

AN INTERNAL VARIABLE CONSTITUTIVE THEORY FOR BUBBLY FLOWS INCORPORATING SURFACE TENSION PHENOMENON

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Abstract. *This work presents a thermodynamical model which consistently incorporates internal surface tension phenomenon in homogeneous two-component two-phase flows, without appealing to additional kinematical variables to describe its microstructure. The liquid and gaseous phases are regarded as a pseudo fluid whose constitutive behavior is obtained from two thermodynamic potentials – the Helmholtz free energy and a pseudo-potential of dissipation. The structure of the flow is assumed to be described solely by the void fraction, which is treated as an internal variable. The constraint associated with it is regarded as a material property, being an effective part of the constitutive equations. Surface tension is taken by the model into account by adding a suitable extra term, with dependence on the void fraction, in the Helmholtz free energy. The capability of the model in describing pertinent physical phenomenon is demonstrated by comparing the analytical predictions of sound speeds in the medium with available experimental data.*

Keywords. *Two-phase flows, surface tension, sound speed, internal variable theory, hyperbolicity.*

1. Introduction

Homogeneous two-phase flows have been extensively investigated from the theoretical and experimental points of view in the past decades due to its significant importance in industrial applications. Fluid flows in heat exchangers with condensation and boiling and pipelines carrying liquid-gas mixtures, in steady and unsteady states, are some of a vast universe of practical engineering problems. An example of practical significance, which in fact has motivated this work, is the case of bubbly liquids flowing in pipelines. Very small gas concentrations by volume are known to alter drastically the sonic velocity. If it is not properly accounted for, the identification of pipeline sections susceptible to mechanical failure may be severely compromised, when structural integrity transient analyses (Freitas Rachid et al, 1994 and 1998) are carried out.

Several distinct two-component two-phase models have been proposed in the literature to describe the dynamics of the fluid flow with different levels of sophistication. Simplifying assumptions currently used in these models encompass homogeneous and isothermal mixtures as well as non viscous flows. On the other hand, sophisticated and relevant features are in general marked by the inclusion in the modeling - through different approaches - of heat transfer, micro-inertia and surface tension effects (Ishii, 1975; Drumheller et al., 1982; Drew and Passman, 1999; Gavriluk and Saurel, 2002).

When at least one of the last two features are taken into consideration, the state of the local structure of the flow is in an indirect or direct fashion accounted for, so that additional variables - along with balance or/and constitutive equations - are in general required. For instance, if the mean radius of the bubbles is taken as an additional kinematical variable in bubbly flows, then the traditional Laplace model is usually employed in the Rayleigh-Plesset equation in order to describe surface tension effects (Drumheller et al., 1982 and Drew and Passman, 1999). However, if, by one hand, the use of an additional variable allows the adoption of a well-known constitutive relation, it has, by the other hand, the disadvantage of increasing the number of variables to deal with as well as the computational effort when numerical solutions are envisaged. Since such a cost-benefit relationship can not be rated unless alternative models be available for comparisons, this argument motivates by itself the search for new ones.

Within this context, instead of using additional variables, surface tension effects are incorporated in the modeling of homogeneous liquid-gas flows proposed herein by considering the void fraction only. The idea of using the void fraction as a unique variable at the macroscopic level to report changes in the microstructure of multi-component flows, describing complex physical phenomena, is not a new proposal. The works of Capriz and Cohen (1983) and Frémond and Nicolas (1987) are good examples of this approach to model micro-inertia effects in the dynamical behavior of bubbly liquids and the sorption-desorption phenomena in saturated porous media, respectively.

This paper presents a macroscopic thermodynamically consistent model which incorporates surface tension effects in homogeneous and isothermal liquid-gas flows without appealing directly to its microstructure. In the model proposed herein the local structure of the flow is only characterized by the void fraction. This parameter is considered as an internal variable so that it and its constraint are treated as material properties, being part of the constitutive equations. Surface tension is taken into account by adding an extra term, with dependence on the void fraction, in the Helmholtz free energy of the mixture. Physical and mathematical features, such as hyperbolicity of the model equations, are then exploited to consistently derive restrictions on the choice of this extra term. The capability of the model in appropriately

reproducing some practical features is illustrated by presenting a particular form for that extra term and computing the wave speeds small disturbances propagate in the medium with and without surface tension effects. Sound speeds in air-water mixtures predicted by a classical and the proposed models are compared with experimental data available in the literature. It is shown that the proposed model present a better agreement with experimental data than the classical one for mixtures with very small contents of gas at low frequencies.

2. Balance equations

Homogeneous flows form a subclass of two-phase flows for which there exists no significant relative motion or slip between the constituents, what is equivalent to consider that the liquid and gas have the same velocities in the entire domain. In addition, when both the liquid and the gas constituents have always the same temperature \mathbf{q} and the flow is isothermal ($\dot{\mathbf{q}}=0$ and $\text{grad } \mathbf{q}=0$), it can be thermo-mechanically described by employing the linear momentum principle along with the first and second laws of the thermodynamics for the mixture as a whole, instead of doing it for each phase separately (Graham, 1969 and Ishii, 1975). As a consequence, the liquid-gas mixture can be regarded as a pseudo fluid sharing thermo-mechanical average properties of the two phases. At a macroscopic level, these constituents are assumed to coexist at every material point and time.

In the model presented here, it is further considered that there is no vapor along with the gas. Moreover, we admit as a basic premise that the gas can not be dissolved in the liquid and vice-versa in the course of the motion. To take these features into account the gas volume fraction \mathbf{a} is considered as an internal variable. The gas volume fraction, or simply void fraction as it is usually referred to, is defined as being the ratio between the volume of gas and the total volume of the mixture. In view of the aforementioned assumptions it is subjected to the constraint, $\mathbf{a} \in (0,1)$. As we shall see later, this restriction is considered in the present model as a constitutive behavior and is properly accounted for by the constitutive equations. With the aid of the void fraction the mass density of the mixture can be expressed as:

$$\mathbf{r} = (1-\mathbf{a})\mathbf{r}_l + \mathbf{a}\mathbf{r}_g \quad (1)$$

in which \mathbf{r}_l and \mathbf{r}_g stand for the mass densities of the liquid and the gas, respectively, both of them are assume to be compressible fluids.

Under suitable regularity assumptions, the following classical forms of the balance equations along with a local version of the Second Law of the Thermodynamics (SLT) suffice to fully describe the thermo-mechanical problem (Germain and Muller, 1995):

$$(1-\mathbf{a})\dot{\mathbf{r}}_l - \mathbf{r}_l\dot{\mathbf{a}} + (1-\mathbf{a})\mathbf{r}_l \text{div } \mathbf{v} = 0 \quad (2)$$

$$\mathbf{a}\dot{\mathbf{r}}_g + \mathbf{r}_g\dot{\mathbf{a}} + \mathbf{a}\mathbf{r}_g \text{div } \mathbf{v} = 0 \quad (3)$$

$$\mathbf{r}\dot{\mathbf{v}} = -\text{grad } p + \text{div } \mathbf{S} + \mathbf{r}\mathbf{g} \quad (4)$$

$$d = -(p + \Psi)\text{div } \mathbf{v} + \mathbf{S} : \mathbf{D} - \dot{\Psi} \geq 0 \quad (5)$$

The above equations, in Eulerian coordinates, represent the balance of mass for each of the constituents, the balance of linear momentum and the Clausius-Duhem inequality for the pseudo fluid as a whole, respectively. As usual, the superimposed dot stands for the material time derivative, \mathbf{v} is the spatial velocity field, p is the thermodynamic pressure, $\mathbf{S} = \mathbf{S}^T$ is the extra stress tensor due to motion, \mathbf{g} is the external body force per unit mass, $\mathbf{D} = \frac{1}{2}[\text{grad } \mathbf{v} + (\text{grad } \mathbf{v})^T]$ is the rate of deformation tensor and Ψ is the Helmholtz free energy of the pseudo fluid per unit volume. Equation (5) is a local version of the SLT which defines the rate of the energy dissipation d and makes a distinction between possible ($d \geq 0$) and impossible ($d < 0$) processes. Processes that do not violate the SLT are classed as reversible ($d = 0$) and irreversible ($d > 0$).

To complete the problem description, we must add the constitutive relationships for the mixture to adequately describe the physical phenomena we are interested in modeling (internal surface tension effects in our case), in such a way that inequality (5) be satisfied no matter the external actions, the initial and the boundary conditions.

3. Constitutive Theory

The constitutive relations describing the macroscopic mechanical behavior of the mixture are derived in the framework of the Thermodynamics of Irreversible Processes. In this theory, once the local state of the material has been characterized by means of an appropriate choice of the set of state variables, two thermodynamical potentials - the Helmholtz free energy and a pseudo-potential of dissipation - are sufficient to derive a complete set of constitutive equations. For this particular problem, we choose as state variables the local mass densities of the liquid \mathbf{r}_l and the gas

\mathbf{r}_g , the void fraction \mathbf{a} and the absolute temperature \mathbf{q} . As we shall see, the restriction associated to \mathbf{a} is treated in this work as a physical property in the constitutive equations. This approach has already been used by Frémond and Nicolas (1987 and 1990) in the modeling of the sorption-desorption problem in saturated porous media and more recently by Freitas Rachid (2003) in the modeling of cavitation in flows of compressible fluids.

At this point, emphasis should be placed in the fact that contrary to the common practice in the modeling of homogeneous two-phase flows, in which explicit microstructural content is used to incorporate internal surface tension effects, the proposed model attempts to emulate such a feature by employing the gas volume fraction only. The constraint associated with \mathbf{a} , $\mathbf{a} \in (0,1)$, will be treated as a material property, being an effective part of the constitutive equations. For the sake of convenience, this constraint is decomposed in two complementary parcels: $\mathbf{a} \in [0,1]$ and $\mathbf{a} \notin \{0,1\}$.

3.1. Helmholtz free energy

Following the classic assumption of the Thermodynamics of Irreversible Processes, the free energy per total unit volume Ψ is supposed to be a function of the state variables \mathbf{r}_l , \mathbf{r}_g , \mathbf{a} and \mathbf{q} . Since the pseudo fluid is regarded as a mixture of two constituents, its behavior is supposed to comprise a combination of the liquid and gas thermo-mechanical properties, taking \mathbf{a} as a weighting factor. Thus, we choose

$$\Psi = \Psi(\mathbf{r}_l, \mathbf{r}_g, \mathbf{a}, \mathbf{q}) = \Psi'(\mathbf{r}_l, \mathbf{r}_g, \mathbf{a}, \mathbf{q}) + I(\mathbf{a}) \quad (6a)$$

in which

$$\Psi'(\mathbf{r}_l, \mathbf{r}_g, \mathbf{a}, \mathbf{q}) = (1-\mathbf{a})\mathbf{r}_l\Psi_l(\mathbf{r}_l, \mathbf{q}) + \mathbf{a}\mathbf{r}_g\Psi_g(\mathbf{r}_g, \mathbf{q}) + \Psi_s(\mathbf{a}, \mathbf{q}) \quad ; \quad I(\mathbf{a}) := \begin{cases} 0, & \text{if } \mathbf{a} \in [0,1] \\ +\infty, & \text{otherwise.} \end{cases} \quad (6b,c)$$

In the above expression, Ψ' is a smooth function which describes the thermo-mechanical properties of the pseudo fluid whereas $I(\mathbf{a})$ represents the indicator function of the convex set $[0,1]$ (Moreau, 1966). The term $I(\mathbf{a})$ is the non-smooth parcel of the free energy and is included to take the part of the internal constraint $\mathbf{a} \in [0,1]$ into account as a constitutive assumption. In other words, it prevents \mathbf{a} from getting out of its admissible interval since it would be required a infinite amount of energy to do this. The other parcel of the internal constraint $\mathbf{a} \notin \{0,1\}$ will be treated later.

The terms Ψ_l and Ψ_g represent the free energies per unit mass of the liquid and the gas constituents, respectively. As suggested by its functional dependence, these free energies are supposed to represent the thermo-mechanical behavior of the liquid and the gas as if they were single constituents. The interaction term between both constituents is represented by the parcel Ψ_s in the free energy of the pseudo fluid and is included to account for internal surface tension effects. For the present moment, we consider that Ψ_s is smooth with regard to \mathbf{a} , for at least $\mathbf{a} \in (0,1)$.

It should be pointed out that we have tacitly assumed that the internal structure of the pseudo fluid is completely characterized by the gas volume fraction. Of course, it is a very strong assumption whose implications impact directly on limitations of the theory. Nevertheless, as we shall see later, the model presented herein is capable to quite well continuously describe the effect of surface tension on the wave speed at low frequencies in homogeneous liquid-gas systems, ranging from bubbly to droplet flows.

The state laws for the pseudo fluid, relating the reversible components of the thermodynamic forces to the state variables, are obtained from the free energy potential and defined as follows:

$$B^{r_l} := \frac{\partial \Psi'}{\partial \mathbf{r}_l} = (1-\mathbf{a})(\Psi_l + \frac{p_l}{\mathbf{r}_l}) \quad ; \quad B^{r_g} := \frac{\partial \Psi'}{\partial \mathbf{r}_g} = \mathbf{a}(\Psi_g + \frac{p_g}{\mathbf{r}_g}) \quad ; \quad B^{\mathbf{a}} := \frac{\partial \Psi'}{\partial \mathbf{a}} + h, \quad \text{with } h \in \partial_{\mathbf{a}} I(\mathbf{a}) \quad (7a,b,c)$$

in which

$$\frac{\partial \Psi'}{\partial \mathbf{a}} = \mathbf{r}_g \Psi_g - \mathbf{r}_l \Psi_l + \frac{\partial \Psi_s}{\partial \mathbf{a}} \quad ; \quad p_l := \mathbf{r}_l \frac{\partial \Psi_l}{\partial \mathbf{r}_l} \quad ; \quad p_g := \mathbf{r}_g \frac{\partial \Psi_g}{\partial \mathbf{r}_g} \quad (7d,e)$$

In the above equations, p_l and p_g stand for the liquid and gas pressures, respectively. The term h in (7c) is an element of the subdifferential set $\partial_{\mathbf{a}} I(\mathbf{a})$ (also called generalized derivative) with respect to \mathbf{a} of the convex function $I(\mathbf{a})$. The subdifferential of the indicator function $I(\mathbf{a})$ at \mathbf{a} is given by the set (Ekeland and Teman, 1976 and Moreau and Panagiotopoulos, 1988);

$$\partial_a I(\mathbf{a}) = \{h \in \mathfrak{R} \mid I(\mathbf{a}^*) - I(\mathbf{a}) \geq h(\mathbf{a}^* - \mathbf{a}); \quad \forall \mathbf{a}^* \in [0,1]\} \quad (8)$$

A straightforward calculation shows that, $\partial_a I(\mathbf{a} = 0) = \mathfrak{R}^-$, $\partial_a I(0 < \mathbf{a} < 1) = \{0\}$, $\partial_a I(\mathbf{a} = 1) = \mathfrak{R}^+$ and $\partial_a I(\mathbf{a}) = \emptyset$ if $\mathbf{a} \notin [0,1]$. It is important to remark that the restriction $\mathbf{a} \in [0,1]$ is effectively taken into account through the constitutive law (7c), since this relation implies that the subdifferential $\partial_a I(\mathbf{a})$ is not empty.

Once a form for Ψ is chosen in Eq. (6), we are able to compute its material time derivative $\dot{\Psi}$ which appears in (5). Keeping in mind that time derivatives must be left derivatives in order to cope with the principle of determinism, it comes out that, for $\Delta t > 0$:

$$\dot{\Psi} = \frac{\partial \Psi'}{\partial \mathbf{r}_l} \dot{\mathbf{r}}_l + \frac{\partial \Psi'}{\partial \mathbf{r}_g} \dot{\mathbf{r}}_g + \frac{\partial \Psi'}{\partial \mathbf{a}} \dot{\mathbf{a}} + \lim_{\Delta t \rightarrow 0} \frac{I(\mathbf{a}(t)) - I(\mathbf{a}(t - \Delta t))}{\Delta t} \quad (9)$$

In computing $\dot{\Psi}$ care should be taken since Ψ is not a smooth function. By using the definition of the subdifferential it can be shown that:

$$\lim_{\Delta t \rightarrow 0} \frac{I(\mathbf{a}(t)) - I(\mathbf{a}(t - \Delta t))}{\Delta t} \leq h \dot{\mathbf{a}}, \quad \forall h \in \partial_a I(\mathbf{a}(t)) \quad (10)$$

When the above result is used along with the state laws (7), Eq.(9) can be written as:

$$\dot{\Psi} \leq B^{r_l} \dot{\mathbf{r}}_l + B^{r_g} \dot{\mathbf{r}}_g + B^a \dot{\mathbf{a}} \quad (11)$$

Finally, inequality (11) can be used to find a lower bound \hat{d} for the dissipation d in Eq.(5) such as:

$$d \geq \hat{d} = -(p + \Psi) \text{div } \mathbf{v} + \mathbf{S} : \mathbf{D} - B^{r_l} \dot{\mathbf{r}}_l - B^{r_g} \dot{\mathbf{r}}_g - B^a \dot{\mathbf{a}} \quad (12)$$

To obtain a complete set of constitutive equations, it suffices to specify a pseudo-potential of dissipation from which complementary laws are derived in such a way that the local version of the second law (5) or (12) is always verified, regardless the initial and boundary conditions.

3.2. Pseudo-potential of dissipation

To introduce the irreversible behavior of the pseudo fluid, and also to ensure that the SLT is always satisfied, we assume that there exists a pseudo-potential of dissipation Φ , which is an objective, convex and differentiable function of $\Phi = \Phi(\mathbf{D}, \dot{\mathbf{a}}; \mathbf{a})$, with the following properties:

$$\Phi(\mathbf{D}, \dot{\mathbf{a}}; \mathbf{a}) \geq 0 \quad \text{and} \quad \Phi(\mathbf{D}, \dot{\mathbf{a}}; \mathbf{a}) = 0, \quad \forall (\mathbf{D}, \dot{\mathbf{a}}; \mathbf{a}) \quad (13)$$

The additional information associated to the dissipative behavior of the mixture is obtained from Φ through the following complementary laws:

$$\mathbf{S} := \frac{\partial \Phi}{\partial \mathbf{D}}, \quad B^a := \frac{\partial \Phi}{\partial \dot{\mathbf{a}}} \quad (14)$$

In addition, if the rate of energy dissipation \hat{d} is supposed to have the form,

$$\hat{d} := \mathbf{S} : \mathbf{D} + B^a \dot{\mathbf{a}} - I(\mathbf{a}) \text{div } \mathbf{v} \quad (15)$$

then we get from the convexity property of Φ that, for any actual evolution:

$$\hat{d} := \mathbf{S} : \mathbf{D} + B^a \dot{\mathbf{a}} \geq \Phi(\mathbf{D}, \dot{\mathbf{a}}; \mathbf{a}) - \Phi(\mathbf{0}, 0; \mathbf{a}) \quad (16)$$

In view of (13), it is easy to see that $\hat{d} \geq 0$ for any actual evolution of the pseudo fluid and so the SLT (5) is always satisfied.

From the mechanical viewpoint, equation (15) establishes that the rate of energy dissipation is in fact the sum of two parcels. The first parcel in the right-hand side of (15) is due to viscous effects and the second one is due to internal changes in mixture. The third term do not express any dissipation for actual evolutions since $I(\mathbf{a}) = 0$ for $\mathbf{a} \in [0,1]$. It is incorporated into the dissipation to give coherence to the model. It means that to force \mathbf{a} to get out of the interval $[0,1]$ either a an infinite energy dissipation would be required or the SLT would be violated according to the sign of the divergence of the spatial velocity field.

The constitutive assumptions made so far are sufficient to completely characterize the mechanical behavior of the pseudo fluid. In fact, since the mass balance equations (2) and (3) define subspaces of the linear space spanned by \mathbf{v} , $\dot{\mathbf{r}}_l$, $\dot{\mathbf{r}}_g$ and $\dot{\mathbf{a}}$, then in order that (12) be equal to (16) for any actual evolution one must have:

$$-(p + \Psi)\text{div } \mathbf{v} - B^{r_l} \dot{\mathbf{r}}_l - B^{r_s} \dot{\mathbf{r}}_g - B^a \dot{\mathbf{a}} = B^a \dot{\mathbf{a}} + \mathbf{h}((1-\mathbf{a})\dot{\mathbf{r}}_l - \mathbf{r}_l \dot{\mathbf{a}} + (1-\mathbf{a})\mathbf{r}_l \text{div } \mathbf{v}) + \mathbf{x}(\mathbf{a}\dot{\mathbf{r}}_g + \mathbf{r}_g \dot{\mathbf{a}} + \mathbf{a}\mathbf{r}_g \text{div } \mathbf{v}) - I(\mathbf{a})\text{div } \mathbf{v} \quad (17)$$

in which \mathbf{h} and \mathbf{x} are Lagrange multipliers. Since Eq. (17) holds for any independent evolution of \mathbf{v} , $\dot{\mathbf{r}}_l$, $\dot{\mathbf{r}}_g$ and $\dot{\mathbf{a}}$, it comes out that:

$$\begin{aligned} -p - \Psi - \mathbf{h}(1-\mathbf{a})\mathbf{r}_l - \mathbf{x}\mathbf{a}\mathbf{r}_g + I(\mathbf{a}) &= 0 \\ -B^{r_l} - (1-\mathbf{a})\mathbf{h} &= 0 \\ -B^{r_s} - \mathbf{a}\mathbf{x} &= 0 \\ -B^a - B^a + \mathbf{h}\mathbf{r}_l - \mathbf{x}\mathbf{r}_g &= 0 \end{aligned} \quad (18)$$

Since $\mathbf{a} \in (0,1)$ by hypothesis, \mathbf{h} and \mathbf{x} can be eliminated from the above equations to render the following relationships among the thermodynamical forces,

$$p = (1-\mathbf{a})p_l - \mathbf{a}p_g - \Psi_s \quad ; \quad B^a = p_g - p_l - \frac{\partial \Psi_s}{\partial \mathbf{a}} \quad (19a,b)$$

Special mention is due to the last terms in the right-hand side of (19a) and (19b), which appear as a consequence of the inclusion of the internal surface tension effects in the model. Equation (19a) shows that the pressure in the mixture is a mean value between the liquid and gas pressures plus an additional term Ψ_s . The presence of this term is unusual and will be discussed later.

3.3. Constitutive laws

The expressions (7),(14) and (19) form a complete set of constitutive laws provide the functions $\Psi_l(\mathbf{r}_l, \mathbf{q})$, $\Psi_g(\mathbf{r}_g, \mathbf{q})$, $\Psi_s(\mathbf{a}, \mathbf{q})$ and $\Phi(\mathbf{D}, \dot{\mathbf{a}}; \mathbf{a})$ are specified.

Without losing generality, if we assume that both constituents behave as Newtonian fluids an appropriate choice for Φ is:

$$\Phi = \frac{I}{2}(\text{tr}(\mathbf{D}))^2 + \mathbf{m}\mathbf{D} : \mathbf{D} + \frac{\mathbf{e}}{2}\dot{\mathbf{a}}^2 \quad (20)$$

where \mathbf{e} is a positive material constant and $I = I(\mathbf{a})$, $\mathbf{m} = \mathbf{m}(\mathbf{a})$ are average properties between, respectively, I_l and I_g and between \mathbf{m}_l and \mathbf{m}_g having \mathbf{a} as weighting factor. These material parameters are such that $\mathbf{m} \geq 0$ and $I + \frac{2}{3}\mathbf{m} \geq 0$. For this specific choice, the state and the complementary laws become:

$$\mathbf{S} = I\text{tr}(\mathbf{D})\mathbf{I} + 2\mathbf{m}\mathbf{D} \quad ; \quad B^a = \mathbf{e}\dot{\mathbf{a}} \quad (21a,b)$$

Equation (21a) is classic and express the behavior of a Newtonian fluid, which in this case is supposed to mix the liquid and gas properties. Expression (21b) characterizes the volume fraction evolution. By combining (21b) with (19b) it

becomes apparent the effect of the internal surface tension on the volume fraction evolution. Before going a step further towards the specific form of the function Ψ_s , it is worth noting some peculiar behaviors this function must attend in order to properly describe the surface tension phenomenon.

Equations (1-4), (7), (19) and (21) completed by suitable boundary and initial conditions are sufficient to describe the isothermal and homogeneous flow of liquid-gas mixtures of Newtonian fluids that automatically satisfies (5). Since the constitutive relation for a Newtonian fluid is well-known we shall from now on focus attention on the internal surface tension effect.

4. Restrictions on the choice of Ψ_s

Although the main structure of the model has been presented, it is not complete yet since the extra term Ψ_s of the Helmholtz free energy has not been specified. As will be shown next, the term Ψ_s must not only account for the constraint $\mathbf{a} \notin \{0,1\}$ but also attend some requisites in order to assign the model physical and mathematical consistency. The parcel of the constraint $\mathbf{a} \notin \{0,1\}$ and the physical consistency will be approached setting up conditions on Ψ_s , and on its first derivative with respect to \mathbf{a} , at the limits of the admissible interval. On the other hand, mathematical consistency of the model will be explored by requiring hyperbolicity of the dynamic fluid flow governing equations.

4.1. Physical features – conditions on the limits

Since $\mathbf{a}=0$ and $\mathbf{a}=1$ are not admissible values as it has been pointed out earlier (i.e., $0 < \mathbf{a} < 1$), such an information must be taken by the model into account. In our case it is considered through relation (7c). Since we have assumed that Ψ_s is smooth, two alternatives are possible. By letting Ψ_s be either infinite as $\mathbf{a} \rightarrow 0^+$ and as $\mathbf{a} \rightarrow 1^-$ or not differentiable with respect to \mathbf{a} at $\mathbf{a}=0$ and at $\mathbf{a}=1$. Since Ψ_s must be finite not only as $\mathbf{a} \rightarrow 0^+$ and as $\mathbf{a} \rightarrow 1^-$ but also for $\mathbf{a} \in (0,1)$ by virtue of (19a), then Ψ_s can not be differentiable at $\mathbf{a}=0$ and at $\mathbf{a}=1$. The presence of Ψ_s in (19a) is non classic is due to the approach proposed herein. If we admit from the knowledge of volume averaging theories (Drew and Passman, 1993) that the term Ψ_s does not exist in fact in (19a) for any actual evolution, then $|\Psi_s|$ should be small when compared to $|(1-\mathbf{a})p_l + \mathbf{a}p_g|$ for all $\mathbf{a} \in (0,1)$. In addition, since we are going to take second order derivatives of Ψ_s with respect to \mathbf{a} , in choosing Ψ_s the following restrictions must be satisfied in order that the model be physically coherent:

$$\Psi_s(\mathbf{a}, \cdot) \in C^2 \quad \text{for} \quad \mathbf{a} \in (0,1) \quad (22a)$$

$$\frac{\partial \Psi_s}{\partial \mathbf{a}}(\mathbf{a}, \cdot) \quad \text{does not exist for} \quad \mathbf{a}=0 \quad \text{and} \quad \mathbf{a}=1 \quad (22b)$$

$$\Psi_s(\mathbf{a}, \cdot) \ll d := |(1-\mathbf{a})p_l + \mathbf{a}p_g| \quad \forall \mathbf{a} \in (0,1) \quad (22c)$$

If expression (7c) obeys condition (22b) the internal constraint $\mathbf{a} \in (0,1)$ is automatically satisfied, which in physical grounds means that the gas can not be dissolved into the liquid and vice-versa.

Conditions (22) are necessary but not sufficient to ensure physical consistency. To establish additional conditions on Ψ_s , we note from (19b) and (21b) that under equilibrium conditions ($\dot{\mathbf{a}}=0$) the partial derivative of Ψ_s with respect to \mathbf{a} equals the pressure difference between the gas and liquid constituents. If we realize that as $\mathbf{a} \rightarrow 0^+$ the pseudo fluid can be identified as being composed of small bubbles of gas in a liquid medium, then one must have $p_g > p_l$. On the other hand, if we realize that as $\mathbf{a} \rightarrow 1^-$ one has droplets of liquid in a gas medium one must have $p_g < p_l$. As a result, the following conditions should be expected:

$$\lim_{\Delta t \rightarrow 0^+} \frac{\partial \Psi_s}{\partial \mathbf{a}} > 0 \quad ; \quad \lim_{\Delta t \rightarrow 1^-} \frac{\partial \Psi_s}{\partial \mathbf{a}} < 0 \quad (23a,b)$$

Another restriction on the choice of the function Ψ_s and its derivative can be established by considering that, at finite volume fraction evolution rates or at equilibrium conditions ($\dot{\mathbf{a}}=0$), one must have $p \rightarrow p_l$ as $\mathbf{a} \rightarrow 0^+$ and

$p \rightarrow p_g$ as $\mathbf{a} \rightarrow \Gamma$. To better characterize these implications, we manipulate relations (19) and (21b) in order to rewrite the pressure of the pseudo fluid as a function of either the liquid pressure or the gas pressure and other quantities as follows, respectively:

$$p = p_l + \mathbf{a} \mathbf{e} \dot{\mathbf{a}} + \mathbf{a} \frac{\partial \Psi_s}{\partial \mathbf{a}} - \Psi_s \quad ; \quad p = p_g - (1 - \mathbf{a}) \mathbf{e} \dot{\mathbf{a}} - (1 - \mathbf{a}) \frac{\partial \Psi_s}{\partial \mathbf{a}} - \Psi_s \quad (24a,b)$$

Now, by applying the conditions set before on the last paragraph we obtain the desired properties:

$$\lim_{\Delta t \rightarrow 0^+} \left[\mathbf{a} \frac{\partial \Psi_s}{\partial \mathbf{a}} - \Psi_s \right] = 0 \quad ; \quad \lim_{\Delta t \rightarrow \Gamma} \left[(1 - \mathbf{a}) \frac{\partial \Psi_s}{\partial \mathbf{a}} + \Psi_s \right] = 0 \quad (25a,b)$$

4.1. Mathematical aspect – hyperbolicity

The physical features explored in the past section have given rise to some particular behaviors the extra term in the Helmholtz free energy Ψ_s and its first derivative with respect to \mathbf{a} should attend in order that the model be coherent. However, a model that is not properly formulated mathematically cannot describe physical phenomena correctly. To ensure mathematical consistency, we shall explore the hyperbolicity of the governing equations, which, as we shall see, will impose restrictions on the second order derivative of Ψ_s with respect to \mathbf{a} .

For the sake of simplicity, the governing equations we are referring to are those associated with the isothermal dynamical non viscous fluid flow of a homogeneous gas-liquid mixture described solely by the balance equations (2),(3) and (4) along with the constitutive relations (7),(19) and (21b). Since no particular form of the Helmholtz free energy potential has been given, including the extra term Ψ_s , some general definitions are required before going a step further.

The wave speed small disturbances propagate isolated in the liquid and in the gas constituents are defined as:

$$c_l^2 := \left. \frac{\partial p_l}{\partial \mathbf{r}_l} \right|_{c=\text{const.}} \quad \text{and} \quad c_g^2 := \left. \frac{\partial p_g}{\partial \mathbf{r}_g} \right|_{c=\text{const.}} \quad (26)$$

If \mathbf{c} is taken as being the entropy, then we have the isentropic wave propagation velocities. However, if it is assumed that \mathbf{c} is the temperature, then wave speeds are associated with a isothermal process. For liquids, the difference between the isentropic and isothermal wave speeds is not significant. Nevertheless, it is not the case when the constituent is a gas. Because of transient heat-transfer effects which occur during the passage of a wave, it is not obvious which path it should be used to compute the wave speeds. It is generally accepted that for rapid compression and expansion (high frequencies) the gas behaves almost isentropically. On the other hand, slow changes (low frequencies) seem to be best represented by a isothermal transformation (Temkin, 1992). Since isothermal processes have been assumed when the balance equations were presented, the forthcoming analysis will be carried out assuming that $\mathbf{c} = \mathbf{q}$.

To proceed with the analysis of the hyperbolicity, we shall assume, for the sake of simplicity, one dimensional flows in, for instance, the x direction. Within this context, a set of partial differential equations having as independent variables the spatial coordinate x and the time t can be written in the following canonical form,

$$\mathbf{A} \frac{\partial \mathbf{U}}{\partial t} + \mathbf{B} \frac{\partial \mathbf{U}}{\partial x} + \mathbf{F} = \mathbf{0} \quad (27)$$

in which $\mathbf{U} := \mathbf{U}(x,t) \in \mathfrak{R}^n$ is the n -dimensional vector of dependent variables, $\mathbf{A} := \mathbf{A}(\mathbf{U})$ and $\mathbf{B} := \mathbf{B}(\mathbf{U})$ are n by n matrices and $\mathbf{F} := \mathbf{F}(\mathbf{U})$ is the n -dimensional vector associated with the sink/source terms. A system like (27) is said to be merely hyperbolic if, providing that \mathbf{A}^{-1} exists, the eigenvalues given by,

$$\det(\mathbf{A}^{-1} \mathbf{B} - \mathbf{I} \mathbf{I}) = 0 \quad (28)$$

are all real (but not necessarily distinct) and the eigenvectors associated with the eigenvalues \mathbf{I} form a set of n linearly independent vectors spanning the space \mathfrak{R}^n (Jeffrey, 1976).

When the dissipation associated with the void fraction evolution is taken into account ($\mathbf{e} \neq 0$ in (21b)), it can easily be shown that the governing equations (2),(3),(4) and (21b) are hyperbolic, whatsoever the nature of the extra term Ψ_s is. However, if such a mechanism of dissipation is negligible, then additional restrictions about the function Ψ_s appear as a consequence of the hyperbolicity of the governing equations. Since this mechanism of dissipation may in fact be non significant, we shall assume hereto after that $\mathbf{e} = 0$ so that there is no dissipation of energy associated to $\dot{\mathbf{a}}$ and consequently $B^{\dot{\mathbf{a}}} = 0$ in (21b). In such a case, neglecting convective terms, (2-4),(19) and (26) can be manipulated and combined in such a way that (2),(3),(4) and (19b) assume the form (27), with $\mathbf{U} = (p_g, p_l, v, \mathbf{a})^T$, $\mathbf{F} = \mathbf{0}$, and:

$$\mathbf{A} = \begin{pmatrix} \frac{\mathbf{a}}{c_g^2} & 0 & 0 & \mathbf{r}_g \\ 0 & \frac{(1-\mathbf{a})}{c_l^2} & 0 & -\mathbf{r}_l \\ 0 & 0 & \mathbf{r} & 0 \\ 1 & -1 & 0 & -\frac{\partial^2 \Psi_s}{\partial \mathbf{a}^2} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 0 & 0 & \mathbf{a} \mathbf{r}_g & 0 \\ 0 & 0 & (1-\mathbf{a}) \mathbf{r}_l & 0 \\ \mathbf{a} & (1-\mathbf{a}) & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (29)$$

In this case, the eigenvalues computed according to (28) give rise to two non propagating wave speeds ($\mathbf{I}^{(1)} = \mathbf{I}^{(2)} = 0$) and other two propagating wave speeds ($\mathbf{I}^{(3)} = -c$ and $\mathbf{I}^{(4)} = +c$), in which:

$$c = \left[\frac{c_l^2 \mathbf{r}_l c_g^2 \mathbf{r}_g + \mathbf{a}(1-\mathbf{a}) \frac{\partial^2 \Psi_s}{\partial \mathbf{a}^2} (c_l^2 \mathbf{r}_l (1-\mathbf{a}) + c_g^2 \mathbf{r}_g \mathbf{a})}{\mathbf{r} \left(c_l^2 \mathbf{r}_l \mathbf{a} + c_g^2 \mathbf{r}_g (1-\mathbf{a}) + \mathbf{a}(1-\mathbf{a}) \frac{\partial^2 \Psi_s}{\partial \mathbf{a}^2} \right)} \right]^{1/2} \quad (30)$$

Due to the presence of the second order derivative of Ψ_s with respect to \mathbf{a} in the numerator and denominator of (30), it can be seen that surface tension affects the speed with which disturbances propagate in the pseudo fluid, as would be expected. Such a result is known and has already been reported by Marchal (1962). Moreover, it can promptly be shown in expression (30) that $c \rightarrow c_l$ and $c \rightarrow c_g$ as $\mathbf{a} \rightarrow 1$ and $\mathbf{a} \rightarrow 0^+$, respectively, whatsoever the function Ψ_s is. In addition, if $\Psi_s \equiv 0$ (what is equivalent to disregard surface tension effects), then (30) reduces to the classical expression of wave speed c_o (Graham, 1969);

$$c_o = \left[\frac{c_l^2 \mathbf{r}_l c_g^2 \mathbf{r}_g}{\mathbf{r} (c_l^2 \mathbf{r}_l \mathbf{a} + c_g^2 \mathbf{r}_g (1-\mathbf{a}))} \right]^{1/2} \quad (31)$$

which has been derived in one of the pioneering works (Wood, 1930).

To ensure hyperbolicity of (27) along with (29) it is first of all necessary that (30) be a real number, what implies the following conditions:

$$-\mathbf{a}(1-\mathbf{a}) \frac{\partial^2 \Psi_s}{\partial \mathbf{a}^2} < a := \frac{c_l^2 \mathbf{r}_l c_g^2 \mathbf{r}_g}{((1-\mathbf{a})c_l^2 \mathbf{r}_l + \mathbf{a}c_g^2 \mathbf{r}_g)} \text{ and } -\mathbf{a}(1-\mathbf{a}) \frac{\partial^2 \Psi_s}{\partial \mathbf{a}^2} < b := \mathbf{a}c_l^2 \mathbf{r}_l + (1-\mathbf{a})c_g^2 \mathbf{r}_g, \quad \forall \mathbf{a} \in (0,1) \quad (32a)$$

Once (32a) and (32b) are satisfied, it is easy to prove that the eigenvectors associated with $\mathbf{I}^{(i)}$, for $i = 1, \dots, 4$ are linearly independent rendering the system (27) along with (29) merely hyperbolic.

5. Model's prediction for a particular choice of Ψ_s

Although the restrictions established in the past section for the material function Ψ_s must be satisfied in order to qualify the model for applications, they are not sufficient to ensure success in reproducing experimental results. In this section it is proposed a particular form for Ψ_s which, as we shall see, is capable to satisfy both requisites.

Whatever the choice of Ψ_s is, expressions (22), (23), (25) and (32) should be satisfied in order that the model be coherent. Of course, these relations do not ensure a unique form for Ψ_s . One possible choice for Ψ_s is the following two-parameter material function :

$$\Psi_s(\mathbf{a}, \mathbf{q}) := -\mathbf{g}[\mathbf{a}(1-\mathbf{a})\ln(\mathbf{k}\mathbf{a}(1-\mathbf{a}))] \quad (33)$$

in which $\mathbf{g} = \mathbf{g}(\mathbf{q})$ and $\mathbf{k} = \mathbf{k}(\mathbf{q})$ are positive material functions, which depend on the temperature. Easy calculations reveal that (33) promptly satisfies the conditions (22a), (22b), (23) and (25), whatever are the values assigned to \mathbf{g} and \mathbf{k} .

For the particular choice expressed by (33) in which it has been assumed that $\mathbf{g} > 0$, it can be shown that the conditions (32), which are related to the hyperbolicity of the governing equations, can be used to establish an upper bound to the material parameter \mathbf{g} :

$$\mathbf{g} \leq \inf_{\mathbf{a} \in (0,1)} \left\{ \frac{\mathbf{a}}{f}, \frac{\mathbf{b}}{f} \right\}, \quad \text{provided} \quad \mathbf{a}(1-\mathbf{a}) \frac{\partial^2 \hat{\Psi}_s}{\partial \mathbf{a}^2} < 0 \quad \text{for} \quad \mathbf{a} \in (0,1) \quad \text{in which} \quad f = \left| \mathbf{a}(1-\mathbf{a}) \frac{\partial^2 \hat{\Psi}_s}{\partial \mathbf{a}^2} \right| \quad (34)$$

Since $\mathbf{a}(1-\mathbf{a})\partial^2 \hat{\Psi}_s / \partial \mathbf{a}^2$ tends to -1 as $\mathbf{a} \rightarrow 0^+$ and $\mathbf{a} \rightarrow 1^-$ for any $\mathbf{k} > 0$, an upper bound for \mathbf{g} according to (34) will always exist and the conditions associated to hyperbolicity of the governing equations will automatically be verified.

The requirements established in the past section concerning the material function Ψ_s are necessary but not sufficient conditions to ensure that the model appropriately describes the physical phenomena related to the surface tension. Although several features may be involved in and so must be evaluated before a model be qualified as a good one, the speed acoustic waves propagate in the mixture is one for which consolidate results are known and available. For instance, Marchal (1962) has shown, by using an analytical model with microstructure appeal, that the net effect of the surface tension in a homogeneous bubbly mixture with a low concentration by volume of gas (small gas bubbles) is to increase the wave speed disturbances propagate in the medium when compared to the wave speed predicted by c_o (Eq. (31)) (in which such phenomenon is not taking into account). When the bubbles are small their compressibility is reduced by the effects of surface tension, assigning to the mixture a larger wave speed than predicted by c_o .

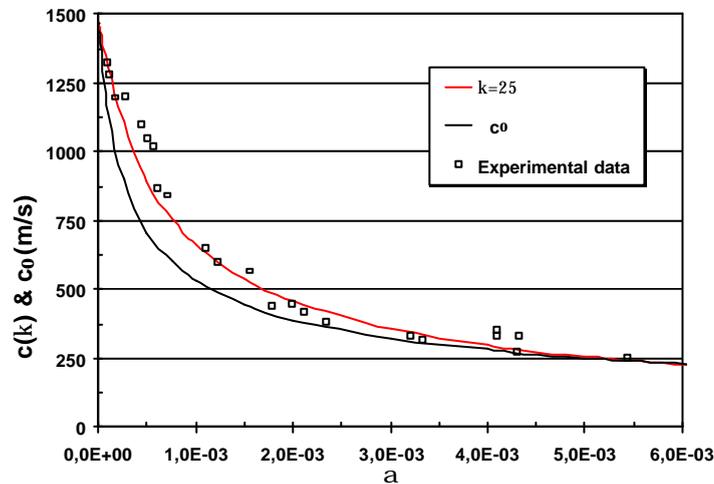


Figure 1: Comparison of the behaviors of the wave speeds against the void fraction \mathbf{a} predicted by the classical c_o (Eq. (31)) and the proposed $c(\mathbf{k})$ (Eq. (30)) models with experimental data of Kobori et al. (1995). The wave speed $c(\mathbf{k})$ is plotted when Ψ_s is given by Eq. (33) with $\mathbf{g} = 130$ kPa and $\mathbf{k} = 25$. Air-water mixture is at 324 kPa and at room temperature.

To corroborate the statement of the past paragraph, it is depicted in Figure 1 a comparison among the theoretical wave speed $c(\mathbf{k})$, given by Eq. (30) along with expression (33), the classical wave speed c_o given by Eq. (31) and the experimental data reported by Kobori et al. (1955). Although many experimental data about sonic velocities in homogeneous two-phase flow systems are available in the literature (Kobori et al. 1955; Karplus, 1961; Semenov and Kosterin, 1964; England et al., 1966 and Henry et al. 1971), only the data of Kobori et al. cover the very small range of

gas volume fractions ($\alpha < 5.0 \times 10^{-3}$]) where internal surface tension effects become relevant. Kobori's data were obtained for air bubbles in a pipeline containing water at 324 kPa at room temperature. Although the pipe-wall elasticity do affect the wave speed in the mixture, it becomes insignificant for small gas volume fractions such as that of the experimental data, allowing the comparison of Eqs. (30) and (31) with Kobori's data. The wave speed response predicted by the proposed model was plotted for $k = 25$ and $g = 130$ kPa, being the upper bound for g given by restriction (34) equal to 290.3 kPa. As expected, small air contents in volume produces a wave speed less than the speed of sound in the air. Such an effect is not only observed in the experimental data but also in both theoretical models. However, it can be clearly seen that the proposed model presents a better agreement with experimental data than the classical one over the whole range of the void fraction observed. Thus, surface tension acts in a mixture with small amounts of gas by attenuating the wave speed reduction predicted by the classical theory (given by Eq. 30). For the range of void fraction shown in Figure 6, it can be shown that $|\Psi_s / d|$ does not exceed 0.45 %, showing that the perturbation term Ψ_s in (19a) is indeed negligible.

5. Concluding remarks

A coherent thermodynamic model which consistently incorporates internal surface tension effects in homogeneous and isothermal two-component two-phase flows has been presented, without appealing to additional kinematical variables to describe the microstructure of the flow. The model is capable to continuously emulate the internal surface tension effects in liquid-gas flows over the whole range of the void fraction, $\alpha \in (0,1)$, without losing the hyperbolicity of the governing equations. For air-water mixtures at atmospheric pressure and room temperature, it is shown that internal surface tension affects the speed of sound in a bubbly flow but does not affect it in a droplet one. When the theoretical predictions of speed of sound based on the classical and proposed models are compared with experimental data for air-water systems, it is shown that the proposed model presents a better agreement than the classical one. The difference observed in the theoretical behaviors may be attributed to the surface tension which tends to reduce the compressibility of the gas at very small concentrations of air by volume.

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7. References

- Capriz, G. and Cohen, H., 1983, "The Bubbly Fluid as a Continuum with Microstructure", *Mechanics Research Communications*, Vol. 10, No. 10, pp. 359-367.
- Drew, D.A. and Passman, S.L., 1999, "Theory of Multicomponent Fluids", Springer-Verlag, New York.
- Drumheller, D.S., Kipp, M.E. and Bedford, A., 1982, "Transient Wave Propagation in Bubbly Liquids", *J. Fluid Mech.*, Vol. 119, pp. 347-365.
- Ekeland, I. and Teman, R., 1976, "Convex Analysis and Variational Problems", North-Holland, Amsterdam.
- England, W.C., Firey, J.C. and Trapp, O.E., 1966, "Additional Velocity of Sound Measurements", *I. & E.C. Proc. Design and Develop.*, Vol. 5, pp. 198-202.
- Freitas Rachid, F.B., 2003, "A Thermodynamically Consistent Model for Cavitating Flows of Compressible Fluids", *Int. J. of Non-Linear Mechanics*, Vol. 38, pp. 1007-1018.
- Freitas Rachid, F.B., Mattos, H.S.C. and Saldanha da Gama, R. M., 1994, "Modelling of Hydraulic Transients in Damageable Elasto-Viscoplastic Piping Systems", *Appl. Math. Modelling*, Vol. 18, pp. 207-215.
- Freitas Rachid, F.B. and Costa Mattos, H., 1998, "Modelling of Pipeline Integrity Taking into Account the Fluid-Structure Interaction", *Int. J. for Num. Methods in Fluids*, Vol. 28, pp. 337-355.
- Frémond, M. and Nicolas, P., 1990, "Macroscopic Thermodynamics of Porous Media", *Continuum Mechanics and Thermodynamics*, Vol. 2, pp. 119-139.
- Gavrilyuk, S. and Saurel, R., 2002, "Mathematical and Numerical Modeling of Two-Phase Compressible Flows with Micro-Inertia", *J. of Comput. Physics*, Vol. 175, pp. 326-360.
- Germain, P. and P. Muller, P., 1995, "Introduction à la Mécanique des Milieux Continus", Masson, Paris.
- Graham, B.W., 1969, "One-Dimensional Two-Phase Flow", McGraw-Hill, New York.
- Henry, R.E. M.A. Grolmes, M.A. and Fauske, H.K., 1971, "Pressure Pulse Propagation in Two-phase One- and Two-component Mixtures", Argonne National Laboratory Rep. 7792.
- Ishii, M., 1975, "Thermo-Fluid Dynamics Theory of Two-Phase Flow", Eyrolles, Paris.
- Jeffrey, A., 1976, "Quasilinear Hyperbolic Systems and Waves", Pitman Publishing, London.

- Karplus, H.B., 1961, "Propagation of a Pressure Wave in a Mixture of Water and Steam", Armour Research Foundation of Illinois Institute of Technology Rep. 4132.
- Kobori, T., Yokoyama, S. and Miyashiro, H., 1955, "Propagation Velocity of Pressure Wave in Pipe Line" Hitachi Hyoron, Vol. 37, No. 10, pp. 345-404.
- Marchal, R., 1962, "Sound Velocity in Bubbly Liquids", Compt. Rend. Acad. Sci., Vol. 254, pp. 2524-2526.
- Moreau, J.J., Panagiotopoulos, P.D. and Strang, G., 1988, "Topics in Non-Smooth Mechanics", Birkhäuser.
- Semenov, N.I. and S.I. Kosterin, S.I., 1964, "Results of Studying the Speed of Sound in Moving Gas-liquid System" Teplonergetika, Vol. 11, pp. 46-51.
- Temkin, S., 1992, "Sound Speeds in Suspension in Thermodynamics Equilibrium", Phys. Fluids A, Vol. 4. No. 11, pp. 2399-2409.

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