Modified Godunov Method for Multicomponent Flow Simulation

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Abstract. The paper deals with the elaboration of the algorithm for multicomponent gas flows simulation in the presence of strong shock waves. In order to deal with strong shock wave properly the exact Riemann solver for multicomponent flow and non-perfect gases is used. Standard finite volume Godunov-type scheme gives the effect of numerical pressure oscillations on a contact discontinuity. In order to fix the situation the convenient modification of double flux method is described and tested. The simplicity and robustness of the method render it as good candidate for the realization in multi-D algorithms.

1. Introduction
In the recent years, the problems associated with the creation of hypersonic aircraft (HA) for long-term atmospheric flight equipped with a supersonic combusting ramjet engine (scramjet) have become increasingly important. If the HA can carry out a sufficiently long gliding flights in the stratosphere, i.e. at altitudes of 20 ÷ 30 km and at a speed of 5 ÷ 12 Mach numbers or more, they may be natural prototypes of new models of military and civilian equipment. In this case, a fundamental role will be played by the combustion processes of fuels of different types, as well as changes in the properties of the air environment due to a deviation from the perfectness, for example, the beginning of the processes of dissociation and chemical reactions, as well as the consequences of a strong increase in temperature behind the shock wave front.

The described phenomena suggest that the medium in question consists of many components, for each of which it is necessary to write out the appropriate balance equations (in the absence of chemical reactions – the laws of mass conservation). Therefore, the basic system of Navier-Stokes equations, firstly, expands due to additional equations of mass balance of components, and, secondly, the corresponding "turbulent coefficients", which are responsible for turbulent viscosity, mixing and other characteristic phenomena, are seriously changed. All of the above requires special care in the design of numerical algorithms for solving this class of problems, especially given the fact that the introduction of additional equations for the components, as is well known, see, for example, [1], leads to a notable complication of the computational model.

This paper is devoted to the study of the properties of the developed model algorithm for solving an extended system of Euler equations for an arbitrary number of components. This algorithm takes into account the possibility of strong jumps in the solutions, which is expressed in the use of accurate solutions to the corresponding Riemann problem, in particular, for non-perfect gases, and also takes into account the appearance of pressure oscillations inherent in algorithms for direct generalization of numerical solution methods to multicomponent systems. The paper considers the simplest one-
dimensional case. In the future, it is supposed to use the developed algorithm first to obtain solutions to the multidimensional extended system of Euler equations, and then on the basis of the splitting method for the complete system of Navier–Stokes equations taking into account turbulence and chemical reactions. The ideology of this briefly described setting is based on a far-reaching generalization of the results of [2], recently obtained by its authors.

2. Mathematical model

The extended system of Euler equations is a system of gas dynamics equations in which conservation laws for additional components are added. Within the general anticipated framework the process of solving Navier–Stokes system with chemical reactions is split into two stages: the solution of the hyperbolic and parabolic parts of the equations of the system. In this paper we are interested in a general algorithm for solving the hyperbolic part using for illustrative purposes the one-dimensional setting. An important element of the algorithm is the exact solution of the Riemann problem for an extended system of Euler equations. Although such a solution was described in [1] for perfect gases, here we will conduct a more systematic review, also including non-perfect gases, since in the presence of strong shock waves when flying HA with scramjet on hypersonic mode, it seems important to rely not on an approximate, but on the exact solution of the Riemann problem.

The extended one-dimensional system of Euler equations has the form of a system of balance laws consisting of $N_{sp} + 2$ equations, where $N_{sp}$ is the number of components in the mixture:

$$\frac{\partial U}{\partial t} + \sum_{m} \frac{\partial F(U)}{\partial x} = G(U,x,t),$$

where $U = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{m+3} \end{pmatrix}$, $F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u E \\ \rho Y_m \end{pmatrix}$, $E = e + u^2/2$.

Here $m = 1,\ldots,N_{sp} - 1$, $e$ – internal energy, $Y_m$ – mass concentration of the component with number $m$, $\sum Y_k = 1$, $k = 1,\ldots,N_{sp}$, function $G$ is the source term, which controls the chemical reactions and energy flows, in the framework of the present study we are not concerned with the specific form of this right-hand term. It is assumed that the mixture of carrier gas and the chemical reactions (in particular, combustion) products obeys the following equation of state (EoS)

$$e = \frac{p + \rho_0 c_0^2}{\rho (\gamma - 1)} - \frac{c_0^2}{\gamma - 1},$$

where $\rho_0, c_0$ are certain parameters. The adiabatic index $\gamma$ is defined as follows

$$\gamma = \frac{C_p}{C_v} = 1 + \frac{R}{C_v}, \quad R = \sum_{m=1}^{N_{sp}-1} Y_m (R_m - R_0) + R_0; \quad C_v = \sum_{m=1}^{N_{sp}-1} Y_m (C_v^m - C_v^0) + C_v^0.$$

Let us note that $\gamma$ is a homogeneous function with respect to conservative unknowns $u_1, u_{3,m}$. This observation further will lead to more simple formulae.

The system (1) is non-strictly hyperbolic, i.e. it has multiple eigenvalues (all real) but complete system of eigenvectors. The eigenvalues of matrix $F'(U)$ are $\lambda_1 = u - c$, $\lambda_2 = \ldots = \lambda_{N_{sp}+1} = u$, $\lambda_{N_{sp}+2} = u + c$, where sound speed equals $c = \sqrt{\gamma p + \rho_0 c_0^2}/\rho$. Note that the sound speed expression
for (1) is quite similar to one for conventional gas dynamics. This fact follows from the homogeneity of $\gamma$ and has been mentioned just above.

Denote $\rho e$ via $\Theta$ and write the expressions for right eigenvectors $\mathbf{r}_i, i = 1, \ldots, N_{sp} + 2$ (naturally, it is possible to write analogous expressions for the left eigenvectors $\mathbf{l}_i$):

\[
\mathbf{r}_i = \left[ 1; u - c; \frac{c^2 - c_0^2}{\gamma - 1} + \frac{u^2}{2} - uc; \left\{ Y_{m} \right\}_{m=1}^{N_{sp}+1} \right], \quad \mathbf{r}_2 = \left[ 1; u; \frac{u^2}{2} - c_0^2 + \Theta_0'; \left\{ 0 \right\}_{m=1}^{N_{sp}+1} \right],
\]

\[
\mathbf{r}_{m+2} = \left( \Theta_0'; u \Theta_0'; 0; \ldots; (\gamma - 1)u^2/2 - c_0^2 - \Theta_0'; 0; \ldots; 0 \right), \quad m = 1, \ldots, N_{sp} - 1,
\]

\[
\mathbf{r}_{N_{sp}+2} = \left( 1; u + c; \frac{c^2 - c_0^2}{\gamma - 1} + \frac{u^2}{2} + uc; \left\{ Y_{m} \right\}_{m=1}^{N_{sp}+1} \right), \quad \gamma_0' = \frac{\partial \gamma}{\partial u_1}, \quad \gamma_m' = \frac{\partial \gamma}{\partial u_{m+3}}.
\]

In the algorithm of the numerical solution of the system (1), which will be described in the next section, we need to obtain a solution of the Riemann problem for (1) under the assumption that the right-hand term is identically zero. To do this, let us study the behavior of the corresponding rarefactions and strong discontinuities.

2.1. Rarefaction waves

The rarefaction waves are generated only by eigenvectors $\mathbf{r}_1, \mathbf{r}_{N_{sp}+2}$ since the rest of the eigenvectors correspond to $\lambda = u$ and the associated simple waves are contact discontinuities. The expressions for the first three components of the eigenvectors $\mathbf{r}_1, \mathbf{r}_{N_{sp}+2}$ coincide with the components of the corresponding eigenvectors for the equations of conventional gas dynamics. Let us show that along the rarefaction waves corresponding to the system (1), the value of $\gamma$ remains constant. Indeed, in the system of equations that describes the rarefaction waves $\dot{\mathbf{U}} \parallel \mathbf{r}_1$ or $\dot{\mathbf{U}} \parallel \mathbf{r}_{N_{sp}+2}$ the relations $du_{m+3} / du_1 = u_{m+3} / u_1, m = 1, \ldots, N_{sp} - 1$ are true. It follows from these relations that $u_i = C_i u_1$ with some constant $C_i$. Further the homogeneity property of $\gamma$ readily produces the required result. Thus, the projection to the subspace $(u_1, u_2, u_3)$ of the rarefaction waves curves in the phase space coincides with the curves for conventional gas dynamics, but with specific value of $\gamma$, which will depend on the initial point from which this curve originates.

2.2. Strong discontinuities

The description of strong discontinuities for (1) follows from Hugoniot relations

\[
s \left( \mathbf{U} - \mathbf{U}^- \right) = \mathbf{F} \left( \mathbf{U} \right) - \mathbf{F} \left( \mathbf{U}^- \right), \quad (2)
\]

where $s$ is the discontinuity speed. Namely, the following formulae are true, $m = 1, \ldots, N_{sp} - 1$. ...
where \( \{ \ldots \}^- \) denotes the expression corresponding to the expression in the considered line but taken at \( U = U^- \). Taking into account the first equation (2) the last \( N_{sp} - 1 \) equations can be written in the form

\[
\left( u_{1} - u_{1}^- \right) \{ u_{1}^0, u_{2}^0, u_{3}^0 \} = 0, m = 1, ..., N_{sp} - 1 \quad (3)
\]

Now it is possible to immediately distinguish two major classes of solutions to the system (3): (a) the solutions, solutions of the first class are such strong discontinuities on which the velocity is continuous, that is, contact discontinuities. In this case, no additional restrictions are imposed on the values of the variables associated with the concentration of the components, and the curve in the phase space for the contact discontinuity is determined from the first three equations (2), i.e. coincides with the contact discontinuity curve in the phase space for conventional gas dynamics. The only difference is that the values of \( \gamma \) to the right and to the left of the contact discontinuity is now determined through the concentrations \( Y_m \) which are different at both sides of the contact discontinuity.

For the solutions of the second class the value of \( \gamma \) is preserved when crossing the discontinuity. Therefore, the first three equations (2) define solutions in the form of shock waves that correspond to the families with minimal and maximal eigenvalue. These trajectories in the phase space will be identical to the trajectories obtained for the conventional gas dynamics for a specific \( \gamma \), which is determined by \( U^- \).

Thus, the solution to the Riemann problem for (1) under the assumption that the source term equals zero can be obtained by appropriate modification of the solution to the Riemann problem for the conventional gas dynamics system.

2.3. Remark on the thermodynamics of non-perfect gases mixture
Let us consider the convenient generalization of perfect gas model

\[
p = (\gamma - 1) \rho e + (\rho - \rho_0) \varepsilon_0^2,
\]

with some constants \( \rho_0, \varepsilon_0 \). Refer to, for example, [3] where the origination of (4) are explained and also the possibility of usage (4) in calculations in order to approximate general EoS.

We are interested in the following question: whether the mixture of gases that each has (4) as EoS will have the EoS of the form (4)? The answer is that this is true only approximately. Let show this.

Using the well-known thermodynamic relation \( T \) is the temperature, \( V = 1/\rho \)

\[
T \left( \frac{\partial p}{\partial T} \right)_\gamma = \left( \frac{\partial e}{\partial V} \right)_\gamma + p,
\]

it is possible to obtain from (4) the thermic equation of state.
\begin{equation}
\rho = \frac{\tilde{R} \cdot T}{V} - \frac{\rho_0 c_0^2}{\gamma}, \quad \gamma - 1 = \frac{\tilde{R}}{C_V},
\end{equation}

here $C_V$ is the specific heat capacity under constant volume condition, $\tilde{R} = R/M$, where $R$ is the universal gas constant and $M$ is the molecular weight for the specific gas under consideration. From (4) and (5) the following form of EoS can be get

\begin{equation}
e = C_v T + V \frac{\rho_0 c_0^2}{\gamma} - \frac{c_0^2}{\gamma - 1},
\end{equation}

Now let us have the equilibrium mixture of $N_{SP}$ non-perfect gases, each gas has the EoS in the form (4) and (5). Then the common temperature $T$ exists and $\rho = \sum m \rho_m$ $m = 1, \ldots, N_{SP}$, here $\rho$ is the mixture density and $\rho_m$ are the densities of the components. Each component has its own EoS, and mixture internal energy $e$ can be expressed via the internal energies of components $e_m$, namely $e = \sum Y_m e_m$, $Y_m = \rho_m / \rho$. Then using the thermodynamic relation $p = -(\partial V / \partial e)_T$ one obtains Dalton’s law $p = \sum p_m$, where $p_m$ are partial pressures.

Further assume that each component in the mixture has the EoS in the form (4), (5), the relevant values and constants will be marked by the index $m$. Using (6) for each component we get

\begin{equation}
e = \sum_{m=1}^{N_{SP}} Y_m e_m = C_v T + V \sum_{m=1}^{N_{SP}} \frac{\rho_0 C_0^2 m}{\gamma_m} - \sum_{m=1}^{N_{SP}} Y_m \frac{c_0^2 m}{\gamma_m - 1},
\end{equation}

where $C_v = \left( \frac{\partial e}{\partial T} \right)_V = \sum_{m=1}^{N_{SP}} Y_m C_{V,m}$. From the equation (5) one infers

\begin{equation}
p = \sum_{m=1}^{N_{SP}} p_m = T \rho \sum_{m=1}^{N_{SP}} \tilde{R}_m Y_m - \sum_{m=1}^{N_{SP}} \frac{\rho_0 C_0^2 m}{\gamma_m} = \tilde{R} \rho - \sum_{m=1}^{N_{SP}} \frac{\rho_0 C_0^2 m}{\gamma_m},
\end{equation}

and $\tilde{R} = \sum_{m=1}^{N_{SP}} \tilde{R}_m Y_m$. So expressing $T$ from the last relation we finally obtain

\begin{equation}
p = (\gamma - 1) \rho e + \rho (\gamma - 1) \sum_{m=1}^{N_{SP}} Y_m \frac{c_0^2 m}{\gamma_m - 1} - \gamma \sum_{m=1}^{N_{SP}} \frac{\rho_0 C_0^2 m}{\gamma_m}.
\end{equation}

If the mixture consists of similar gases then (7) naturally comes to (4). If we somehow neglect the dependence of the second term in (7) on $Y_m$ then we again come to the form (4). Thus the mixture of non-perfect gases (each gas satisfies the EoS of the form (4)) satisfies (4) only as approximation. The algorithm for the exact solution of the Riemann problem for two different gases with the EoS of the form (4) is given in [3] and is used by us further.

3. Brief description of numerical solution method
For the numerical solution of the system (1) with zero source term the Godunov type scheme [4] is used:

\begin{equation}
\frac{U_i^{k+1} - U_i^{k}}{\tau_k} + \frac{F(U_i^{k+1/2}) - F(U_i^{k-1/2})}{h} = 0, \quad i = 1, \ldots, N.
\end{equation}
The calculation of fluxes is performed via the exact solution of the Riemann problem described in the previous section; the boundary conditions are posed by standard methods; parameters notations are the same as in [3].

The well-known issue of schemes of Godunov type for the equations of multicomponent gas dynamics is the occurrence of oscillations of the pressure at the contact boundary between the gases with substantially different parameters [5–10] (similar problems arise in a variety of methods, requiring a clear definition of the boundary between substances [11, 12]).

There are several approaches to solving this problem, associated either with the adjustment of the mathematical model and the rejection of its divergent form, for example, [7] or with the adjustment of the computational scheme. In this paper we use the convenient modification of the so-called "double flux method" [6], a similar approach was successfully used in [10]. The modification concerns the multicomponent gas dynamics with strong shock waves. The point of this method is the splitting of the procedure of Godunov flux calculating for the energy equation. As a result, the energy is calculated according to the "predictor-corrector" scheme with the calculation of the pressure at the predictor stage. In the first step of the scheme, the value of the total energy in the cell is calculated using the fluxes calculated at a fixed \( \gamma \) for a given cell, i.e. in each grid node with a number \( n = i + 1/2 \) two different fluxes are calculated, the left "L" with \( \gamma_i \) and the right "R" with \( \gamma_{i+1} \). This allows for each cell to locally satisfy the non-oscillating condition for the pressure. The corresponding stencil is shown in Figure 1.

\[
\begin{align*}
\text{Figure 1. The “double flux” method for the cell } n &= i+1/2. \\
&= \begin{array}{c}
\gamma_i \\
\gamma_{i+1}
\end{array}
\end{align*}
\]

After that, at the second step of the algorithm, the pressure is calculated in accordance with already obtained energy value for the cell via the EoS used with the same fixed \( \gamma \). Next, the correction of the total energy field is carried out using the internal energy value recalculated from the obtained pressure field and the values of \( \gamma \) obtained from the calculated values \( \gamma_{i+1} \). Now the corrected Godunov scheme using the "double flux" method for cell \( i \) is written as follows:

- Step 1.

\[
\begin{bmatrix}
\rho^{i+1} \\
(\rho u)^{i+1} \\
(\rho E)^{i+1} \\
(\rho Y_m)^{i+1}
\end{bmatrix}
= \begin{bmatrix}
\rho^i \\
(\rho u)^i \\
(\rho E)^i \\
(\rho Y_m)^i
\end{bmatrix}
- \frac{\tau_k}{h} \left[ F^L \left( U_{i+1/2}^k, \gamma_i \right) - F^R \left( U_{i-1/2}^k, \gamma_i \right) \right].
\]
• Step 2.

\[
p_i^{k+1} = \left(\gamma_i - 1\right) \left(\rho E_i^k - \frac{1}{2} (\rho u_i^k)^2\right) + \left(c_{i,j}^k\right)^2 \left(\rho_i^{k+1} - \rho_{0,i}^k\right),
\]

\[
\gamma_i^{k+1} = \gamma \left(y_i^{k+1}\right), \quad c_{i,j}^{k+1} = c_0 \left(y_i^{k+1}\right), \quad \rho_i^{k+1} = \rho_0 \left(y_i^{k+1}\right),
\]

\[
(\rho E)_i^{k+1} = \frac{p_i^{k+1} + \left(c_{i,j}^{k+1}\right)^2 \left(\rho_i^{k+1} - \rho_{0,i}^{k+1}\right)}{\left(\gamma_i^{k+1} - 1\right)} + \frac{1}{2} (\rho u_i^k)^2.
\]

The error in the balance of total energy, which inevitably occurs when using the double flux method, as practice shows, does not have in most cases a significant impact on the final solution of the problem. The papers [6, 12] are devoted to the analysis of this question. Moreover, in the cited papers for computation of numerical fluxes an approximate Riemann solver was used twice for each face (with fixed value of gamma corresponding to left or right state in adjacent cell). In the present work the Riemann problem is solved exactly and only once with left and right states with different \(\gamma\). This in turn both increases the accuracy of the simulations and reduces the computational costs due to the mass character of flux computational operation.

4. The results of test simulations

In order to verify the developed technique, the implemented algorithms were tested on three test problems: the Sod problem on the shock tube, the modified Sod problem and the problem on the propagation of two shock waves. A detailed description of each of these problems and the results of the calculations are given in this section. Let us note that all tests just mentioned are the classical ones and assume perfect gas EoS – but all simulation presented in this section were performed using general approach described in the sections above which assumes non-perfect gas behavior.

The testing methodology corresponds to the one proposed in [13]. In addition to the visual comparison of the calculation results with the known reference solutions, the absolute and relative \(L_1\) error norm were also compared, calculated using the following formula

\[
\|\Delta f\| = \sum_{i=1}^{N} \|\Delta f_i\| \cdot h_i / \sum_{i=1}^{N} h_i, \quad \|\varepsilon_j\| = \sum_{i=1}^{N} |\Delta f_i| \cdot h_i / \sum_{i=1}^{N} f_i \cdot h_i,
\]

where \(f_i\) – calculated value of certain variable in the mesh cell \(i\) and \(\tilde{f}_i\) – known value of the same variable in the same cell, \(N\) – the number of cells in the mesh, \(h_i\) – the cell size, \(\Delta f_i = f_i - \tilde{f}_i\).

Also the order of convergence of the numerical solution under the condition of reduction the computational grid cells sizes was also estimated. For this purpose, four uniform grids of sizes \(N = 500, 1000, 2000\) and \(4000\) cells were used. The following formula for uniform grids was used to estimate the order of convergence

\[
\sigma(f) = \sigma(f : N_i, N_j) = \ln \frac{\|\Delta f^{(N_i)}\|}{\|\Delta f^{(N_j)}\|} / \ln \frac{h_i}{h_j}.
\]

The time step \(\tau_k\) was given by

\[
\tau_k = CFL \cdot \tau_{\max}, \quad \tau_{\max} = \frac{h}{\max_{i} \{\sqrt{1 + c_i^k}\}},
\]

where \(h\) – the cell size for mesh, \(k\) – the index of current time step, \(i = 1, \ldots, N\). All calculations were performed for a fixed CFL = 0.5.
Good results were obtained for all three problems. The relative error for each of the basic gas-dynamic values did not exceed 5% at \(N = 500\) and 2% at \(N = 4000\). In addition, the obtained convergence orders exceeded the expected value \(\sigma = 1/2\) for the schemes of the first order of accuracy [14].

4.1. Sod problem

As a first test example, we consider the Sod problem, which is of interest from the point of view of modeling the flows with shock waves that arise at the contact boundaries of gases with the same adiabatic indexes. The problem is described in detail in [13, 15] and is put as follows. The segment \(0 \leq x \leq 1\) contains two identical perfect gases separated at the initial moment of time:

\[
(\rho, u, p, \gamma)_{t=0} = \begin{cases} 
1.0, & 0.0, 1.0, 1.4 \text{ as } 0 \leq x \leq 0.5, \\
0.125, & 0.0, 0.1, 1.4 \text{ as } 0.5 < x \leq 1.
\end{cases}
\]

Let us denote the gas to the left of initial discontinuity by the index “I” and the gas to the right – by the index “II”.

A solid wall condition is assumed at the segment boundaries. The value \(t = 0.2\) is used as a reference time moment. The corresponding Riemann problem has the solution where the resulting flow contains five subdomains, schematically depicted in figure 2.

![Figure 2. The flow domains at \(t = 0.2\).](image)

- the domain 0: \(0 \leq x < X_{RW1}\) – the gas I with initial parameters \(\rho_I, u_I, p_I\);
- the domain 1: \(X_{RW1} \leq x < X_{RW2}\) – the gas I under the rarefaction wave with the parameters \(\rho_I, u_I, p_I\);
- the domain 2: \(X_{RW2} \leq x < X_I\) – the gas I before contact discontinuity, through which the rarefaction wave has passed, with the parameters \(\rho_1, u_1, p_1\);
- the domain 3: \(X_I \leq x < X_{SW}\) – the gas II after contact discontinuity, through which the shock wave has passed, with the parameters \(\rho_2, u_2, p_2\), at this \(p_3 = p_2, u_3 = u_2\);
- the domain 4: \(X_{SW} \leq x \leq 1\) – the gas II with initial parameters \(\rho_H, u_H, p_H\),

where \(X_{RW1}\) is the position of forward front of rarefaction wave, \(X_{RW2}\) is the position of backward front of rarefaction wave, \(X_I\) is the position of contact discontinuity, \(X_{SW}\) is the position of shock wave. The analytic solution of this problem [15] is used as reference solution.

Numerical calculations were carried out on uniform grids containing 500, 1000, 2000 and 4000 cells, respectively. In the figure 3 the profiles of density, pressure, internal energy and velocity at time \(t = 0.2\) are given for the calculations on the coarsest and finest grids in comparison with the reference solution. In tables 1 and 2 the numerical values of absolute and relative \(L_1\) errors (the difference between the calculated and the reference solution) are given.
Figure 3. Sod problem: reference solution and calculated values at $t = 0.2$
(profiles of density, pressure, internal energy and velocity).

Table 1. Sod problem: absolute $L_1$ error at time moment $t = 0.2$.

| $\Delta L_1$ | 500  | 1000 | 2000 | 4000 | $\sigma$ |
|--------------|------|------|------|------|---------|
| $p \cdot 10^3$ | 5.3817 | 3.1701 | 1.8240 | 1.0459 | 0.7878 |
| $\rho \cdot 10^3$ | 6.9116 | 4.3833 | 2.7502 | 1.7418 | 0.6628 |
| $e \cdot 10^2$ | 2.6482 | 1.7432 | 1.1440 | 0.7629 | 0.5985 |
| $u \cdot 10^2$ | 1.0160 | 0.5748 | 0.3045 | 0.1671 | 0.8681 |

Table 2. Sod problem: relative $L_1$ error at time moment $t = 0.2$.

| $\varepsilon_{L_1}$ [%] | 500  | 1000 | 2000 | 4000 |
|------------------------|------|------|------|------|
| $p$                    | 1.03 | 0.61 | 0.35 | 0.20 |
| $\rho$                 | 1.23 | 0.78 | 0.49 | 0.31 |
| $e$                    | 1.17 | 0.77 | 0.51 | 0.34 |
| $u$                    | 2.30 | 1.30 | 0.69 | 0.38 |
4.2. Modified Sod problem

Further let us consider modified Sod problem, which differs from the subsection 4.1 by the presence of contact boundary between the gases with different adiabatic indexes. The problem is described in [13, 16] and is put as follows. The segment $0 \leq x \leq 1$ contains two different perfect gases separated at the initial moment of time:

$$(\rho, u, p, \gamma)|_{t=0} = \begin{cases} 
1.0, & 0.0, 2.0, 2.0 \text{ as } 0 \leq x \leq 0.5, \\
0.125, & 0.0, 0.1, 1.4 \text{ as } 0.5 < x \leq 1.
\end{cases}$$

Let us again denote the gas to the left of initial discontinuity by the index “I” and the gas to the right – by the index “II”.

A solid wall condition is assumed at the segment boundaries. The value $t = 0.2$ is used as a reference time moment. The corresponding Riemann problem has the solution where the resulting flow contains five subdomains similarly to subsection 4.1, see Figure 2. The analytic solution of this problem [17] is used as reference solution.

Numerical calculations were carried out on uniform grids containing 500, 1000, 2000 and 4000 cells, respectively. In the Figure 4 the profiles of density, pressure, internal energy and velocity at time $t = 0.2$ are given for the calculations on the coarsest and finest grids in comparison with the reference solution. In tables 3 and 4 the numerical values of absolute and relative $L_1$ errors (the difference between the calculated and the reference solution) are given.

| $\Delta_{L_1}$ | 500   | 1000  | 2000  | 4000  | $\sigma$ |
|----------------|-------|-------|-------|-------|---------|
| $p \cdot 10^{-2}$ | 1.3555 | 0.8000 | 0.4559 | 0.2642 | 0.7863  |
| $\rho \cdot 10^{-3}$ | 7.8724 | 4.9130 | 3.0133 | 1.9110 | 0.6808  |
| $e \cdot 10^{-2}$ | 6.7964 | 4.6920 | 3.1518 | 2.1406 | 0.5556  |
| $u \cdot 10^{-2}$ | 1.7293 | 0.9864 | 0.5153 | 0.3001 | 0.8409  |

| $\varepsilon_{L_1}$ [%] | 500   | 1000  | 2000  | 4000  |
|-------------------------|-------|-------|-------|-------|
| $p$                     | 1.69  | 1.00  | 0.57  | 0.33  |
| $\rho$                  | 1.40  | 0.87  | 0.54  | 0.34  |
| $e$                     | 4.01  | 2.76  | 1.86  | 1.26  |
| $u$                     | 2.18  | 1.24  | 0.65  | 0.38  |

4.3. The problem with two shock waves

The last example is the problem with two shock waves, which is of interest from the point of view of modeling the flows with shock waves that arise at the contact boundaries of gases with the different adiabatic indexes. The problem was proposed in [18] and in another form was shown in [13]. It is put as follows. The segment $0 \leq x \leq 1$ contains two perfect gases, in one of them the shock wave is present:

$$(\rho, u, p, \gamma)|_{t=0} = \begin{cases} 
2.7647, & 1.4833, 4.4468, 1.35 \text{ as } -0.37 \leq x \leq 0.1, \\
1.0, & 0.0, 1.0, 1.35 \text{ as } 0.1 \leq x \leq 0.5, \\
1.9, & 0.0, 1.0, 5.0 \text{ as } 0.5 < x \leq 1.
\end{cases}$$
Figure 4. Modified Sod problem: reference solution and calculated values at $t = 0.2$ (profiles of density, pressure, internal energy and velocity).

Let us denote the gas to the left of initial discontinuity by the index “I” and the gas to the right – by the index “II”. Denote also initial state for $-0.37 \leq x \leq 0.1$ as “I0” and for $0.1 \leq x \leq 0.5$ as “I1”.

On the left boundary of the segment the momentum, mass and energy flows are given with respect to the values at the shock wave; right boundary is the rigid wall. The value $t = 0.25$ is used as a reference point of time.

The initial shock wave reaches the contact boundary between the gases. As a result of the corresponding Riemann problem, two shock waves are formed that are propagating to the right and to the left of the contact boundary between the gases, the contact boundary moves to the right. The resulting flow contains four areas schematically depicted in figure 5:

- the domain $0$: $-0.37 \leq x < X_{SWL}$ – the gas I with initial shock wave and with the parameters $\rho_I^*, u_I^*, p_I^*$.
the domain 1: $X_{SWl} \leq x < X_I$ – the gas I after the shock wave reflected from the contact boundary and going to the left with the parameters $\rho_1, u_1, p_1$;

the domain 2: $X_I \leq x < X_{SWr}$ – the gas II, through which the shock wave has passed, with the parameters $\rho_2, u_2, p_2$, at this $p_2 = p_1, u_2 = u_I$;

the domain 3: $X_{SWr} \leq x \leq 1$ – the gas II with initial parameters $\rho_{II}, u_{II}, p_{II}$,

where $X_{SWl}$ and $X_{SWr}$ are the positions of shock waves, $X_I$ is the position of contact discontinuity. The analytic solution of this problem [18] is used as reference solution.

Numerical calculations were carried out on uniform grids containing 500, 1000, 2000 and 4000 cells, respectively. In the figure 6 the profiles of density, pressure, internal energy and velocity at time $t = 0.25$ are given for the calculations on the coarsest and finest grids in comparison with the reference solution. In tables 5 and 6 the numerical values of absolute and relative $L_1$ errors (the difference between the calculated and the reference solution) are given.

Figure 6. Two shocks problem: reference solution and calculated values at $t = 0.25$ (profiles of density, pressure, internal energy and velocity).
5. Conclusions
The paper presents an explicit Godunov-type scheme for the calculation of multicomponent gas-
dynamic flows, modified to prevent pressure oscillations at the contact boundaries. The developed
scheme takes into account the possibilities of strong shock waves in non-perfect gases. The convenient
modification of "double flux method" used shows quite good results in accuracy and convergence of
calculations both on contact discontinuities and on strong shock waves. This method, due to its
simplicity and robustness, is suitable for implementation in multidimensional algorithms and further
calculations of high-speed flows arising in practical problems of hypersonic aircraft flight with scramjet.

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References
[1] Laroutourou B, Fezoui L 2006 On the Equations of Multi-Component Perfect or Real Gas
Inviscid Flow In Nonlinear hyperbolic problems, Lecture Notes in Math. Springer 1402
69 – 97
[2] Zhukov V T, Zabrodin A V, Feodoritova O B 1993 The Solution Method for 2D Equations of
Heat Conductive Gas Dynamics in the Domains of Complex Shape Comput. Math. Math.
Phys. 33 8 1099 – 1108
[3] Kulikovsky A G, Pogorelov N V, Semenov A Yu 2012 Mathematical Questions of Numerical
Solutions to Hyperbolic Systems of Equations (2nd ed.) (Fizmatlit) ISBN 978-5-9221-1198-0
(in Russian)
[4] Godunov S K 1959 Difference method of numerical calculation of discontinuous solutions of
hydrodynamics equations. Mat. Sh. 47 89 271 – 306 (in Russian)
[5] Abgrall R 1988 Generalisation of the ROE Scheme for the Computation of Mixture of Perfect
Gases Rech. Aerosp. 6
[6] Billet G, Abgrall R 2003 An Adaptive Shock-Capturing Algorithm for Solving Unsteady
Reactive Flows Computers & Fluids 32 (10) 1473 – 1495
[7] Abgrall R 1994 How to Prevent Pressure Oscillations in Multicomponent Flow Calculations: a
Quasi Conservative Approach RR-2372 INRIA
[8] Tunik Y V 2017 Instability of Contact Surface in Cylindrical Explosive Waves Fluid Mech.
Open Acc. 4 168

[9] Gidaspov V Yu, Ivanov I E, Kryukov I A, Naboko I M, Petukhov V A, Strel'tsov V Yu 2004 Investigation of buster waves moves in cumulating cavity Matem. Mod. 16 6 118 – 122 (in Russian)

[10] Ivanov I E, Kryukov I A 2007 Numerical modeling of multicomponent gas flows with strong discontinuities of medium properties Matem. Mod. 19 (12) 89 – 100 (in Russian)

[11] Saurel R, Abgrall R 1999 A Multiphase Godunov Method for Compressible Multifluid and Multiphase Flows J. of Computational Physics 150 425 – 467

[12] Ma P C, Lv Yu Ihme M 2017 An Entropy-Stable Hybrid Scheme for Simulations of Transcritical Real-Fluid Flows J. of Computational Physics 340 330 – 357

[13] Yanilkin Yu V, Bondarenko Yu A, Goncharov E A et al. 2017 Tests for Hydrocodes, which Model the Flows with Shock Waves in Multicomponent Media vol. 1 (Sarov: FGUP “RFYaC-VNIIEF”) ISBN 978-5-9515-0351-0 (in Russian)

[14] Ivanov M Ya, Korecki V V, Kurochkina N Ya 1980 The Investigation of Properties of High Order Accuracy Numerical Schemes Chislennye metody mechaniki sploshnoi sredy 11 (4) 88 – 103 (in Russian)

[15] Sod G 1978 A Survey of Several Finite Difference Methods for Systems of Nonlinear Hyperbolic Conservation Laws J. Comp. Phys. 27 1 – 31

[16] Barlow A 2001 A New Lagrangian Scheme for Multimaterial Cells In Proceedings of European Congress on Computation Methods in Applied Science and Engineering ECCOMAS computational Fluid Dynamics Conf., Swansea, Wales, U.K. 235 – 294

[17] Shashkov M J 2007 Close Models for Multimaterial Cells in Arbitrary Lagrangian-Eulerian Hydrocodes Int. J. Numer. Meth. Fluids 56 1497 – 1504

[18] Banks J W, Schwendeman D W, Kapila A K, Henshaw W D 2007 A High-Resolution Godunov Method for Compressible Multi-Material Flow on Overlapping Grids J. Comp. Phys. 223 262 – 297