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A compressible mixture model with phase transition

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HIGHLIGHTS

- We introduce a thermodynamically consistent model for multi-phase flows.
- The model allows for phase transitions and chemical reactions.
- We investigate physically admissible sharp interface limits.
- The limit is an Allen–Cahn/Euler system with admissible interfacial conditions.
- The model allows for two phase equilibria with surface tension in the leading order.

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ABSTRACT

We introduce a new thermodynamically consistent diffuse interface model of Allen–Cahn/Navier–Stokes type for multi-component flows with phase transitions and chemical reactions. For the introduced diffuse interface model, we investigate physically admissible sharp interface limits by matched asymptotic techniques. We consider two scaling regimes, i.e. a non-dissipative and a dissipative regime, where we recover in the sharp interface limit a generalized Allen–Cahn/Euler system for mixtures with chemical reactions in the bulk phases equipped with admissible interfacial conditions. The interfacial conditions satisfy, for instance, a Young–Laplace and a Stefan type law.

1. Introduction

In this study, we propose a model for chemically reacting viscous fluid mixtures that may develop a transition between a liquid and a vapor phase. The mixture consists of N constituents and is described by N partial mass balance equations and a single equation of balance for the barycentric momentum. We exclusively consider isothermal evolutions. To describe the phase transition, we introduce an artificial phase field indicating the present phase by assigning the values 1 and -1 to the liquid and the vapor phase, respectively. Within the transition layer between two adjacent phases, the phase field smoothly changes between 1 and -1. However, usually the transition layers are very thin leading to steep gradients of the phase field.

This model belongs to the class of diffuse interface models. An alternative model class, that likewise represents phase transitions in fluid mixtures, contains sharp interface models. From the modeling point of view, sharp interface models have a simpler physical basis than diffuse interface models. For this reason, there arises always the non-trivial question if the sharp interface limits of a given diffuse model lead to admissible sharp interface models. The main concern of this paper is a careful discussion of this problem.

While diffuse interface models solve partial differential equations in the transition region, sharp interface models deal with jump conditions across the interface between the phases. Sometimes the jump conditions are mixed with geometric partial differential equations.

For two phases without chemical reactions, our compressible model reduces to an Allen–Cahn/Navier–Stokes type model, which is quite similar to the model derived by Blesgen [1]. Blesgen's model has been investigated analytically in [2,3], where existence

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of strong local-in-time solutions and weak solutions has been shown.

We would like to emphasize that the thermodynamical approaches of Blesgen's system and our derived model are different. For instance, the phase field variable χ in Blesgen's model, which satisfies the Allen–Cahn equation, is a physical quantity, namely the local mass fraction of one phase, whereas in our proposed model χ simply indicates the present phase. In addition, the function h that interpolates between the phases, which will be described later, is linear in Blesgen's model. This means that, in contrast to our proposed model, in general the equilibria depend on the chosen interpolation function h, which implies that Blesgen's system runs into different equilibria. Our approach with χ as an artificial phase field variable permits to obtain physical meaningful jump conditions at the interface agreeing with classical laws of thermodynamics.

A modified version of Blesgen's model can be found in [4]. In contrast to [1] and our introduced model, Witterstein [4] describes a mixture of two compressible fluids, which physically differ, exclusively by different Lamé coefficients which are assumed to depend on the phase field parameter and the mass density. Witterstein's model [4] also differs in the choice of the free energy, which contains two length scales. Moreover, the minima of the double well potential in the free energy have to be of different heights. This implies that the energy can only be controlled for transition regions with fixed width but not in the sharp interface limit.

Related to our work are diffuse interface models for incompressible and quasi-incompressible fluids. A diffuse interface model of Navier–Stokes–Cahn–Hilliard type for two incompressible, viscous Newtonian fluids, having the same densities, has been introduced by Hohenberg and Halperin in [5]. That model has been modified in several thermodynamically consistent ways such that different densities are allowed, see e.g. [6–8]. For existence results of strong local-in-time solutions and weak solutions, we refer to [9–11]. A diffuse interface model for two incompressible constituents which permits the transfer of mass between the phases due to diffusion and phase transitions has been proposed in [12,13]. The densities of the fluids may be different, which leads to quasi-incompressibility of the mixture.

Our newly introduced diffuse interface model is given by the following system of PDEs for $(\rho, \rho_{\alpha=1,\dots,N-1}, \boldsymbol{v}, \chi)$ in $[0, T_f) \times \Omega$, $\Omega \subset \mathbb{R}^d$:

$$\partial_t \rho + \operatorname{div}(\rho \boldsymbol{v}) = 0,$$

$$\partial_t \rho_\alpha + \operatorname{div}(\rho_\alpha \boldsymbol{v}) - \operatorname{div}\left(\sum_{\beta=1}^{N-1} M_{\alpha\beta} \nabla(\mu_\alpha - \mu_N)\right)$$

$$= \sum_{i=1}^{N_R} \gamma_\alpha^i m_\alpha M_r^i \left(1 - \exp\left(\frac{A^i}{kT}\right)\right),$$

$$\partial_t(\rho \boldsymbol{v}) + \operatorname{div}(\rho \boldsymbol{v} \otimes \boldsymbol{v}) + \nabla p + \operatorname{div}\left(\gamma \nabla \chi \otimes \nabla \chi - \boldsymbol{\sigma}_{NS}\right) = 0,$$

$$\rho \partial_t \chi + \rho \boldsymbol{v} \cdot \nabla \chi = -M_p \left(\frac{\partial \rho \psi}{\partial \chi} - \gamma \Delta \chi\right),$$

where p is the pressure, T the temperature, m_α the atomic mass of constituent α, k the Boltzmann constant,

$$\rho \psi = W(\chi) + \frac{\gamma}{2} |\nabla \chi|^2 + \rho f(\rho_1, \dots, \rho_N, \chi) \quad \text{and}$$

$$\mu_\alpha = \frac{\partial(\rho\psi)}{\partial \rho_\alpha}$$

with $\rho f(\rho_1, \dots, \rho_N, \chi) := h(\chi) \rho \psi_L(\rho_1, \dots, \rho_N) + (1 - h(\chi)) \rho \psi_V(\rho_1, \dots, \rho_N)$. In addition, γ_α^i are the stoichiometric coefficients of N_R possible chemical reactions, A^i the affinities and $M_{\alpha\beta}$, M_r^i and M_p the mobilities.

The work is organized as follows. In the upcoming section we derive the thermodynamically consistent model for multicomponent flows with phase transitions and chemical reactions. Section 3 is devoted to the non-dimensionalization, the introduction of two interesting scaling regimes of the system and the setting of asymptotic analysis. Finally, in Sections 4 and 5, we determine the sharp interface limits for the two different scaling regimes introduced previously. We would like to emphasize that Section 4.2 contains a conjecture on the incapability of viscous diffuse models to generate viscous sharp models.

2. The mixture model

2.1. Constituents and phases

We consider a fluid mixture consisting of N constituents $A_1, A_2, \dots, A_N$ indexed by $\alpha = 1, 2, \dots, N$. The constituents may be subjected to chemical reactions. There are N_R reactions, indexed by $i = 1, 2, \dots, N_R$, of the general type

$$a_1^i A_1 + a_2^i A_2 + \cdots + a_N^i A_N \rightleftarrows b_1^i A_1 + b_2^i A_2 + \cdots + b_N^i A_N. \tag{2.1}$$

Thus, there are forward (f) as well as backward (b) reactions. The constants $(a_\alpha^i)_{\alpha=1,2,\dots,N}$ and $(b_\alpha^i)_{\alpha=1,2,\dots,N}$ are positive integers and $\gamma_\alpha^i = b_\alpha^i - a_\alpha^i$ denotes the stoichiometric coefficient of constituent α in the reaction $i = 1, \dots, N_R$.

The fluid mixture may exist in the two phases, liquid (L) and vapor (V). The two phases may coexist. In this paper, we describe the phases in the diffuse interface setting, where the interface between adjacent liquid and vapor phases is modeled by a thin layer. Within the layer, certain thermodynamic quantities smoothly change from values in one phase to different values in the adjacent phase. However, usually steep gradients occur.

2.2. Introduction of basic quantities and basic variables

Two phase mixtures can be modeled within three different model classes, i.e. Classes I–III. Class I considers as basic variables the mass densities $(\rho_\alpha)_{\alpha=1,2,\dots,N}$ of the constituents, the barycentric velocity $\boldsymbol{v}$, the temperature T and the phase field χ, which is used to indicate the present phase at $(t, \boldsymbol{x})$. It assumes values in the interval $[-1, 1]$ with $\chi = 1$ in the liquid and $\chi = -1$ in the vapor. The basic variables of Class II are the mass densities $(\rho_\alpha)_{\alpha=1,2,\dots,N}$, the velocities $(\boldsymbol{v}_\alpha)_{\alpha=1,2,\dots,N}$ of the constituents, the temperature T and the phase field χ. Finally, in Class III we have the mass densities $(\rho_\alpha)_{\alpha=1,2,\dots,N}$, the velocities $(\boldsymbol{v}_\alpha)_{\alpha=1,2,\dots,N}$, the temperatures $(T_\alpha)_{\alpha=1,2,\dots,N}$ of the constituents and the phase field χ. In this study, we choose a description within Class I. The mixture occupies a region $\Omega \subset \mathbb{R}^d$. At any time $t \geq 0$, the thermodynamic state of Ω is described by N partial mass densities $(\rho_\alpha)_{\alpha=1,2,\dots,N}$, the barycentric velocity and by the temperature T of the mixture. These quantities may be functions of time $t \geq 0$ and space $\boldsymbol{x} = (x^i)_{i=1,\dots,d} = (x^1, \dots, x^d) \in \Omega$. However, we restrict ourselves to isothermal processes so that T appears only as a constant parameter in the equations.

Partial mass densities and partial velocities are used to define the total mass density ρ of the mixture and its barycentric velocity $\boldsymbol{v}$

$$\rho := \sum_{\alpha=1}^N \rho_\alpha, \qquad \boldsymbol{v} := \frac{1}{\rho} \sum_{\alpha=1}^N \rho_\alpha \boldsymbol{v}_\alpha. \tag{2.2}$$

The diffusion velocities $\boldsymbol{u}_\alpha$ and the corresponding diffusion fluxes $\boldsymbol{J}_\alpha$ are defined by

$$\boldsymbol{u}_\alpha := \boldsymbol{v}_\alpha - \boldsymbol{v}, \qquad \boldsymbol{J}_\alpha := \rho_\alpha \boldsymbol{u}_\alpha \quad \text{with} \quad \sum_{\alpha=1}^N \boldsymbol{J}_\alpha = 0\,. \tag{2.3}$$