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ABOUT ONE NUMERICAL METHOD OF COMPRESSIBLE MULTIFLUID FLOW MODELING IN EULER FORMULATION

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ABSTRACT

A numerical algorithm for modelling a mixture of viscous compressible non reacting gas flow in transonic regimes is presented. Method is based on the finite volume approach together with the implementation of the regularized, or quasi gas dynamics equations. Simulations examples of a nonstationary supersonic air flow interactions with light and heavy gas bubbles are shown.

Keywords: gas mixture, regularized gas dynamic equations, quasi gas dynamic equations, supersonic flow.

INTRODUCTION

Quasi gas dynamic (QGD), or regularized gas dynamic equations for description of different kinds of flows and the effective methods for its numerical implementation are now used in a number of test and imitational engineering problems. Especially the QGD approach is effective for numerical simulation of nonstationary or time-dependent gas flows. The wide use of this approach is supported by the fact, that quasi gas dynamic algorithms are now implemented in the open international used program platform OpenFOAM, and it is available to a wide range of users all over the world.

It seems to be natural to enlarge the existing QGD gas dynamic models for nonstationary flows of gas mixtures. The first attempts were made for rarefied and dense gas mixtures in Elizarova T *et al.*, 2001 and Elizarova T *et al.*, 2019. In this paper we present a new variant of the algorithm for non-rarefied flows, closely related with the mentioned above, but more robust and numerically stable. Particularly, this method can be used in modeling of gas mixing jets in engine cameras, jet issues in gas pipes damages, definitions of boundary positions between different sorts of nonstationary gas layers and in other simulations. This method was firstly tested in Shilnikov EV, Elizarova TG, 2019 on the modeling of extremely slow process of Rayleigh-Taylor instability development. This paper presents the first attempts in using our method for supersonic flows simulation.

Opposite to the previous QGD algorithms for gas mixtures, the mathematical structure of the new method is similar to the basing QGD method, implemented earlier as new computational QGD kernel in complex OpenFOAM, see, for example Kraposhin MV *et al.*, 2017 and Kraposhin MV *et al.*, 2018. This important feature of the new algorithm would facilitate its implementation in OpenFOAM library and would allow to connect it with other developed computational nodes of OpenFOAM (see OpenFOAM User Guide). For example, with computational nodes describing chemical reactions between mixture components. All these points explain the actuality of the work.

The structure of the paper is the following: in the first part the popular mathematical model for gas mixture flows without chemical reactions is presented. As a model among others we choose the variant, which describes a gas mixture as a system of equations for densities of each gas component, without explicit border selection and additional mass fraction equation. For simplicity reasons we are limited by a binary gas mixture. In the second part the regularized analog of the gas mixture system is presented. The third part is devoted to the examples of numerical modeling of the well-known unsteady mixture flow together with the brief presentation of numerical realization of the QGD system. Particularly, the simulation of supersonic gas flow in a tube containing gas bubbles of different densities under shock-wave impact is presented in details and compared with other numerical results and experimental data. In conclusion some possible generalizations and implementations of the method are mentioned.

EQUATION SYSTEM FOR A GAS MIXTURE

Let us consider a gas mixture without chemical reactions. As a basis, we choose a well-known model written for densities of individual components. Mutual diffusion of gases is not taken into account. The model is based on the assumption that the interaction of gas particles occurs quickly compared to hydrodynamic time, so mixture components have common velocity and temperature. Therefore, the equation of momentum and total energy for the mixture is not split into separate components. The processes of viscosity and thermal conductivity in a mixture are considered at the level of the entire mixture as a whole and are determined by the coefficients of viscosity and thermal conductivity for the mixture.

The system of equations does not include an explicit definition of interphase boundaries. Thus, boundaries between components of the mixture are formed automatically in zones of large gradients of component densities. So a separate equation to determine the position of the boundaries is not used.

This variant of a gases mixture model is very common. In particular, it is used in many works, see, for example, Quirk J, Karni S, 1996, Abgrall R, 1996, Abgrall R, Karni S, 2001, Billet G, Abgrall R, 2003. For this kind of model a lot of effort was taken to suppress oscillations at the interface between the fluids in the calculations employed schemes with high order of approximation. For this purpose, Double Flux modification of widely used numerical methods such as TVD-MUSCL schemes (Abgrall R, Karni S, 2001), discontinuous Galerkin method (Billet G, Ryan J, 2011), and Godunov-type schemes (Saurel R, Abgrall R, 1999, Borisov VE, Rykov Yu, 2019) was used. In contrast to the model described above, in Saurel R, Abgrall R, 1999, a multi-fluid model is considered, when each fluid has not only its own density, but also its own velocity and pressure. This leads to the presence of exchange and non-conservative terms in the right-hand side parts of equations. This model copes well with modeling flows of a mixture of liquids and gases. However, the presence of exchange terms leads to the need to solve a generally rigid system of ordinary differential equations at each computational time step, which sufficiently complicates the algorithm. In modeling the reacting gases flows, such a system must be solved in one way or another (Borisov VE, Rykov Yu, 2019, Lian YS, Xu K, 2000). But in the absence of chemical reactions, it seems more desirable to avoid this complication.

For brevity, here we consider a mixture of two gases. For this case the mentioned above equation system has the following form:

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

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

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \mathrm{div}(\rho(\mathbf{u} \otimes \mathbf{u})) + \nabla p = \mathrm{div}\,\Pi_{\mathrm{NS}} + \rho \mathbf{F}, \tag{3}$$

$$\frac{\partial E}{\partial t} + \mathrm{div}((E+p)\mathbf{u}) = -\mathrm{div}\,\mathbf{q}_{\mathrm{NS}} + \mathrm{div}(\Pi_{\mathrm{NS}} \cdot \mathbf{u}) + \rho(\mathbf{u} \cdot \mathbf{F}) + Q, \tag{4}$$

Here a common definitions for gas dynamic quantities are used. Additionally, vector **F** and scalar *Q* are an external force and a source or a drain of external energy, respectively. The shear stress tensor Π_{NS} and the heat flax vector $\mathbf{q}_{\mathrm{NS}}$ are

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

with I being the unity matrix. We suppose that a gas mixture has a common velocity **u** and temperature *T,* and a mixture density, pressure and the specific total energy are defined as

$$\rho = \rho_a + \rho_b, \; p = p_a + p_b, \; E = \rho\varepsilon + \rho \mathbf{u}^2/2.$$

Additionally, a mixture obeys the usual relations for ideal polytropic gas:

$$p = \rho R T = \rho\varepsilon(\gamma - 1),$$

where γ is the adiabatic index, *R* is a gas constant and ε is the specific internal energy of the mixture:

$$R = \frac{R_a \rho_a + R_b \rho_b}{\rho} = c_{\mathrm{p}} - c_{\mathrm{V}}, \quad \gamma = \frac{c_{\mathrm{p}}}{c_{\mathrm{V}}}, \quad \gamma - 1 = \frac{R}{c_{\mathrm{V}}}.$$

$$\varepsilon = \frac{\varepsilon_a \rho_a + \varepsilon_b \rho_b}{\rho} = c_{\mathrm{V}} T, \quad c_{\mathrm{V}} = \frac{c_{\mathrm{V}a} \rho_a + c_{\mathrm{V}b} \rho_b}{\rho},$$

Mention, that gas dynamic values for the mixture are defined as weighted values of gas component values and depend of the fractions of a mixture components in each time-space point (*x*,*t*). The sound speed can be calculated from one of the following formulae:

$$c_{\mathrm{s}}^2 = \gamma R T, \text{ or } \rho c_{\mathrm{s}}^2 = \gamma_a p_a + \gamma_b p_b.$$

A generalization of this model to the case of a mixture of more than two gases is not difficult.

REGULARIZED EQUATION SYSTEM FOR A GAS MIXTURE

Regularized equation system for ideal polytropic gas has the following form (Elizarova TG, 2009 and Sheretov Yu, 2009):

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho(\mathbf{u} - \mathbf{w})) = 0, \tag{5}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \mathrm{div}(\rho(\mathbf{u} - \mathbf{w}) \otimes \mathbf{u}) + \nabla p = \mathrm{div}\,\Pi + (\rho - \tau\,\mathrm{div}(\rho \mathbf{u}))\mathbf{F}, \tag{6}$$

$$\frac{\partial E}{\partial t} + \mathrm{div}((E+p)(\mathbf{u} - \mathbf{w})) = -\mathrm{div}\,\mathbf{q} + \mathrm{div}(\Pi \cdot \mathbf{u}) + \rho(\mathbf{u} - \mathbf{w}) \cdot \mathbf{F} + Q. \tag{7}$$

This system contains regularizing additives having the form

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

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

$$\mathbf{q} = \mathbf{q}_{\mathrm{NS}} + \mathbf{q}^{\tau}, \tag{10}$$

$$\Pi = \Pi_{\mathrm{NS}} + \rho\mathbf{u}\otimes\hat{\mathbf{w}} + \tau(\mathbf{u}\nabla p + \gamma p\,\mathrm{div}\,\mathbf{u} - (\gamma-1)Q), \tag{11}$$

$$-\mathbf{q}^{\tau} = \tau\rho\mathbf{u}\left(\mathbf{u}\nabla\varepsilon + p(\mathbf{u}\nabla)\left(\frac{1}{\rho}\right) - \frac{Q}{\rho}\right). \tag{12}$$

They are proportional to the coefficient τ that has the dimension of time

$$\tau = l/c, \tag{13}$$

where c is a speed of sound and l is some characteristic size of the flow under consideration. In the most computational problems it may be taken proportional to a local space step:

$$\tau = \alpha h/c, \tag{14}$$

with a numerical coefficient $\alpha \le 1$ adjusted in calculations for the accuracy and stability requirements. This coefficient defines the level of subgrid dissipation. Note, that here the additives are introduced to the velocity vector $\mathbf{u}$, to the shear stress tensor Π_{NS} and to the heat flax vector $\mathbf{q}_{\mathrm{NS}}$.

By analogy with these equations we construct the regularized equations for the mixture. In the same way as in the system Eq. (1) – Eq. (4) we set $\rho = \rho_a + \rho_b$ and split the density equation Eq. (5) for the separate equations for the mixture components ρ_a and ρ_b. In the same way we split the regularizing additives in density equations. Taking into account that the mixture components have the same velocity, we suppose, that the regularizing additives to the velocity components are also equal to each other $\mathbf{w}_a = \mathbf{w}_b = \mathbf{w}$. Then the regularized gas mixture equations would have the form

$$\frac{\partial\rho_a}{\partial t} + div(\rho_a(\mathbf{u}-\mathbf{w})) = 0, \tag{15}$$

$$\frac{\partial\rho_b}{\partial t} + div(\rho_b(\mathbf{u}-\mathbf{w})) = 0, \tag{16}$$

$$\frac{\partial\rho\mathbf{u}}{\partial t} + div(\rho(\mathbf{u}-\mathbf{w})\otimes\mathbf{u}) + \nabla p = div\Pi + (\rho - \tau div(\rho\mathbf{u}))\mathbf{F}, \tag{17}$$

$$\frac{\partial E}{\partial t} + div((E+p)(\mathbf{u}-\mathbf{w})) = -div\mathbf{q} + div(\Pi\cdot\mathbf{u}) + \rho(\mathbf{u}-\mathbf{w})\cdot\mathbf{F} + Q \tag{18}$$

with the same regularizing additives Eq. (8) – Eq. (12). A sound speed for the gas mixture c_s is used here to calculate the coefficient τ in Eq. (13) and Eq. (14).

TEST PROBLEM FORMULATION

The test problem consists in simulation of the shock-bubble interaction described in experimental paper Haas JF and Sturtevant B., 1987 and numerically investigated in Quirk J, Karni S, 1996, Abgrall R, 1996 and Ivanov IE, Kryukov IA, 2007. A rectangular 2D region filled with air is considered (Figure 1). A planar shock wave, moving through air, falls on a cylindrical bubble of either helium or Refrigerant 22 (CHCIF2). A bubble with radius $R = 0.025$ is placed in the air with the bubble centre at the point $(x_c, y_c) = (0.32, 0)$.

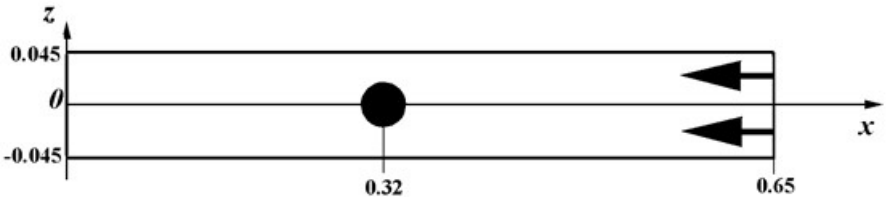

Fig. 1 - Scheme of the computational region

All gas components are regarded as perfect gases. We neglect the physical viscosity μ and the heat conductivity κ of the gases and use mixture equations in Euler formulation. External force **F** and heat source Q are supposed to be equal to zero. The initial equilibrium parameters of gases in the computational region are:

$$(\rho, u, v, p, \gamma)\big|_{t=0} = \begin{cases} 1.0, \quad 0.0,\ 0.0,\ 10^5,\ 1.4 & -\,air \\ 0.182,\ 0.0,\ 0.0,\ 10^5,\ 1.6667 & -\,bubble \end{cases}$$

for the helium bubble and

$$(\rho, u, v, p, \gamma)\big|_{t=0} = \begin{cases} 1.0, \quad 0.0,\ 0.0,\ 10^5,\ 1.4 & -\,air \\ 3.1538,\ 0.0,\ 0.0,\ 10^5,\ 1.249 & -\,bubble \end{cases}$$

for the R22 bubble. At the right boundary, the condition for the inflow of air is set with the parameters behind the shock wave moving from the right through the air at a speed corresponding to Mach number $M_s = 1.22$:

$$(\rho, u, v, p, \gamma)\big|_{\text{right}} = (1.3764, -124.82414,\ 0.0,\ 156983.9256,\ 1.4).$$

All other boundaries of the region are treated as solid walls with slip boundary conditions. The calculations are carried out on a uniform grid consisting of 1300×178 cells with a spatial step $h = 5 \cdot 10^{-4}$ in both directions and on a finer grid consisting of 2600×356 cells.

For numerical implementation of QGD system Eq. (15) - Eq. (18) 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 centres. Their values at the centers of the cell faces are calculated using the linear interpolation. The stability condition for this scheme has a Courant type and the time step is defined by the formula

$$\Delta t = \beta \cdot \min_i \frac{h_i}{c_i + |\mathbf{u}_i|} \tag{19}$$

where minimum is taken over all grid cells, β is a numerical coefficient (Courant number) which does not depend on the spatial step size.

The final time is taken equal to $t_{\text{fin}} = 1.4\times10^{-3}$ for helium bubble and $t_{\text{fin}} = 1.1\times10^{-3}$ for R22 bubble.

CALCULATION RESULTS

Calculation results for the case of R22 bubble with $\alpha = 0.4$ and Courant number $\beta = 0.5$ are presented in Figure 2.

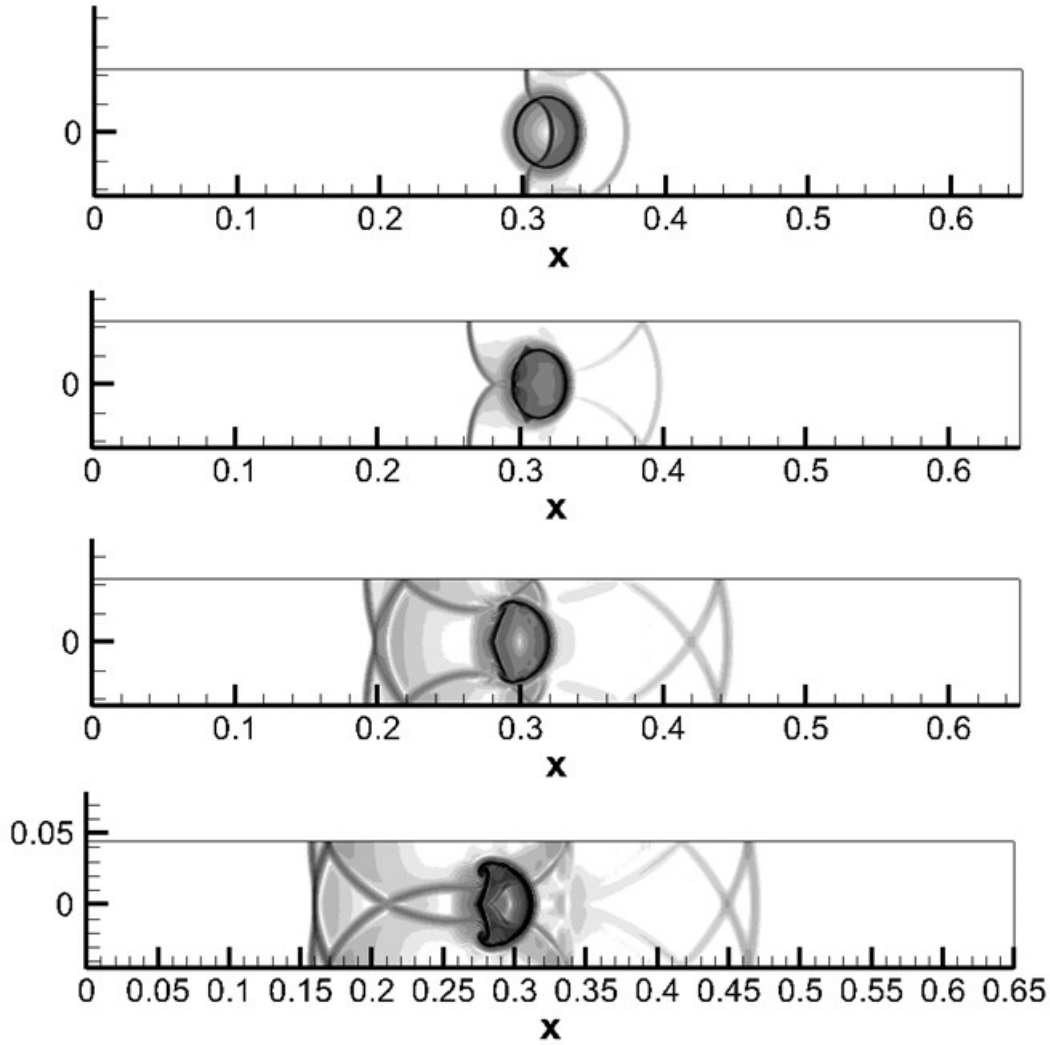

Fig. 2 - R22 bubble. Numerical schlieren images at successive time moments (from top to bottom):
$t = 7.61\cdot10^{-4}$, $t = 8.47\cdot10^{-4}$, $t = 1.01\cdot10^{-3}$, $t = 1.1\cdot10^{-3}$

After the incident shock wave hits the bubble, the later begins to move to the left direction and is deformed. At the top picture, corresponding to the time $t = 7.61\cdot10^{-4}$, one can see the incident shock as two vertical fragments near the top and bottom of the bubble. The refracted shock running inside the bubble is curved because its central region moves with lower speed than the incident wave. This is because the speed of sound in R22 is much less than in the air. At the same time the outer ends of the refracted shock move with the inner ends of the incident shock fragments. A curved reflected shock which is much weaker than the incident and refracted shocks moves to the right outside the bubble. The incident and reflected shocks are

joint by two weak waves reflected from the horizontal walls. The diffraction of the shock around the bubble leads to a strong bubble deformation. At the next pictures in Figure 2 the formation and development of two roll-ups where vorticity is generated is seen. After some time the incident shock fragments are connected, passing the bubble, and moves further to the left as a whole. The lagging point of the connection of the shock fragments gradually catches up with its external ends and the wave front is straightened. All these effects are in good correspondence with the experiment and the numerical results of other authors.

The comparison of the bubble form at the final time moment obtained in our calculations with the numerical (Quirk J, Karni S, 1996) and experimental (Haas JF, Sturtevant B, 1987) results are shown in Figure 3. It should be noted that both the evolution of the bubble shape and the general structure of a complex flow with a large number of waves of different types coincide with the results of other authors.

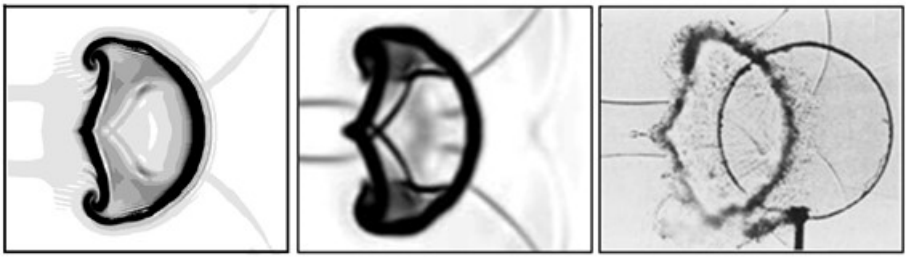

Fig. 3 - R22 bubble. Bubble form at the time moment $t = 1.1 \cdot 10^{-3}$. Our results (left), results from Quirk J., Karni S., 1996 (middle) and experiment from Haas JF, Sturtevant B., 1987 (right)

Calculation results for the case of helium bubble with $\alpha = 0.4$ and Courant number $\beta = 0.2$ are presented in Figure 4.

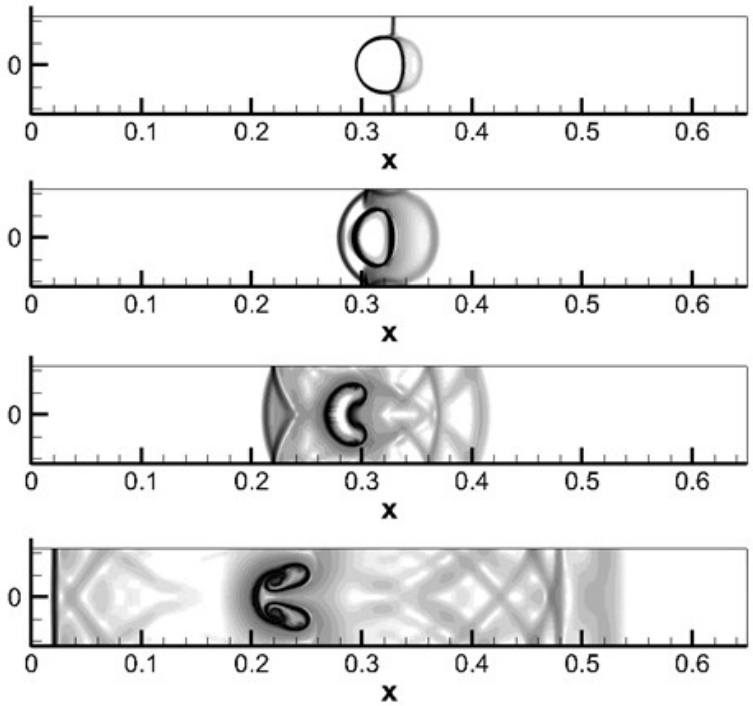

Fig. 4 - Helium bubble. Numerical schlieren images at successive time moments (from top to bottom): $t = 7.04 \cdot 10^{-4}$, $t = 7.52 \cdot 10^{-4}$, $t = 9.13 \cdot 10^{-4}$, $t = 1.342 \cdot 10^{-3}$

Whereas the helium bubble is lighter than the surrounding air and so acts as a divergent acoustic lens, the R22 bubble is heavier and therefore acts as a convergent acoustic lens. These two cases lead to very different flow behavior.

As for previous case after incident shock hits the bubble a curved refracted shock is formed inside the bubble. However, this shock moves faster than the incident one because the sound speed in helium is higher than in the air. One more difference from the previous case is the fact that the reflected wave here is much weaker and it is not a shock wave, but is an expansion wave. The further deformation of the helium bubble is much stronger than for R22 and it moves to the left faster than heavy R22 bubble.

The comparison of the bubble form at the final time moment obtained in our calculations with the same results as for R22 case are shown in Figure 5.

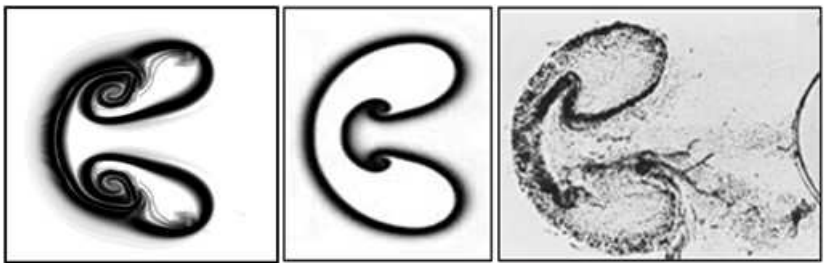

Fig. 5 - Helium bubble. Bubble form at time moment $t = 1.342 \cdot 10^{-3}$. Our results (left), results from Quirk J, Karni S, 1996 (middle) and experiment from Haas JF, Sturtevant B, 1987 (right)

The obtained calculations results show good properties of the numerical approach used here. The overall flow pictures and main characteristic features of the complicated flows are in a good correlation as with the experiment and with numerical results of other authors. It is worth noting that the numerical solution has a proper symmetry. The improvement of its quality is quite visible with the spatial grid refinement.

CONCLUSION

The paper presents an extension of the previously constructed numerical algorithm using regularized or quasi-gas-dynamic (QGD) equations for numerical modeling of chemically non-reactive gas mixtures.

The method was tested on a series of well-known problems concerning the interaction of an incoming shock wave with gas droplets located in a gas stream of a different density.

The constructed algorithm can be naturally generalized to a multicomponent mixture of ideal gases by generalizing the formulae for pressure, density, and other parameters of the mixture to the desired number of components.

The algorithm is similar in structure to the previously implemented QGD algorithms and is therefore convenient for its inclusion in the OpenFOAM package.

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