Application of the Riemann problem with complex equations of state for modeling three-dimensional flows of real media

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Abstract: The paper considers the numerical simulation of spatial flows of real media in safety valves on the basis of the problem of an arbitrary discontinuity breakdown with complex equations of state. The solution is constructed by means of the developed numerical method, which is a modification of the classical scheme by S. K. Godunov and includes various complex equations of state of matter. The Van der Waals equations of state were used to model the flow of real gases, and the Mie-Grüneisen equation was used to describe the flow of a real weakly compressible fluid. It is shown that the proposed numerical schemes allow for modeling fluid and gas dynamic processes in real fluids and gases with shock waves and contact discontinuities and can be used both in areas of classical medium behavior and in areas with non-classical behavior.

1. Introduction

The equation of state is an equation that relates the variables that describe the state of matter for a given set of physical conditions. This equation is one of equations that close the system of conservation equations in mathematical modeling of fluid motion. In the case of describing the behavior of gaseous well-compressible substances, the ideal gas equation of state is most commonly used. When we study the motion of absolutely incompressible fluids, the equation of state for the constant density of the substance leads to a new mathematical model of an incompressible fluid, which excludes the density of the medium from the list of unknown quantities. However, there are special modes of media motion, when the above models do not allow us to obtain reliable results. In the case of compressible media, such modes include areas of non-classical gas behavior near their critical state, and in the case of fluids, these are the modes in which the density change cannot be neglected, for example, at extremely high pressures.

In these cases, special equations of state are used for modeling [1-7], among which the Van der Waals, Redlich-Kwong, Peng-Robinson, Kamerling-Hones, Martin-Howe, and Jones-Wilkins-Lee equations of state can be distinguished. The Van der Waals equation [7], which allows for taking into account intermolecular interactions and the real intrinsic volume of molecules, is the most widely used for modeling the behavior of real gases. This equation is applied to describe the flows of high molecular weight substances characterized by a large value of specific heat capacity [1, 6], dense gases and chemically reacting gases in the local thermodynamic equilibrium, for numerical studies of flows and heat exchange in near-critical media under spaceflight conditions [8]. The issues of modeling the
flow of weakly compressible real fluids, as well as the corresponding equations of state, are considered in [2, 9-11]. The Mie-Grüneisen equation of state together with the Hugonio equation has been used to calculate intense shock waves in multiphase problems of condensed media [10, 11].

This paper presents the results of solving the test problem of an arbitrary discontinuity breakdown using the numerical method by S. K. Godunov in the media described by the Van der Waals equation of state for a real gas and the Mie-Grüneisen equation of state for a weakly compressible fluid. The numerical method is generalized for the three-dimensional case of the flow of real media by the example of a direct-acting safety valve.

2. Mathematical model
The solution of an arbitrary discontinuity breakdown problem is given within two approaches: for a compressible gas based on the Van der Waals equation and for a weakly compressible fluid based on the Mie-Grüneisen equation. The medium flow is described by conservation equations (mass, momentum and energy) with equations of state in the form of Van der Waals equation [1] for gaseous media

\[\varepsilon(p, \rho) = \frac{1 - b\rho}{d} \left(\frac{p}{\rho} + ap\right)\] (1)

and the Mie-Grüneisen equation [10] for weakly compressible media

\[\varepsilon(p, \rho) = \frac{\rho - \rho_c c_k^2 \delta}{\mu - 1} \left[\frac{\gamma - 1}{\delta - 1} + \frac{\gamma - \mu}{\mu} \left(1 - \delta^\mu\right)\right] \rho^{-\gamma - 1} (\gamma - 1)\] (2)

In equations (1), (2) the following designations are used: \(R\) is the specific gas constant, \(a\) and \(b\) are dimensional Van der Waals gas constants, \(d = R/c_s^2\), \(c_s\) is the specific heat capacity at the constant volume, constants with the index 0 correspond to a certain initial (original) gas state, \(\varepsilon\) is the specific energy, \(S\) is the entropy, \(\rho\) is the density, \(\delta = \rho/\rho_c\), \(\gamma = 1.638\), \(\mu = 5\) are constants of the Mie-Grüneisen model, \(\rho_c = 1180.5 \text{kg/m}^3, c_k = 2090.1 \text{m/s}\).

For the convenience of constructing calculation schemes and algorithms [13, 14], the system of equations used is reduced to a dimensionless form with respect to the critical parameters of matter: \(p_c, \rho_c, T_c\). The flow velocity is related to the value of \(\sqrt{p_c/\rho_c}\), while the internal energy relates to the ratio \(\rho_c/\rho\). The coefficients of the equation in this case do not depend on the matter in question: \(A = 3, B = 1/3\) with the equation of state \(\varepsilon = \frac{8BT}{d} - A\rho\).

For the Mie-Grüneisen equation the density is related to the value of the stagnation density \(\rho_{00}\), corresponding to the known stagnation parameters for the flow \(p_{00}, T_{00}\). The velocity is related to the speed of sound \(c_{00}\), the pressure is related to the value of \(\rho_{00} c_{00}^2\), while the internal energy is related to \(c_{00}^2\).

The solution of the resulting system of equations is made by the method of S. K. Godunov [11]. In this case, the initial approximation of the equation of state by a two-member equation of state allows us to find the initial approximation of variables for solving the resulting system of equations.

The issues of forming mathematical models of the flow of a real gas and real weakly compressible fluid, as well as the issues of developing numerical schemes and algorithms are considered in detail in [12, 15]. The specified approbation and verification of numerical schemes and algorithms are given in [13-17].
The developed mathematical models are used to carry out test calculations for the flow of real media in a shock tube, as well as to simulate flows in a complex three-dimensional area of a safety valve (Figure 1).

The no-flow condition is used on solid surfaces, the symmetry condition is used on the symmetry boundary, and the parameter extrapolation is used on the outlet boundary. The enthalpy of stagnation and constant entropy condition are given at the inlet boundary [15].

3. Van der Waals equation for real gas flow modeling
The necessity of transition to Van der Waals equation of state is caused by impossibility to describe the medium behavior in the non-classical area with the help of the ideal gas equation of state. This area is near the critical point of the saturation curve of the substance and is characterized by negative values of the fundamental derivative [17]

\[ G(p, \rho) = \frac{(d+1)(d+2)\rho^2 \left( \frac{p + A\rho^2}{1 - B\rho} \right)^2 - 6A\rho^2}{2(d+1)\rho^2 \left( \frac{p + A\rho^2}{1 - B\rho} \right)^2 - 4A\rho^2} \]

Test calculations are performed for the classical problem of an arbitrary discontinuity breakdown as well as for the problem with non-classical behavior. In the first case, the initial distribution of parameters is given as follows

\[ p_1 = 1, u_1 = 0, \rho_1 = 0.5 \text{ for } x < 0, \quad p_2 = 0.75, u_2 = 0, \rho_2 = 0.125 \text{ for } x > 0. \]
The substance with the ratio of the specific gas constant to the specific heat capacity equal to 0.329 is in the area of the critical state (Fig. 2a). In the second case, the substance with a large specific heat capacity with respect to its molecular mass with \( d = 0.0128 \) is considered:

\[
p_1 = 3, u_1 = 0, \rho_1 = 1.818 \quad \text{for} \quad x < 0, \quad p_2 = 0.575, u_2 = 0, \rho_2 = 0.275 \quad \text{for} \quad x > 0.
\]

On the left side, gas parameters correspond to the area of non-classical behavior (Figure 2b). Figure 2a shows the precise and numerical solution of the Riemann problem. The agreement of the calculated parameters and the values given in [2] confirms the legitimacy of the approach used for modeling the flow of real gases. The peculiarities of the gas flow in the non-classical area can be estimated from the results shown in Figure 2b. In this case, the shock wave is smoothened, while the rarefaction wave at negative values of \( G(p, \rho) \) forms a rarefaction jump and the steepness of the flow parameter curves increases.

![Figure 2. Solution of discontinuity breakdown problem](image)

(a) classical, (b) non-classical gas behaviour.

The results of modeling of the three-dimensional flow of a real gas are shown in Fig. 3. Two areas of initial distribution of dimensionless physical quantities - the area up to the narrow gap with parameters \( p_1 = 1.09, u_1 = 0, \rho_1 = 0.879 \) and the area behind the gap with parameters \( p_2 = 0.885, u_2 = 0, \rho_2 = 0.562 \) - are defined as initial conditions. The calculations were performed for a high-molecular weight substance with index \( d = 0.0128 \). Figure 3 shows the flow lines and the pressure field in the gas when the disk is raised to a height of 10 mm.

![Figure 3. Flow of a real gas in the valve](image)

(a) current lines, b) changes in parameters along the flux.

The flow pattern (Figure 3a) shows the predominant influence of geometry on the fluid and gas dynamics in the valve. It can be seen that the operation of the safety valve is associated with the process of intensive vortex formation. In the central area of the valve two circulation zones are formed: under and over the disk. As a result, the flow is divided into two parts that do not intersect each other until they exit the spigot. The geometrical expansion of the valve outlet channel contributes to the creation of another vortex area in the upper part of the spigot. The maximum gas velocity
exceeds the sound velocity by more than twice in the area below the disk. The obtained results indicate the non-uniform dynamic mode of gas passage through the internal cavity of the valve. Figure 3b shows the change in the main flow parameters along the flux. After the critical section, the character of changes in values becomes non-uniform.

4. Mie–Grüneisen equation for weakly compressible fluid flow modeling

In cases of droplet fluids operating at extreme pressures, the change in density of the medium cannot be neglected. In this case, the Mie-Grüneisen equation of state, which describes the relationship between fluid pressure and volume at a given temperature, can be used. Parameters of the Mie-Grüneisen equation were obtained by approximation of the known table and analytical relations [15]. As a test of the algorithm, the Riemann discontinuity breakdown problem with the following parameters at the initial moment of time was solved by the example of water (Figure 4):

\[
p_1 = 0.13, u_1 = 0, \rho_1 = 1 \quad \text{for} \quad x < 0, \quad p_2 = 0.0013, u_2 = 0, \rho_2 = 0.9 \quad \text{for} \quad x > 0.
\]

Figure 4. Solution of the Riemann problem for water.

A comparison of the precise and numerical solutions is shown in Figure 5. The largest error is observed for the rarefaction wave. The shock waves are approximated with good accuracy. Thus, the approach used is applicable to the calculation of weakly compressible fluids by the Godunov method using the Mie-Grüneisen equation of state.

The results of modeling the three-dimensional flow of a weakly compressible fluid are shown in Figure 5. As the initial conditions, two areas of initial distribution of dimensionless physical quantities are defined: the area up to the narrow gap with parameters \( p_1 = 0.13139, u_1 = 0, \rho_1 = 1 \) and the area behind the gap with parameters \( p_2 = 0.1319 \times 10^{-4}, u_1 = 0, \rho_1 = 0.9 \). Calculations were performed for water. Figure 5a shows the flow lines and the pressure field in the gas when the disk is raised to a height of 10 mm.

Figure 5. Flow of a weakly compressible fluid in a valve: (a) flow lines and (b) changes in flow parameters along the flux.
The structure of the fluid flow in the safety valve cavity is comparable to the flow of a real gas. Formation of vortex extended flows along the body and their behavior in the outlet spigot are also caused by geometrical features of internal channels of the valve. In stagnation zones, the flow mode close to the classical flow in a cavity is implemented.

The change of dimensionless parameters along the flux is shown in Figure 5b. The character of gas dynamic parameters variation is characterized by the essential non-uniformity.

5. Conclusion
The paper presents the results of numerical simulation of the flow of real media obtained by S.K. Godunov method using complex equations of state. The carried out test calculations for the Riemann problem on the arbitrary discontinuity breakdown showed that the Godunov scheme with the local approximation of the Van der Waals and Mic-Grüneisen equation of state by a two-member equation allows modeling the fluid and gas dynamics processes in real fluids and gases with shock waves and contact discontinuities and can be used both in areas of classical gas behavior and in areas with non-classical behavior. The method was generalized to the three-dimensional case of the flow in the safety valve cavity. As a result of comparison of the obtained data, it was revealed that the structure of flows of gases and fluids are similar in many respects and are mainly caused by the geometry of elements of the device: the casing, disk, and outlet spigot.

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