties of the QGD approach and the numerical algorithm based on it. Here we present the results of modeling the outflow of a gas jet into a space filled with air. This problem can be considered as the simplest model of gas leakage during a breakthrough of an underground gas pipeline.

Some gas flows through a hole (1 m by 1 m) in the horizontal plane, at some speed into the area above it, filled with stationary air under normal conditions. The computational region is presented in Fig. 1. Boundary conditions are the following: no slip conditions are set at the bottom plane; overpressure one half an atmosphere and outflow vertical velocity 2 m/s in the hole; zero normal derivatives for all variables are imposed at the rest boundaries.

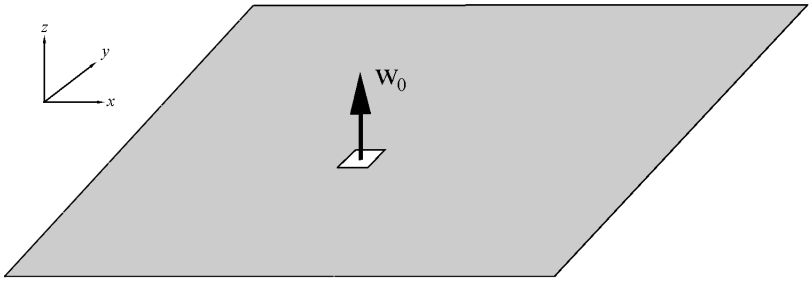

Figure 1. Computational region

For numerical implementation we use the explicit-in-time finite-volume scheme with an approximation of all space derivatives by second-order central differences. All gas dynamic variables are addressed to the cell centers. Their values at the centers of the cell faces are calculated using the linear interpolation.

In the first set of calculations, the outflowing gas is methane which adiabatic index $\gamma = 1.304$ and molecule mass $M = 16.04$. Figure 2 presents the methane mass concentration evolution in the vertical symmetry plane of the computational region. Mass concentration of inflowing gas is indicated by T in all pictures. The outer isoline corresponds to the boundary of the explosive concentration of methane gas in the air. This boundary moves with the speed approximately 5 m/c that is two and a half times more than outflow velocity.

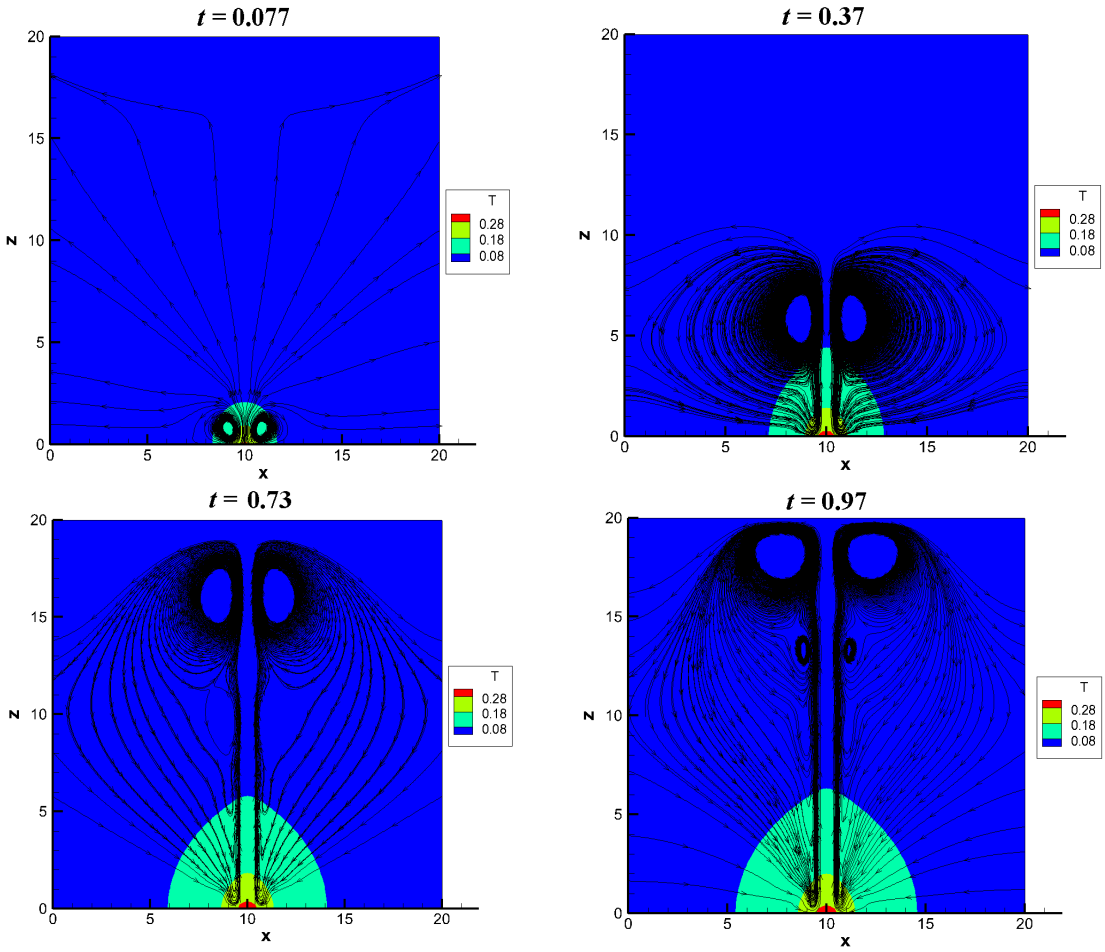

Figure 2. Instant stream traces on the background of the methane concentration at different time moments (still air)

The calculations are held for the same problem in the presence of horizontal wind in the air with the speed 5 m/c. The results are presented in Fig. 3. One can see the shift of the gas mass concentration distribution in the wind direction.

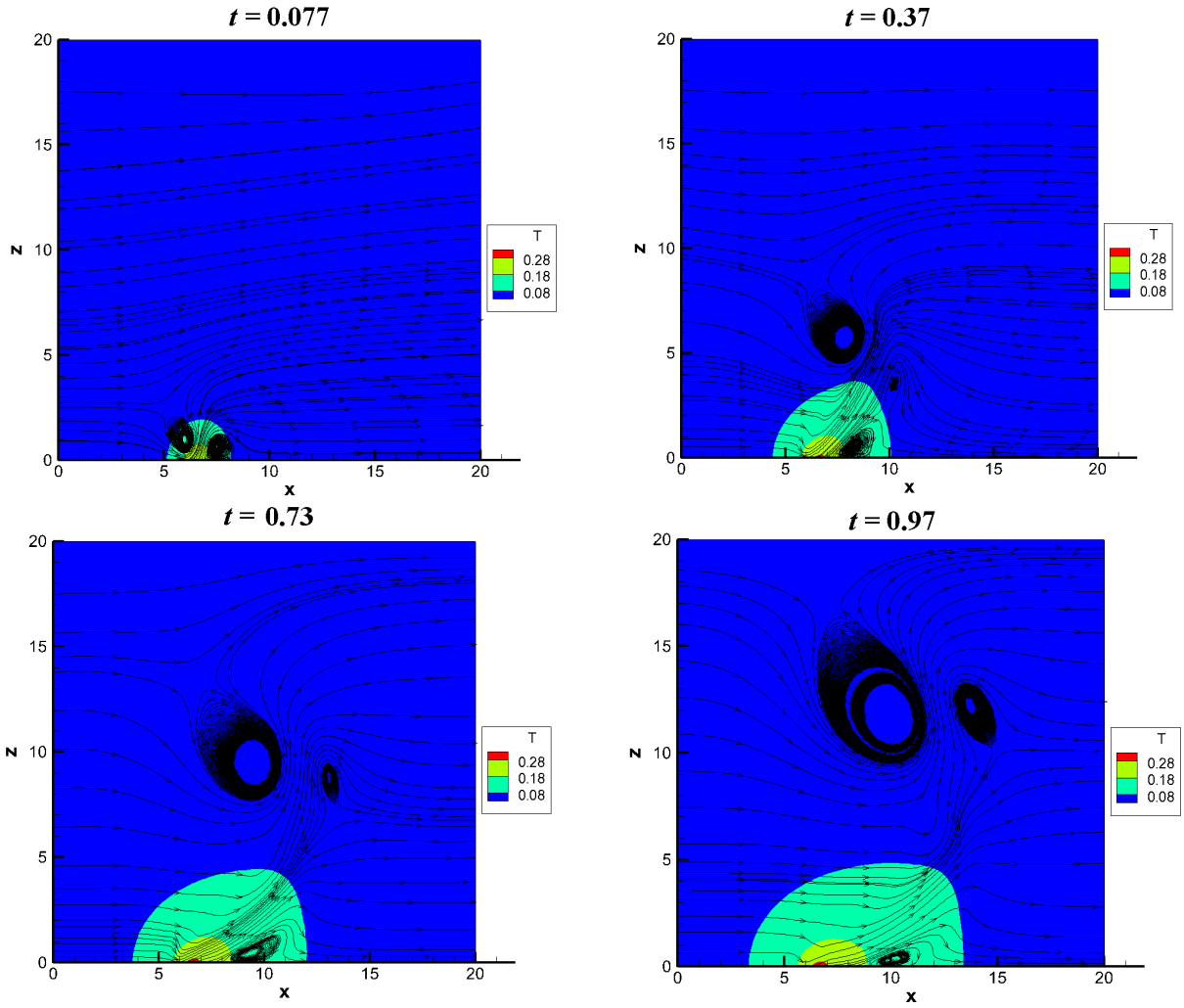

Figure 3. Instant stream traces on the background of the methane concentration at different time moments (wind in the air)

Next calculations are held for other gases. At first, we consider light gas helium (see Fig. 4). For helium $\gamma = 5/3$, $M = 4.003$. Overall picture is similar, but the propagation speed is much greater, that is quite natural for 4 times lighter gas jet.

The flow picture for much more heavy gas butane ($\gamma = 1.094$, $M = 58.12$) is presented in Fig. 5. It differs from previous ones. Heavy butane molecules in the jet have a higher kinetic energy than methane molecules. Therefore, their speed is less damped when interacting with the surrounding air. As a result, butane rises higher and then sinks down, being heavier than air. Therefore, the jet behaves like a fountain.

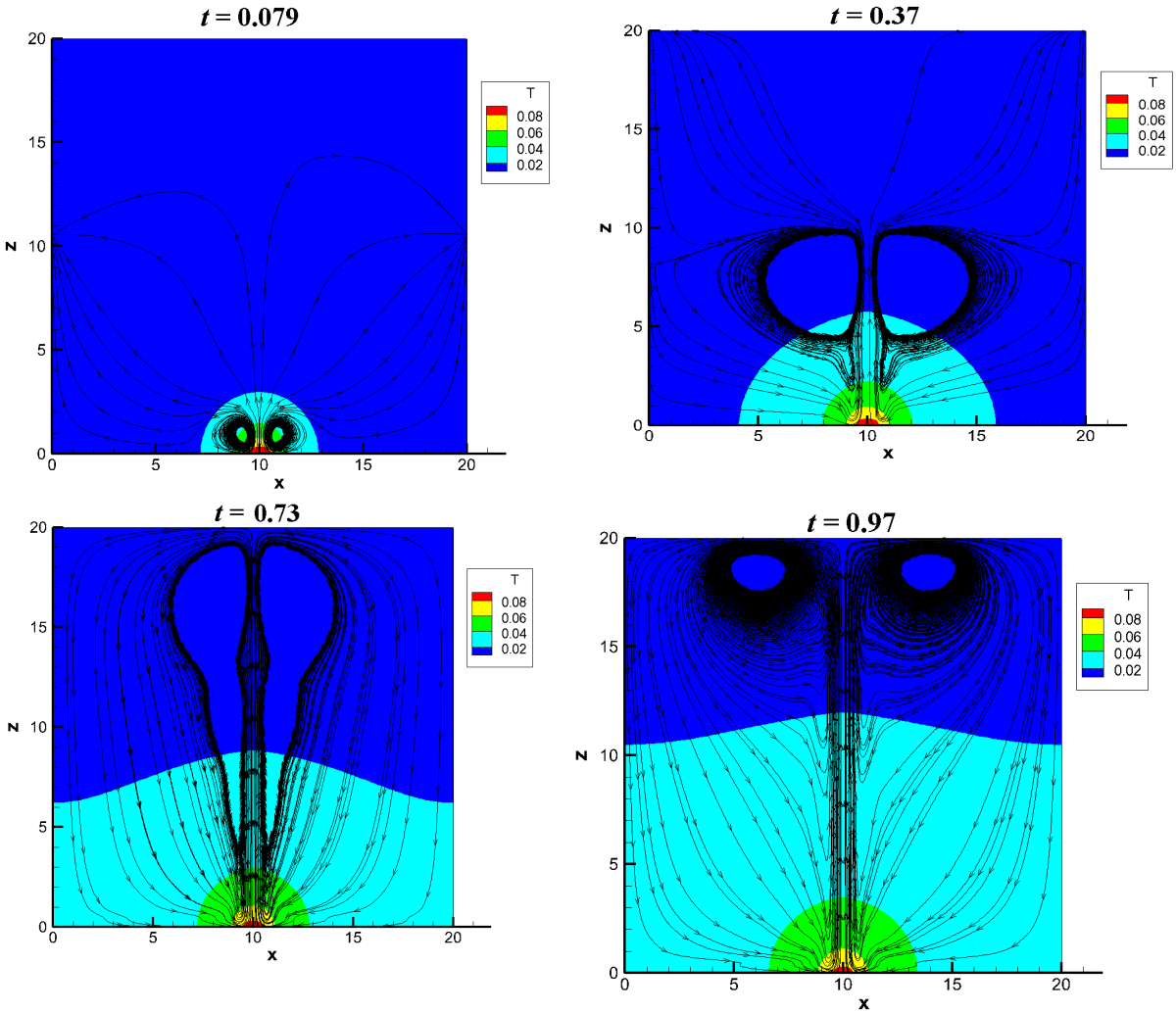

Figure 4. Instant stream traces on the background of the helium concentration at different time moments

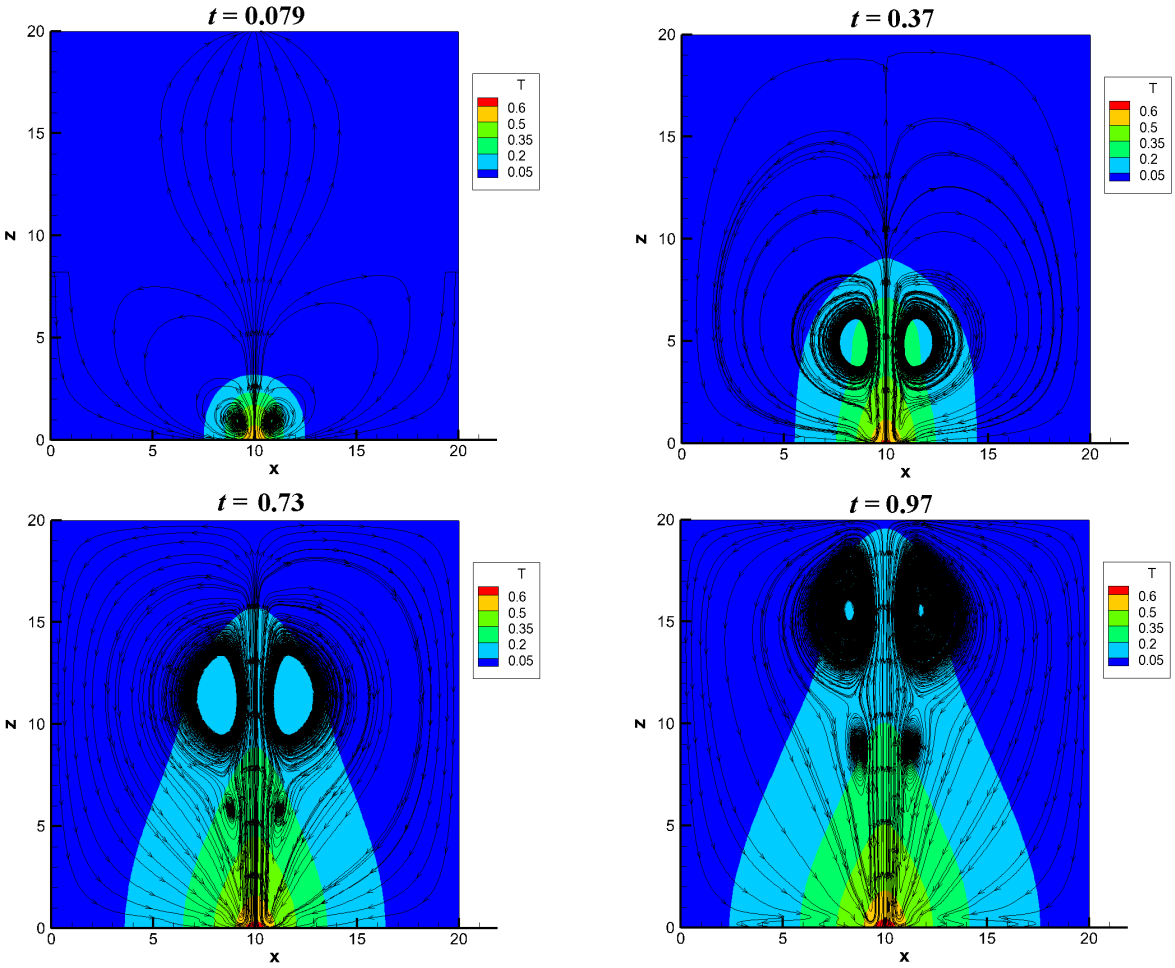

Figure 5. Instant stream traces on the background of the butane concentration at different time moments

Stability Investigation

As a test for studying the stability of the algorithm, we solve the one-dimensional Riemann problem for two different gases initially in non-equilibrium gas-dynamic state. The problem statement is taken from [11]. Initial conditions are: helium ($\rho_{He} = 14.54903$, $p_{He} = 10^7$) in the left half of the region $0 \le x \le 0.5$, and air ($\rho_{Air} = 1.16355$, $p_{Air} = 10^5$) in its right half. The initial velocity in the entire region is equal to zero. The size of the calculated area and the final time of the calculation ($t_{fin} = 2.0 \cdot 10^{-4}$) are coordinated in such a way that the perturbations do not reach the boundaries. Therefore, the conditions of constancy of all gas-dynamic parameters are set at the region boundaries. We neglect the physical viscosity μ and thermal conductivity κ of gases and use the mixture equations in the Euler formulation.

The calculations show the formation of small oscillations in the region behind the contact discontinuity, where the density of one of the components of the mixture is close to zero. They are clearly visible in Figure 6 (a). In the calculations of the gas outflow given above in this paper, no such oscillations were detected. However, such fluctuations were observed in multidimensional calculations [10], but there they were barely noticeable against the background of shock waves. It should be noted that the suppression of such non-physical oscillations, as a result of which the densities of some components can become negative in areas where these densities are small, is given much attention in the scientific literature. Thus, in [8, 12], the double flux method is used for this purpose, when special modifications of the numerical methods are used to approximate convective fluxes at the cell boundaries. We managed to completely suppress the fluctuations and avoid the occurrence of negative densities of the gas components by using a modified scheme in which the

convective flux in equation (1) for air is approximated by upwind difference. The result of the calculation using such modified scheme is shown in Fig. 6 (b). All other scheme parameters are the same.

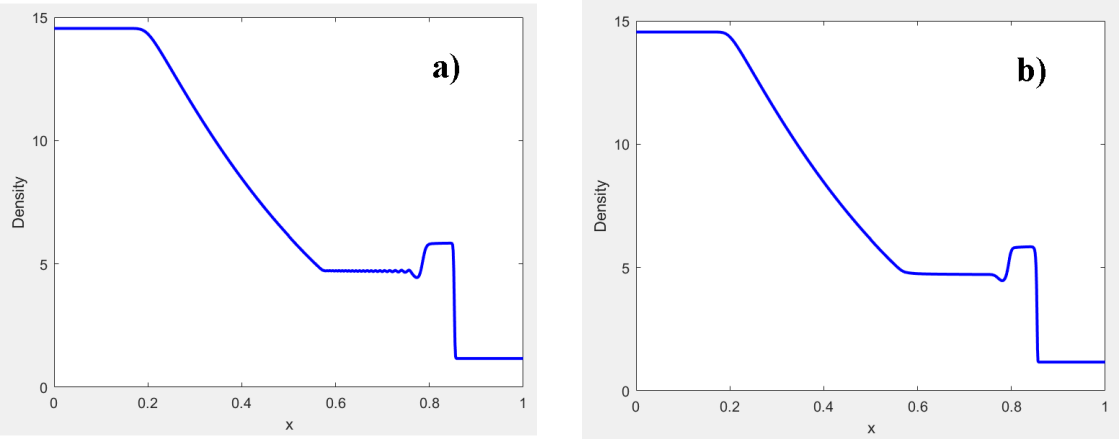

Figure 6. Riemann problem solution by use of scheme [10] (a) and modified scheme (b)

In order to investigate the stability of the scheme, calculations are performed with different time and space steps for different α values . For each selected value of α, a series of calculations are performed with different Courant numbers β in the formula

$$\Delta t = \beta \cdot \min_i \frac{h}{c_i + |u_i|}, \tag{11}$$

where the minimum is taken for all grid cells at a given time, i is the cell number. The maximum value of β is chosen, at which the solution of the problem remains stable. When calculating according to the initial scheme from [10], the study of stability is complicated by the presence in the numerical solution of oscillations mentioned above, which must be distinguished from instability. In this case, the calculation is considered stable at such a value of β, at which the amplitude of the oscillations ceased to change when it decreased. The results of the calculations are shown in Figs. 7-8.

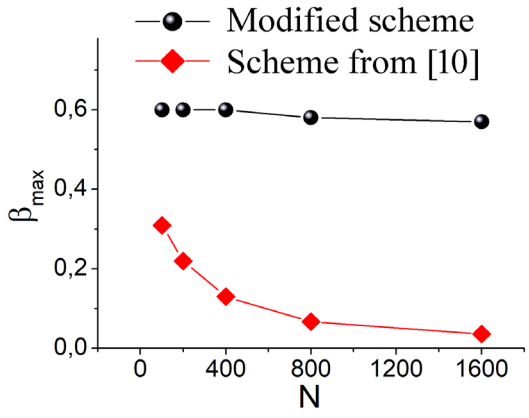

Figure 7. Grid size influence on the acceptable Courant number. $\alpha = 0.3$

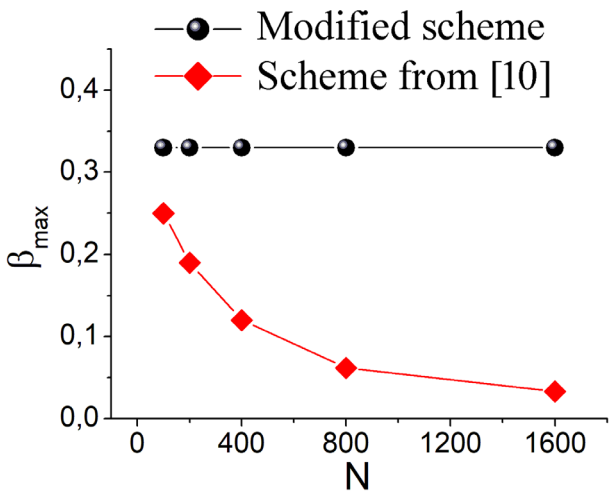

Figure 8. Grid size influence on the acceptable Courant number. $\alpha = 0.13$

The following conclusions can be drawn from these figures.

- The modified scheme allows calculating with a higher value of the Courant number β.
- The stability of the modified scheme is really determined by the Courant condition (11), in contrast to the scheme from [10], for which the maximum allowable value of β decreases markedly with a decrease in the space step.
- The allowable Courant number in the calculations according to the modified scheme depends more strongly on the regularization parameter α than in the calculations according to the scheme [10]. So, for shown in Fig. 7 and 8 values of α, the allowable values of β for the modified scheme differ almost twice, while for the scheme [10] the differences do not exceed 10%.

Figure 9 shows the dependence of the allowable Courant number for the modified scheme on the parameter α. It is typical for schemes based on QGD systems of equations.

It can be seen from this figure that the best stability level is observed at the values of α lying in the range $0.2 \div 0.3$. However, under such conditions, the dissipation introduced by the QGD regularizers is quite large, which worsens the quality of the resulting solution. Therefore, the smallest values of α are usually used, which provide sufficient stability. Most of our calculations are carried out with $\alpha = 0.13$, at which the maximum allowable Courant number $\beta = 0.33$.

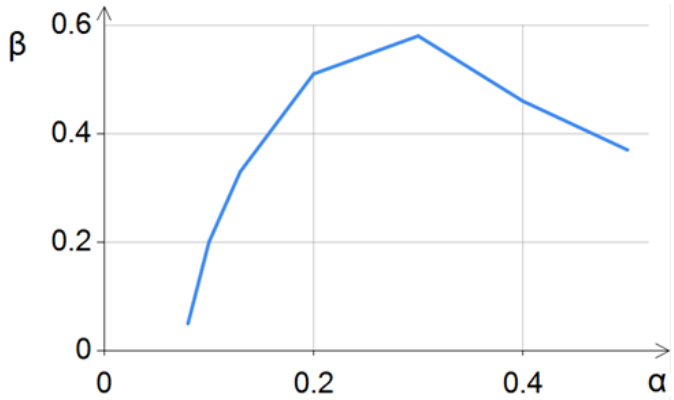

Figure 9. The dependence of the acceptable Courant number β on the regularization parameter α when using the modified scheme

Summary

Numerical method based on the QGD equations allows performing numerical simulation of jet flows with gases with very different particle masses. Obtained results are qualitatively reasonable. Numerical solution has proper symmetry. The quality improvement with the spatial grid refinement is shown. The computational method stability is investigated, the Courant type stability condition is confirmed.

Developed technique can be applied to vide variety of problems connected with different gas mixtures. In the future we plan to include the developed algorithm into the open software complex OpenFOAM.

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