Numerical simulation of gravity instabilities in gas flows by use of the quasi gas dynamic equation system

E Shilnikov¹,²,³ and T Elizarova¹

¹Keldysh Institute of Applied Mathematics of RAS, 4, Miusskaya sq., 125047, Moscow, Russia
²Moscow Automobile and Road Construction Technical University, 64, Leningradsky av., 125319, Moscow, Russia
³E-mail: shilnikov@imamod.ru

Abstract. Paper presents two models for gravity instability simulations using compressible gas formulations, and especially, using regularised gas dynamic equations, or, in other words, the quasi-gas dynamic (QGD) equation system. The first part of the paper describes the layer flow for a single-component gas and the second one is one-fluid approximation for a gas mixture. Here a density equation for a mixture is split in two equations for each gas species. Momentum and energy equations are presented for a mixture with unified velocity and temperature and aggregated density and pressure. Examples of numerical calculations of Rayleigh-Taylor instability for different Atwood numbers are shown. The obtained results correspond to the well-known behaviour features of the Rayleigh-Taylor instability.

1. Introduction
The problems related with gravity, or Rayleigh-Taylor instabilities in layer gas flows arise in aerodynamic, engineering and environmental applications. However, for the numerical modelling incompressible flow models are commonly applied, beginning from the very first papers e.g., [1]. Detailed description of Rayleigh-Taylor instability simulation in compressible flow may be found in [2]. The review [3] contains a significant amount of information about both Rayleigh–Taylor and Richtmyer–Meshkov instabilities, including analytical investigations, experimental as well as computational results.

In this paper we show two models for gravity instability simulations using compressible gas formulations, and especially, using regularized gas dynamic equations, or, in other words, the quasi-gas dynamic (QGD) equation system. One of the advantages of this system is the nice possibilities for numerical modelling of strongly non stationary flows. The QGD system can be interpreted as the Navier-Stokes equation system averaged or smoothed over some small time and space intervals. This smoothing leads to the appearance of the strongly non-linear additional dissipation terms proportional to the small parameter $\tau$ which has a dimension of time. The first variants of the system have been published more than three decades ago by Chetverushkin, Elizarova and Sheretov. Over these years the QGD system was used to construct numerical algorithms for simulations of wide variety of gas dynamic problems. The obtained results may be found in, e.g., [4, 5] and in the recent papers, such as [6]. A number of theoretical results such as the close relations between QGD and Navier-Stokes equation systems and exact solutions of QGD system have been established in [5]. Theoretical investigations presented in [7] permit to establish Petrovskii parabolicity and linearized stability of...
equilibrium solutions of the QGD equation system. In the present paper the QGD system is examined in simulation of the Relay-Taylor instabilities in single gas and in a mixture of two different non-reacting gases.

2. Single gas convection in QGD formulation

For gravity flows of ideal polytropic gas QGD equations in Cartesian coordinates have the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} J_i = 0,$$  \hspace{1cm} (1)

$$\frac{\partial}{\partial t} \rho u_j + \frac{\partial}{\partial x_j} p = \rho F_i + \frac{\partial}{\partial x_j} \Pi_j,$$  \hspace{1cm} (2)

$$\frac{\partial}{\partial t} E + \frac{\partial}{\partial x_j} J_j \left( \frac{E + p}{\rho} \right) + \frac{\partial}{\partial x_j} q_j = J_j F_j + \frac{\partial}{\partial x_j} \Pi_j u_j.$$  \hspace{1cm} (3)

Here $E = \rho \left( u_i^2/2 + e \right)$ is the total energy per unit volume, $F_i = -g \delta^{i3}$ is the gravity force with $g$ is the gravity acceleration, $\delta^{ij}$ is the Kronecker delta. Here we use the notations:

$$J_i = \rho (u_i - w_i), \hspace{0.5cm} w_i = \frac{\tau}{\rho} \left( \frac{\partial}{\partial x_j} \rho u_j + \frac{\partial}{\partial x_j} p - \rho F_i \right), \hspace{0.5cm} \rho_s = \rho - \tau \frac{\partial}{\partial x_i} \rho u_i.$$  \hspace{1cm} (4)

The viscous stress tensor $\Pi$ and the vector of heat flux $q$ are given by

$$\Pi_{ij} = \Pi_{ij}^{NS} + \tau \rho u_i \left( u_k \frac{\partial}{\partial x_k} u_j + \frac{1}{\rho} \frac{\partial}{\partial x_j} p - F_j \right) + \tau \delta_{ij} \left( u_k \frac{\partial}{\partial x_k} p + \gamma p \frac{\partial}{\partial x_i} u_k \right).$$  \hspace{1cm} (5)

$$q_i = q_i^{NS} - \tau \rho u_i u_j \left( \frac{\partial}{\partial x_j} p + \frac{1}{\rho} \frac{\partial}{\partial x_i} \rho \right).$$  \hspace{1cm} (6)

Navier-Stokes expressions for the viscous stress tensor $\Pi^{NS}$ and the heat flux vector $q^{NS}$ are

$$\Pi_{ij}^{NS} = \mu \left( \frac{\partial}{\partial x_i} u_j + \frac{\partial}{\partial x_j} u_i - \frac{2}{3} \delta^{ij} \frac{\partial}{\partial x_k} u_k \right), \hspace{0.5cm} q_i^{NS} = -\kappa \frac{\partial}{\partial x_i} T.$$  \hspace{1cm} (7)

Here the indices $i, j, k$, taking values 1, 2 and 3, denote Cartesian coordinates. The closing relations and the heat conductivity coefficient are given by

$$p = \rho RT, \hspace{0.5cm} \varepsilon = \frac{RT}{\gamma - 1}, \hspace{0.5cm} \kappa = \mu \frac{\gamma R}{(\gamma - 1) Pr},$$  \hspace{1cm} (8)

where Pr is the Prandtl number, $R$ is a gas constant and $\gamma = c_p/c_v$ is the adiabatic index. The gas viscosity coefficient $\mu$, appearing in expressions for the viscous stress tensor and the heat flux, is defined by a temperature power-law [8]

$$\mu = \mu_0 \left( \frac{T}{T_0} \right)^\omega.$$  \hspace{1cm} (9)

Here $\omega$ value is related to the intermolecular potential for gas molecules. The bulk viscosity is supposed to be zero. The relaxation parameter $\tau$ appearing in formulae (4) – (6) is defined as
\[ \tau = \alpha \cdot h / c, \quad c = \sqrt{\gamma RT}, \]  

(10)

where \( c \) is the sound speed and \( h \) is the grid resolution, estimated locally. The value of \( \tau \) defines the time required for a perturbation to travel across a grid cell and the coefficient \( \alpha \), which is adjusted experimentally, defines the level of subgrid dissipation. According to numerical practice its value is restricted in the interval 0.1-1.0. The coefficient \( \alpha \) is the only tuning parameter of the QGD computational model.

3. Gas mixture convection. One-fluid model

In one-fluid model for a binary gas mixture simulation (gas a and gas b) we suppose that velocities and temperatures of gas components are in equilibrium with each other and are equal, so \( u^a = u^b = u \) and \( T^a = T^b = T \). One-fluid approximation for a binary gas mixture in QGD formulation was proposed and tested for rarefied flows in e.g., [4, 9]. However this approach loses the applicability for dense gas simulations. One of the reasons is the large density and pressure gradients of the components \( \rho^a \) and \( \rho^b \) near the interface of domains, occupied by separated gas species. It means that the density of a gas component may change significantly, while the aggregated density \( \rho^a + \rho^b \) conserves near a constant value.

Here we propose a new QGD formulation for a dense binary gas mixture. In contrast to the equation (1) the density equation is split into two equations for each species (a and b)

\[ \frac{\partial \rho^a}{\partial t} + \frac{\partial J^a_i}{\partial x_i} = 0, \quad \frac{\partial \rho^b}{\partial t} + \frac{\partial J^b_i}{\partial x_i} = 0, \]  

(11)

where mass flux for each gas component is presented in the form

\[ J^\alpha_i = \rho^\alpha (u_i - w_i), \quad \alpha = a, b. \]  

(12)

The additional velocity components \( w_i \) (4) and momentum and energy equations for gas mixture are similar to equations (2) - (6), but include gas mixture parameters with aggregate values of density, pressure and mass fluxes. Note, that here \( \mathbf{J} = \mathbf{J}^a + \mathbf{J}^b \). In mixture gas equations gas parameters \( \gamma \) and \( R \) depend on the mass fractions of the species and are calculated as averaged values by:

\[ \gamma = \frac{\gamma^a \rho^a + \gamma^b \rho^b}{\rho}, \quad R = \frac{R^a \rho^a + R^b \rho^b}{\rho}, \quad \rho = \rho^a + \rho^b. \]  

(13)

Viscosity and heat conductivity coefficients \( \mu \) and \( k \) are calculated for the mixture as the sum of corresponding species values.

4. Numerical algorithm and computational results

For numerical implementation of QGD system we use the explicit-in-time finite-volume scheme with an approximation of all space derivatives by second-order central differences on a rectangular grid.

The calculation process is organized as follows: we calculate densities using (11). Then we found the mixture parameters and calculate the common velocity components \( u_i \) and total energy \( E \). Using first two equations (8) and supposing that the temperatures of gases are equal \( T^a = T^b = T \) we found the temperature and the mixture pressure \( p \).

The first test is a flow simulation of the behavior of two cold and hot single gas layers in a cavity. Such flows strongly depend on the value of Atwood number, that characterizes a density difference \( \rho_1 \) and \( \rho_2 \) in the layers

\[ A = (\rho_1 - \rho_2) / (\rho_1 + \rho_2). \]  

(14)

We consider a following problem. A rectangular container \( 14 \text{cm} \times 14 \text{cm} \times 20 \text{cm} \) is filled with argon under atmospheric pressure \( p = 101325 \text{ Pa} \). The gas in the lower half of the container is hot.
with the density $\rho_1 = 1.62 \text{ kg/m}^3$ and the upper half is filled with cold gas with the density $\rho_2$. Two numerical experiments were held for different values of $\rho_2$. This density was taken equal to $\rho_2 = 3 \text{ kg/m}^3$, which corresponds to the Atwood number $A = 0.3$ (variant 1) and $\rho_2 = 5 \text{ kg/m}^3$ with $A = 0.51$ (variant 2). Gas viscosity was taken equal to $\mu_0 = 2.26 \cdot 10^{-3} \text{ N} \cdot \text{s/m}^2$ for $T_0 = 273 \text{ K}$, viscosity index $\omega = 0.81$, $\gamma = 5/3$, molecular mass 39.9166 and Prandtl number $Pr = 0.67$ [8]. At the beginning of the simulations the velocities in the whole computational region are equal to zero, except the boundary surface between the hot and cold gases. In this surface the vertical velocity has a sinusoidal profile with the amplitude of 0.2 m/s. The no slip boundary conditions are set at all borders. Figure 1 shows the computational domain with the density distributions along the walls (left) and the temperature distribution in the middle section (right) for variant 1. Figure 2 demonstrates the density lines together with the stream function lines in the middle section of the domain for variant 1 (left) and 2 (right).

![Figure 1](image1.png)

**Figure 1.** Density distributions along the walls (left picture) and the temperature distribution in the middle section (right picture) for variant 1, $A=0.3$, $t = 0.7 \text{ s}$.

![Figure 2](image2.png)

**Figure 2.** Density distributions together with the streamfunction lines in the middle section of the domain for variant 1, $A=0.3$ (left picture) and variant 2, $A=0.51$ (right picture), $t = 0.7 \text{ s}$.
It is seen that the increasing of Atwood number leads in changing the flow picture with "mushroom" form to the picture with "knife" form of falling down streams of heavy gas.

Both calculations were carried out until the time moment \( t_{\text{fin}} = 0.7 \) s with the coefficient in regularization parameter in (10) \( \alpha = 0.2 \) and the Courant number \( \beta = 0.4 \). It corresponds to a time step \( \Delta t = 2 \times 10^{-4} \) s. The calculation grid contains 80×80×120 cells.

The second test problem is similar to previous one but two gases in the container are different. For the sake of simplicity we solved this problem in 2D formulation. A rectangular container 12.5 cm × 50 cm is considered. Its upper half is filled with heavy gas sulfur hexafluoride (SF\(_6\), \( \gamma = 1.094, \) Pr = 0.736, molecular mass 146.0554). The gas in the lower half is light. We considered two variants of the light gas: argon (Ar, it's parameters are mentioned above) and helium (He, \( \gamma = 5/3, \) Pr = 0.67, molecular mass 4.003). The corresponding Atwood numbers are equal to \( A = 0.57 \) for Ar – SF\(_6\) and \( A = 0.95 \) for He – SF\(_6\). The initial state of the gases at time \( t = 0 \) is determined by hydrostatic equilibrium assuming adiabaticity and zero gas velocities. The normal atmospheric pressure and temperature (as in the first problem) are set at the interface surface. In this surface the vertical velocity has a sinusoidal profile with larger amplitude of 10 m/s. The boundary conditions are: no slip conditions are set at the bottom, slip conditions at the vertical walls and constant pressure and zero vertical derivatives for the rest variables are imposed at the upper boundary. Such conditions allow perturbations of the solution to leave the calculation region through the upper boundary.

Figure 3 demonstrates the distributions of the flow parameters at the advanced stage of flow development in the Ar – SF\(_6\) mixture. The mushroom shape of the emerging bubbles of light gas and the downward bubbles of heavy gas is clearly visible, while the edges of the bubbles twist inward and become thinner over time. Acoustic disturbances forming in the gas-dynamic fields of light and heavy gases in the process of their evolution are also clearly visible.

An increase in temperature is observed on the temperature distribution, near the boundaries of the bubbles, which is associated with the light gas heating during its compression in the structures formed. Over time, the picture of gravitational mixing of gases becomes more and more complex, and more and more small details and vortex formations appear in it. Ultimately, these new details become comparable in size with the spatial grid, which leads to the termination of the calculations.

The results of calculations for a mixture of He-SF\(_6\) are presented in figures 4 and 5. Comparison with the previous calculation shows that, in general, the overall picture of the instability development persists. However, with an increase in Atwood number all processes proceed with a significantly greater speeds, the formation of bubbles-fungi occurs more intensely, the magnitude of acoustic disturbances increases. One can see a sharp lowering of heavy gas into the zone of very light helium.

**Figure 3.** Distributions of the light gas density \( \rho_a \) (left picture), heavy gas density \( \rho_b \) (center picture) and the temperature \( T \) (right picture) for the Ar – SF\(_6\) mixture at the time moment \( t = 0.2 \) s.
gas, which forms a thin stream of heavy gas. At the ends of SF₆ jets mushroom-like formations occur, while the jets themselves tend to split and form drops. In addition, a rapid heating of helium due to its compression is observed under the action of heavy gas, which plays the role of a piston.

**Figure 4.** Density distributions of SF₆ at time moments \( t = 0.05 \) s (left) and \( t = 0.15 \) s (right).

**Figure 5.** Density distributions of He at time moments \( t = 0.05 \) s (left) and \( t = 0.15 \) s (right).

The calculations were held on the uniform spatial grid containing 125×400 cells. To analyze the dependence of the numerical solution on the grid size the calculations were held for the Ar–SF₆ mixture on the grids 60×200 and 250×800 nodes. Figure 6 shows the results obtained on these three spatial grids for the same time moment \( t = 0.12 \) s.

**Figure 6.** Aggregate density distributions obtained on different spatial grids: 60×200 (left picture), 125×400 (center picture) and 250×800 (right picture), At=0.57.

These results clearly show that even on rough mesh the overall picture flow is obtained, with the exception of a specific curving shape of the boundaries between the gases, since this boundary contains only one or several grid cells. When the mesh is refined, additional finer effects are revealed.
It is known that numerical modeling of such problems with high Atwood numbers present serious difficulties due to the huge difference in gas densities and high speed processes. As an advantage of the algorithm used here it is worth noting that the symmetry properties of the numerical solution with respect to $x$ - axis are preserved with high accuracy.

5. Conclusion
Presented here a new numerical method based on the QGD equations, allows to perform numerical simulation of Rayleigh-Taylor type instability problems in a wide range of Atwood numbers. The results obtained are qualitatively consistent with those known in the literature. Numerical solution has proper symmetry. The improvement of its quality is shown with the spatial grid refinement. The numerical algorithm is constructed to simulate the 3D flows. 2D calculations described in the paper are performed by use of 3D code with the minimum number of nodes in the third direction.

In the future we plan to work on the inclusion of the developed algorithm for the gas mixtures flow simulation into the open software complex OpenFOAM [10]. In addition, the developed technique can be applied to other problems connected with gas mixtures flows, including jets, both in subsonic and supersonic modes, as well as to geophysical flows at atmospheric scales.

Acknowledgements
This work was supported by Russian Foundation for Basic Research, grants No 19-01-00262, 18-01-00587 and 18-01-00405.

References
[1] Taylor G I 1950 Proc. of Roy. Soc. A 201 192
[2] Reckinger S J, Livescu D and Vasilyev O V 2016 J. Comput. Phys. 313 181–208
[3] Zhou Y 2017 Phys. Reports 723–725 1–160
[4] Elizarova T G 2009 Quasi-Gas Dynamic Equations (Berlin: Springer-Verlag)
[5] Sheretov Yu 2009 Continuum dynamics under spatiotemporal averaging (Moscow-Izhevsk: R&C Dynamics) in Russian
[6] Shirokov I A and Elizarova T G 2014 Journ. of Turb. 15 707–30
[7] Zlotnik A A 2010 Dokl. Math. 82 811–5
[8] Bird G A 1994 Molecular Gas Dynamic and the Direct Simulation of Gas Flows (Oxford: Clarendon Press)
[9] Elizarova T G, Graur I A and Lengrand J C 2001 European Journal of Mechanics B 3 351–69
[10] Kraposhin M V, Smirnova E V, Elizarova T G and Istomina M A 2018 Computers & Fluids 166 163–75