

EQUILIBRIUM CONDITIONS AND SOUND VELOCITIES IN TWO-PHASE FLOWS*

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ABSTRACT. We consider a hierarchy of hyperbolic models describing single-component two-phase flows in pipelines, with applications to CO₂ capture and storage. The hierarchy is characterized by the number of equilibrium assumptions made. We present a formal proof that every additional level of enforced equilibrium lowers the propagation velocity of pressure waves. This subcharacteristic condition holds for arbitrary thermodynamic state equations. We present numerical examples relevant for CO₂ transport, and argue the importance for pipeline integrity simulations.

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1. INTRODUCTION

Two-phase pipe flow simulations have a number of industrial applications, including nuclear reactor safety analysis [1, 16], petroleum production [2, 8] and CO₂ capture and storage [10, 11]. In order to obtain models sufficiently tractable for such large-scale industrial simulations, some simplifying assumptions must be made. In particular, most relevant flow models are averaged in space to yield one-dimensional systems of hyperbolic balance laws, expressible in the form:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial x} + \mathbf{B} \frac{\partial \mathbf{W}(\mathbf{U})}{\partial x} = \mathbf{S}(\mathbf{U}), \quad (1)$$

to be solved for the unknown M -vector \mathbf{U} .

Furthermore, dynamical two-phase flow processes will generally not take place in thermodynamic equilibrium. However, the relaxation time towards equilibrium may for several practical purposes be small. For such cases, the equilibrium assumption may be a valid approximation.

In this paper, we are interested in studying how the assumptions of mechanical, thermal, and phase equilibrium influence the propagation of pressure waves in the resulting fluid-mechanical models. For smooth solutions, the models may be written in the general *relaxation* form [13]:

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{U}}{\partial x} = \frac{1}{\varepsilon} \mathbf{Q}(\mathbf{U}), \quad (2)$$

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where

$$\mathbf{A} = \frac{\partial \mathbf{F}(\mathbf{U})}{\partial \mathbf{U}} + \mathbf{B} \frac{\partial \mathbf{W}(\mathbf{U})}{\partial \mathbf{U}}. \quad (3)$$

The relaxation term \mathbf{Q} is assumed to be endowed with a constant linear operator \mathbf{P} with rank $m < M$ such that

$$\mathbf{P}\mathbf{Q}(\mathbf{U}) = 0. \quad (4)$$

This yields n homogeneous equations

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{P}\mathbf{A} \frac{\partial \mathbf{U}}{\partial x} = 0 \quad (5)$$

in the reduced variable

$$\mathbf{V} = \mathbf{P}\mathbf{U}. \quad (6)$$

We further assume that each \mathbf{V} uniquely determines a local equilibrium value $\mathbf{U} = \mathcal{E}(\mathbf{V})$, satisfying $\mathbf{Q}(\mathcal{E}(\mathbf{V})) = 0$ as well as

$$\mathbf{P}\mathcal{E}(\mathbf{V}) = \mathbf{V}. \quad (7)$$

One may then close the system (5) by imposing the equilibrium condition for \mathbf{U} :

$$\mathbf{U} = \mathcal{E}(\mathbf{V}). \quad (8)$$

As $\varepsilon \rightarrow 0$, the solutions to the relaxation system (2) are expected to approach the solutions to the relaxed system (5).

1.1. The Subcharacteristic Condition. A main issue in the study of such hyperbolic relaxation systems is the question of stability of the reduced solution \mathbf{V} . Central to this question is the *subcharacteristic condition*, a concept introduced by Liu [9]. This may be interpreted as a causality principle – the wave velocities of the relaxed system must be interlaced between the wave velocities of the relaxing system. A general, precise definition is stated by Chen et al. [3]:

Definition 1. *Let the M eigenvalues of the relaxing system (2) be given by*

$$\lambda_1 \leq \dots \leq \lambda_k \leq \lambda_{k+1} \leq \dots \leq \lambda_M \quad (9)$$

and the m eigenvalues of the relaxed system (5) and (8) be given by

$$\tilde{\lambda}_1 \leq \dots \leq \tilde{\lambda}_j \leq \tilde{\lambda}_{j+1} \leq \dots \leq \tilde{\lambda}_m. \quad (10)$$

Herein, the relaxation system (2) is applied to a local equilibrium state $\mathbf{U} = \mathcal{E}(\mathbf{V})$ such that

$$\lambda_k = \lambda_k(\mathcal{E}(\mathbf{V})), \quad \tilde{\lambda}_j = \tilde{\lambda}_j(\mathbf{V}). \quad (11)$$

*Now let the $\tilde{\lambda}_j$ be interlaced with λ_k in the following sense: Each $\tilde{\lambda}_j$ lies in the closed interval $[\lambda_j, \lambda_{j+M-m}]$. Then the relaxed system (5) is said to satisfy the **subcharacteristic condition** with respect to (2).*

1.2. Outline of This Paper. The purpose of this paper is to investigate the eigenvalues of relaxation two-phase flow models, with a particular focus on the subcharacteristic condition. The relaxation models we consider are highly related to the models presented by Saurel et al. [14]. Furthermore, exact expressions for the eigenvalues of these models already abound in the literature [6, 7, 15, 14]. However, these expressions typically involve different thermodynamic variables, making a direct comparison between them difficult.

The original contribution of this paper is expressing the eigenvalues in a form suitable for directly proving the subcharacteristic condition. In particular, for each new level n of equilibrium condition added, we are able to express the mixture sound velocity as

$$\hat{c}_{n+1}^{-2} = \hat{c}_n^{-2} + S_n, \quad (12)$$

where S_n can be written as a positive sum of squares. From this, the subcharacteristic condition follows directly.

Our paper is organized as follows: in Section 2, we describe the basic relaxation model of our hierarchy. Here no thermodynamic equilibrium assumptions are made.

In Section 3, we make our first equilibrium assumption; we instantaneously impose equal pressures for both phases. In Section 4, we add instantaneous temperature equilibrium to this model. Finally, in Section 5, we assume full thermodynamic equilibrium, including phase transitions.

Our work is briefly summarized in Section 7.

2. THE BASIC MODEL

Our starting point is the following relaxation two-phase flow model:

- *Mass conservation:*

$$\frac{\partial}{\partial t}(\rho_g \alpha_g) + \frac{\partial}{\partial x}(\rho_g \alpha_g v) = \mathcal{K}(\mu_\ell - \mu_g), \quad (13)$$

$$\frac{\partial}{\partial t}(\rho_\ell \alpha_\ell) + \frac{\partial}{\partial x}(\rho_\ell \alpha_\ell v) = \mathcal{K}(\mu_g - \mu_\ell). \quad (14)$$

- *Volume advection:*

$$\frac{\partial \alpha_g}{\partial t} + v \frac{\partial \alpha_g}{\partial x} = \mathcal{J}(p_g - p_\ell). \quad (15)$$

- *Momentum conservation:*

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v^2 + \alpha_g p_g + \alpha_\ell p_\ell) = 0. \quad (16)$$

- *Energy balance:*

$$\begin{aligned} \frac{\partial E_g}{\partial t} + \frac{\partial}{\partial x}(v(E_g + \alpha_g p_g)) + \frac{v}{\rho} \left(\rho_g \alpha_g \frac{\partial}{\partial x}(\alpha_\ell p_\ell) - \rho_\ell \alpha_\ell \frac{\partial}{\partial x}(\alpha_g p_g) \right) \\ = \mathcal{H}(T_\ell - T_g) + p^* \mathcal{J}(p_\ell - p_g) + \mu^* \mathcal{K}(\mu_\ell - \mu_g), \end{aligned} \quad (17)$$

$$\begin{aligned} \frac{\partial E_\ell}{\partial t} + \frac{\partial}{\partial x}(v(E_\ell + \alpha_\ell p_\ell)) + \frac{v}{\rho} \left(\rho_\ell \alpha_\ell \frac{\partial}{\partial x}(\alpha_g p_g) - \rho_g \alpha_g \frac{\partial}{\partial x}(\alpha_\ell p_\ell) \right) \\ = \mathcal{H}(T_g - T_\ell) + p^* \mathcal{J}(p_g - p_\ell) + \mu^* \mathcal{K}(\mu_g - \mu_\ell). \end{aligned} \quad (18)$$

Herein, we use the following nomenclature for phase $k \in \{g, \ell\}$:

- ρ_k - density of phase k ,
- p - pressure of phase k ,
- v - velocity common to both phases,
- α_k - volume fraction of phase k ,
- E_k - total energy density of phase k ,
- μ_k - chemical potential of phase k ,
- T_k - temperature of phase k ,
- p^* - effective pressure at the gas-liquid interface,
- μ^* - effective chemical potential at the gas-liquid interface,
- \mathcal{H} - temperature relaxation coefficient,
- \mathcal{J} - pressure relaxation coefficient,
- \mathcal{K} - phase transfer relaxation coefficient.

We here assume that the relaxation coefficients satisfy

$$\mathcal{H} \geq 0, \quad (19)$$

$$\mathcal{J} \geq 0, \quad (20)$$

$$\mathcal{K} \geq 0. \quad (21)$$

Furthermore, we have used the following abbreviations:

$$\rho = \rho_g \alpha_g + \rho_\ell \alpha_\ell, \quad (22)$$

$$E_g = \rho_g \alpha_g \left(e_g + \frac{1}{2} v^2 \right), \quad (23)$$

$$E_\ell = \rho_\ell \alpha_\ell \left(e_\ell + \frac{1}{2} v^2 \right) \quad (24)$$

$$(25)$$

where e_k is the specific internal energy of phase k .

Proposition 1. *The relaxation model (13)–(18) respects conservation of total mass, momentum and energy.*

Proof. Add (13) and (14) to obtain

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 0, \quad (26)$$

giving conservation of total mass. Conservation of total momentum follows directly from (16). Add (17) and (18) to obtain

$$\frac{\partial}{\partial t}(E_g + E_\ell) + \frac{\partial}{\partial x}(v(E_g + E_\ell + \alpha_g p_g + \alpha_\ell p_\ell)) = 0, \quad (27)$$

giving conservation of total energy. \square

Lemma 1. *The internal energy evolution equations can be written as:*

$$\frac{\partial}{\partial t}(\rho_g \alpha_g e_g) + \frac{\partial}{\partial x}(\rho_g \alpha_g e_g v) + \alpha_g p_g \frac{\partial v}{\partial x} = \mathcal{H}(T_\ell - T_g) + p^* \mathcal{J}(p_\ell - p_g) + \mu^* \mathcal{K}(\mu_\ell - \mu_g) \quad (28)$$

and

$$\frac{\partial}{\partial t}(\rho_\ell \alpha_\ell e_\ell) + \frac{\partial}{\partial x}(\rho_\ell \alpha_\ell e_\ell v) + \alpha_\ell p_\ell \frac{\partial v}{\partial x} = \mathcal{H}(T_g - T_\ell) + p^* \mathcal{J}(p_g - p_\ell) + \mu^* \mathcal{K}(\mu_g - \mu_\ell). \quad (29)$$

Proof. We may write (16) as

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} + \frac{1}{\rho} \frac{\partial}{\partial x} (\alpha_g p_g + \alpha_\ell p_\ell) = 0. \quad (30)$$

This yields the kinetic energy evolution equations:

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{1}{2} \rho_g \alpha_g v^2 \right) + \frac{\partial}{\partial x} \left(\frac{1}{2} \rho_g \alpha_g v^3 \right) + v \frac{\partial}{\partial x} (\alpha_g p_g) \\ + \frac{v}{\rho} \left(\rho_g \alpha_g \frac{\partial}{\partial x} (\alpha_\ell p_\ell) - \rho_\ell \alpha_\ell \frac{\partial}{\partial x} (\alpha_g p_g) \right) = 0 \end{aligned} \quad (31)$$

and

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{1}{2} \rho_\ell \alpha_\ell v^2 \right) + \frac{\partial}{\partial x} \left(\frac{1}{2} \rho_\ell \alpha_\ell v^3 \right) + v \frac{\partial}{\partial x} (\alpha_\ell p_\ell) \\ + \frac{v}{\rho} \left(\rho_\ell \alpha_\ell \frac{\partial}{\partial x} (\alpha_g p_g) - \rho_g \alpha_g \frac{\partial}{\partial x} (\alpha_\ell p_\ell) \right) = 0. \end{aligned} \quad (32)$$

Using (31)–(32) as well as (23)–(24) in (17)–(18), we recover (28)–(29). \square

Proposition 2. *Assume that the effective pressure and chemical potential can be written as convex combinations of the gas and liquid states as follows:*

$$p^* = \beta_p p_g + (1 - \beta_p) p_\ell, \quad (33)$$

$$\mu^* = \beta_\mu \mu_g + (1 - \beta_\mu) \mu_\ell, \quad (34)$$

where

$$\beta_p \in [0, 1], \quad (35)$$

$$\beta_\mu \in [0, 1]. \quad (36)$$

Then the relaxation model (13)–(18) satisfies the second law of thermodynamics.

Proof. We introduce the material derivative:

$$D_t = \frac{\partial}{\partial t} + v \frac{\partial}{\partial x}, \quad (37)$$

and we can write the fundamental thermodynamic differential as

$$D_t e_k = T_k D_t s_k + \frac{p_k}{\rho_k^2} D_t \rho_k, \quad (38)$$

where s_k is the specific entropy of phase k . By (38), as well as (13)–(15), we can rewrite (28)–(29) as entropy evolution equations:

$$D_t s_g = \frac{\mathcal{H}}{\rho_g \alpha_g} \frac{T_\ell - T_g}{T_g} + \frac{p^* - p_g}{\rho_g \alpha_g T_g} \mathcal{J}(p_\ell - p_g) + \left(\frac{\mu^* - \mu_g}{T_g} - s_g \right) \frac{\mathcal{K}}{\rho_g \alpha_g} (\mu_\ell - \mu_g), \quad (39)$$

$$D_t s_\ell = \frac{\mathcal{H}}{\rho_\ell \alpha_\ell} \frac{T_g - T_\ell}{T_\ell} + \frac{p^* - p_\ell}{\rho_\ell \alpha_\ell T_\ell} \mathcal{J}(p_g - p_\ell) + \left(\frac{\mu^* - \mu_\ell}{T_\ell} - s_\ell \right) \frac{\mathcal{K}}{\rho_\ell \alpha_\ell} (\mu_g - \mu_\ell), \quad (40)$$

through expansion of derivatives. Using the mass equations (13)–(14), we can write these as

$$\frac{\partial}{\partial t}(\rho_g \alpha_g s_g) + \frac{\partial}{\partial x}(\rho_g \alpha_g s_g v) = \mathcal{H} \frac{T_\ell - T_g}{T_g} + \frac{p^* - p_g}{T_g} \mathcal{J}(p_\ell - p_g) + \frac{\mu^* - \mu_g}{T_g} \mathcal{K}(\mu_\ell - \mu_g), \quad (41)$$

$$\frac{\partial}{\partial t}(\rho_\ell \alpha_\ell s_\ell) + \frac{\partial}{\partial x}(\rho_\ell \alpha_\ell s_\ell v) = \mathcal{H} \frac{T_g - T_\ell}{T_\ell} + \frac{p^* - p_\ell}{T_\ell} \mathcal{J}(p_g - p_\ell) + \frac{\mu^* - \mu_\ell}{T_\ell} \mathcal{K}(\mu_g - \mu_\ell), \quad (42)$$

By summing (41)–(42), we obtain an equation for the total entropy $S = \rho_g \alpha_g s_g + \rho_\ell \alpha_\ell s_\ell$:

$$\begin{aligned} \frac{\partial S}{\partial t} + \frac{\partial}{\partial x}(Sv) &= \mathcal{H} \frac{(T_\ell - T_g)^2}{T_g T_\ell} + \left(\frac{p_1 - p^*}{T_1} + \frac{p^* - p_2}{T_2} \right) \mathcal{J}(p_1 - p_2) \\ &\quad + \left(\frac{\mu_1 - \mu^*}{T_1} + \frac{\mu^* - \mu_2}{T_2} \right) \mathcal{K}(\mu_1 - \mu_2), \end{aligned} \quad (43)$$

or from (33)–(34):

$$\begin{aligned} \frac{\partial S}{\partial t} + \frac{\partial}{\partial x}(Sv) &= \mathcal{H} \frac{(T_\ell - T_g)^2}{T_g T_\ell} + \left(\frac{1 - \beta_p}{T_1} + \frac{\beta_p}{T_2} \right) \mathcal{J}(p_1 - p_2)^2 \\ &\quad + \left(\frac{1 - \beta_\mu}{T_1} + \frac{\beta_\mu}{T_2} \right) \mathcal{K}(\mu_1 - \mu_2)^2. \end{aligned} \quad (44)$$

It now follows from (35)–(36) that

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial x}(Sv) \geq 0. \quad (45)$$

□

Throughout this paper, we will assume that (33)–(36) are satisfied.

2.1. Wave Velocities. We now derive the wave velocities of the above basic model. We will first find it convenient to express the model in an equivalent form.

Lemma 2. *The relaxation model (13)–(18) can be equivalently expressed as:*

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 0, \quad (46)$$

$$D_t Y = \frac{\mathcal{K}}{\rho} (\mu_\ell - \mu_g), \quad (47)$$

$$D_t \alpha_g = \mathcal{J}(p_g - p_\ell), \quad (48)$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v^2 + \alpha_g p_g + \alpha_\ell p_\ell) = 0, \quad (49)$$

$$D_t s_g = \frac{\mathcal{H}}{\rho_g \alpha_g} \frac{T_\ell - T_g}{T_g} + \frac{p^* - p_g}{\rho_g \alpha_g T_g} \mathcal{J}(p_\ell - p_g) + \left(\frac{\mu^* - \mu_g}{T_g} - s_g \right) \frac{\mathcal{K}}{\rho_g \alpha_g} (\mu_\ell - \mu_g), \quad (50)$$

$$D_t s_\ell = \frac{\mathcal{H}}{\rho_\ell \alpha_\ell} \frac{T_g - T_\ell}{T_\ell} + \frac{p^* - p_\ell}{\rho_\ell \alpha_\ell T_\ell} \mathcal{J}(p_g - p_\ell) + \left(\frac{\mu^* - \mu_\ell}{T_\ell} - s_\ell \right) \frac{\mathcal{K}}{\rho_\ell \alpha_\ell} (\mu_g - \mu_\ell), \quad (51)$$

where

$$Y = \frac{\rho_g \alpha_g}{\rho}. \quad (52)$$

Proof. The equations (46) and (48)–(51) are simply restatements of (26), (15)–(16) and (39)–(40). To obtain (47), write (13) as

$$\frac{\partial}{\partial t}(\rho Y) + \frac{\partial}{\partial x}(\rho Y v) = \mathcal{K}(\mu_\ell - \mu_g) \quad (53)$$

and use (46). \square

Proposition 3. *The vector of eigenvalues of the basic relaxation model (13)–(18) is given by*

$$\mathbf{\Lambda}_0 = \begin{bmatrix} v - \hat{c}_0 \\ v \\ v \\ v \\ v \\ v + \hat{c}_0 \end{bmatrix}, \quad (54)$$

where

$$\hat{c}_0^2 = \alpha_g c_g^2 + \alpha_\ell c_\ell^2, \quad (55)$$

$$c_k = \left(\frac{\partial p}{\partial \rho_k} \right)_{s_k} \quad \forall k \in \{g, \ell\}. \quad (56)$$

Proof. From (47)–(48) and (39)–(40), we see directly that $(Y, \alpha_g, s_g, s_\ell)$ are characteristic variables corresponding to an eigenvalue with magnitude v . Now if we set $dY = d\alpha_g = ds_g = ds_\ell = 0$, we obtain the following reduced model:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 0, \quad (57)$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v^2 + \alpha_g p_g + \alpha_\ell p_\ell) = 0. \quad (58)$$

$$(59)$$

This can be written in quasilinear form:

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho v \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ \hat{c}_0^2 - v^2 & 2v \end{bmatrix} \frac{\partial}{\partial x} \begin{bmatrix} \rho \\ \rho v \end{bmatrix} = 0, \quad (60)$$

where

$$\hat{c}_0^2 = \left(\frac{\partial}{\partial \rho} (\alpha_g p_g + \alpha_\ell p_\ell) \right)_{Y, \alpha_g, s_g, s_\ell}. \quad (61)$$

Hence the two missing waves of the full model are sound waves with velocities $v \pm \hat{c}_0$. It now remains to determine \hat{c}_0 . The assumption of constant entropies gives us

$$dp_g = c_g^2 d\rho_g, \quad (62)$$

$$dp_\ell = c_\ell^2 d\rho_\ell. \quad (63)$$

Furthermore, the assumption of constant volume and mass fractions gives us

$$dY = \frac{\alpha_g}{\rho} (d\rho_g - d\rho) = \frac{\alpha_\ell}{\rho} (d\rho - d\rho_\ell) = 0, \quad (64)$$

Hence

$$d\rho = d\rho_g = d\rho_\ell. \quad (65)$$

We now recover (55) by using (62)–(63) and (65) in (61). \square

3. PRESSURE RELAXATION

We are now interested in the limit of *instantaneous pressure relaxation* in the model (13)–(18). We consider the the limit

$$\mathcal{J} \rightarrow \infty \quad (66)$$

and replace (15) with the assumption

$$p_g = p_\ell = p. \quad (67)$$

Furthermore, following (33) we write:

$$p^* = p. \quad (68)$$

In this limit, the energy equations (17)–(18) can be rewritten as

$$\begin{aligned} \frac{\partial E_g}{\partial t} + \frac{\partial}{\partial x}(vE_g) + \frac{\rho_g \alpha_g}{\rho} v \frac{\partial p}{\partial x} + p \left(\frac{\partial \alpha_g}{\partial t} + \frac{\partial}{\partial x}(\alpha_g v) \right) \\ = \mathcal{H}(T_\ell - T_g) + \mu^* \mathcal{K}(\mu_\ell - \mu_g), \end{aligned} \quad (69)$$

$$\begin{aligned} \frac{\partial E_\ell}{\partial t} + \frac{\partial}{\partial x}(vE_\ell) + \frac{\rho_\ell \alpha_\ell}{\rho} v \frac{\partial p}{\partial x} + p \left(\frac{\partial \alpha_\ell}{\partial t} + \frac{\partial}{\partial x}(\alpha_\ell v) \right) \\ = \mathcal{H}(T_g - T_\ell) + \mu^* \mathcal{K}(\mu_g - \mu_\ell). \end{aligned} \quad (70)$$

Furthermore, following the approach detailed in [6], we can derive volume fraction evolution equations:

$$\begin{aligned} \frac{\partial \alpha_g}{\partial t} + \frac{\partial}{\partial x}(\alpha_g v) - \alpha_g \frac{\rho \hat{c}_1^2}{\rho_g c_g^2} \frac{\partial v}{\partial x} = \frac{\rho \hat{c}_1^2}{\rho_g c_g^2 \rho_\ell c_\ell^2} (\alpha_g \Gamma_\ell + \alpha_\ell \Gamma_g) \mathcal{H}(T_\ell - T_g) \\ + \frac{\rho \hat{c}_1^2}{\rho_g c_g^2 \rho_\ell c_\ell^2} (\alpha_g (\Gamma_\ell \mu^* - \Gamma_\ell h_\ell - c_\ell^2) + \alpha_\ell (\Gamma_g \mu^* - \Gamma_g h_g - c_g^2)) \mathcal{K}(\mu_\ell - \mu_g) \end{aligned} \quad (71)$$

and

$$\begin{aligned} \frac{\partial \alpha_\ell}{\partial t} + \frac{\partial}{\partial x}(\alpha_\ell v) - \alpha_\ell \frac{\rho \hat{c}_1^2}{\rho_\ell c_\ell^2} \frac{\partial v}{\partial x} = \frac{\rho \hat{c}_1^2}{\rho_g c_g^2 \rho_\ell c_\ell^2} (\alpha_g \Gamma_\ell + \alpha_\ell \Gamma_g) \mathcal{H}(T_g - T_\ell) \\ + \frac{\rho \hat{c}_1^2}{\rho_g c_g^2 \rho_\ell c_\ell^2} (\alpha_g (\Gamma_\ell \mu^* - \Gamma_\ell h_\ell - c_\ell^2) + \alpha_\ell (\Gamma_g \mu^* - \Gamma_g h_g - c_g^2)) \mathcal{K}(\mu_g - \mu_\ell), \end{aligned} \quad (72)$$

where

$$h_k = e_k + \frac{p}{\rho_k} \quad \forall k \in \{g, \ell\}, \quad (73)$$

Γ_k is the *Grüneisen coefficient*:

$$\Gamma_k = \frac{1}{\rho_k} \left(\frac{\partial p}{\partial e_k} \right)_{\rho_k}, \quad (74)$$

and

$$\hat{c}_1^{-2} = \rho \left(\frac{\alpha_g}{\rho_g c_g^2} + \frac{\alpha_\ell}{\rho_\ell c_\ell^2} \right). \quad (75)$$

Proposition 4. *The pressure relaxed model corresponding to the limit $\mathcal{J} \rightarrow \infty$ in (13)–(18) can be written as:*

- Mass conservation:

$$\frac{\partial}{\partial t}(\rho_g \alpha_g) + \frac{\partial}{\partial x}(\rho_g \alpha_g v) = \mathcal{K}(\mu_\ell - \mu_g), \quad (76)$$

$$\frac{\partial}{\partial t}(\rho_\ell \alpha_\ell) + \frac{\partial}{\partial x}(\rho_\ell \alpha_\ell v) = \mathcal{K}(\mu_g - \mu_\ell). \quad (77)$$

- Momentum conservation:

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v^2 + p) = 0. \quad (78)$$

- Energy balance:

$$\begin{aligned} \frac{\partial E_g}{\partial t} + \frac{\partial}{\partial x}(v E_g) + \frac{\rho_g \alpha_g}{\rho} v \frac{\partial p}{\partial x} + p \alpha_g \frac{\rho \hat{c}_1^2}{\rho_g c_g^2} \frac{\partial v}{\partial x} \\ = \left(1 - p \frac{\alpha_g \Gamma_\ell + \alpha_\ell \Gamma_g}{\rho_g \alpha_\ell c_g^2 + \rho_\ell \alpha_g c_\ell^2}\right) \mathcal{H}(T_\ell - T_g) \\ + \left(1 - \frac{p}{\mu^*} \frac{\alpha_g(\Gamma_\ell \mu^* - \Gamma_\ell h_\ell - c_\ell^2) + \alpha_\ell(\Gamma_g \mu^* - \Gamma_g h_g - c_g^2)}{\rho_g \alpha_\ell c_g^2 + \rho_\ell \alpha_g c_\ell^2}\right) \mu^* \mathcal{K}(\mu_\ell - \mu_g), \end{aligned} \quad (79)$$

$$\begin{aligned} \frac{\partial E_\ell}{\partial t} + \frac{\partial}{\partial x}(v E_\ell) + \frac{\rho_\ell \alpha_\ell}{\rho} v \frac{\partial p}{\partial x} + p \alpha_\ell \frac{\rho \hat{c}_1^2}{\rho_\ell c_\ell^2} \frac{\partial v}{\partial x} \\ = \left(1 - p \frac{\alpha_g \Gamma_\ell + \alpha_\ell \Gamma_g}{\rho_g \alpha_\ell c_g^2 + \rho_\ell \alpha_g c_\ell^2}\right) \mathcal{H}(T_g - T_\ell) \\ + \left(1 - \frac{p}{\mu^*} \frac{\alpha_g(\Gamma_\ell \mu^* - \Gamma_\ell h_\ell - c_\ell^2) + \alpha_\ell(\Gamma_g \mu^* - \Gamma_g h_g - c_g^2)}{\rho_g \alpha_\ell c_g^2 + \rho_\ell \alpha_g c_\ell^2}\right) \mu^* \mathcal{K}(\mu_g - \mu_\ell). \end{aligned} \quad (80)$$

Proof. The equations (76)–(78) are simply restatements of (13)–(14) and (16). Substituting (71)–(72) into (69)–(70), we recover (79) and (80). \square

3.1. Wave Velocities. The wave structure of this model has been extensively analyzed in [6]. In particular, the vector of eigenvalues was found to be

$$\Lambda_1 = \begin{bmatrix} v - \hat{c}_1 \\ v \\ v \\ v \\ v + \hat{c}_1 \end{bmatrix}, \quad (81)$$

where the waves corresponding to the eigenvalue v represent one mass fraction wave and one entropy wave for each phase.

Proposition 5. *The relaxed model (76)–(80) satisfies the subcharacteristic condition with respect to the relaxation model (13)–(18), subject only to the natural conditions*

$$\rho_k > 0, \quad (82)$$

$$c_k > 0 \quad (83)$$

for $k \in \{g, \ell\}$. In particular, we have

$$\hat{c}_1^{-2} = \hat{c}_0^{-2} (1 + \alpha_g \alpha_\ell Z), \quad (84)$$

where

$$Z = \alpha_g \left[\left(\frac{c_\ell}{c_g} - \sqrt{\frac{\rho_\ell}{\rho_g}} \right)^2 + \left(2\sqrt{\frac{\rho_\ell c_\ell^2}{\rho_g c_g^2}} + 1 \right) \left(\sqrt{\frac{\rho_g c_g^2}{\rho_\ell c_\ell^2}} - 1 \right)^2 \right] \\ + \alpha_\ell \left[\left(\frac{c_g}{c_\ell} - \sqrt{\frac{\rho_g}{\rho_\ell}} \right)^2 + \left(2\sqrt{\frac{\rho_g c_g^2}{\rho_\ell c_\ell^2}} + 1 \right) \left(\sqrt{\frac{\rho_\ell c_\ell^2}{\rho_g c_g^2}} - 1 \right)^2 \right], \quad (85)$$

and it follows that $\hat{c}_1 \leq \hat{c}_0$.

Proof. By (54) and (81), it follows from Definition 1 that the subcharacteristic condition reduces to

$$\hat{c}_1 \leq \hat{c}_0. \quad (86)$$

Now note that

$$\hat{c}_0^2 \hat{c}_1^{-2} = (\alpha_g c_g^2 + \alpha_\ell c_\ell^2) (\alpha_g \rho_g + \alpha_\ell \rho_\ell) \left(\frac{\alpha_g}{\rho_g c_g^2} + \frac{\alpha_\ell}{\rho_\ell c_\ell^2} \right). \quad (87)$$

Expanding and using $\alpha_g + \alpha_\ell = 1$, we can write this as

$$\hat{c}_0^2 \hat{c}_1^{-2} - 1 = \alpha_g^2 \alpha_\ell \left(\frac{\rho_g c_g^2}{\rho_\ell c_\ell^2} + \frac{c_\ell^2}{c_g^2} + \frac{\rho_\ell}{\rho_g} - 3 \right) + \alpha_\ell^2 \alpha_g \left(\frac{\rho_\ell c_\ell^2}{\rho_g c_g^2} + \frac{c_g^2}{c_\ell^2} + \frac{\rho_g}{\rho_\ell} - 3 \right) = \alpha_g \alpha_\ell Z, \quad (88)$$

and (84) follows. \square

4. TEMPERATURE RELAXATION

We now focus on the limit of *instantaneous relaxation* of both the pressure and temperature in the model (13)–(18). We take as our starting point the model (76)–(80) and consider the limit

$$\mathcal{H} \rightarrow \infty. \quad (89)$$

In this limit, we replace (79)–(80) with their sum

$$\frac{\partial}{\partial t} (E_g + E_\ell) + \frac{\partial}{\partial x} (v(E_g + E_\ell + p)) = 0 \quad (90)$$

and make the assumption

$$T_g = T_\ell = T. \quad (91)$$

4.1. Wave Velocities. This model was analyzed in [6]. In particular, the vector of eigenvalues was found to be

$$\Lambda_2 = \begin{bmatrix} v - \hat{c}_2 \\ v \\ v \\ v + \hat{c}_2 \end{bmatrix}, \quad (92)$$

where the waves corresponding to the eigenvalue v represent one mass fraction wave and one mixture entropy wave. Furthermore, the mixture sound velocity was found as

$$\hat{c}_2^{-2} = \hat{c}_1^{-2} + \frac{\rho}{T} \frac{C_{p,g} C_{p,\ell} (\zeta_\ell - \zeta_g)^2}{C_{p,g} + C_{p,\ell}}, \quad (93)$$

where for $k \in \{g, \ell\}$, ζ_k is defined as

$$\zeta_k = \left(\frac{\partial T}{\partial p} \right)_{s_k} \quad (94)$$

and $C_{p,k}$ are the extensive heat capacities

$$C_{p,k} = \rho_k \alpha_k c_{p,k}, \quad (95)$$

where

$$c_{p,k} = T \left(\frac{\partial s_k}{\partial T} \right)_p. \quad (96)$$

Proposition 6. *The temperature relaxed model (76)–(78) augmented with (90)–(91) satisfies the subcharacteristic condition with respect to the relaxation model (76)–(80), subject only to the natural constraints*

$$\rho \geq 0, \quad (97)$$

$$T > 0, \quad (98)$$

$$C_{p,k} > 0. \quad (99)$$

Proof. By (81) and (92), it follows from Definition 1 that the subcharacteristic condition reduces to

$$\hat{c}_2 \leq \hat{c}_1, \quad (100)$$

which follows directly from (93) and (97)–(99). \square

5. PHASE TRANSFER RELAXATION

We now consider the case of simultaneous instantaneous relaxation of both the pressure, temperature and chemical potential. In the context of the model of Section 4, this corresponds to the limit

$$\mathcal{K} \rightarrow \infty. \quad (101)$$

In this limit, we may replace (76)–(77) with their sum, and make the additional assumption

$$\mu_g = \mu_\ell = \mu. \quad (102)$$

Assuming (34), we may also write

$$\mu^* = \mu. \quad (103)$$

The model thus obtained may be restated as follows:

- *Mass conservation:*

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) = 0 \quad (104)$$

- *Momentum conservation:*

$$\frac{\partial}{\partial t} (\rho v) + \frac{\partial}{\partial x} (\rho v^2 + p) = 0. \quad (105)$$

- *Energy conservation:*

$$\frac{\partial}{\partial t} (E_g + E_\ell) + \frac{\partial}{\partial x} (v(E_g + E_\ell + p)) = 0, \quad (106)$$

which we recognize as the *homogeneous equilibrium model*.

5.1. Wave Velocities. The wave structure of the homogeneous equilibrium model is well known, and the vector of eigenvalues can be written as

$$\Lambda_3 = \begin{bmatrix} v - \hat{c}_3 \\ v \\ v + \hat{c}_3 \end{bmatrix}, \quad (107)$$

where

$$\hat{c}_3 = \left(\frac{\partial p}{\partial \rho} \right)_s \quad (108)$$

and s is the mixture entropy. Saurel et al. [14] state the following expression for \hat{c}_3 :

$$\hat{c}_3^{-2} = \hat{c}_1^{-2} + \rho T \left[\frac{\rho_g \alpha_g}{c_{p,g}} \left(\frac{\partial s_g}{\partial p} \right)_{\text{sat}}^2 + \frac{\rho_\ell \alpha_\ell}{c_{p,\ell}} \left(\frac{\partial s_\ell}{\partial p} \right)_{\text{sat}}^2 \right], \quad (109)$$

where $(\cdot)_{\text{sat}}$ denotes differentiation along the boiling point curve, where

$$\mu_g = \mu_\ell. \quad (110)$$

Proposition 7. *The relaxed model (104)–(106) satisfies the subcharacteristic condition with respect to the relaxation model of Section 4, subject only to the natural conditions*

$$\rho_k > 0, \quad (111)$$

$$T > 0, \quad (112)$$

$$C_k > 0 \quad (113)$$

for $k \in \{g, \ell\}$. In particular, we have

$$\hat{c}_3^{-2} = \hat{c}_2^{-2} + \rho T (C_{p,g} + C_{p,\ell}) \left(\frac{\rho_\ell - \rho_g}{\rho_g \rho_\ell (h_\ell - h_g)} + \frac{\zeta_g C_{p,g} + \zeta_\ell C_{p,\ell}}{T (C_{p,g} + C_{p,\ell})} \right)^2, \quad (114)$$

and it follows that $\hat{c}_3 \leq \hat{c}_2$.

Proof. By (92) and (107), it follows from Definition 1 that the subcharacteristic condition reduces to

$$\hat{c}_3 \leq \hat{c}_2. \quad (115)$$

From the Clausius-Clapeyron relation we obtain

$$\left(\frac{\partial s_k}{\partial p} \right)_{\text{sat}} = -c_{p,k} \left(\frac{\zeta_k}{T} + \frac{\rho_\ell - \rho_g}{\rho_g \rho_\ell (h_\ell - h_g)} \right). \quad (116)$$

Substituting in (109) and using (93) we recover (114). \square

6. APPLICATION TO CO₂ TRANSPORT

In this section, we wish to illustrate the relevance of these results for simulating the transport of CO₂ in pipelines. For pipeline integrity simulations, a correct modelling of the propagation velocity of pressure waves is important in order to capture the dynamics of a rapid depressurization. For CO₂ at the boiling point at

$T = 273$ K, the following physical parameters apply:

$$c_g = 205 \text{ m/s}, \quad (117)$$

$$c_\ell = 441 \text{ m/s}, \quad (118)$$

$$\rho_g = 135 \text{ kg/m}^3, \quad (119)$$

$$\rho_\ell = 861 \text{ kg/m}^3, \quad (120)$$

$$c_{p,g} = 2556 \text{ J/(kg} \cdot \text{K)}, \quad (121)$$

$$c_{p,\ell} = 2996 \text{ J/(kg} \cdot \text{K)}. \quad (122)$$

The sound velocities \hat{c}_1 , \hat{c}_2 and \hat{c}_3 are plotted in Figure 1.

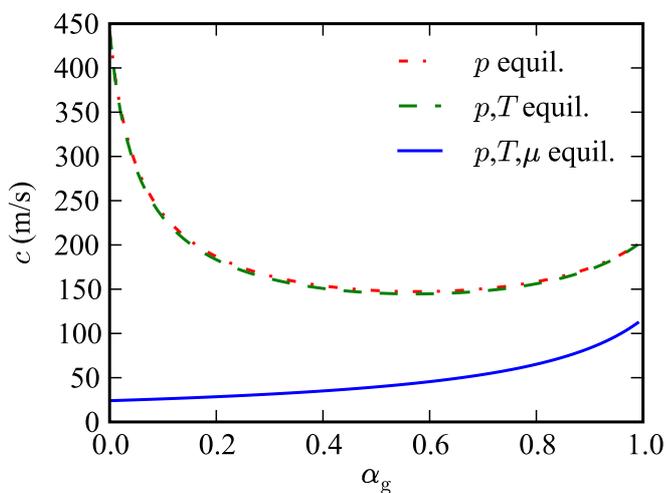


FIGURE 1. Mixture sound velocity of two-phase CO_2 as a function of gas fraction.

We note that \hat{c}_1 and \hat{c}_2 are virtually indistinguishable to plotting accuracy. However, the phase transfer equilibrium velocity \hat{c}_3 is significantly lower; note also that we do not recover the one-phase sound velocities (117) and (118) in the limits $\alpha_k \rightarrow 1$.

The low values of \hat{c}_3 predicted by the homogeneous equilibrium model are unphysical, a fact that has been previously noted by several authors [7, 12, 15]. On the other hand, the values \hat{c}_1 and \hat{c}_2 predicted by the models of Sections 3 and 4 agree well with experiments [4, 5].

This indicates that the pressure and temperature relaxed models described in Sections 3–4 should be used for numerical simulations of CO_2 pipeline transport. The full equilibrium model of Section 5 would yield an unphysically slow propagation of pressure pulses.

7. SUMMARY

We have investigated a hierarchy of *relaxation models* for two-phase flow. In particular, we have studied models with equilibrium assumptions imposed in the following order:

- (1) pressure equilibrium (p equil.)
- (2) temperature equilibrium (p, T equil.)
- (3) phase transfer equilibrium (p, T, μ equil.)

We have shown that the mixture sound velocities of these models satisfy the inequalities

$$\hat{c}_3 \leq \hat{c}_2 \leq \hat{c}_1 \leq \hat{c}_0. \quad (123)$$

In particular, we may write \hat{c} as

$$\hat{c}_{n+1}^{-2} = \hat{c}_n^{-2} + S_n \quad (124)$$

where the parameters $S_n \geq 0$ are given by

$$S_0 = \hat{c}_0^{-2} \alpha_g \alpha_\ell Z, \quad (125)$$

$$S_1 = \frac{\rho}{T} \frac{C_{p,g} C_{p,\ell} (\zeta_\ell - \zeta_g)^2}{C_{p,g} + C_{p,\ell}}, \quad (126)$$

$$S_2 = \rho T (C_{p,g} + C_{p,\ell}) \left(\frac{\rho_\ell - \rho_g}{\rho_g \rho_\ell (h_\ell - h_g)} + \frac{\zeta_g C_{p,g} + \zeta_\ell C_{p,\ell}}{T(C_{p,g} + C_{p,\ell})} \right)^2, \quad (127)$$

and Z is given by (85).

We have argued that these observations are highly relevant for simulations of pipeline integrity for CO₂ transport. In particular, the assumption of instantaneous phase equilibrium leads to a severe underestimation of the propagation velocity of pressure pulses.

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