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Jean Bussac

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# A NON-EQUILIBRIUM MULTI-COMPONENT MODEL WITH MISCIBLE CONDITIONS

J. BUSSAC

ABSTRACT. This paper concerns the study of a full non-equilibrium model for a compressible mixture of any number of phases. Miscible conditions are considered in one phase, that lead to non symmetric constraints on the statistical fractions. These models are subject to the choice of interfacial and source terms. We show that under a classical assumption on the interfacial velocity, the interfacial pressures are uniquely defined. The model is hyperbolic and symmetrizable under non-resonance conditions. Classes of entropy-consistent source terms are then proposed.

## 1. INTRODUCTION

The present paper concerns the modelling of multiphase compressible flows which arise in many industrial applications, especially in the nuclear safety framework. Among several scenarios that are studied (see IRSN website [18]), the Loss Of Coolant Accident (LOCA) involves these types of flow. It is a brutal rupture in the coolant circuit that creates phase transition waves in the loop and leads to the appearance of vapor inside the liquid, these phases interacting with the ambient air. Other types of accidents require to consider more phases, for instance in vapor explosion type scenarios [3]. Consequently, a model must account for the dynamical and the thermodynamical disequilibrium.

A wide range of multiphase flow models has been proposed since decades, especially in the two-phase flow situation, see for instance [1, 4, 7, 14, 19] for the Baer-Nunziato two-fluid approach and [2, 16, 21] for the homogeneous (in terms of velocity) models. More recently, three-phase flows have been investigated with full non-equilibrium models in the immiscible [9, 10, 11] and miscible [12] conditions, and also with homogeneous models [2, 16, 21]. Among all these models, two classes can be distinguished: the majority of them is based on the multifluid approach [1, 4, 9, 14, 10, 12, 19], where each component has its own velocity field. The second one are the homogeneous models [2, 17, 21] where all the component share the same velocity.

In the multifluid approach, the dynamics of each component is described by an Euler-type model and the different systems are coupled through interfacial non-conservative terms and source terms which model the return to the equilibrium. Closure conditions have been investigated in the immiscible case in [4, 10] respectively for two-phase and three-phase flow. Analysis of this model for a two-phase flow has been done for instance in [6, 8], and a generalization with all these features has been proposed in [22]. More recently, these type of results have been investigated with miscible conditions in [14, 12].

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For the sake of clarity, let us precise that the term "phase" refers to a state of the matter, "component" to a chemical substance and "field" to a component in a given phase. For instance, an hybrid mixture of liquid water, vapor water and an inert gas is composed of three fields, two phases and two components.

The present work focuses on the modelling of a  $N$ -phase mixture of  $M$  fields, with  $N \leq M$ , where all the miscible part of the fluid is contained in the  $N$ th phase. That is a physically relevant situation where this latter phase would be the gaseous phase, and no miscibility can be observed for another state of the matter. These miscible components are then supposed to be perfectly intricate like ideal gases, and so all their statistical fractions are equal

$$(1) \quad \forall k \geq N, \alpha_k = \alpha_N.$$

Since we consider that no void can occur, the global volume constraint is

$$(2) \quad \sum_{k=1}^N \alpha_k = 1,$$

with  $\alpha_k \in [0; 1]$  for all  $k = 1, \dots, N$ .

The outline of the article is the following.

The first part presents the model by introducing the thermodynamical framework, the system of equations and the evolution equation of the mixture entropy. Then we demonstrate the uniqueness of the pressure interfacial terms under classical hypotheses concerning the interfacial velocity. In the third part, the analysis of the convective system is investigated, by studying its hyperbolicity and the symmetrization. Finally, admissible forms of source terms are detailed, in order to satisfy the second principle of thermodynamics.

## 2. MODEL

**2.1. Thermodynamical framework.** The fluid is composed of  $N \geq 2$  phases that are immiscible, where only the  $N$ th phase can contain several components of number  $K \geq 1$ . The fluid is then composed of  $M = N + K - 1$  fields. In other words, we consider a mixture of  $N$  phases and  $M$  fields, where the phase  $N$  contains all the miscible components of the fluid. We define  $\mathcal{K}$  the set of fields, and thus we have  $\#\mathcal{K} = M$ .

1	2	3	...	N, N+1, ..., M
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**2.1.1. Equations of state.** Each field  $k \in \mathcal{K}$  is depicted by its phasic specific volume  $\tau_k > 0$  and its specific energy  $e_k > 0$ . The thermodynamical behaviour of each phase  $k$  is fully described by its intensive entropy function  $(\tau_k, e_k) \mapsto s_k(\tau_k, e_k)$  defined on  $\Omega_k \subset (\mathbb{R}_*^+)^2$ , that is a complete EoS. By adopting the Gibbs formalism, each entropy function  $s_k$  complies with the following differential form

$$(3) \quad T_k ds_k = de_k + p_k d\tau_k,$$

where the phasic temperature  $T_k = T_k(\tau_k, e_k)$  and pressure  $p_k = p_k(\tau_k, e_k)$  are defined by

$$(4) \quad \frac{1}{T_k} = \left. \frac{\partial s_k}{\partial e_k} \right|_{\tau_k}, \quad p_k = T_k \left. \frac{\partial s_k}{\partial \tau_k} \right|_{e_k},$$

and the phasic chemical potential by the relation

$$(5) \quad \mu_k = -T_k s_k + p_k \tau_k + e_k.$$

2.1.2. *Volume constraints and mixture entropy.* We now turn to the description of the thermodynamical behaviour of the mixture. The volume conservation plus the miscibility hypotheses give the following relations on the statistical fractions

$$(6) \quad \begin{cases} \sum_{k=1}^N \alpha_k = 1 \\ \alpha_k = \alpha_N \text{ for } k \geq N \end{cases},$$

thus the derivatives verify

$$(7) \quad \sum_{k=1}^{N-1} \partial_x \alpha_k = -\partial_x \alpha_N.$$

These constraints are fundamental to manage the different mathematical proofs. We define the state vector of the field  $k$  by

$$\mathbf{Y}_k = (\alpha_k, \rho_k, v_k, e_k),$$

where  $\rho_k = 1/\tau_k$  and  $v_k$  is the phasic velocity. For a given mixture state  $(\tau, e)$ , the mixture entropy is defined as a combination of the phasic entropies with weights  $m_k = \alpha_k \rho_k$ . Denoting  $\mathbf{Y} = \bigcup_{k \in \mathcal{K}} \mathbf{Y}_k$ , it reads

$$(8) \quad \sigma(\mathbf{Y}) = \sum_{k \in \mathcal{K}} m_k s_k(\mathbf{Y}_k).$$

Finally, the specific total energy of the phase  $k$  is noted  $E_k = e_k + v_k^2/2$ .

2.2. **Set of partial differential equations.** Following the models in [14, 10, 12, 22], the fluid equations contain  $N$  transport equations on  $\alpha_k$ , for  $k = 1, \dots, N$

$$(9) \quad \partial_t \alpha_k + V_I(\mathbf{Y}) \partial_x \alpha_k = \Phi_k(\mathbf{Y}),$$

plus, for  $k \in \mathcal{K}$ , the following Euler-type systems

$$(10) \quad \partial_t (m_k) + \partial_x (m_k v_k) = \Gamma_k(\mathbf{Y}),$$

$$(11) \quad \partial_t (m_k v_k) + \partial_x (m_k v_k^2 + \alpha_k p_k) + \sum_{\substack{l \in \mathcal{K} \\ l \neq k}} P_{k,l}(\mathbf{Y}) \partial_x \alpha_l = S_{q,k}(\mathbf{Y}),$$

$$(12) \quad \partial_t (m_k E_k) + \partial_x (m_k v_k (E_k + \frac{p_k}{\rho_k})) + \sum_{\substack{l \in \mathcal{K} \\ l \neq k}} P_{k,l}(\mathbf{Y}) V_I(\mathbf{Y}) \partial_x \alpha_l = S_{E,k}(\mathbf{Y}),$$

Source terms  $\Phi_k$ ,  $\Gamma_k$ ,  $S_{q,k}$ ,  $S_{E,k}$  must be chosen in agreement with the second law of thermodynamics. Let us emphasize at the  $(\Phi_k)_{k=1, \dots, N}$  are only defined for the  $N$  first statistical fractions.

Exchanges between the different fields are accounted by non conservative terms in equations (9), (11) and (12), involving interfacial velocity  $V_I$  and interfacial

pressures  $(P_{k,l})$ , defined for  $k \neq l$ . These terms must be specified in order to close the system, which will be done in Section 2.3.

**Remark 1.** *Following recent works [14, 12], we consider that source terms and interfacial closures only depend on  $\mathbf{Y}$ . These could depend on the derivatives of  $\mathbf{Y}$ , as suggested for instance in [15, 24].*

Since we consider a closed system, the total mass, momentum and energy exchanges must balance, thus the source terms must verify

$$(13) \quad \sum_{k \in \mathcal{K}} \Gamma_k(\mathbf{Y}) = 0, \quad \sum_{k \in \mathcal{K}} S_{q,k}(\mathbf{Y}) = 0, \quad \sum_{k \in \mathcal{K}} S_{E,k}(\mathbf{Y}) = 0.$$

Moreover, as we consider no vacuum occurrence, the source terms on the void fractions verify

$$(14) \quad \sum_{k=1}^N \Phi_k(\mathbf{Y}) = 0.$$

Besides, the interfacial pressure terms  $(P_{k,l})$  should cancel each other

$$(15) \quad \sum_{k \in \mathcal{K}} \sum_{\substack{l \in \mathcal{K} \\ l \neq k}} P_{k,l}(\mathbf{Y}) \partial_x \alpha_l = 0,$$

in order to preserve the mixture conservative equations on momentum and energy.

2.2.1. *Entropy production.* The mixture entropy has been defined in (8), and it is well known [14, 12] that it verifies the following equation

$$(16) \quad \partial_t \sigma(\mathbf{Y}) + \partial_x f_\sigma(\mathbf{Y}) = \mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) + RHS_\sigma(\mathbf{Y}),$$

where  $f_\sigma(\mathbf{Y}) = \sum_{k \in \mathcal{K}} m_k s_k v_k$  is the entropy flux and the production terms are defined by

$$(17) \quad \mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) = \sum_{k \in \mathcal{K}} \frac{1}{T_k} (v_k - V_I) \left( \sum_{\substack{l \in \mathcal{K} \\ l \neq k}} P_{k,l}(\mathbf{Y}) \partial_x \alpha_l + p_k \partial_x \alpha_k \right),$$

that correspond to the interfacial contribution, and

$$\begin{aligned} RHS_\sigma(\mathbf{Y}) = & \sum_{k \in \mathcal{K}} \frac{1}{T_k} \left( S_{E,k}(\mathbf{Y}) - \Gamma_k(\mathbf{Y}) e_k - v_k (S_{q,k}(\mathbf{Y}) \right. \\ & \left. - \frac{1}{2} \Gamma_k(\mathbf{Y}) v_k) + \rho_k \frac{\partial e_k}{\partial \rho_k} (\rho_k \Phi_k(\mathbf{Y}) - \Gamma_k(\mathbf{Y})) \right) \\ & + \sum_{k \in \mathcal{K}} \left( s_k \Gamma_k(\mathbf{Y}) + \rho_k \frac{\partial s_k}{\partial \rho_k} (\Gamma_k(\mathbf{Y}) - \rho_k \Phi_k(\mathbf{Y})) \right), \end{aligned}$$

which correspond to the source terms contribution. According to the second law of thermodynamics, these production terms have to be non-negative. By following

the work in [4, 10] in the two and three-phase flow context, our concern here is to determine constraints such as

$$(18) \quad \mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) = 0,$$

corresponding to the minimal entropy dissipation model, which is the subject of the following section. The second term  $RHS_\sigma$  relies on the source terms, that we will study later on, see 4.

**2.3. Definition of the interfacial pressures.** The system of partial derivative equations (9)-(12) requires a unique definition of the pressure interfacial terms. The work has been done for immiscible two, three and then  $N$ -phase flow in [4, 10, 22], or more recently for hybrid mixtures in [14, 12].

For this purpose, we postulate that the interfacial velocity is a convex combination (using Galilean invariance) of the phasic velocities

$$(19) \quad V_I(\mathbf{Y}) = \sum_{k \in \mathcal{K}} \beta_k(\mathbf{Y}) v_k,$$

with

$$(20) \quad \begin{cases} \sum_{k \in \mathcal{K}} \beta_k(\mathbf{Y}) = 1 \\ \beta_k(\mathbf{Y}) \geq 0 \quad \forall k \in \mathcal{K} \end{cases}.$$

Determining the interfacial pressures ( $P_{k,l}$ ) as it is done in [22] is out of reach due to reasons coming from the miscibility constraints. However, these constraints allow to consider another set of pressure terms that we define here.

Let us introduce the interfacial terms ( $K_{k,l}$ ), defined for  $k = 1, \dots, M$  and  $l = 1, \dots, N - 1$ . For the sake of clarity, we allow ourselves to write the initial pressure terms ( $P_{k,l}$ ) for  $k = l$ . The definition is then

$$(21) \quad K_{k,l} = P_{k,l}(1 - \delta_{k,l}) - \sum_{j=N}^M P_{k,j}(1 - \delta_{k,j}),$$

and the following notation for the same indices

$$(22) \quad \chi_{k,l} = \delta_{k,l} - \sum_{j=N}^M \delta_{k,j} = \begin{cases} 0 & \text{if } k \leq N - 1 \text{ and } k \neq l, \\ 1 & \text{if } k = l, \\ -1 & \text{if } k \geq N \text{ for all } l \leq N - 1, \end{cases}.$$

where  $\delta_{k,l}$  is the Kronecker symbol. We now introduce the following lemma that contains fundamental rewriting techniques used in this paper.

**Lemma 1.** *For all  $k = 1, \dots, M$  and  $l = 1, \dots, N - 1$ , we have the two relations*

$$(23) \quad \sum_{\substack{l \in \mathcal{K} \\ l \neq k}} P_{k,l} \partial_x \alpha_l = \sum_{l=1}^{N-1} K_{k,l} \partial_x \alpha_l,$$

$$(24) \quad \sum_{\substack{l \in \mathcal{K} \\ l \neq k}} P_{k,l} \partial_x \alpha_l + p_k \partial_x \alpha_k = \sum_{l=1}^{N-1} (K_{k,l} + \chi_{k,l} p_k) \partial_x \alpha_l,$$

*Proof.* By using miscibility constraints (6) and relation (7), we can rewrite the sum as

$$(25) \quad \begin{aligned} \sum_{\substack{l \in \mathcal{K} \\ l \neq k}} P_{k,l} \partial_x \alpha_l &= \sum_{l=1}^{N-1} P_{k,l} (1 - \delta_{k,l}) \partial_x \alpha_l + \sum_{j=N}^M P_{k,j} (1 - \delta_{k,j}) \partial_x \alpha_j \\ &= \sum_{l=1}^{N-1} P_{k,l} (1 - \delta_{k,l}) \partial_x \alpha_l + \partial_x \alpha_N \sum_{j=N}^M P_{k,j} (1 - \delta_{k,j}) \\ &= \sum_{l=1}^{N-1} P_{k,l} (1 - \delta_{k,l}) \partial_x \alpha_l - \sum_{l=1}^{N-1} \partial_x \alpha_l \sum_{j=N}^M P_{k,j} (1 - \delta_{k,j}) \\ &= \sum_{l=1}^{N-1} \left( P_{k,l} (1 - \delta_{k,l}) - \sum_{j=N}^M P_{k,j} (1 - \delta_{k,j}) \right) \partial_x \alpha_l \\ &= \sum_{l=1}^{N-1} K_{k,l} \partial_x \alpha_l, \end{aligned}$$

where  $K_{k,l}$  has been defined in (21).

The second relation can be deduced by the first one, we just need to express the term  $p_k \partial_x \alpha_k$  in function of the  $(\partial_x \alpha_l)_{1 \leq l \leq N-1}$ , that is

$$(26) \quad p_k \partial_x \alpha_k = \sum_{l=1}^{N-1} \chi_{k,l} p_k \partial_x \alpha_l,$$

where  $\chi_{k,l}$  is defined by (22). Then we deduce the relation (24).  $\square$

These relations allow us to rewrite any expression involving  $(\partial_x \alpha_l)_{1 \leq l \leq M}$  in terms of the first  $N - 1$  quantities  $(\partial_x \alpha_l)_{l \leq N-1}$ .

Using Lemma 1, the momentum and energy equations (11)-(12) can be rewritten

$$(27) \quad \partial_t (\alpha_k \rho_k v_k) + \partial_x (\alpha_k \rho_k v_k^2 + \alpha_k p_k) + \sum_{k=1}^{N-1} K_{k,l} \partial_x \alpha_l = 0,$$

$$(28) \quad \partial_t (\alpha_k \rho_k E_k) + \partial_x (\alpha_k \rho_k v_k (E_k + p_k / \rho_k)) + \sum_{k=1}^{N-1} K_{k,l} V_I \partial_x \alpha_l = 0,$$

Thereby, we have reduced the number of interfacial unknowns. Indeed, there was  $M(M-1)$  coefficients  $(P_{k,l})$  and now there are  $M(N-1)$  effective coefficients  $(K_{k,l})$ . We can now rewrite the minimal entropy dissipation condition (18) in function of the  $(K_{k,l})$ .

**Lemma 2.** *The term  $\mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y})$  reads*

$$(29) \quad \mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) = \sum_{k \in \mathcal{K}} \frac{1}{T_k} (v_k - V_I) \sum_{l=1}^{N-1} (K_{k,l} + \chi_{k,l} p_k) \partial_x \alpha_l,$$

with  $(\chi)_{k,l}$  defined by (22).

*Proof.* It consists in rewriting (18) in function of the  $N - 1$  firsts  $(\partial_x \alpha_k)$ , using Lemma 1.  $\square$

Let us now give the main result of this paper.

**Proposition 1.** *(Minimal entropy production due to the interfacial states) Let us assume that (15) hold true. If all the phasic temperatures are positive, then for any convex combination (19), the interfacial pressure terms  $(K_{k,l})$  are uniquely defined.*

*Proof.* The idea of the proof is very similar to [22]. We determine equations thanks to

- (1) The independence of the derivatives  $(\partial_x \alpha_k)$
- (2) The independence of the relative velocities  $(v_{k+1} - v_k)$

Then we obtain  $N - 1$  linear systems, one for each  $l = 1, \dots, N - 1$ , in the variables  $(K_{k,l})_{k=1, \dots, M}$ .

According to (6), the  $(\partial_x \alpha_l)_{1 \leq l \leq N-1}$  must be independant. Using this and Lemma 2, imposing  $\mathcal{A}_\sigma(\mathbf{Y}, \partial_x \mathbf{Y}) = 0$  is equivalent to write for  $l = 1, \dots, N - 1$  the following relations

$$(30) \quad \sum_{k \in \mathcal{K}} \frac{1}{T_k} (v_k - V_I) (K_{k,l} + \chi_{k,l} p_k) = 0.$$

Using the convex combination (19), we rewrite the difference  $v_k - V_I$  as

$$(31) \quad v_k - V_I = \sum_{i=1}^{k-1} \sum_{j=1}^i (-\beta_j) (v_i - v_{i+1}) + \sum_{i=k}^{M-1} \sum_{j=i+1}^M (\beta_j) (v_i - v_{i+1}),$$

that allows us to rearrange (30) in terms of the independant differences  $(v_i - v_{i+1})$ . Introducing  $c_i = \sum_{j=1}^i \beta_j$ ,  $c^i = \sum_{j=i+1}^M \beta_j$ , for  $i = 1, \dots, M - 1$ , we obtain the following relations

$$(32) \quad \sum_{k=1}^i \frac{1}{T_k} c^i K_{k,l} - \sum_{k=i+1}^M \frac{1}{T_k} c_i K_{k,l} = \sum_{k=1}^i \frac{1}{T_k} c^i \chi_{k,l} p_k - \sum_{k=i+1}^M \frac{1}{T_k} c_i \chi_{k,l} p_k,$$

for  $l = 1, \dots, N - 1$  and  $i = 1, \dots, M - 1$ . We define for the same indices

$$d_l^i = \sum_{k=1}^i a_k c^i \chi_{k,l} p_k - \sum_{k=i+1}^M a_k c_i \chi_{k,l} p_k \quad \text{and} \quad a_i = \frac{1}{T_i}.$$

We obtain the final system defined by the following equations for  $l = 1, \dots, N - 1$  and  $i = 1, \dots, M - 1$

$$(33) \quad \sum_{k=1}^i c^i a_k K_{k,l} - \sum_{k=i+1}^M c_i a_k K_{k,l} = d_l^i.$$

In other words, for any  $l = 1, \dots, N-1$ , there are  $M-1$  equations for  $M$  unknowns that are the  $(K_{k,l})_{1 \leq k \leq M}$ . This can be compensated by adding the constraint (15) that gives, using (21) and the independence of  $(\partial_x \alpha_l)_{l \leq N-1}$ , for  $l = 1, \dots, N-1$

$$(34) \quad \sum_{k \in \mathcal{K}} K_{k,l} = 0.$$

Then we have  $N-1$  linear systems of size  $M \times M$ , for each  $l \in \{1, \dots, N-1\}$ , that are

$$(35) \quad \mathbf{A} \mathbf{K}_l = \mathbf{d}_l,$$

with

$$\bullet \mathbf{A} = \begin{pmatrix} c^1 a_1 & -c_1 a_2 & -c_1 a_3 & \cdots & -c_1 a_M \\ c^2 a_1 & c^2 a_2 & -c_2 a_3 & \cdots & -c_2 a_M \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c^{M-1} a_1 & c^{M-1} a_2 & \cdots & c^{M-1} a_{M-1} & -c_{M-1} a_M \\ 1 & 1 & \cdots & \cdots & 1 \end{pmatrix},$$

- $\mathbf{K}_l = (K_{1,l}, K_{2,l}, \dots, K_{M,l})^\top$ ,
- $\mathbf{d}_l = (d_l^1, d_l^2, \dots, d_l^M)^\top$ .

Finally, we need to show that  $\mathbf{A}$  is regular so the  $(K_{k,l})$  are uniquely determined.

Let us note  $D = \det \mathbf{A}$ . The idea of the proof is to develop this determinant on the last row, then express the minors of size  $M-1$  with a second order determinant thanks to  $M-3$  developments.

We remind here two relations that we will need. For  $i = 1, \dots, M-1$ , we have

$$(36) \quad c_i + c^i = 1, \quad c^{i+1} - c^i = -\beta_i.$$

By developing  $D$  on the last row and factorizing by  $\bar{a}_i$ , we get

$$(37) \quad D = \sum_{i=1}^M (-1)^{M+i} \bar{a}_i D_i,$$

where  $D_i$  is the minor formed by deleting the last row and the  $i$ th column, and  $\bar{a}_i = \prod_{j \neq i}^M a_j$ . For  $i = 1, \dots, M-1$ , we have

$$(38) \quad D_i = \det \begin{pmatrix} c^1 & -c_1 & \cdots & -c_1 & -c_1 & \cdots & -c_1 \\ c^2 & c^2 & & \cdots & \cdots & & -c_2 \\ & & \ddots & -c_{i-1} & -c_{i-2} & & \\ \vdots & & & \ddots & c^{i-1} & -c_{i-1} & \vdots \\ & & & & c^i & -c_i & \\ & & & & c^{i+1} & c^{i+1} & \\ & & & & \vdots & \vdots & \ddots \\ c^{M-1} & c^{M-1} & \cdots & c^{M-1} & c^{M-1} & \cdots & -c_{M-1} \end{pmatrix},$$

that we can rewrite with the columns  $\mathcal{C}_j = (-c_1, \dots, -c_{j-1}, c^j, \dots, c^{M-1})^\top \in \mathbb{R}^{M-1}$  as

$$(39) \quad D_i = \det (\mathcal{C}_1 \quad \mathcal{C}_2 \quad \dots \quad \mathcal{C}_{i-1} \quad \mathcal{C}_{i+1} \dots \quad \mathcal{C}_M).$$

Then,  $D_i$  can be reduced to a second order determinant with  $M - 3$  operations:

- $\mathcal{C}_1 \leftarrow \mathcal{C}_1 - \mathcal{C}_2$  and a development along  $\mathcal{C}_1$  is done  $i - 2$  times,
- $\mathcal{C}_n \leftarrow \mathcal{C}_n - \mathcal{C}_{n-1}$  and a development along  $\mathcal{C}_n$  is done  $M - (i + 1)$  times, where  $n$  is the size of the considered minor.

It appears a factor  $(-1)$  for each second type operation, thus we have

$$(40) \quad D_i = (-1)^{M-(i+1)} \det \begin{pmatrix} c^{i-1} & -c_{i-1} \\ c^i & -c_i \end{pmatrix},$$

so, thanks to relations (36), we can express the latter determinant as

$$(41) \quad \begin{aligned} D_i &= (-1)^{M-(i+1)} (-\beta_i) \\ &= (-1)^{M-i} \beta_i, \end{aligned}$$

for  $i = 2, \dots, M - 1$ . On the other hand, the cases  $i = 1$  and  $i = M$  give  $D_1 = c_1$  and  $D_M = c^{M-1}$ .

Coming back to (37), we get

$$(42) \quad D = \bar{a}_1 c_1 + \bar{a}_M c^{M-1} + \sum_{i=2}^{M-1} (-1)^{M+i} \bar{a}_i (-1)^{M-i} \beta_i,$$

that simplifies into

$$(43) \quad D = \bar{a}_1 c_1 + \bar{a}_M c^{M-1} + \sum_{i=2}^{M-1} \bar{a}_i \beta_i > 0.$$

Since  $\sum_i \beta_i = 1$  and  $a_i > 0$  for all  $i = 1, \dots, M$ , then  $\det \mathbf{A} > 0$  and the interfacial terms  $(K_{k,l})$  are fully determined.  $\square$

**Remark 2.** *Even if the approach differs from [14, 12], we verified at different stages of the proof that the results were in agreement with these references.*

**Remark 3.** (*Preservation of the pressure equilibria*) An important feature is the preservation of an initial steady state where the fluid is supposed to be at the thermodynamical equilibrium : the phasic pressures verify the Dalton's law, the phasic temperatures are equal to each other and the velocities are equal to zero. A detailed explanation is given in [13]. This must be verified, but it seems difficult to achieve without an explicit expression of the interfacial pressure terms.

### 3. ANALYSIS

In this section, we investigate the hyperbolicity and the symmetrization of the system.

**3.1. Hyperbolicity.** First, we consider the convective system associated to (9)-(12) and rewrite it in the primitive variables  $w = (\alpha_1, \dots, \alpha_{N-1}, w_1, \dots, w_M)$ , where  $w_k = (\rho_k, v_k, p_k)$ . For  $k = 1, \dots, N$  we have

$$(44) \quad \partial_t \alpha_k + V_I \partial_x \alpha_k = 0,$$

and for  $k \in \mathcal{K}$

$$(45) \quad \partial_t \rho_k + \frac{\rho_k}{\alpha_k} (v_k - V_I) \partial_x \alpha_k + v_k \partial_x \rho_k + \rho_k \partial_x v_k = 0,$$

$$(46) \quad \partial_t v_k + \frac{1}{\alpha_k \rho_k} \left( \sum_{l \in \mathcal{K}} P_{k,l} \partial_x \alpha_l + p_k \partial_x \alpha_k \right) + v_k \partial_x v_k + \frac{1}{\rho_k} \partial_x p_k = 0,$$

$$(47) \quad \partial_t p_k + \frac{\rho_k}{\alpha_k} (v_k - V_I) \sum_{\substack{l \in \mathcal{K} \\ l \neq k}} C_{k,l}^2 \partial_x \alpha_l + \rho_k c_k^2 \partial_x v_k + v_k \partial_x p_k = 0,$$

where  $C_{k,l}$  and  $c_k$  are respectively the interfacial sound speed and the phasic sound speed, defined by

$$(48) \quad \begin{aligned} C_{k,l}^2 &= -((\partial p_k / \partial e_k) P_{k,l} / \rho_k^2 + (\partial p_k / \partial \rho_k)), \\ c_k^2 &= \partial p_k / \partial \rho_k + p_k / \rho_k + p_k / \rho_k^2 (\partial p_k / \partial e_k). \end{aligned}$$

Then, we express the  $(\partial_x \alpha_l)_{1 \leq l \leq M}$  in function of the  $(\partial_x \alpha_l)_{l \leq N-1}$  by using Lemma 1, it reads

$$(49) \quad \partial_t \alpha_k + V_I \partial_x \alpha_k = 0,$$

$$(50) \quad \partial_t \rho_k + \frac{\rho_k}{\alpha_k} (v_k - V_I) \left( \left( 1 - \sum_{j=N}^M \delta_{k,j} \right) \partial_x \alpha_k - \left( \sum_{j=N}^M \delta_{k,j} \right) \sum_{l=1}^{N-1} \partial_x \alpha_l \right) + v_k \partial_x \rho_k + \rho_k \partial_x v_k = 0$$

$$(51) \quad \partial_t v_k + \frac{1}{\alpha_k \rho_k} \sum_{l=1}^{N-1} (K_{k,l} + \chi_{k,l} p_k) \partial_x \alpha_l + v_k \partial_x v_k + \frac{1}{\rho_k} \partial_x p_k = 0$$

$$(52) \quad \partial_t p_k + \rho_k c_k^2 \partial_x v_k + \frac{\rho_k}{\alpha_k} (v_k - V_I) \sum_{l=1}^{N-1} \gamma_{k,l} \partial_x \alpha_l + v_k \partial_x p_k = 0,$$

with  $\gamma_{k,l} = C_{k,l}^2 (1 - \delta_{k,l}) - \sum_{j=N}^M C_{k,j}^2 (1 - \delta_{k,j})$  and  $K_{k,l}$  defined by (21). Note that we used the argument from Lemma 2 for the velocity equation.

Thus we have the following quasi-linear system

$$(53) \quad \partial_t \mathbf{w} + \mathbf{B}(\mathbf{w}) \partial_x \mathbf{w} = 0,$$

where  $\mathbf{B}(\mathbf{w}) \in \mathcal{M}_{N-1+3M}(\mathbb{R})$  is the block matrix

$$(54) \quad \mathbf{B}(\mathbf{w}) = \left( \begin{array}{c|ccc} V_I \mathbf{I}_{N-1} & 0 & \dots & 0 \\ \mathbf{A}_1 & \mathbf{B}_1 & & \\ \dots & & \dots & \\ \mathbf{A}_M & & & \mathbf{B}_M \end{array} \right).$$

The matrices  $\mathbf{A}_k \in \mathcal{M}_{3,N-1}(\mathbb{R})$  and  $\mathbf{B}_k \in \mathcal{M}_3(\mathbb{R})$  are defined by

$$(55) \quad \mathbf{A}_k = \begin{pmatrix} \frac{\rho_k}{\alpha_k} (v_k - V_I) (\mathbf{e}_k^\top (1 - \sum_{j=N}^M \delta_{k,j}) - \mathbf{1}_{N-1}^\top \sum_{j=N}^M \delta_{k,j}) \\ \frac{1}{\alpha_k \rho_k} \boldsymbol{\beta}_k^\top \\ \frac{\rho_k}{\alpha_k} (v_k - V_I) \boldsymbol{\gamma}_k^\top \end{pmatrix},$$

$$(56) \quad \mathbf{B}_k = \begin{pmatrix} v_k & \rho_k & 0 \\ 0 & v_k & 1/\rho_k \\ 0 & \rho_k c_k^2 & v_k \end{pmatrix},$$

where

- $\mathbf{e}_k$  is the  $k$ th unit vector in  $\mathbb{R}^{N-1}$ , with the convention  $\mathbf{e}_k = \mathbf{0}$  if  $k \geq N$ ,
- $\mathbf{1}_{N-1}$  is the vector in  $\mathbb{R}^{N-1}$  whose components are all equal to 1,
- the vectors  $\boldsymbol{\beta}_k, \boldsymbol{\gamma}_k \in \mathbb{R}^{N-1}$  are defined, for  $l = 1, \dots, N-1$ , by

$$(57) \quad \boldsymbol{\beta}_k = (K_{k,1} + \chi_{k,1} p_k, \dots, K_{k,N-1} + \chi_{k,N-1} p_k)^\top$$

$$(58) \quad \boldsymbol{\gamma}_k = (\gamma_{k,1}, \dots, \gamma_{k,N-1})^\top.$$

We remark that the phasic matrices  $\mathbf{B}_k$  do not differ from the immiscible case [22], but the  $\mathbf{A}_k$  matrices do change. The eigenstructure of  $\mathbf{B}$  is exactly the same than in this latter case, thus we only remind here the elements and refer to [22] for more details.

The eigenvalues are:

- $\lambda_{I,k} = V_I$ ,  $k = 1, \dots, N-1$
- $\lambda_k = v_k$  and  $\lambda_{k,\pm} = v_k \pm c_k$ ,  $k = 1, \dots, M$ .

**Remark 4.** *The nature and properties of these characteristic fields are as expected, see [8] for their analysis in the two-phase framework. We emphasize that the nature of  $V_I$  remains unknown, and so its Riemann invariants, that obviously depend on its definition. One can refer to [4] where different closures for  $V_I$  are investigated for a two-phase mixture, allowing to define unique jump relations.*

We now turn to the determination of the eigenvectors. The matrix  $\mathbf{R}$  composed of the right eigenvectors has a block structure and reads

$$(59) \quad \mathbf{R} = \left( \begin{array}{c|ccc} \mathbf{R}_I^0 & 0 & \dots & 0 \\ \mathbf{R}_I^1 & \mathbf{R}_1 & & \\ \dots & & \dots & \\ \mathbf{R}_I^M & & & \mathbf{R}_M \end{array} \right),$$

The phasic problems are well known and so  $\mathbf{R}_k$  is. For  $\mathbf{R}_I^k$ , we introduce the following notations

$$(60) \quad \kappa_0 = \prod_{l=1}^M \alpha_l \sigma_l, \quad \kappa_k = \prod_{l=1, l \neq k}^M \alpha_l \sigma_l, \quad k = 1, \dots, M$$

$$(61) \quad \sigma_k = \delta_k^2 - c_k^2 \text{ and } \delta_k = v_k - V_I.$$

Thus we have

$$(62) \quad \mathbf{R}_I^k = \kappa_k \rho_k \left( \begin{array}{c} \alpha_k c_k^2 \boldsymbol{\beta}_k^\top - \delta_k^2 \boldsymbol{\gamma}_k^\top \\ -(\alpha_k \boldsymbol{\beta}_k^\top - \boldsymbol{\gamma}_k^\top) \delta_k / \rho_k \\ -\sigma_k (\mathbf{e}_k^\top (1 - \sum_{j=N}^M \delta_{k,j}) - \mathbf{1}_{N-1}^\top \sum_{j=N}^M \delta_{k,j}) + \alpha_k \boldsymbol{\beta}_k^\top - \boldsymbol{\gamma}_k^\top \end{array} \right),$$

$$(63) \quad \mathbf{R}_I^0 = \kappa_0 \mathbf{I}_{N-1}, \quad \mathbf{R}_k = \begin{pmatrix} 1 & 1 & 1 \\ -c_k/\rho_k & 0 & c_k/\rho_k \\ c_k^2 & 0 & c_k^2 \end{pmatrix}.$$

The matrix  $\mathbf{R}$  is regular under the following well known condition

$$(64) \quad \sigma_k \neq 0, \iff V_I \neq v_k \pm c_k \quad \forall k = 1, \dots, M$$

called the *non-resonance condition*.

**Proposition 2.** *The system (9)-(12) is hyperbolic under the non-resonance condition (64).*

The non-resonance condition appears when a genuinely non linear field associated to  $v_k \pm c_k$  overlaps the coupling wave  $V_I$ . In such a situation, the vector space is not anymore spanned by the eigenvectors.

**3.2. Symmetrization.** The proof of the symmetrization relies on the same arguments than in [6, 14] and is exactly the same than in the generalized immiscible case of  $N$  phases [22]. We build a symmetric positive definite matrix  $\mathbf{P} = \mathbf{P}(\mathbf{w})$  such that  $\mathbf{P}\mathbf{B}$  is symmetric, by using the block structure of  $\mathbf{B}$  and its left and right eigenvectors matrices. We remind here the general idea.

First we define  $\mathbf{P}_k$  the symmetrizer of the phasic problem by

$$(65) \quad \mathbf{P}_k = \begin{pmatrix} 1 & 0 & -1/c_k^2 \\ 0 & 0.5(\rho_k/c_k)^2 & 0 \\ -1/c_k^2 & 0 & 1.5/c_k^4 \end{pmatrix},$$

that is a symmetric positive definite matrix. Moreover it is such that  $\mathbf{P}_k \mathbf{B}_k$  symmetric. We then define  $\mathbf{P}_{k,\alpha}$  under the non-resonance condition (64) by

$$(66) \quad \mathbf{P}_{k,\alpha} = \mathbf{L}_k^\top (\boldsymbol{\Lambda}_k - V_I \mathbf{I}_3)^{-1} \mathbf{R}_k^\top \mathbf{P}_k \mathbf{A}_k,$$

where  $\mathbf{L}_k$  is the left eigenvectors matrix of  $\mathbf{B}_k$  and  $\boldsymbol{\Lambda}_k$  is the eigenvalues matrix of  $\mathbf{B}_k$ . We remind that these matrices verify  $\mathbf{L}_k \mathbf{B}_k \mathbf{R}_k = \boldsymbol{\Lambda}_k$  and  $\mathbf{L}_k \mathbf{R}_k = \mathbf{I}_3$ . Thus we can define the symmetrizer for  $\mathbf{B}$ , that is

$$(67) \quad \mathbf{P} = \left( \begin{array}{c|ccc} NP_\alpha \mathbf{I}_{N-1} & \mathbf{P}_{1,\alpha}^\top & \dots & \mathbf{P}_{M,\alpha}^\top \\ \hline \mathbf{P}_{1,\alpha} & \mathbf{P}_1 & & \\ \dots & & \dots & \\ \mathbf{P}_{M,\alpha} & & & \mathbf{P}_M \end{array} \right),$$

where  $P_\alpha \mathbf{I}_{N-1}$  must be specified.

The cornerstone is that  $(V_I \mathbf{P}_{k,\alpha} + \mathbf{P}_k \mathbf{A}_k)^\top = \mathbf{P}_{k,\alpha}^\top \mathbf{B}_k$ , that traduces the symmetry of the first row and column of block of  $\mathbf{P} \mathbf{B}$ .

It relies on the fact than  $\mathbf{P}_{k,\alpha}^\top \mathbf{A}_k$  is a symmetric matrix, since  $\mathbf{P}_k^\top \mathbf{R}_k = \mathbf{L}_k^\top$ .

Now we prove that  $\mathbf{P}$  is positive definite. Let  $\mathbf{a} \in \mathbb{R}^{N-1+3M}$  such as  $\mathbf{a} = (\mathbf{a}_\alpha, \mathbf{a}_1, \dots, \mathbf{a}_M)$ , with  $\mathbf{a}_\alpha \in \mathbb{R}^{N-1}$ .

$$(68) \quad \mathbf{a}^\top \mathbf{P} \mathbf{a} = P_\alpha \sum_{k=1}^{N-1} \sum_{i=1}^{N-1} \left( a_{\alpha,i} + (\mathbf{P}_{k,\alpha}^\top \mathbf{a}_k)_i / P_\alpha \right)^2 + \sum_{k=1}^M \frac{1}{P_\alpha} \mathbf{a}_k^\top \mathbf{Q} \mathbf{a}_k,$$

where  $\mathbf{Q} = P_\alpha \mathbf{P}_k - \mathbf{P}_{k,\alpha} \mathbf{P}_{k,\alpha}^\top$ . Let us determine a condition on  $P_\alpha$  such as the terms  $\mathbf{a}_k^\top \mathbf{Q} \mathbf{a}_k$  are non-negative.

We consider the Cholesky decomposition of  $\mathbf{P}_k = \mathbf{C}_k \mathbf{C}_k^\top$  and we define  $\mathbf{E}_k = \mathbf{C}_k^{-1} \mathbf{P}_{k,\alpha}^\top \mathbf{P}_{k,\alpha} \mathbf{C}_k^\top$ , that is a symmetric matrix. Thus, there exists  $\mathbf{T}_k$  such that  $\mathbf{T}_k \mathbf{E}_k \mathbf{T}_k^\top = \mathbf{D}_k = \text{diag}(\mu_1^k, \mu_2^k, \mu_3^k)$ , where  $(\mu_i^k)_{1 \leq i \leq 3}$  are the eigenvalues of  $\mathbf{E}_k$ . Thus we have

$$(69) \quad \mathbf{a}_k^\top \mathbf{Q} \mathbf{a}_k = \mathbf{b}_k^\top (P_\alpha \mathbf{I}_3 - \mathbf{D}_k) \mathbf{b}_k = \sum_{i=1}^3 b_{k,i} (P_\alpha - \mu_i^k),$$

with  $\mathbf{b}_k = \mathbf{T}_k^\top \mathbf{C}_k^\top \mathbf{a}_k$ . Choosing  $P_\alpha > \max_{i,k} |\mu_i^k| > 0$  the term  $\mathbf{a}_k^\top \mathbf{Q} \mathbf{a}_k$  is non-negative and is positive for  $\mathbf{a}_k \neq 0$ , so  $\mathbf{a}^\top \mathbf{P} \mathbf{a}$  is.

Finally, the system (49)-(52) is symmetrizable and according to Kato's theorem [20], there exists a local-in-time smooth solution to the associated Cauchy problem.

#### 4. ADMISSIBLE SOURCE TERMS

We investigate in this section some conditions on the source terms in order to satisfy the second principle of thermodynamics.

We omit the dependence in  $\mathbf{Y}$  of the source terms for the sake of readability. We first give the form of each source term, and then we determine conditions on each contribution.

Firstly, let us remark that the mechanical transfer source terms  $\Phi_k$  verify

$$(70) \quad \forall k \geq N, \Phi_k = \Phi_N, \quad \sum_{k=1}^N \Phi_k = 0,$$

that is a consequence of the miscibility and saturation constraints. This allows us to use a similar rewriting than (23) and (24), which will be useful later.

The mass transfer term  $\Gamma_k$  is defined as a sum of dyadic contributions

$$(71) \quad \Gamma_k = \sum_{\substack{l \in \mathcal{K} \\ l \neq k}} \Gamma_{kl},$$

where  $\Gamma_{kl}$  represents the mass transfer from phase  $k$  towards phase  $l$ . In practical modelling, some of these terms may be equal to zero, for example if the phase  $k$  is a non-condensable gas.

The momentum contribution is decomposed into a drag term and a mass transfer term

$$(72) \quad S_{q,k} = \sum_{l \neq k} D_{kl} + \sum_{l \neq k} \Gamma_{kl} v_{kl}.$$

Last, the total energy source term contains thermal transfer, drag effects and mass transfer

$$(73) \quad S_{E,k} = \sum_{l \neq k} \Psi_{kl} + \sum_{l \neq k} v_{kl} D_{kl} + \sum_{l \neq k} \Gamma_{kl} H_{kl} + \sum_{l \neq k} P_{k,l} \Phi_l,$$

plus this last term, coming from the choice of modelling we made at the beginning of the paper. Indeed, by choosing the derivatives in space for  $\alpha_l$  in the energy equation (12), the associated source term  $S_{E,k}$  contains a mechanical contribution, that is not the case for example in [14, 12].

Let us remark some relations on these contributions. First, the dyadic contributions of (71), (72) and (73) must verify

$$(74) \quad \Gamma_{kl} = -\Gamma_{lk}, \quad D_{kl} = -D_{lk}, \quad \Psi_{kl} = -\Psi_{lk}.$$

Those from (73) give

$$v_{kl} D_{kl} = -v_{lk} D_{lk},$$

that impose  $v_{kl} = v_{lk}$ , thanks to the independance of the  $D_{kl}$ . Similarly, we have  $H_{kl} = H_{lk}$ .

Now we can regroup the contributions according to their nature

$$(75) \quad RHS_\sigma = RHS_\sigma^\Phi + RHS_\sigma^\Gamma + RHS_\sigma^D + RHS_\sigma^\Psi.$$

In order to ensure the entropy growth, each of these four term must be positive.

- **Admissible mechanical contribution  $\Phi$**

$$\begin{aligned}
RHS_\sigma^\Phi &= \sum_{k \in \mathcal{K}} a_k \left( \sum_{l \neq k} P_{k,l} \Phi_l + \rho_k^2 \frac{\partial e_k}{\partial \rho_k} \Phi_k \right) - \rho_k^2 \frac{\partial s_k}{\partial \rho_k} \Phi_k \\
&= \sum_{k \in \mathcal{K}} a_k \left( \sum_{l \neq k} P_{k,l} \Phi_l + p_k \Phi_k \right) \\
&= \sum_{k \in \mathcal{K}} a_k \left( \sum_{l \leq N-1} (K_{k,l} + \chi_{k,l} p_k) \Phi_l \right) \\
&= \sum_{l=1}^{N-1} \left( \sum_{k=1}^M a_k (K_{k,l} + \chi_{k,l} p_k) \right) \Phi_l.
\end{aligned}$$

We obtain the condition, for all  $l = 1, \dots, N-1$

$$(76) \quad \left( \sum_{k=1}^M a_k (K_{k,l} + \chi_{k,l} p_k) \right) \Phi_l \geq 0.$$

- **Amissible mass transfer contribution  $\Gamma$**

By using the relation  $\mu_k = e_k - T_k s_k + p_k / \tau_k$ , we have

$$RHS_\sigma^\Gamma = \sum_k a_k \sum_{l \neq k} (H_{kl} + \frac{v_k^2}{2} - v_k v_{kl}) \Gamma_{kl} - \sum_k \sum_{l \neq k} a_k \mu_k \Gamma_{kl}.$$

By setting  $H_{kl} = \frac{v_k v_l}{2}$  and  $v_{kl} = \frac{v_k + v_l}{2}$ , the first sum is equal to zero. Hence, it imposes

$$(77) \quad \forall k \neq l, (a_k \mu_k - a_l \mu_l) \Gamma_{kl} \geq 0,$$

that is equivalent to

$$(78) \quad \forall k \neq l, \left( \frac{T_l}{\mu_l} - \frac{T_k}{\mu_k} \right) \Gamma_{kl} \geq 0,$$

- **Admissible drag effects contribution**

$$RHS_\sigma^D = \sum_{k \in \mathcal{K}} a_k \left( \sum_{l \neq k} v_{kl} D_{kl} - v_k \sum_{l \neq k} D_{kl} \right).$$

We assume the following form for  $v_{kl}$  to comply with the Galilean invariance principle

$$v_{kl} = \beta_{kl} v_k + (1 - \beta_{kl}) v_l, \text{ with } \beta_{kl} + \beta_{lk} = 1 \text{ and } \beta_{kl} \in [0; 1].$$

Then we impose for  $k \neq l$

$$\begin{aligned}
&a_k (1 - \beta_{kl} + a_l (1 - \beta_{lk})) (v_l - v_k) D_{kl} \geq 0 \\
\iff &a_k (\beta_{lk} + a_l (1 - \beta_{lk})) (v_l - v_k) D_{kl} \geq 0.
\end{aligned}$$

Knowing that  $a_k (\beta_{lk} + a_l (1 - \beta_{lk})) > 0$ , the final condition is

$$(79) \quad (v_l - v_k)D_{kl} \geq 0.$$

• **Admissible thermal transfer contribution**

$$RHS_\sigma^\Psi = \sum_{k \in \mathcal{K}} \sum_{l > k} \Psi_{kl}(a_k - a_l),$$

and so the constraint is that for  $k \neq l$ ,

$$(80) \quad \Psi_{kl}(T_l - T_k) \geq 0.$$

Finally, these class of source terms comply with the second principle of thermodynamics. In practical cases, see [14, 12] for instance, the condition on the mechanical contribution  $\Phi_l$  can be given more precisely, and we refer to these papers for more details.

## 5. CONCLUSION

We have addressed in this paper the study of a Baer-Nunziato-like model for a compressible  $N$ -phase flow with miscibility conditions. The main result concerns the closure laws of the pressure interfacial terms. We demonstrate that under classical conditions on the interfacial velocity, the interfacial pressure terms are uniquely defined. Explicit expressions of these terms can be given in practical situations for given values of  $M$  and  $N$ , see for instance [14, 12].

Then, the hyperbolicity and symmetrization of the convective system have been investigated. The system is hyperbolic under the classical non-resonance condition. The symmetrization gives the local-in-time existence of a smooth solution.

Finally, we have determined constraints on the source terms in order to satisfy the second principle of thermodynamics. Results are the same than in practical models where  $M$  and  $N$  are given. The missing explicit expressions of the interfacial terms  $\Phi_k$  may be overcome in practical situations, see [14, 12].

If we turn to approximation of solutions of system (9)-(12), recent works investigated relaxation schemes dedicated to the two-phase Baer-Nunziato model with strong properties, see [5], and also in the three-phase immiscible barotrope case [23]. It would be interesting to extend these works to the two-phase three-field case and to begin a numerical study.

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NANTES UNIVERSITÉ, CNRS, LABORATOIRE DE MATHÉMATIQUES JEAN LERAY, LMJL, F-44000  
NANTES, FRANCE  
*Email address:* `jean.bussac@univ-nantes.fr`