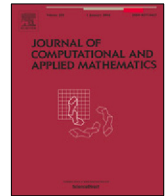




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A new method to discretize a model for isothermal flow with a multi-component equation of state

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ABSTRACT

In this paper we will discuss numerical problems in a phase function model with a multi-component equation of state. It is a sub-model of a diffuse interface model, using a phase field equation, that was introduced by Dreyer et al. in 2014. This model was proposed to describe chemically reacting fluid mixtures consisting of N constituents where phase transitions between a liquid and a vapor phase may occur. The phase field indicates the present phase or the transition layer. The discretization of the model with shock capturing methods for the hyperbolic sub-part is a challenge. One difficulty is that the equation of state has a steep gradient in the density. Moreover, numerical viscosity in diffusive interface computations leads to intermediate values that are unphysical. Our sub-model contains these problems in a nutshell. We develop a solution strategy and apply the new method to several test cases.

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1. Introduction

Two-phase multi-component flows, where the components may be present in the gas or in the liquid phase, have a wide range of applications. To model the interactions of the fluids, especially the exchange of mass and energy due to phase transitions and chemical reactions, is a challenge. Several types of models with different pros and cons are available in the literature.

Models of Baer–Nunziato type typically require a large number of equations that increase numerical cost substantially. Usually these models are not in divergence form. Accordingly special attention has to be given to the discretization. Moreover, the form of the exchange term is not known, but has to be derived for the special situation at hand. For more details see [1,2].

Sharp interface models need only a smaller number of equations. Instead, the interface, more or less, has to be resolved exactly. Accordingly, a very fine grid resolution is required. Alternatively, the computations have to be performed on a moving mesh or using front-tracking on a fixed mesh. Both methods are computationally challenging especially involving changes in interface topology. Interesting results on this can be found in [3–5].

To overcome the above mentioned disadvantages of the referred types of models, one can deal with so-called phase field models. Here a phase field parameter is introduced. This parameter takes two distinct values to indicate the phases.

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It smoothly changes in the interfacial region which is a zone of finite width. Phase field models enjoy a growing interest in research.

For chemical reactions the equations are modified by reaction sources. For their discretization an ODE-solver has to be coupled to the numerical method. We are not aware of any problems caused by such a coupling to numerical methods for sharp or diffusive interface models.

For phase transitions the situation is completely different. In Baer–Nunziato type models, the phase transition is modeled by source terms, e.g. of relaxation type, see [6–8]. Sharp interface models use kinetic relations, see [9–11]. The advantage of a phase field model is that the phase transition is handled by the PDE for the phase field quantity.

Numerical methods for a sub-model of a phase field model derived by Dreyer, Giesselmann and Kraus [12] are the main focus of this paper. We will introduce both models in the following section. They are isothermal models. So, they are suitable for chemical reactions and phase transitions since the latent heat released or adsorbed in these processes is transported with infinite velocity. Therefore, these models do not need an extra energy balance equation. In the third section, we discuss the discretization of the sub-model. It turns out that some unexpected difficulties appear. These difficulties are also relevant for discretizations of the full model, since they are due to the nature of the equation of state. It is identical for both models. In the subsequent section, we develop a strategy to overcome these problems. We give some numerical examples and finally make some remarks on future work.

2. The model

In [12] Dreyer et al. consider an N -component mixture. Each of the constituents $\alpha = 1, \dots, N$ has its own partial density ρ_α . The density ρ of the mixture is given by

$$\rho = \sum_{\alpha=1}^N \rho_\alpha.$$

Accordingly, only N of these densities have to be determined by partial differential equations.

The compressible N -component two-phase model introduced by Dreyer et al. [12] is given by the following system of partial differential equations

$$\begin{aligned} \partial_t \rho + \operatorname{div}(\rho \mathbf{v}) &= 0 \\ \partial_t \rho_\alpha + \operatorname{div}(\rho_\alpha \mathbf{v}) - \operatorname{div} \left(\sum_{\beta=1}^{N-1} M_{\alpha\beta} \nabla(\mu_\alpha - \mu_N) \right) &= \sum_{i=1}^{N_R} \gamma_\alpha^i m_\alpha M_r^i \left(1 - \exp \left(\frac{A^i}{kT} \right) \right) \\ \partial_t(\rho \mathbf{v}) + \operatorname{div}(\rho \mathbf{v} \otimes \mathbf{v}) + \nabla p + \operatorname{div}(\gamma \nabla \chi \otimes \nabla \chi - \sigma_{NS}) &= 0 \\ \rho \partial_t \chi + \rho \mathbf{v} \cdot \nabla \chi &= -M_p \left(\frac{\partial \rho \psi}{\partial \chi} - \gamma \Delta \chi \right) \end{aligned}$$

for the mixture density ρ , the partial densities ρ_α , $\alpha = 1, \dots, N - 1$, the mixture velocity \mathbf{v} and the phase field χ in $[0, T) \times \Omega$, $\Omega \subset \mathbb{R}^d$. Here p denotes the pressure, T the temperature, m_α the atomic mass of component α , k the Boltzmann constant, $\rho \psi$ the free energy density of the mixture and μ_α the chemical potential of constituent α . Further, γ_α^i are the stoichiometric coefficients of N_R possible chemical reactions, A^i the affinities and $M_{\alpha\beta}$, M_r^i , M_p the mobilities.

The phase field quantity χ denotes the present phase. It takes values in the interval $[-1, 1]$. Here $\chi = 1$ indicates pure liquid, while $\chi = -1$ indicates a pure vapor phase. Values in $] - 1, 1[$ indicate a transition layer.

This model considers isothermal chemically reacting viscous liquid–vapor flows of N constituents with phase transitions in d space dimensions. However, to solve such systems numerically one typically uses splitting methods. This means, that the system is split into two sub-problems. On the one hand one considers the flow part of the system, on the other the reacting part by integrating the source terms. In this work we will focus on the flow part and neglect the diffusive and reaction terms. This is justified because any numerical method for the full problem must compute the flow part correctly. The diffusive terms will not correct any errors in the advective terms. Actually, the method may not work at all, due to the nature of the equation of state, as we will see below. Therefore, our model is well suited to study and overcome the numerical problems associated with the multi-component equation of state.

Accordingly, in the following, we restrict ourselves to the 1- d homogeneous subsystem of first order terms that is given by

$$\partial_t \rho_\alpha + \partial_x(\rho_\alpha v) = 0 \quad \alpha = 1, \dots, N \tag{1a}$$

$$\partial_t(\rho v) + \partial_x(\rho v^2 + p) = 0 \tag{1b}$$

$$\rho \partial_t \chi + \rho v \partial_x \chi = 0. \tag{1c}$$

For convenience, we replaced the balance of mass for the mixture density $\rho = \sum_{\alpha=1}^N \rho_\alpha$ by the equivalent mass balance equation for constituent N . We refer to this model as hyperbolic system (1). This system can also be viewed as an augmentation of the isothermal Euler equation with a phase function in order to compute two-phase flows.

Equation of state. The pressure p is a constitutive quantity that is related to the phase function variable χ and the partial densities ρ_α , $\alpha = 1, \dots, N$ of the components by an equation of state $p = p(\chi, \rho_1, \dots, \rho_N)$. This equation of state is derived from the free energy density

$$\rho\psi = W(\chi) + h(\chi)\rho\psi_L(\rho_1, \dots, \rho_N) + (1 - h(\chi))\rho\psi_V(\rho_1, \dots, \rho_N),$$

of the mixture, where $W(\chi) = w_0(\chi - 1)^2(\chi + 1)^2$ denotes the double well potential and $\rho\psi_L$ and $\rho\psi_V$ are the free energy density functions of the liquid and the vapor phases, resp.

There is some degree of freedom in choosing h and the free energy densities. We follow Dreyer et al. [12] and choose $h : \mathbb{R} \rightarrow [0, 1]$ to be

$$h(\chi) = \begin{cases} 0 & \chi \leq -1 \\ (-\frac{1}{4}\chi + \frac{1}{2})(\chi + 1)^2 & -1 < \chi < 1 \\ 1 & \chi \geq 1 \end{cases}.$$

This is the simplest smooth interpolation function satisfying

$$h(-1) = 0 \quad h(1) = 1 \quad \text{and} \quad h'(\chi) = 0 \quad \text{for} \quad |\chi| \geq 1.$$

For the free energy density functions

$$\rho\psi_L = \sum_{\alpha=1}^N \rho_\alpha \psi_{L\alpha} \quad \text{and} \quad \rho\psi_V = \sum_{\alpha=1}^N \rho_\alpha \psi_{V\alpha},$$

we proceed as follows. We use the partial free energy density functions $\psi_{k\alpha}$, $k \in \{L, V\}$, $\alpha = 1, \dots, N$ such that in pure phases in the single component case we end up with the stiffened gas law. For more details see Dreyer and Bothe [13]. This leads to

$$p(\chi, \rho_1, \dots, \rho_N) = -W(\chi) + h(\chi) \sum_{\alpha=1}^N p_{L\alpha}(\rho_\alpha) + (1 - h(\chi)) \sum_{\alpha=1}^N p_{V\alpha}(\rho_\alpha) \tag{2}$$

with $p_{k\alpha}(\rho_\alpha) = a_{k\alpha}^2 \rho_\alpha + d_{k\alpha}$. Here $a_{k\alpha}$ is the isothermal sound speed of component α in phase $k \in \{L, V\}$. The parameter $d_{k\alpha}$ equals zero for ideal gases.

The double well function moderates the mass transfer between the phases due to condensation and evaporation. The interpolation function h allows to describe mixtures of the vapor and the liquid phase.

3. Discretization

Basic properties of the system. It is easy to verify that for any N the system (1) is hyperbolic with eigenvalues $\lambda_0 = v - A$, $\lambda_{N+1} = v + A$ and the N -fold eigenvalue $\lambda_1 = \dots = \lambda_N = v$. The quantity A with

$$A^2 = \frac{1}{\rho} \sum_{\alpha=1}^N \rho_\alpha \frac{\partial p}{\partial \rho_\alpha} = \frac{1}{\rho} \sum_{\alpha=1}^N \rho_\alpha (h(\chi)a_{L\alpha}^2 + (1 - h(\chi))a_{V\alpha}^2)$$

is related to the sound speeds of the single components.

We use the abbreviation

$$B := \partial_\chi p = -W'(\chi) + h'(\chi) \sum_{\alpha=1}^N (a_{L\alpha}^2 \rho_\alpha + d_{L\alpha}) - h'(\chi) \sum_{\alpha=1}^N a_{V\alpha}^2 \rho_\alpha. \tag{3}$$

If $B \neq 0$ we find the full system of linearly independent eigenvectors

$$\mathbf{k}_0 = \begin{pmatrix} 0 \\ -\rho_1 \\ \vdots \\ \vdots \\ -\rho_N \\ A \end{pmatrix}, \quad \mathbf{k}_1 = \begin{pmatrix} -A_1^2 \\ B \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \quad \dots, \quad \mathbf{k}_N = \begin{pmatrix} -A_N^2 \\ 0 \\ \vdots \\ 0 \\ B \\ 0 \end{pmatrix}, \quad \mathbf{k}_{N+1} = \begin{pmatrix} 0 \\ \rho_1 \\ \vdots \\ \vdots \\ \rho_N \\ A \end{pmatrix}. \tag{4}$$

On the other hand, if $B = 0$ the eigenvector basis is given by

$$\mathbf{k}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \mathbf{k}_2 = \begin{pmatrix} 0 \\ -A_2^2 \\ A_1^2 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \dots, \mathbf{k}_N = \begin{pmatrix} 0 \\ -A_3^2 \\ 0 \\ A_1^2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \mathbf{k}_{N+1} = \begin{pmatrix} 0 \\ -A_N^2 \\ 0 \\ \vdots \\ 0 \\ A_1^2 \\ 0 \end{pmatrix} \tag{5}$$

and \mathbf{k}_0 and \mathbf{k}_{N+1} as before.

The characteristic fields related to λ_0 and λ_{N+1} are non-linear, while the field related to the multiple eigenvalue is linearly degenerate. The exact solution for a Riemann problem consists of 4 constant states separated by three waves. The middle wave is a contact discontinuity resp. phase boundary, the outer waves are shock waves or rarefactions. For more details see Hantke et. al [14]. Note that for $N = 1$ and pure phases the system (1) reduces to the isothermal Euler equations for two phases discussed in Hantke et. al [11].

Discretization and Riemann solver. In this work we use the computational domain $[0, 1] \times [0, T]$. The spatial domain $[0, 1]$ is discretized into uniform cells with width Δx . The time step Δt is determined via the CFL-condition where we use the CFL-number $C_{CFL} = 0.9$.

Due to the very simple structure of the Riemann solutions to the hyperbolic system (1), the HLL-Riemann solver seems to be an appropriate choice for the conserved quantities of the system, namely $\rho_\alpha, \alpha = 1, \dots, N$ and ρv . However, the particular choice of the solver is not essential for the problems we will meet.

The phase function χ , indicating the present phase, is an artificial quantity introduced by Dreyer et. al [12]. In contrast to volume or mass fractions in other fluid models it is not related to further physical quantities. So the phase function here is an indicator function with no additional physical meaning and it is not conserved. Accordingly, rewriting the transport equation for the phase function (1c) in divergence form and using a conservative discretization for χ does not make any sense. Hence it is questionable what is an appropriate discretization of Eq. (1c). An analogous difficulty is known from the discretization of the non-conservative terms in the Baer–Nunziato model, see Saurel and Abgrall [15] as well as the following section. Anyway, for the moment we use an upwind discretization for Eq. (1c).

Problems and interpretation. Starting some simulation for a proper set of Riemann initial data for a liquid and a vapor phase with significant differences in the phase densities the computation immediately breaks down, even for $N = 1$. The reason is: On the one hand, usually the phase interface moves and does not coincide with any cell boundary after a certain time. On the other hand all quantities will smear out during the calculations. Accordingly mixture cells evolve. One can observe that the pressure becomes negative in most of the mixture cells.

At first glance this seems to be surprising because phase function models are developed to deal with phase mixtures. In particular, due to the design of the equation of state one may expect that mixture cells can be handled.

We illustrate the situation in Fig. 1 for pure water at room temperature. Here the pressure is represented as a function of the density and the phase function. The states on the left boundary correspond to pure vapor whereas the states on the right boundary indicate pure liquid water. One can see that for most states (χ, ρ) in the phase plane the pressure is negative. This means that these states are not meaningful.

Solving a Riemann problem for initially pure phases means that states on the left boundary are connected to the right boundary. In the exact Riemann solution the intermediate state lies in the reasonable part of the mixture region in between. The crucial point is that a feasible numerical solver has to preserve this property. This is not the case for any standard Riemann solver.

In the following we equip our solver with a consistency condition to guarantee that the numerical solution lies in the physical region of the phase plane.

4. The related problem and a pressure estimator

Computing solutions for systems of conservation laws one chooses the set of conserved variables and a conservative discretization. Other choices usually lead to wrong propagation speeds of discontinuities that are typically present in the solution. In other words, non-conservative methods do not converge to the exact solution.

Our system (1) consists of $N + 1$ conservation laws for the mass densities and the momentum and the transport equation (1c) for the phase function. The latter is no conservation law. Accordingly it is not clear how to discretize this equation.

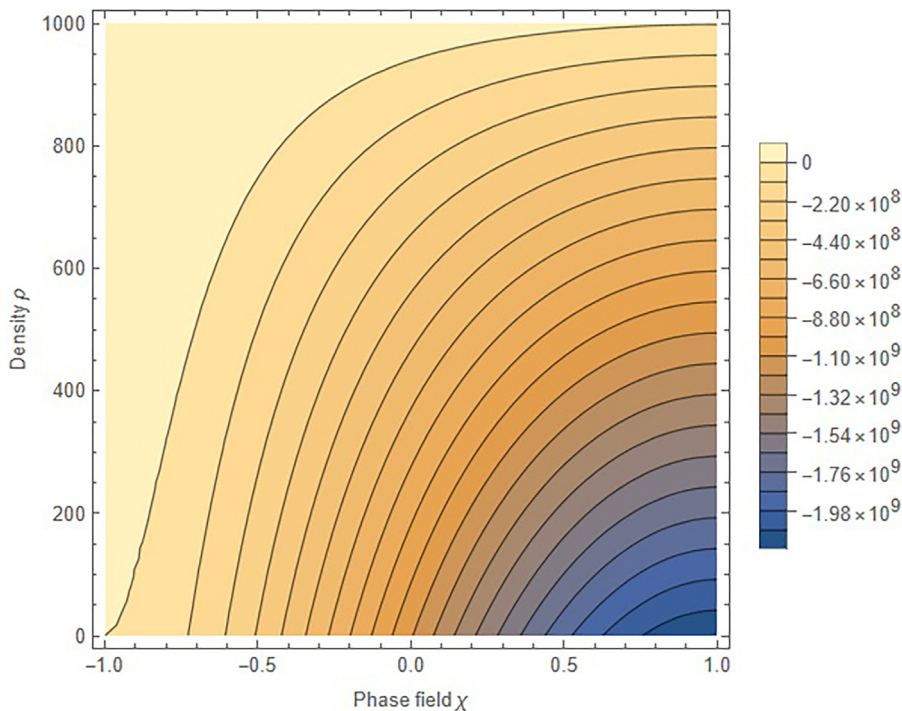


Fig. 1. Pressure p depending on phase function χ and density ρ .

Table 1
Riemann initial data Example 1.

| | Left | Right | | Parameters |
|--------|----------|----------|-------|-------------------------|
| χ | -1 | 1 | a_v | 367.8 m/s |
| p | 2300 Pa | 1000 Pa | a_L | 1478.4 m/s |
| v | -100 m/s | -100 m/s | d_L | $-2.1817 \cdot 10^9$ Pa |

Abgrall trick. As already mentioned a similar situation is known from the discretization of the non-conservative terms in the two-phase Baer–Nunziato model. In [15] Saurel and Abgrall suggested to use a special upwind discretization determined by maintaining that certain constant solutions remain constant. The idea is based on the knowledge of the properties of the exact Riemann solution. In this model pressures and velocities are constant across the phase interface. So the discretization has to be carried out in such a way that homogeneous pressure and velocity fields are preserved. The specific design of the discretization depends on the Riemann solver applied.

Strategy. Unfortunately we are not able to copy this strategy to our system. Nevertheless we will use the insight about the exact Riemann solution of system (1) to develop a solution strategy.

Let a set of initial data for the phase function χ , the mass densities of the components ρ_α and the velocity v of the mixture be given. Then by applying a finite volume scheme one can easily find proper values for the densities and the velocity after a single time step. With respect to the equation of state (2) it is equivalent to evolve the phase function or the pressure, resp. This yields the idea to obtain the new pressure from an acceptable pressure estimator and then to compute the phase function using the equation of state.

We illustrate the procedural method with the help of the following single component example that is taken from Hantke et. al [11], see Table 1, where the exact solution is known. This Riemann problem is solved numerically using the HLL Riemann solver on a very coarse grid with $\Delta x = \frac{1}{100}$. Of course we do not estimate the pressure but use the pressure from the exact solution in every computational cell. Afterwards we calculate the phase function χ using the equation of state (2) by Newton’s method (see Fig. 2).

In fact, we obtain a moderate numerical solution. The phase boundary is smeared over an array of grid cells. Nevertheless, refining the grid we observe convergence to the exact solution. The convergence rates are given in the following Table 2. We achieve almost order 1 as expected. This calculation shows that, if one is able to estimate the pressure fairly well, this is sufficient to compute suitable numerical solutions. So our aim is to develop a pressure estimator for system (1).

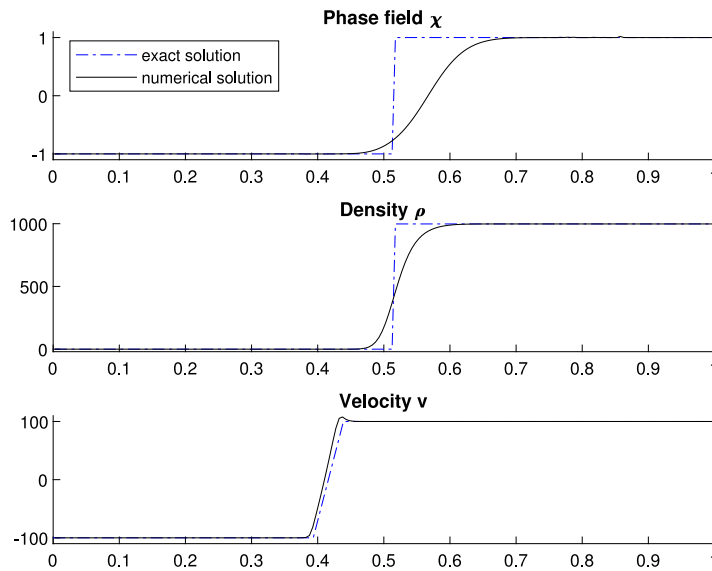


Fig. 2. Exact and numerical solution of Example 1.

Table 2
Experimental order of convergence for Example 1.

| Number of cells | 600 | 700 | 800 | 900 | 1000 |
|-----------------|--------|--------|--------|--------|--------|
| EOC | 0.8095 | 0.8348 | 0.9011 | 0.9491 | 0.8692 |

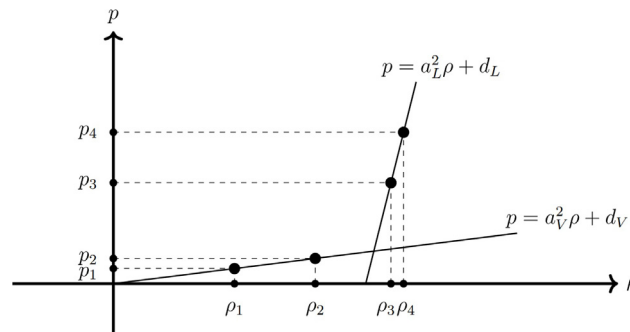


Fig. 3. Pressure differences depending on density changes.

Pressure estimator and related problem. Considering a flow of a liquid and a vapor phase one can observe that most of the changes occur in the gas. The reason is that the liquid – compared to the gas – is almost incompressible. This means that a small change in the pressure causes a big difference in the density of the gas phase. In contrast to that a big change in the pressure in the liquid phase could be barely noticed and causes a very small difference in the density. This fact is illustrated in Fig. 3.

In the following we will take advantage of this instance to find a related problem with a solution approximating the solution of the Riemann problem under consideration. Once again we study Example 1 which is nothing else than a piston problem, see Fig. 4.

As mentioned before in the exact Riemann solution changes in the pressure are negligibly small. Accordingly it seems to be a reasonable simplification to treat the liquid phase as a solid wall, see Fig. 5. Note that the velocity difference between the phases is 200 m/s. We use Galilean invariance to assume that the liquid is a solid wall at rest while the vapor moves at $v_R = v_V - v_L = -200$ m/s.

Boundary value problems resulting from this simplifying assumptions will be referred to as *related problems*. For the original and the related problem we have the solution structure depicted in Fig. 6. Note that in the original problem we have $p(\rho_V^*) = p(\rho_L^*) =: p^*$. The related problem can be solved explicitly using Theorem 6.2 in Hantke et. al [11].

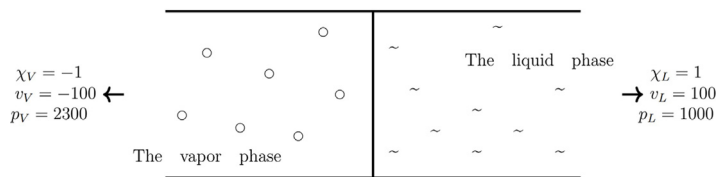


Fig. 4. The piston problem Example 1.



Fig. 5. The related wall problem.

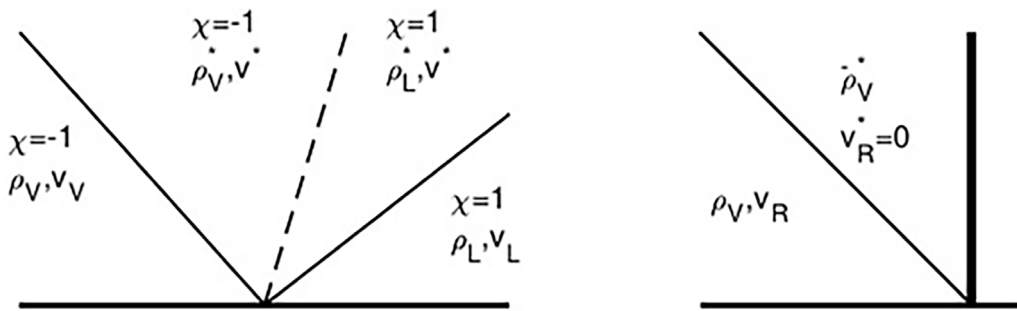


Fig. 6. The solution structure of the original problem (left) and the related problem (right), cf. Section 3.

In particular, let the density ρ_V , the sound speed a_V and the relative velocity v_R of the vapor phase be given. Then for the intermediate pressure $p(\bar{\rho}_V^*)$ of the related problem we have

$$p(\bar{\rho}_V^*) = \begin{cases} a_V^2 \rho_V \left(\frac{v_R}{2a_V} + \sqrt{\frac{v_R^2}{4a_V^2} + 1} \right)^2 & v_R > 0 \\ \exp\left(\frac{v_R}{a_V} + \log(\rho_V a_V^2)\right) & v_R \leq 0 \end{cases} \tag{6}$$

We expect, that the intermediate pressure $p(\bar{\rho}_V^*)$ of the related problem is a good approximation for the intermediate pressure p^* of the original problem. It will be used as an estimation for the intermediate pressure of the original problem in our numerical simulations.

Extension to multi-components. The idea explained in the last paragraph can easily be extended to multi-components because of the simple structure of the exact Riemann solution, cf. Section 3. Let us assume that the gas phase consists of N components. Then we modify formula (6) in the following way.

$$p(\bar{\rho}_M^*) = \begin{cases} a_M^2 \rho_M \left(\frac{v_R}{2a_M} + \sqrt{\frac{v_R^2}{4a_M^2} + 1} \right)^2 & v_R > 0 \\ \exp\left(\frac{v_R}{a_M} + \log(\rho_M a_M^2)\right) & v_R \leq 0 \end{cases} \tag{7}$$

Here $\rho_M = \sum_{j=1}^N \rho_j$ denotes the density of the gas mixture that is the sum of the partial gas densities. The quantity a_M approximates the sound speed of the mixture. The pressure p_M of the gas mixture is given by

$$p_M = \sum_{j=1}^N p_j = \sum_{j=1}^N a_{Vj}^2 \rho_j.$$

Table 3
Riemann initial data Example 2, cf. Example 2 in [11].

| | Left | Right | | Parameters |
|--------|-----------|------------|-------|-------------------------|
| χ | -1 | 1 | a_v | 467.3 m/s |
| p | 60 000 Pa | 100 000 Pa | a_L | 1143.9 m/s |
| v | -200 m/s | -50 m/s | d_L | $-1.1299 \cdot 10^9$ Pa |

Table 4
Riemann initial data Example 3.

| | Left | Right | | Parameters | Parameters | |
|----------|---------------------------|-----------------------------|----------|-----------------------|------------|-------------|
| χ | -1 | 1 | a_{v1} | 500 m/s | a_{v2} | 400 m/s |
| ρ_1 | 0.0336 kg/m ³ | 833.3375 kg/m ³ | a_{L1} | 1200 m/s | d_{L2} | 1000 m/s |
| ρ_2 | 0.00583 kg/m ³ | 1000.0003 kg/m ³ | d_{L1} | $-1.2 \cdot 10^9$ m/s | d_{L2} | -10^9 m/s |
| v | 53.558 m/s | 19.998 m/s | | | | |

Table 5
Approximated pressure and exact pressure.

| | Approximated pressure | Exact pressure |
|-----------|-----------------------|----------------|
| Example 1 | 1335.3208 Pa | 1335.3199 Pa |
| Example 2 | 43 526 Pa | 43 531 Pa |
| Example 3 | 10 000.0375 Pa | 10 000 Pa |

This motivates the relation

$$a_M^2 = \frac{p_M}{\rho_M}. \tag{8}$$

5. Numerical examples

In this section we first test the pressure estimator introduced in the previous section considering three different examples to find the pressure in the intermediate region. After that we use the pressure estimator in the numerical solver.

The initial data and the parameters for Example 1 are already given in Table 1. In Tables 3 and 4 the data for Example 2 and 3 are given. Example 2 is also a single component example. The parameters correspond to water at a temperature of $T = 473.15$ K. Note that this is a very high temperature where liquid water is much more compressible than at standard temperature as in Example 1. Example 3 is a two component example with arbitrary parameters. This example is considered in order to test the extended version of the pressure estimator.

Estimating the pressure by solving the related problem. For all the three examples we use the pressure estimator from the previous section to approximate the pressure in the intermediate region. We compare the results to the exact values in Table 5

One can observe that the exact pressures and the approximated pressures are in very good agreement. The largest discrepancy appears in Example 2. This is not surprising due to the more intense compressibility of the liquid phase that comes along with the very high temperature.

Numerical solver. Finally the pressure estimator has to be integrated into the numerical solver. This Riemann solver is based on the idea that the solution of a general initial value problem is a superposition of local Riemann problems that appear between neighboring computational cells.

For all local Riemann problems we estimate the pressure. As a consequence for every computational cell we obtain two pressure estimations, a left and a right sided value. The estimator gives very good approximations for the pressure, cf. Table 5. On the other hand, it neglects the wave propagating through the liquid phase, see Fig. 6. Accordingly the left sided approximations will be used in the vapor and in the mixture region while the right sided estimations are used in the liquid. Alternatively one can use some averaged value.

The overall algorithm for a single time step can be summarized as follows.

- use any Riemann solver to evolve the conserved quantities
- solve the related problem at every inner cell boundary
- update the pressure
- calculate the corresponding phase function value

Numerical results. Using the above algorithm we solve Examples 1 and 2. The computations used a coarse grid with $\Delta x = \frac{1}{150}$. The phase boundary is smeared. This is not surprising due to the very large density gradient at the phase

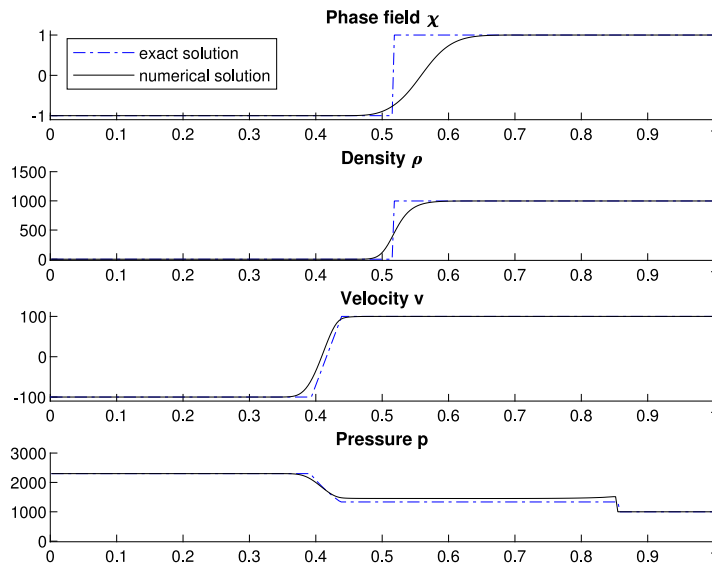


Fig. 7. Exact and numerical solution of Example 1.

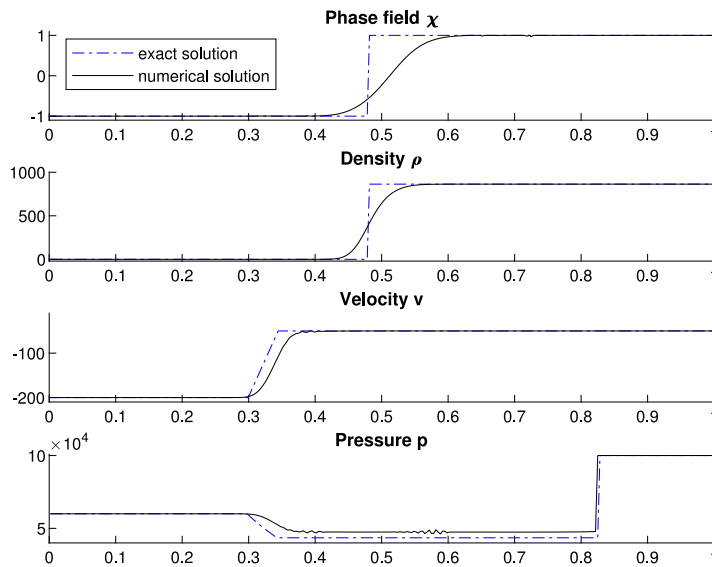


Fig. 8. Exact and numerical solution of Example 2.

boundary. The wave speeds are fitted very well. Nevertheless one can observe that the pressure is slightly overestimated (see Fig. 7).

Using a volume based mean value instead for the pressure estimation the pressure in the intermediate region will be in perfect agreement to the exact pressure. But then the shock speed will be underestimated.

Refining the grid the numerical solution converges. The order of convergence is almost the same as in Table 2.

The numerical solution of Example 2 behaves similar. There is some deviance in the left rarefaction. This discrepancy disappears when the grid is refined (see Fig. 8).

6. Conclusion and outlook

Summary. We developed a method to discretize the phase function model (1) that avoids expensive techniques like interface tracking. The new method uses an unsophisticated pressure estimator that is very cheap because it does not require an iterative procedure. This approach may also be used when discretizing the original model of Dreyer et al. [12].

The results presented are satisfactory. They show that this strategy is a promising concept. Furthermore, this concept can easily be extended to a multi-component flow. Nevertheless, there is some potential for improvements. In particular, although the pressure estimator gives nearly perfect results the numerical solver slightly overestimates the pressures in our examples. Here some more research is required how to incorporate the pressure estimator into the numerical solver.

Remarks. The investigations on the discretization of the model (1) are still at the beginning. Accordingly we restricted ourselves to a first order discretization. However, we want to point out that the method presented is also compatible with a second order reconstruction algorithm. The important matter is that the reconstruction has to be carried out for the primitive variables in order to preserve the constant pressure and velocity states across the phase interface.

A further remark applies to the phase function. Even if one does not need the quantity χ for estimating the pressure, this quantity becomes important when solving the full model.

Future work. The weakness of the results is caused by the fact that changes in the liquid phase are neglected when estimating the pressure using the solid wall approximation. Accordingly, the main focus in prospective research should lie on the integration of the pressure estimator into the numerical solver to overcome this.

As a next step the full model should be considered. A further interesting topic is the question whether it is possible to extend the introduced strategy to other models where large density gradients lead to difficulties in the discretization.

Data availability

No data was used for the research described in the article.

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