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Interface Capturing Method Based on the Cahn–Hilliard Equation for Two-Phase Flows

I. S. Menshov[a,b,c,*] and C. Zhang[d,]**

[a] *Keldysh Institute of Applied Mathematics, Russian Academy of Sciences, Moscow, 125047 Russia*
[b] *Scientific Research Institute for System Analysis, Moscow, 117218 Russia*
[c] *Dukhov Automatics Research Institute, Moscow, 127055 Russia*
[d] *Moscow State University, Moscow, 119992 Russia*
**e-mail: menshov@kiam.ru*
***e-mail: zhang-c@mail.ru*

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Abstract—A numerical method for flows of heterogeneous two-phase compressible media is considered. The main problem in the construction of such a method is to find the interface between the components with different physical and mechanical properties. An efficient method for solving this problem that gives a good spatial resolution of the interfaces is proposed. This method is based on the use of the Cahn–Hilliard equation. To describe the flow of the two-phase medium, the single-velocity five-equation model is used; in this model, the Cahn–Hilliard equation is used as the equation for the order function. This makes it possible to significantly decrease the domain of the interface numerical smearing. Numerical results confirm the high accuracy and effectiveness of the proposed method.

Keywords: two-phase flow, Cahn–Hilliard equation, resolution of phase interfaces

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1. INTRODUCTION

An important problem in the simulation of a flow of a multicomponent heterogeneous medium is to determine the location of the interface between the components with different physical and mechanical properties. The numerical methods for calculating the flow of a heterogeneous medium with an interface can be divided into two groups. The first group includes the methods in which the interface is explicitly tracked in a special way so that the interface is represented by a surface at each point in time [1–5]. The second group consists of diffuse interface methods [6–11], in which the interface is determined by a narrow spatial domain with a sharp variation of the characteristic function or the order parameter specifying the spatial distribution of the components.

In each of the two approaches, a number of models for describing the dynamics of the phase interface have been proposed. In the methods of the first group, the interface is the discontinuity surface of the characteristic function, and its position is computed at each time step. This is a relatively easy task if the interface coincides with a line of the computational grid. However, this can lead to strong distortions of the computational grid cells if the interface undergoes large deformations. Alternative approaches do not explicitly relate the interface tracking method to the computational grid. Among them are the arbitrary Lagrangian–Eulerian (ALE) method [1], the level set method [2], and the front-tracking method [3]. The main drawback of these methods is the violation of conservativeness of the method in a neighborhood of the interface.

The methods in the second group make it possible to overcome the main drawbacks of the methods based on the direct computation of the interface. In the literature, they are called the diffuse interface methods [6–11]. The idea underlying these methods is to consider the medium consisting of different components as a homogeneous effective medium the properties of which depend on the characteristic function—the order parameter—that determines the spatial distribution of constituting components. For example, the volume fraction of a component may be used as such a function. In this case, the interface between the phases is not explicitly distinguished; rather, it is represented by a zone in which the value of the volume fraction varies continuously from zero to one.

Note that, in addition to the models based on the characteristic function [6, 7, 9–11], approaches that do not use special equations for resolving the interface between the components are considered. They use equations for the mass concentrations of individual components and balance equations for the total momentum and energy of the mixture [12, 13].

The interface smearing domain in the diffuse interface methods inevitably increases with time due to numerical dissipation. Even high-order schemes on fixed grids cannot completely eliminate the numerical dissipation; the initial jump in the distribution of the volume fraction gets a smooth profile with time. In this domain, the medium is a mixture of different components, and the interface motion is determined by the adopted physical model of the mixture. The less this zone, the less is the influence of the mixture numerical model and the more accurately the interface position is determined. For this reason, in the development of a diffuse interface method, a tradeoff should be found by allowing the controllable interface smearing; i.e., the numerical smearing should be allowed only within certain limits.

The aim of this paper is to construct a controllable resolution technology for diffuse interface models. The main idea is to use the Cahn–Hilliard equation [14, 15] for correcting the order function smearing.

The Cahn–Hilliard equation is derived from thermodynamic considerations for the order parameter that determines the phase transition in the two-phase system. This equation is based on the assumption that the free energy of the system has the form

$$\psi(\phi, \nabla\phi) = f(\phi) + \frac{\chi^2}{2}|\nabla\phi|^2, \tag{1}$$

where ψ is the free energy density, ϕ is the order parameter (typically, it is the difference of the phase concentrations), χ is a positive constant related to the linear size of the diffuse interface domain, and $f(\phi)$ is the coarse-grain component of the free energy corresponding to the phase separation.

The total free energy is given by the formula

$$\Psi(\phi) = \int_\Omega \psi(\phi, \nabla\phi) d\mathbf{x}, \tag{2}$$

where Ω is the spatial domain occupied by the system.

Formally, the variation $\Psi(\phi)$ with respect to the order parameter ϕ is

$$\delta\Psi(\phi) = \int_\Omega [f'(\phi) - \chi^2\Delta\phi]\delta\phi d\mathbf{x} = \int_\Omega \mu\delta\phi d\mathbf{x}, \tag{3}$$

where

$$\mu(\phi) := \frac{\delta\Psi(\phi)}{\delta\phi} = f'(\phi) - \chi^2\Delta\phi$$

is the first variation of the system free energy, which has the meaning of chemical potential.

The process of relaxation in the direction of equilibrium is described by the balance equation [14, 15]

$$\frac{\partial\phi}{\partial t} = \nabla\cdot(M(\phi)\nabla\mu), \tag{4}$$

where the positive function $M(\phi) \geq 0$ is called the *mobility* of the system. In this paper, we assume that it is equal to 1.

The coarse-grain component of the free energy $f(\phi)$ is a function with two local minimums, and in the majority of studies it is approximated by the fourth-degree polynomial

$$f(\phi) = \frac{1}{4}(\phi^2 - 1)^2. \tag{5}$$

Approximation (5) does not guarantee the physically feasible range of variation of ϕ. Solution (4) can be outside the interval $[-1, 1]$, which corresponds to negative values of the phase densities. For this reason, we use the logarithmic Flory–Huggins approximation [16]

$$f(\phi) = f_0(\phi) - \frac{\theta_0}{2}\phi^2, \quad f_0(\phi) = (1+\phi)\ln(1+\phi) + (1-\phi)\ln(1-\phi), \tag{6}$$

where θ_0 is the parameter controlling the phase interface zone; this parameter is related to the thickness of the interface.

Thus, we obtain the following equation for the evolution of the order parameter ϕ, which will be used in the diffusive interface model for the flows of two-phase media:

$$\frac{\partial \phi}{\partial t} = \Delta \mu(\phi),$$
$$\mu(\phi) = \ln(1+\phi) - \ln(1-\phi) - \theta_0 \phi - \chi^2 \Delta \phi. \tag{7}$$

In model (7), the size of the diffusive zone of the interface is controlled by two parameters χ and θ_0. The dependence of the equilibrium distribution of ϕ on the parameters χ and θ_0 is described below in the section in which numerical results are discussed.

The paper is organized as follows. In Section 2, the governing equations of the mathematical model used to describe the flows of the two-phase heterogeneous medium are considered. In Section 3, we discuss the model of resolving the interphase interface based on the solution to the Cahn–Hilliard equation. Section 4 describes a numerical method for solving the system of governing equations and the equation for the order function. Section 5 is devoted to the results of numerical verification of the proposed methods. In the last section, we draw brief conclusions.

2. GOVERNING EQUATIONS OF THE MODEL

We consider the flow of a two-phase heterogeneous mixture consisting of two immiscible fluids. To describe this flow, we use the single-velocity five-equation model [9–11], which can be written as

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \operatorname{div}(\alpha_1 \rho_1 \mathbf{u}) = \rho_1 R(\alpha),$$
$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \operatorname{div}(\alpha_2 \rho_2 \mathbf{u}) = -\rho_2 R(\alpha),$$
$$\frac{\partial \rho \mathbf{u}}{\partial t} + \operatorname{div}(\rho \mathbf{u}\mathbf{u} + P\mathbf{I}) = R(\alpha)(\rho_1 - \rho_2)\mathbf{u}, \tag{8}$$
$$\frac{\partial \rho e}{\partial t} + \operatorname{div}(\rho H \mathbf{u}) = R(\alpha)[(\rho_1 - \rho_2)k + (\rho_1 \varepsilon_1 - \rho_2 \varepsilon_2)],$$
$$\frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \operatorname{grad} \alpha = H(\alpha) + R(\alpha),$$

where α_i is the volume fraction of the component i, $\rho = \sum_{i=1}^{2} \alpha_i \rho_i$ is the mixture density, $P = \sum_{i=1}^{2} \alpha_i P_i$ is the mixture pressure, $\rho\varepsilon = \sum_{i=1}^{2} \alpha_i \rho_i \varepsilon_i$ is the mixture internal energy, $\rho h = \sum_{i=1}^{2} \alpha_i \rho_i h_i$ is the mixture enthalpy, $e = \varepsilon + |\mathbf{u}|^2/2$ is the mixture specific total energy, $k = |\mathbf{u}|^2/2$ is the specific kinetic energy, $H = e + P/\rho$ is the mixture specific total enthalpy, $\alpha = \alpha_1$, $H(\alpha) = \alpha_1 \alpha_2 (C_2 - C_1)/(\alpha_1 C_2 + \alpha_2 C_1)$, $C_i = \rho_i c_i^2$, and c_i is the speed of sound in the component i.

The introduction of nonconservative terms with $R(\alpha)$ into the right-hand side of the system of equations (8) was proposed in [10]; it is a special numerical regularization aimed at a more accurate resolution of the interface. Actually, this nonconservative addition works only in a narrow domain in the vicinity of the interface. As the grid becomes finer, this domain shrinks to the interface surface, and the effect of the nonconservative addition should disappear. The main purpose of this paper is to derive an expression for $R(\alpha)$ by considering an analogy with the Cahn–Hilliard interface thermodynamics. Note that regularized fluid dynamics equations are used fairly often (e.g., see [17, 18]).

Let us make some remarks concerning the governing equations. The system of equations (8) is hyperbolic, and it describes the equilibrium (with respect to velocity and pressure) fluid dynamic model of the two-phase medium. This model can be formally derived from the more general nonequilibrium Baer-Nunziato model based on the asymptotic analysis with respect to the relaxation parameters describing how the mechanical equilibrium of the two-phase system with respect to the velocity and pressure is reached. Theoretically, if the flow of two immiscible fluids is considered ($\alpha_i = 1$, $\mathbf{x} \in \Omega_i$ and $\alpha_i = 0$, $\mathbf{x} \notin \Omega_i$), then $H(\alpha) = 0$. If Eq. (7) is used for the interface capturing computation of the flow of two-phase fluid, then $H(\alpha) \neq 0$ in the diffuse domain of the interface. In [9], the term $H(\alpha)$ on the right-

hand side of the equation for the volume fraction was estimated, and it was shown that this term may be neglected, and the simplified model with $H(\alpha) = 0$ may be used. Below, we use this approximation.

To describe the thermodynamic properties of the phases, we use the generalized Van der Waals equation of state, which has the form

$$P_i(\rho_i, \rho_i\varepsilon_i) = \left(\frac{\gamma_i - 1}{1 - b_i\rho_i}\right)(\rho_i\varepsilon_i - \pi_i + a_i\rho_i^2) - (\pi_i + a_i\rho_i^2), \quad i = 1, 2, \tag{9}$$

where γ_i is the adiabatic coefficient, the coefficient a_i takes into account the attraction forces between molecules (Pa m^6/mol^2), the correction b_i is the total volume of the gas molecules (m^3/mol), and π_i is a semi-empirical constant obtained by analyzing experimental data (Pa).

The isobaric closure of the system of equations (8) — $P_1 = P_2 = P$ — yields the following equation for the mixture state:

$$P(\rho_1, \rho_2, \rho\varepsilon, z) = \left[\sum_{i=1}^{2} z_i\xi_i(\rho_i)\right]^{-1}\left\{\rho\varepsilon + \sum_{i=1}^{2} z_i\left[(a_i\rho_i^2 - \pi_i) - \xi_i(\rho_i)(a_i\rho_i^2 + \pi_i)\right]\right\}, \tag{10}$$

where

$$\xi_i(\rho_i) = \frac{1 - b_i\rho_i}{\gamma_i - 1}.$$

The speeds of sound in the phases are found by the formula

$$c_i = \sqrt{(h_i - \delta_i)/\xi_i}, \tag{11}$$

where

$$\delta_i(\rho_i) = 2a_i\rho_i[\xi_i(\rho_i) - 1] - \frac{b_i}{\gamma_i - 1}\left(P_i + \pi_i + a_i\rho_i^2\right).$$

The speed of sound in the mixture in the model under consideration is determined by the relation

$$c = \sqrt{\sum_{i=1}^{2} y_i\xi_i(\rho_i)c_i^2 \Big/ \xi(\rho_1, \rho_2, z)}. \tag{12}$$

Remark. In this paper, we use the isobaric closure for the following reasons. First, in many dynamical processes, the mechanical relaxation with respect to pressure and velocity is much faster than the temperature relaxation; e.g., in explosive processes or shock waves (also see [11] for estimating the time taken by relaxation processes). With the isobaric closure, model (8) admits different phase temperatures. In addition, it was noted in [9] that the isothermal closure (when the temperatures of the phases are equal) gives a less stable model, which manifests itself in nonphysical oscillations in numerical solutions.

3. THE INTERFACE RESOLUTION METHOD

It has already been mentioned above that, in order to improve the accuracy of resolving the interface between the components, special terms are added to the right-hand side of the system of governing equations (7); this terms are determined by the function $R(\alpha)$. We now give an interpretation of this function in the framework of the thermodynamic interface theory (the Cahn–Hilliard equation).

In this theory, the order parameter ϕ determines the distribution of phases; it is defined as

$$\phi = m_1 - m_2, \tag{13}$$

where m_i is the volume fraction and $m_i = \alpha_i\rho_i/\rho$. It can also be considered as a function of the volume fraction

$$\phi(\alpha) = \frac{\alpha(\rho_1 + \rho_2) - \rho_2}{\alpha(\rho_1 - \rho_2) + \rho_2}. \tag{14}$$

We split the volume fraction equation in model (8) into two parts—convective transfer and numerical regularization for the more accurate resolution of the interface; i.e.,

$$\frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \operatorname{grad} \alpha = 0, \tag{15}$$

$$\frac{\partial \alpha}{\partial t} = R(\alpha). \tag{16}$$

The main idea of the proposed technique is to coordinate the numerical regularization (16) with the Cahn–Hilliard equation (7), which describes the thermodynamically consistent model of the diffuse interface. By substituting (14) into Eq. (7), we obtain

$$\frac{\partial \alpha}{\partial t} = r(\alpha)\Delta\mu(\phi), \tag{17}$$

where

$$r(\alpha) = \frac{\partial \alpha}{\partial \phi} = \frac{\rho^2}{2\rho_1\rho_2} = \frac{[\alpha(\rho_1 - \rho_2) + \rho_2]^2}{2\rho_1\rho_2}. \tag{18}$$

Here we assume that the phase densities ρ_1 and ρ_2 remain unchanged at the step of numerical regularization.

By comparing Eqs. (16) and (17), we obtain

$$R(\alpha) = r(\alpha)\Delta\mu(\phi) = r(\alpha)\frac{\partial \phi}{\partial t}, \tag{19}$$

which closes the governing system of equations (8). Thus, in the proposed model of the flow of the two-phase mixture of immiscible fluids, the governing equations consist of the system of equations (8) and Eq. (7) for the order function, which is used to calculate the regularizing function $R(\alpha)$.

4. NUMERICAL METHOD

For the integration of the system of equations (8), we use the principle of splitting by physical processes; more precisely, we decompose the problem into two subproblems—one of them is related to solving the basic hyperbolic part, and the other requires the integration of the regularizing correction:

$$\begin{gathered}\frac{\partial \alpha_1\rho_1}{\partial t} + \operatorname{div}(\alpha_1\rho_1\mathbf{u}) = 0, \quad \frac{\partial \alpha_2\rho_2}{\partial t} + \operatorname{div}(\alpha_2\rho_2\mathbf{u}) = 0, \quad \frac{\partial \rho\mathbf{u}}{\partial t} + \operatorname{div}(\rho\mathbf{u}\mathbf{u} + P\mathbf{I}) = 0, \\ \frac{\partial \rho e}{\partial t} + \operatorname{div}(\rho H\mathbf{u}) = 0, \quad \frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \operatorname{grad} \alpha = 0,\end{gathered} \tag{20a}$$

$$\begin{gathered}\frac{\partial \alpha_1\rho_1}{\partial t} = \rho_1 R(\alpha), \quad \frac{\partial \alpha_2\rho_2}{\partial t} = -\rho_2 R(\alpha), \quad \frac{\partial \rho\mathbf{u}}{\partial t} = R(\alpha)(\rho_1 - \rho_2)\mathbf{u}, \\ \frac{\partial \rho e}{\partial t} = R(\alpha)[(\rho_1 - \rho_2)k + (\rho_1\varepsilon_1 - \rho_2\varepsilon_2)], \quad \frac{\partial \alpha}{\partial t} = R(\alpha).\end{gathered} \tag{20b}$$

Let us consider these two problems in more detail.

4.1. Hyperbolic System

The last equation in (20a) is the advection equation for the volume fraction, and it can be written in the quasi-conservative form

$$\frac{\partial \alpha}{\partial t} + \operatorname{div}(\mathbf{u}\alpha) = \alpha \operatorname{div}(\mathbf{u}). \tag{21}$$

We will use Eq. (21) for the development of the numerical scheme because this allows us to exactly satisfy the important balancing condition at the discrete level; under this condition, the diffusion of the interface between two fluids with the same pressure equals the mixture pressure [6, 9].

We write the system of equations (20a) in the Cartesian coordinate system (x^1, x^2, x^3) in vector form as

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{q})}{\partial x^1} + \frac{\partial \mathbf{g}(\mathbf{q})}{\partial x^2} + \frac{\partial \mathbf{h}(\mathbf{q})}{\partial x^3} = \mathbf{s}(\mathbf{q}), \tag{22}$$

where $\mathbf{q} = [\rho_1\alpha_1\ \ \rho_2\alpha_2\ \ \rho u\ \ \rho v\ \ \rho w\ \ \rho e\ \ z]^{\mathrm{T}}$, $\mathbf{s}(\mathbf{q}) = [0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ \alpha\,\mathrm{div}(\mathbf{u})]^{\mathrm{T}}$, and $\mathbf{f}$, $\mathbf{g}$, and $\mathbf{h}$ are flows in the directions x^1, x^2, and x^3, respectively.

The system of equations (22) is discretized with respect to space on the Cartesian grid using the finite volume method:

$$\frac{d\overline{\mathbf{q}}_{i,j,k}}{dt} = \frac{1}{\Delta x_i^1}\left(\mathbf{f}_{i-1/2,j,k} - \mathbf{f}_{i+1/2,j,k}\right) + \frac{1}{\Delta x_j^2}\left(\mathbf{g}_{i,j-1/2,k} - \mathbf{g}_{i,j+1/2,k}\right) + \frac{1}{\Delta x_k^3}\left(\mathbf{h}_{i,j,k-1/2} - \mathbf{h}_{i,j,k+1/2}\right) + \mathbf{s}_{i,j,k}.$$

The right-hand side of Eq. (22) is approximated as

$$s_{i,j,k} = \alpha_{i,j,k}\left[\frac{1}{\Delta x_i^1}\left(u_{i+1/2,j,k} - u_{i-1/2,j,k}\right) + \frac{1}{\Delta x_j^2}\left(v_{i,j+1/2,k} - v_{i,j-1/2,k}\right) + \frac{1}{\Delta x_k^3}\left(w_{i,j,k+1/2} - w_{i,j,k-1/2}\right)\right].$$

The numerical flows on the cell boundaries $\mathbf{f}_{i\pm1/2,j,k}$, $\mathbf{g}_{i\pm1/2,j,k}$, $\mathbf{h}_{i\pm1/2,j,k}$ and, respectively, the velocities on the faces $u_{i+1/2,j,k}$, $v_{i,j+1/2,k}$ and $w_{i,j,k+1/2}$ are calculated using Godunov's method [19] with the approximate Riemann problem solver HLLC [20].

The second-order scheme is implemented using the MUSCL scheme. The derivatives of the primitive variables $(\alpha_1\rho_1,\ \alpha_2\rho_2,\ P,\ u,\ \alpha_1)$ are calculated using the limiters MINMOD. The interpolated primitive variables on the left and on the right of the cell edges are determined by

$$a_{i+1/2}^R = a_{i+1} - \frac{1}{2}\min\mathrm{mod}\left(\Delta a_{i+3/2}, \Delta a_{i+1/2}\right),$$

$$a_{i+1/2}^L = a_i + \frac{1}{2}\min\mathrm{mod}\left(\Delta a_{i+1/2}, \Delta a_{i-1/2}\right),$$

where $a = \alpha_1\rho_1$, $\alpha_2\rho_2$, P, u, α, $a_{i+1/2}^L$, and $a_{i+1/2}^R$ are the interpolated values on the left and on the right of the edge $i + 1/2$, respectively, $\Delta a_{i+1/2} = a_{i+1} - a_i$, and $\min\mathrm{mod}(x, y) = \mathrm{sign}(x)\max\{0, \min[|x|, y\,\mathrm{sign}(x)]\}$.

In the MUSCL scheme, the following initial data are used to solve the local Riemann problem in Godunov's method:

$$a = \begin{cases} a_{i+1/2}^L, & x < 0, \\ a_{i+1/2}^R, & x > 0. \end{cases}$$

The numerical flux through the edge $i + 1/2$ is determined by approximately solving the Riemann problem (using the scheme HLLC).

4.2. The System of Equations of the Phase Interface

The system of ordinary differential equations (20b) for each cell of the grid is solved by the Euler method. The last equation must be solved together with Eq. (7).

Equation (7) includes the fourth-order derivative with respect to the order parameter ϕ; therefore, the use of an explicit scheme can require a too hard restriction on the time step. For this reason, we consider for this equation the implicit scheme

$$\begin{gathered} \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{\mu_{i+1}^{n+1} - 2\mu_i^{n+1} + \mu_{i-1}^{n+1}}{\Delta x^2}, \\ \mu_i^{n+1} - \ln(1 + \phi_i^{n+1}) + \ln(1 - \phi_i^{n+1}) + \chi^2\frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} + \theta_0\phi_i^n = 0. \end{gathered} \tag{23}$$

This is a system of nonlinear equations for $\mathbf{Z}_i^{n+1} = (\phi_i^{n+1}, \mu_i^{n+1})$. It is solved by Newton's method. The system of linear equations for the iteration residual $\delta\mathbf{Z}_i = \mathbf{Z}_i^{(k+1)} - \mathbf{Z}_i^{(k)}$ (where k is the iteration index) is solved by the conjugate gradient method.

After computing ϕ_i^{n+1} in this way, we can then find $R(\alpha)$ by the rule

$$R(\alpha_i^n) = r(\alpha_i^n)\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t}. \tag{24}$$

An alternative approach is to calculate the function $R(\alpha)$ on the basis of the volume fraction from the discretization of the last equation in (20b):

$$R(\alpha_i^n) = \frac{\alpha_i^{n+1} - \alpha_i^n}{\Delta t}. \tag{25}$$

Here, α_i^{n+1} is determined from Eq. (13) given the value ϕ_i^{n+1}:

$$\alpha_i^{n+1} = \frac{(1+\phi_i^{n+1})\rho_2}{\rho_1(1-\phi_i^{n+1}) + \rho_2(1+\phi_i^{n+1})}.$$

The first four equations in (20b) determine the variation of the other parameters at the regularization stage. As has been mentioned above, the phase densities do not change at this stage; actually, the solution to system (20b) corrects the values of velocity, pressure, and internal energy in the vicinity of the diffuse interface. The corresponding equations are integrated using the conventional explicit first-order scheme.

5. NUMERICAL RESULTS

To verify the proposed method, we performed a series of computations in which we checked the dependence of the diffuse interface resolution domain on the parameters of the Cahn–Hilliard model θ_0 and χ, and also demonstrated the efficiency and accuracy of the method for the computation of two-phase flows with an interface. We compare these results with those obtained by the computations without the regularizing correction (the standard five-equation model [9]).

5.1. Evolution of the Diffuse Interface in the Cahn–Hilliard Model

First, we consider the model problem of the diffuse interface relaxation according to the Cahn–Hilliard equation. The nonstationary one-dimensional equations (7) are solved with respect to time subject to the initial distribution

$$\phi = \tanh[2.0(x - 0.5)], \quad x \in [0,1]$$

on the grid with 100 uniformly distributed cells. On the basis of the solution for the order function, the evolution of the volume fraction α in time is calculated. The implicit scheme (23) is used. The time step is $\Delta t = 1.0$. It is assumed that the phase densities are identical: $\rho_1 = \rho_2$.

Figure 1a illustrates the computation results with the parameters $\chi = 2\Delta x$ and $\theta_0 = 7.0$ for the first five time steps. It is seen that the numerical values of the volume fraction are within the physically feasible range between 0 and 1.

Figure 1b illustrates the computation results with the parameter $\theta_0 = 7.0$ for the time $t = 5.0$ for various values of the parameter χ. This parameter controls the width of the diffuse interface. It is clear that the less χ, the less is the diffuse interface width. The parameter χ actually determines the number of points N_d in the diffuse zone—$N_d \approx \chi/\Delta x$.

Figure 1c illustrates the computation results with the parameter $\chi = 5\Delta x$ for the time $t = 5.0$ for various values of the parameter θ_0. The decrease of this parameter increases the smearing width of the diffuse interface. However, we see that for $\theta_0 \geq 5$ there is saturation; i.e., the dependence on the parameter becomes weaker and almost disappears.

On the basis of these results, we have chosen $\chi = 2\Delta x$ and $\theta_0 = 7.0$ for the computations of two-phase flows that will be discussed below. At such parameters, the diffuse interface width should be controlled by the model in the range of 2–3 cells.

5.2. Shock Tube

In this section, we consider a standard benchmark for two-phase flows—the one-dimensional flow in a shock tube. The medium consists of two fluids with different equations of state the parameters of which

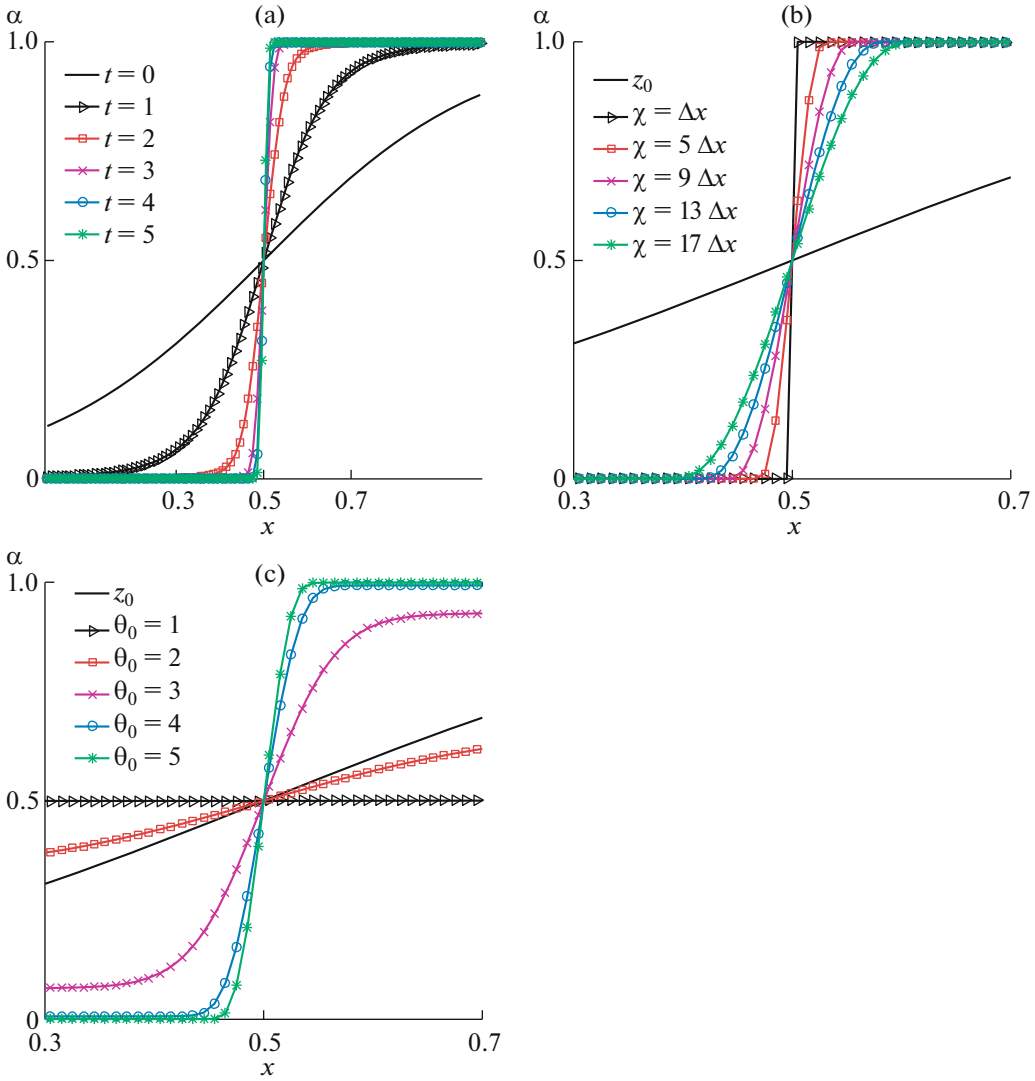

Fig. 1. Numerical solutions for the distribution of the volume fraction α: (a) evolution with time, $\chi = 2\Delta x$, $\theta_0 = 7.0$; (b) dependence on the parameter χ, $\theta_0 = 7.0$; (c) dependence on the parameter θ_0, $\chi = 5\Delta x$.

are shown in Table 1. The length of the computation domain is 1 m. At the initial point in time, fluid 1 is on the left and fluid 2 is on the right of the phase interface, which is at the point $x = 0.7$ m.

The initial data are

$$[\rho_1\ \ \rho_2\ \ u\ \ P\ \ \alpha] = \begin{cases} [1000\ \ 50\ \ 0\ \ 10^9\ \ 1\text{–}10^{-6}], & 0 \le x \le 0.7 \text{ m}, \\ [1000\ \ 50\ \ 0\ \ 10^5\ \ 10^{-6}], & 0.7 < x \le 1.0 \text{ m}, \end{cases}$$

where α is the volume fraction of fluid 1.

Figure 2 illustrates the numerical results obtained without controlling the correction $R(\alpha) = 0$ on grids consisting of 100 and 5000 cells and the results with the controlling correction $R(\alpha)$ on a grid consisting

Table 1. Parameters of the equations of state

Fluid	γ	a ((Pa m^6)/kg)	b (m^3/kg)	π (Pa)
1	4.400	0	0	6×10^8
2	1.400	5	10^{-3}	0

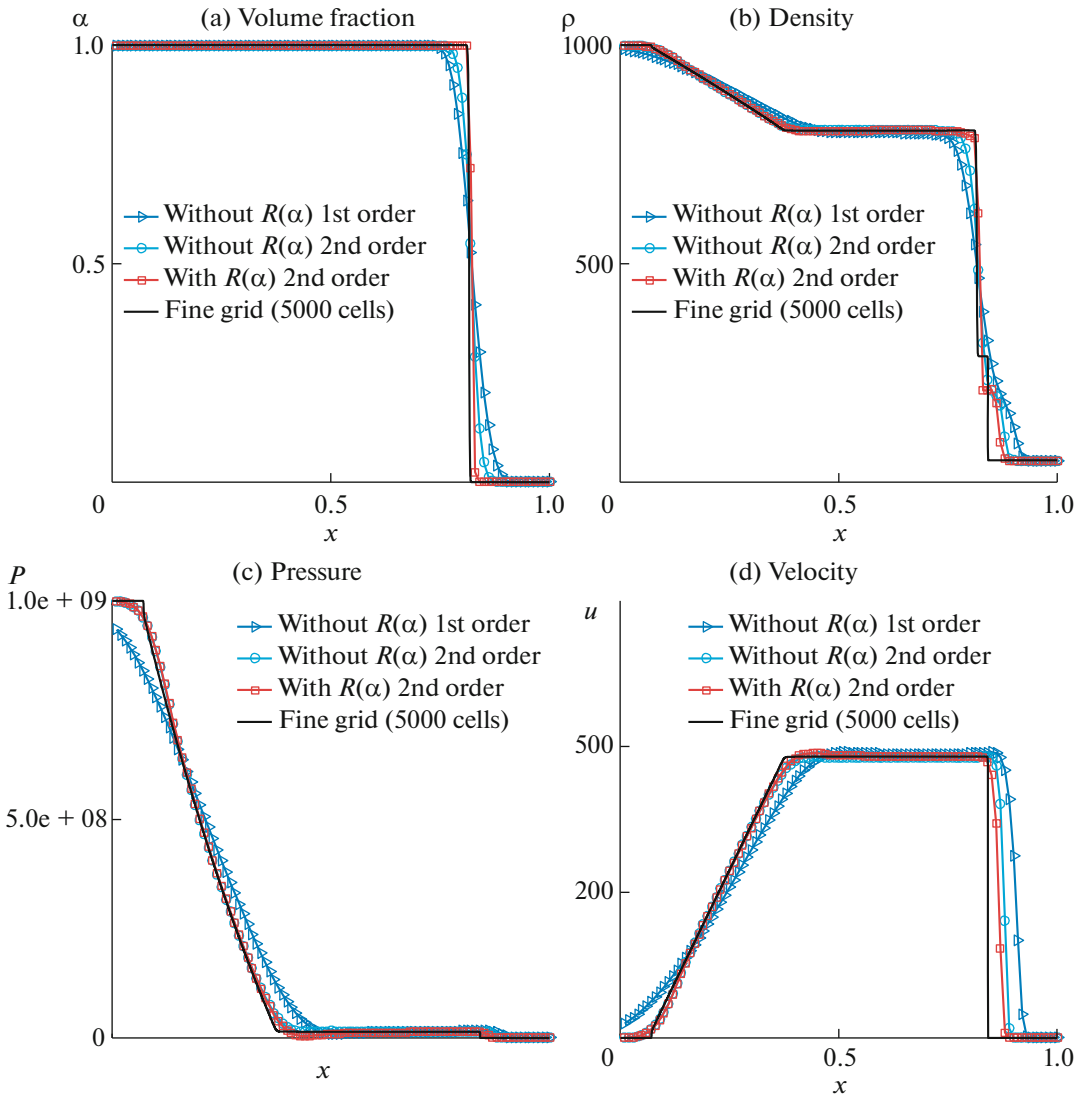

Fig. 2. Numerical solutions of the shock tube problem.

of 100 cells. The result on the grid with 5000 cells was obtained using the second-order MUSCL scheme. It is seen that the numerical dissipation in the computations with $R(\alpha)$ is much lower than in the computations without $R(\alpha)$.

The cost for introducing the regularizing correction in the model is a violation of conservativeness. The system of governing equations generally does not have the form of conservation laws (it has such a form only in the limiting case when the width of the diffuse interface contracts to a point). Therefore, a natural question is how large is the cost of introducing this correction, i.e., how much is the change of the total mass and energy of the system.

To answer this question and estimate the order of nonconservativeness of the scheme with $R(\alpha)$, we introduce the following parameters: the total mass $M = \sum_{i=1}^{n} \rho_i \Delta x$ and the total energy $E = \sum_{i=1}^{n} \rho_i e_i \Delta x$, where i is the cell index. Then, the error due to nonconservativeness can be estimated by the quantity

$$\mathrm{err}(W) = \frac{|W_{\mathrm{end}} - W_0|}{W_0}, \quad W = M, E,$$

Table 2. Error depending on the number of grid cells

Number of cells	100	200	400
err(M)	1.72e–03	1.24e–03	8.40e–04
err(E)	6.08e–04	3.38e–04	1.78e–04

where W_0 and W_{end} are the values of the parameter at the beginning and end of the computation, respectively. Table 2 shows how the error depends on the number of cells. It is seen that the error decreases when the grid becomes finer.

5.3. Interaction of the Shock Wave with a Gas Bubble

In this section, we consider the two-dimensional problem on the interaction of a shock wave with a gas bubble [9]. Similar benchmark problems were also considered in [21, 22]. The two-phase medium is similar to the medium considered in Section 5.2. Fluid 2 is the gas inside the bubble, and fluid 1 is the fluid outside the bubble. The computation domain is shown in Fig. 3. The geometric size of the domain is as follows: $x_0 = 0.70$ m, $x_1 = 0.95$ m, $x_2 = 1.20$ m, $y_0 = 0.50$ m, $y_1 = 1.00$ m, and $r_0 = 0.20$ m.

The initial data are given by

$$[\rho_1\ \rho_2\ u\ v\ P\ \alpha] = \begin{cases} [1.2\ 1230\ -432.69\ 0\ 10^9\ 10^{-6}], & x \in \Omega_1, \\ [1.2\ 1000\ 0\ 0\ 10^5\ 1\text{–}10^{-6}], & x \in \Omega_2, \\ [1.2\ 1000\ 0\ 0\ 10^9\ 10^{-6}], & x \in \Omega_3, \end{cases}$$

where α is the volume fraction of fluid 2.

The computation domain was discretized with respect to space by a uniform Cartesian grid consisting of 120 × 100 cells. The computations on this grid were performed using the standard model without the controlling correction, i.e., $R(\alpha) = 0$ and using the proposed model with a controllable diffuse interface zone.

The computation results are presented in Figs. 4 and 5, where the distribution of the volume fraction and the field of the density gradient (the numerical schlieren), respectively, are shown for two characteristic points in time—$t = 100$ μs and $t = 300$ μs, which correspond to the times when the shock wave passes through the bubble and to the later time when the bubble is fragmented.

It is seen that the main characteristics of the flow occurring when the shock wave diffracts over the deformable gas bubble are well reproduced in both computations. Under the shock wave, the bubble surface takes the characteristic two-petal shape. A wave pattern consisting of the incident, reflected, and refracted inside the bubble shock waves is formed. According to the Cahn–Hilliard equation, the intro-

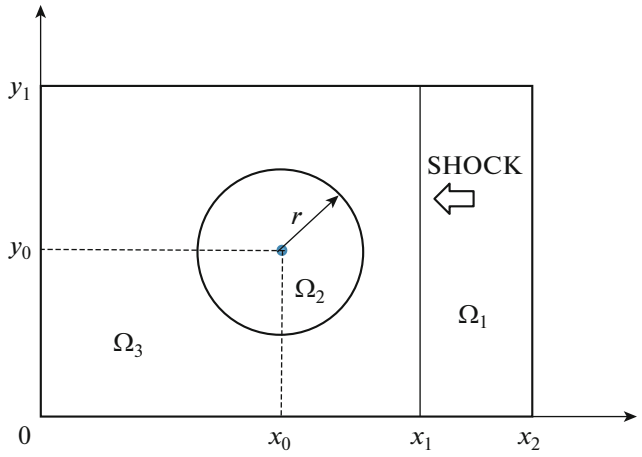

Fig. 3. Diagram of the problem of a shock wave interaction with a gas bubble.

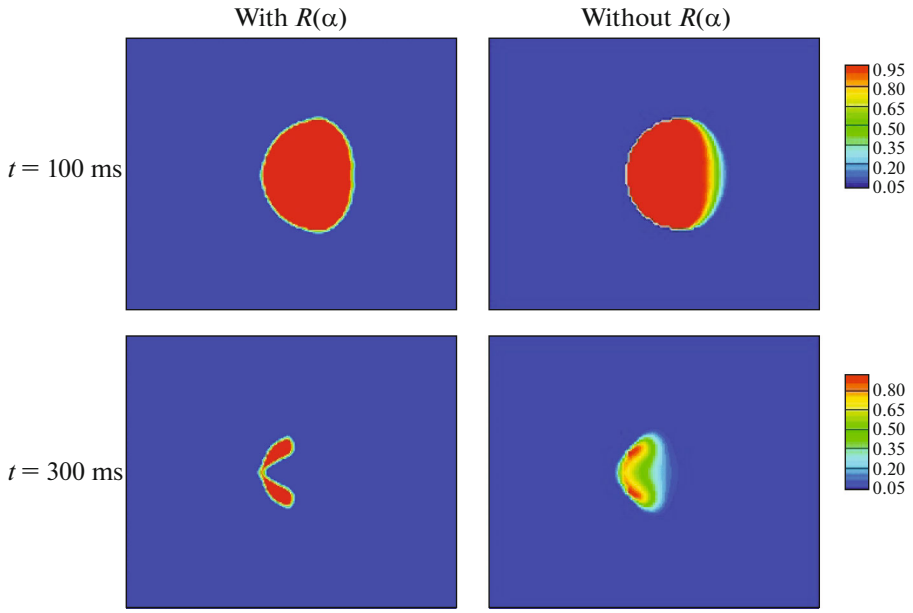

Fig. 4. Distribution of the volume fraction of gas in the problem of a shock wave interaction with a gas bubble.

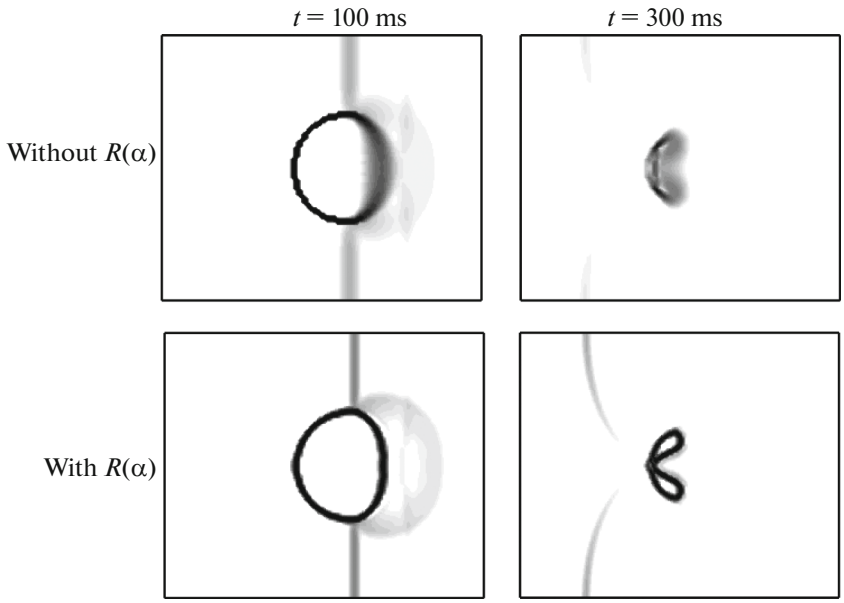

Fig. 5. The field of the gradient density (numerical schlieren) in the problem of a shock wave interaction with a gas bubble.

duction of the regularizing correction $R(\alpha)$ demonstrates the significant improvement in the resolution of the diffuse interface between the components. The characteristic diffuse interface domain (shown in yellow in Fig. 4) does not almost increases with time by contrast with the standard case without $R(\alpha)$.

CONCLUSIONS

A numerical method that ensures the high-quality and controllable spatial resolution of the interface between the phases in the simulation of flows of heterogeneous two-phase compressible media is proposed and implemented. The single-velocity five-equation model with a regularizing correction on the right-hand side is used as a model of the two-phase medium. It is shown that the regularizing correction

can be found using the thermodynamic Cahn–Hilliard model of the interface zone. As a result, a numerical model of the diffuse interface zone with two parameters controlling the zone width is obtained. The dependence of the numerical solutions (the interface zone size) on the controlling parameters is analyzed. Some benchmark problems are numerically solved, and the results show a considerable improvement in the resolution of interfaces between the phases due to using the Cahn–Hilliard equation.

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