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NUMERICAL MODELING OF TWO-PHASE FLOWS USING THE TWO-FLUID TWO-PRESSURE APPROACH

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The present paper is devoted to the computation of two-phase flows using the two-fluid approach. The overall model is hyperbolic and has no conservative form. No instantaneous local equilibrium between phases is assumed, which results in a two-velocity two-pressure model. Original closure laws for interfacial velocity and interfacial pressure are proposed. These closures allow to deal with discontinuous solutions such as shock waves and contact discontinuities without ambiguity for the definition of Rankine-Hugoniot jump relations. Each field of the convective system is investigated, providing that the maximum principle for the volume fraction and the positivity of densities and internal energies are ensured when focusing on the Riemann problem. Two Finite Volume methods are presented, based on the Rusanov scheme and on an approximate Godunov scheme. Relaxation terms are taken into account using a fractional step method. Eventually, numerical tests illustrate the ability of both methods to compute two-phase flows.

Keywords: two-phase flow, hyperbolic system, non-conservative terms, resonance, Finite Volume

AMS Subject Classification: 76T10, 35F25, 35L67, 76M12

1. Introduction

Computation of two-phase flows has been generally based on the homogeneous approach in order to compute either gas-solid flows or gas-liquid flows^{14,19,52}. When focusing on the two-fluid approach, the problem becomes intricate, due to the fact that two-fluid models with an equilibrium pressure assumption have some well-known drawbacks. One of them is that these systems contain non-conservative

terms (which is an serious difficulty^{7,36,11,44}). Furthermore, such models do not necessarily remain hyperbolic in all situations, which means that the initial value problem may be "ill-posed" for a large class of initial conditions. Last but not least, it clearly appears that the maximum principle for the volume fraction does not necessarily hold in general even for smooth solutions, except perhaps in some situations corresponding to the modeling of gas particle flows including granular pressure effects^{8,22,28,49}).

Some recent ideas have been proposed to cope with this kind of system. Roughly speaking, one way to deal with these is based on the use of developments with respect to a small parameter (for instance the relative velocity 52,53, the volume fraction 43 or the density ratio). Other ways to deal with these are based on use of an extension of the notion of upwinding²¹ or of the use of fractional step techniques^{9,8,31}. Though numerical results are rather encouraging, one may still wonder whether the lack of hyperbolicity has not been enforced by some failure in closure assumptions. Some time ago, V.H. Ransom and D.L. Hicks⁴⁰ suggested to use a two-pressure model based on a eight-equation model. More recently, M.R. Baer and J.W. Nunziato suggested in Ref. ² to adopt a similar approach. Their model has been studied and extended by A.K. Kapila et al.³⁵ and S. Gavrilyuk and R. Saurel²⁰. Other two-pressure models have been proposed by J. Glimm and co-workers^{23,24} and by K.A. Gonthier and J.M. Powers²⁹. Here, the system is composed by seven partial differential equations: one transport equation for the volume fraction, two for the mass of each fluid, two for the momentum of each fluid and two for the energy of each fluid. Several definitions of the interfacial velocity and of the interfacial pressure have been proposed in references mentioned above. The present paper adopts an original approach, based on the analysis of the one-dimensional Riemann problem and on the definition of discontinuous solutions in order to deal with nonconservative products and to ensure the maximum principle for the volume fraction, as presented in Ref. ¹⁰. We restrict ourselves to the one-dimensional framework.

The present paper is organized as follows. The first section presents the model devoted to the computation of two-phase flows, using the two-fluid approach. No assumption towards pressure equilibrium is required here and the overall model is unconditionally hyperbolic and non-conservative. Properties of smooth solutions are investigated. Several closures for the interfacial velocity and the interfacial pressure are then proposed. Assuming that the interface between two mixtures of fluids remains infinitely thin when restricting to convective effects, three different forms of interfacial velocity are exhibited. In other words, these closures for the interfacial velocity permit to obtain a linearly degenerate field associated with the wave which initially separates two mixtures. The definition of the interfacial pressure is strongly related to the closure of the non-conservative terms. A first definition enables to complement the system with a natural entropy inequality and a field by field study of the solution of the one-dimensional Riemann problem is provided. Another way of closure for the interfacial pressure is proposed, but is not investigated here. We discuss afterwards about the approximation of solutions of

the system. The approximation of convective terms and source terms is cast into two different steps using a splitting method. The convective part is computed using Finite Volume schemes adapted to the non-conservative frame. Two methods, based on the Rusanov scheme⁴² and on the VFRoe-ncv scheme⁴, are tested here. The latter scheme is a Finite Volume linearised method, like the Roe scheme⁴¹, but using a non-conservative variable for the linearisation (VFRoe-ncv: Volumes Finis Roe - non-conservative variable). Concerning the relaxation terms (drag force and pressure relaxation), we propose an approximation in agreement with the properties satisfied by smooth solutions. Eventually, several numerical tests are performed to compare the robustness and the accuracy of both methods when computing shock tube test cases as well as the water faucet problem.

2. The two-fluid two-pressure model

We present here the global two-fluid system. We focus our analysis on the convective part of the system. The different properties of this system are investigated for smooth solutions before studying the associated Riemann problem.

2.1. Governing equations

The governing set of equations contains convective terms, source terms and diffusive terms. It takes the form for $t > 0, x \in \mathbb{R}$:

$$(Id + D(W))\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial W}{\partial x} = S(W) + \frac{\partial}{\partial x}\left(E(W)\frac{\partial W}{\partial x}\right), \quad (2.1)$$

where W = W(t, x) is the unknown function from $\mathbb{R}_+ \times \mathbb{R}$ to Ω (with Ω a subset of \mathbb{R}^7), F, and S are functions from Ω to \mathbb{R}^7 , while C, D and E are functions from Ω to $\mathbb{R}^{7\times7}$ and Id is the identity matrix of $\mathbb{R}^{7\times7}$. Of course, the extension of (2.1) to a multidimensional framework is classical. The so called conservative variable W is

$$W = {}^{T}(\alpha_1, \alpha_1 \rho_1, \alpha_1 \rho_1 U_1, \alpha_1 E_1, \alpha_2 \rho_2, \alpha_2 \rho_2 U_2, \alpha_2 E_2),$$

where α_k is the volume fraction of phase k, ρ_k , U_k and E_k are respectively the density, the velocity and the total energy of phase k, k = 1, 2. We also define the mass fraction $m_k = \alpha_k \rho_k$ and the pressure P_k of phase k. Let $\Omega = \{W \in \mathbb{R}^7; \alpha_1 \in \mathbb{R}^7 \}$ $(0,1), m_k > 0, E_k/\rho_k - (U_k)^2/2 > 0, k = 1,2$ be the set of admissible states. The convective part (i.e. the left handside) of system (2.1) is defined by

$$D(W)\frac{\partial W}{\partial t} = \begin{pmatrix} 0\\0\\0\\P_{i}\partial_{t}\alpha_{1}\\0\\0\\P_{i}\partial_{t}\alpha_{2} \end{pmatrix}, F(W) = \begin{pmatrix} 0\\\alpha_{1}\rho_{1}U_{1}\\\alpha_{1}(\rho_{1}U_{1}^{2} + P_{1})\\\alpha_{1}U_{1}(E_{1} + P_{1})\\\alpha_{2}\rho_{2}U_{2}\\\alpha_{2}(\rho_{2}U_{2}^{2} + P_{2})\\\alpha_{2}U_{2}(E_{2} + P_{2}) \end{pmatrix}, C(W)\frac{\partial W}{\partial x} = \begin{pmatrix} V_{i}\partial_{x}\alpha_{1}\\0\\-P_{i}\partial_{x}\alpha_{1}\\0\\0\\+P_{i}\partial_{x}\alpha_{1}\\0 \end{pmatrix}$$

where $V_i(W)$ and $P_i(W)$ are the interfacial velocity and the interfacial pressure. Source terms S may be written⁴⁵:

$$S(W) = {}^{T}(K_{P}(P_{1} - P_{2}),$$

$$\dot{m}, -K_{U}(U_{1} - U_{2}) + \dot{m}V_{i}, -K_{U}V_{i}(U_{1} - U_{2}) + \dot{m}E_{i},$$

$$-\dot{m}, +K_{U}(U_{1} - U_{2}) - \dot{m}V_{i}, +K_{U}V_{i}(U_{1} - U_{2}) - \dot{m}E_{i})$$

where we note $K_U(W)$ and $K_P(W)$ the positive functions of velocity and pressure relaxation, $\dot{m}(W)$ the mass transfer and $E_i(W)$ the interfacial energy. Note that terms $K_U(W)(U_1 - U_2)$ correspond to drag force effects. Viscous terms are accounted for through a contribution concerning E(W):

$$E(W)\frac{\partial W}{\partial x} = \begin{pmatrix} 0, \\ 0, \\ \partial_x(\mu_1 \Gamma(U_1)) \\ \partial_x(\mu_1 \Gamma(U_1)U_1) + \partial_x(\kappa_1 \partial_x T_1) \\ 0, \\ \partial_x(\mu_2 \Gamma(U_2)) \\ \partial_x(\mu_2 \Gamma(U_2)U_2) + \partial_x(\kappa_2 \partial_x T_2) \end{pmatrix}, \text{ with } \Gamma(U_k) = \frac{4}{3}\partial_x U_k, \quad (2.2)$$

where T is the temperature $T = P/\rho$, and μ_k and κ_k refer to the laminar viscosity and the conductivity coefficient of phase k, k = 1, 2. The coefficient 4/3 in the definition of the viscous stress tensor Γ is provided from the 3D framework.

The system (2.1) is associated with an initial datum $W_0 \in \Omega$:

$$W(t=0,x) = W_0(x), \quad x \in \mathbb{R}, \tag{2.3}$$

and must be complemented by some closure laws. The volume fractions must comply with

$$\alpha_1 + \alpha_2 = 1$$
.

Moreover, the total energies E_k follow from

$$E_k = \rho_k e_k + \rho_k (U_k)^2 / 2, \quad k = 1, 2,$$

where the internal energies e_k satisfy the equations of state (also called the thermodynamics laws)

$$e_k = \varepsilon_k(P_k, \rho_k), \quad k = 1, 2.$$

Remark 1. The system (2.1) is obtained after an averaging process (see Ref. ³⁴) and variables considered here are mean values. Initially, phases are separated one from another, and a thermodynamics law is available in each phase. Usually, laws which link thermodynamical variables after the averaging process may differ from initial laws. However, basic laws, such as the perfect gas equation of state or the Tammann equation of state, which satisfy

$$\rho_k \varepsilon_k(P_k, \rho_k) = g_k P_k + b_k \rho_k + c_k \tag{2.4}$$

(where $g_k > 0$, b_k and c_k are real constants) remain unchanged after the averaging process unlike more complex thermodynamical laws such as Van der Waals equation of state (see appendix A of Ref. ¹⁵ for more details).

One still needs to detail both the interfacial pressure P_i and the interfacial velocity V_i . We assume that V_i satisfies

$$V_i(W) = \beta(W)U_1 + (1 - \beta(W))U_2 \tag{2.5}$$

The scalar dimensionless function β is non-negative and bounded by 1. Definition (2.5) enables us to account for kinematic equilibrium since $U_2 = U_1$ implies $V_i =$ $U_1 = U_2$. Concerning P_i , one may expect that the relation

$$U_1 = U_2 \text{ and } P_1 = P_2 \implies P_i = P_1 = P_2$$
 (2.6)

holds. Of course, equation (2.5) and relation (2.6) are too general to deduce at this stage explicit forms of V_i and P_i . Nonetheless, several properties for the convective part of the system (2.1) are available.

2.2. Some properties of the convective system

Though system (2.1) is not completely closed (V_i and P_i have not been explicited), some properties are exposed below to determine whether this system is relevant to describe two-phase flows. Hyperbolicity, the maximum principle and the positivity requirement are investigated. The isentropic framework is briefly dealt with too. We emphasize that all the following results are independent from the closure of interfacial pressure P_i and interfacial velocity V_i .

The homogeneous problem associated with (2.1) may be written under the following form for t > 0 and $x \in \mathbb{R}$:

$$\partial_t(\alpha_1) + V_i(W) \,\partial_x \alpha_1 = 0, \tag{2.7a}$$

$$\partial_t(\alpha_1 \rho_1) + \partial_x(\alpha_1 \rho_1 U_1) = 0, \tag{2.7b}$$

$$\partial_t(\alpha_2 \rho_2) + \partial_x(\alpha_2 \rho_2 U_2) = 0, \tag{2.7c}$$

$$\partial_t(\alpha_1 \rho_1 U_1) + \partial_x \left(\alpha_1 \rho_1 U_1^2 + \alpha_1 P_1\right) - P_i(W) \,\partial_x \alpha_1 = 0,\tag{2.7d}$$

$$\partial_t(\alpha_2 \rho_2 U_2) + \partial_x \left(\alpha_2 \rho_2 U_2^2 + \alpha_2 P_2\right) + P_i(W) \,\partial_x \alpha_1 = 0,\tag{2.7e}$$

$$\partial_t(\alpha_1 E_1) + \partial_x(\alpha_1 U_1(E_1 + P_1)) - V_i(W)P_i(W)\partial_x \alpha_1 = 0, \tag{2.7f}$$

$$\partial_t(\alpha_2 E_2) + \partial_x(\alpha_2 U_2(E_2 + P_2)) + V_i(W)P_i(W)\partial_x \alpha_1 = 0. \tag{2.7g}$$

We define the celerity c_k and the coefficient $\hat{\gamma}_k$ of phase k by

$$\rho_k(c_k)^2 = \left(\frac{P_k}{\rho_k} - \rho_k \frac{\partial \varepsilon_k}{\partial \rho_k}\right) \left(\frac{\partial \varepsilon_k}{\partial P_k}\right)^{-1}, \text{ and } \rho_k(c_k)^2 = \hat{\gamma}_k P_k,$$

and the partial specific entropy s_k of phase k, k = 1, 2, by $s_k = \varsigma_k(P_k, \rho_k)$, where ς_k complies with

$$\hat{\gamma}_k P_k \frac{\partial \varsigma_k}{\partial P_k} + \rho_k \frac{\partial \varsigma_k}{\partial \rho_k} = 0.$$

The following proposition holds:

Proposition 1. The homogeneous problem (2.7) is non-strictly hyperbolic on Ω , in the sense that it admits real eigenvalues and the right eigenvectors span the whole space \mathbb{R}^7 , except when some eigenvalues coincide. These eigenvalues are simply:

$$\begin{array}{ccc} \lambda_1 = V_i, \\ \lambda_2 = U_1 - c_1, & \lambda_3 = U_1, & \lambda_4 = U_1 + c_1, \\ \lambda_5 = U_2 - c_2, & \lambda_6 = U_2, & \lambda_7 = U_2 + c_2. \end{array}$$

Moreover, the fields associated with the waves λ_2 , λ_4 , λ_5 and λ_7 are genuinely non-linear and the fields associated with the waves λ_3 and λ_6 are linearly degenerate.

Refer to Ref. 26 for the definition of genuinely non-linear or linearly degenerate fields.

Proof. Let us define the vector

$$Y = {}^{T}(\alpha_1, s_1, U_1, P_1, s_2, U_2, P_2).$$

The study of the hyperbolicity of system (2.7) does not depend on the use of W or Y. The system (2.7) may be written with respect to Y, which gives for regular solutions in Ω

$$\frac{\partial Y}{\partial t} + B(Y)\frac{\partial Y}{\partial x} = 0,$$

where

$$B(Y) = \begin{pmatrix} V_i & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta_2(Y) & U_1 & 0 & 0 & 0 & 0 & 0 \\ \beta_3(Y) & 0 & U_1 & \tau_1 & 0 & 0 & 0 \\ \beta_4(Y) & 0 & \hat{\gamma}_1 P_1 & U_1 & 0 & 0 & 0 \\ \beta_5(Y) & 0 & 0 & 0 & U_2 & 0 & 0 \\ \beta_6(Y) & 0 & 0 & 0 & 0 & U_2 & \tau_2 \\ \beta_7(Y) & 0 & 0 & 0 & 0 & \hat{\gamma}_2 P_2 & U_2 \end{pmatrix}.$$
 (2.8)

The coefficients β_p , p = 2, ..., 7 can be written as

$$\begin{split} \beta_{3k-1}(Y) &= (-1)^k \frac{(U_k - V_i)(P_k - P_i)}{\alpha_k \rho_k} \left(\frac{\partial \varepsilon_k}{\partial P_k}\right)^{-1} \frac{\partial \varsigma_k}{\partial P_k}, \\ \beta_{3k}(Y) &= (-1)^{k+1} \frac{P_k - P_i}{\alpha_k \rho_k}, \\ \beta_{3k+1}(Y) &= (-1)^{k+1} \frac{U_k - V_i}{\alpha_k \rho_k} \left(P_i - \rho_k^2 \frac{\partial \varepsilon_k}{\partial \rho_k}\right) \left(\frac{\partial \varepsilon_k}{\partial P_k}\right)^{-1}, \end{split}$$

and we note $\tau_k = 1/\rho_k$, k = 1, 2.

The hyperbolicity of system (2.7) is then proved by a classical analysis of the matrix B. We focus now on the right eigenvectors of B. The matrix R of right eigenvectors

of B is

$$R(Y) = \begin{pmatrix} r_1^{(1)}(Y) & 0 & 0 & 0 & 0 & 0 & 0 \\ r_1^{(2)}(Y) & 1 & 0 & 0 & 0 & 0 & 0 \\ r_1^{(3)}(Y) & 0 & \tau_1 & \tau_1 & 0 & 0 & 0 \\ r_1^{(4)}(Y) & 0 & -c_1 & c_1 & 0 & 0 & 0 \\ r_1^{(5)}(Y) & 0 & 0 & 0 & 1 & 0 & 0 \\ r_1^{(6)}(Y) & 0 & 0 & 0 & 0 & \tau_2 & \tau_2 \\ r_1^{(7)}(Y) & 0 & 0 & 0 & 0 & -c_2 & c_2 \end{pmatrix}$$

$$(2.9)$$

where $r_1^{(p)}$ is the p^{th} component of the first right eigenvector of matrix B, that is

$$r_1(Y) = {}^{T} \left(1, \frac{-\beta_2}{U_1 - V_i}, \frac{\tau_1 \beta_4 - (U_1 - V_i)\beta_3}{(U_1 - V_i)^2 - c_1^2}, \frac{c_1^2 \beta_3 - \tau_1 (U_1 - V_i)\beta_4}{\tau_1 ((U_1 - V_i)^2 - c_1^2)}, \frac{-\beta_5}{U_2 - V_i}, \frac{\tau_2 \beta_7 - (U_2 - V_i)\beta_6}{(U_2 - V_i)^2 - c_2^2}, \frac{c_2^2 \beta_6 - \tau_2 (U_2 - V_i)\beta_7}{\tau_2 ((U_2 - V_i)^2 - c_2^2)} \right).$$

Then, we can provide the following conditions ensuring that the right eigenvectors of B span \mathbb{R}^7

$$\lambda_1 \neq \lambda_p, \quad p = 2, 4, 5, 7.$$
 (2.10)

If the conditions (2.10) are satisfied, then the right eigenvectors of B(Y) are linearly independent one to the other (see Ref. ⁵⁰ for the nature of the fields associated with the waves λ_p , p = 2, ..., 7). \square

Let us emphasize that the result on the hyperbolicity of system (2.7) is very important when dealing with two-fluid models. Indeed, no condition is required here on the initial datum (2.3) to obtain real eigenvalues, contrary to the classical twofluid one-pressure framework. This property is merely due to the partial differential equation for the volume fraction α_1 , which allows to replace non-conservative terms $P_i \partial_t \alpha_k$ by $-P_i V_i \partial_x \alpha_k$ for k=1,2. Note that the hyperbolicity is non-strict, which means that some eigenvalues may coincide. In this case, a resonant behaviour may $occur^{25,33,48,51}$

Concerning the structure of matrix B and matrix R, one may see that phases 1 and 2 are only coupled by the first column, corresponding to $\partial_x \alpha_1$ in B and related to the wave $\lambda_1 = V_i$. This largely reduces the complexity of the study of the convective system (2.7) since phases evolve independently on each side of the 1-wave. Nevertheless, the nature of the field associated with λ_1 remains unknown, since V_i is not still defined.

We now focus on the maximum principle for the volume fraction α_1 and on the positivity constraint for partial masses m_k , k=1,2. The study which follows is restricted to smooth solutions of system (2.7). The Riemann problem is presented afterwards and the maximum principle and the positivity requirements through elementary waves are investigated in order to extend these properties to discontinuous solutions.

First, let us consider the maximum principle on the volume fraction α_1 . The partial differential equation associated with α_1 is written with a general relaxation term in pressure:

$$\frac{\partial \alpha_1}{\partial t} + V_i(W) \frac{\partial \alpha_1}{\partial x} = \frac{\alpha_1 \alpha_2}{\theta(W)} \frac{P_1 - P_2}{P_1 + P_2}, \quad t \in [0, T], x \in [0, L], \tag{2.11}$$

where θ is a positive real function of W, which may become small. It simply represents a time scale which governs the return to pressure equilibrium. Note that the right-hand side of (2.11) provides an exponentially decreasing relaxation. The maximum principle is stated by the following proposition:

Proposition 2. Let L and T be two positive real constants. Assume that V_i , $\partial_x V_i$ and $(\alpha_1 - \alpha_2)/\theta$ belong to $L^{\infty}([0,T] \times [0,L])$. Then, equation (2.11) on the volume fraction α_1 associated with admissible inlet boundary conditions, that is $\alpha_1(t, x = 0)$ and $\alpha_1(t, x = L)$ in (0,1) for all t in [0,T], leads to

$$0 \le \alpha_1(t, x) \le 1, \quad \forall (t, x) \in [0, T] \times [0, L],$$
 (2.12)

when restrict ourselves to regular solutions and assume that $P_k > 0$, k = 1, 2.

Of course, the maximum principle on α_2 is also satisfied, which follows from (2.12) and the closure relation $\alpha_1 + \alpha_2 = 1$. Moreover, the same result obviously holds if the relaxation term is null as in equation (2.7a).

A property of positivity for $m_k = \alpha_k \rho_k$, k = 1, 2, may be proved for smooth solutions as well. The related partial differential equations is

$$\frac{\partial m_k}{\partial t} + U_k \frac{\partial m_k}{\partial x} + m_k \frac{\partial U_k}{\partial x} = 0, \quad k = 1, 2.$$
 (2.13)

Furthermore, we may state the following proposition:

Proposition 3. Let L and T be positive real constants. Assume that U_k and $\partial_x U_k$ belong to $L^{\infty}([0,T]\times[0,L])$, k=1,2. Then, for k=1,2, equation (2.13) on the partial mass m_k associated with admissible inlet boundary conditions, that is $m_k(t,x=0)$ and $m_k(t,x=L)$ positive for all t in [0,T], leads to

$$m_k(t, x) \ge 0, \quad \forall (t, x) \in [0, T] \times [0, L],$$
 (2.14)

when restrict ourselves to regular solutions.

We recall now the partial differential equation associated with pressure P_k , k = 1, 2:

$$\frac{\partial P_k}{\partial t} + U_k \frac{\partial P_k}{\partial x} + \hat{\gamma}_k P_k \frac{\partial U_k}{\partial x} + (U_k - V_i) \hat{\gamma}_{ik} P_k \frac{\partial \operatorname{Log}(\alpha_k)}{\partial x} = 0, \tag{2.15}$$

where

$$\hat{\gamma}_{ik} = \hat{\gamma}_k + (P_i - P_k) \left(\rho_k P_k \frac{\partial \varepsilon_k}{\partial P_k} \right)^{-1}.$$

Proposition 4. Let L and T be positive real constants. Assume that U_k and $\partial_x U_k$ belong to $L^{\infty}([0,T] \times [0,L])$, k = 1,2. Assume moreover that $\hat{\gamma}_{ik}$ and $\partial_x \operatorname{Log}(\alpha_k)$

belong to $L^{\infty}([0,T]\times[0,L])$, k=1,2. Then, for k=1,2, equation (2.15) on the pressures P_k associated with admissible inlet boundary conditions, that is $P_k(t, x =$ 0) and $P_k(t, x = L)$ positive for all t in [0, T], leads to

$$P_k(t,x) \ge 0, \quad \forall (t,x) \in [0,T] \times [0,L],$$
 (2.16)

when restrict ourselves to regular solutions.

The proof of these three lemmas is "classical" and recalled in Appendix B of Ref. 15.

Eventually, we restrict ourselves to a smooth solution W of (2.7) which satisfies the assumptions described in propositions 2, 3 and 4, complemented by a smooth initial datum W_0 . It follows the *invariant domain* property:

$$W_0 \in \Omega \implies W \in \overline{\Omega}.$$

Such an important property is not satisfied by classical two-fluid models using instantaneous local pressure equilibrium. This is an important step before investigating the Riemann problem and the numerical approximation of system (2.7).

We provide herein a result concerning the isentropic framework. The following proposition holds:

Proposition 5. We restrict ourselves once more to smooth solutions of the system (2.7). Assume that the function P_k may be written in the form $P_k(t,x) =$ $\varphi_k(\rho_k(t,x))$, where φ_k is a monotone non-decreasing function. Then, P_k is a solution of (2.15) if and only if

$$\rho_k \varphi_k'(\rho_k) = \hat{\gamma}_k P_k \tag{2.17}$$

and
$$P_k = P_i$$
, (2.18)

assuming that, for k = 1, 2, the product $(U_k - V_i)\partial_x \alpha_k$ does not vanish.

Proof. Using the equations of pressure P_k and density ρ_k , some easy calculations lead to relations (2.17) and (2.18). Relation (2.17) is the counterpart of the relation when dealing with classical Euler system and (2.18) is derived from terms in $\partial_x \alpha_k$, appearing in the equations of pressure and density. \square

Remark 2. a — Assume first that $\beta(1-\beta) \neq 0$ in (2.5). Then, if there exists a function $P_1 = \varphi_1(\rho_1)$ which is an integral solution of (2.15) with k = 1, then no solution of (2.15) with k=2 of the form $P_2=\varphi_2(\rho_2)$ may be found (except under pressure equilibrium $P_1 = P_2 = P_i$). This means that an isentropic form of system (2.7) for both phases does not exist far from the thermodynamical equilibrium, when using classical isentropic curves.

b — Assume now that $\beta = 1$ (respectively $\beta = 0$), that is $V_i = U_1$ (resp. $V_i = U_2$), then one may find $P_k = \varphi_k(\rho_k)$, k = 1, 2, solutions of (2.15) if and only if $P_i = P_2$ (resp. $P_i = P_1$). Note that these closures for V_i and P_i have been proposed in Ref. 2 .

2.3. Field by field study and closure relations for the interfacial pressure and for the interfacial velocity

We turn now to closure laws for P_i and V_i . Additional properties of the convective system, in particular when focusing on the Riemann problem, and the parametrisation through the wave V_i strongly depend on the definition of P_i and V_i . A Riemann problem corresponds to a Cauchy problem for system (2.7) with

$$W(t = 0, x) = \begin{cases} W_L, & \text{if } x < 0, \\ W_R, & \text{if } x > 0, \end{cases}$$
 (2.19)

where W_L and W_R belong to Ω . We restrict our study to self-similar solutions composed by constant states separated by elementary waves. Moreover, we assume that the initial condition (2.19) does not provide a non-diagonalizable convective matrix (see conditions (2.10)). At this stage, though P_i and V_i remain unknown, some information is available on p-waves, p=2,...,7. Actually, since α_1 is constant on each side of the 1-wave, the system (2.7) locally reduces to two conservative Euler systems. Hence, related Riemann invariants and Rankine-Hugoniot jump relations are locally well defined for all p-waves, p=2,...,7, and their parametrisation is classical (see for instance Ref. ⁵⁰ for a complete description). First, noting $I^p(W)$ the vector of p-Riemann invariants, we have:

$$\begin{split} I^2(W) &= \ ^T \left(\tau_2, u_2, p_2, \alpha_1, s_1, u_1 + f_1(s_1, \rho_1) \right), \\ I^3(W) &= \ ^T \left(\tau_2, u_2, p_2, \alpha_1, p_1, u_1 \right), \\ I^4(W) &= \ ^T \left(\tau_2, u_2, p_2, \alpha_1, s_1, u_1 - f_1(s_1, \rho_1) \right), \\ I^5(W) &= \ ^T \left(\tau_1, u_1, p_1, \alpha_1, s_2, u_2 + f_2(s_2, \rho_2) \right), \\ I^6(W) &= \ ^T \left(\tau_1, u_1, p_1, \alpha_1, p_2, u_2 \right), \\ I^7(W) &= \ ^T \left(\tau_1, u_1, p_1, \alpha_1, s_2, u_2 - f_2(s_2, \rho_2) \right), \end{split}$$

where f_1 and f_2 are defined by $\partial f_k/\partial \rho_k = c_k/\rho_k$, k=1,2. Since the system is locally conservative, p-Riemann invariants and jump relations for linearly degenerate p-fields, *i.e.* for p=3,6, coincide. Concerning the genuinely non-linear fields, the Rankine-Hugoniot jump relations across a discontinuity of speed σ are:

$$\begin{split} & [\alpha_k] = 0 \,, \\ & [m_k(u_k - \sigma)] = 0 \,, \\ & [m_k u_k(u_k - \sigma) + \alpha_k p_k] = 0 \,, \\ & [\alpha_k E_k(u_k - \sigma) + \alpha_k p_k u_k] = 0 \,, \\ & [\tau_{k'}] = 0 \,, \quad [u_{k'}] = 0 \,, \quad [p_{k'}] = 0 \,, \end{split}$$

where for p = 2, 4, we have k = 1 and k' = 2, and for p = 5, 7, we have k = 2 and k' = 1. Moreover, brackets [.] denote the difference between the state at the right of the discontinuity and the state at the left of the discontinuity. Noting W_l

(respectively W_r) the constant state just on the left side (resp. the right side) of the 1-wave, the previous Riemann invariants and Rankine-Hugoniot jump relations allow to link W_L to W_l and W_R to W_r . A first result is the following:

Proposition 6. The Riemann problem (2.7), (2.19) has a unique entropy consistent solution involving constant states separated by shocks, rarefaction waves and contact discontinuities, provided the initial datum (2.3) is in agreement with

$$|(U_k)_R - (U_k)_L| < \frac{2}{\gamma_k - 1}((c_k)_L + (c_k)_R),$$
 (2.20)

k = 1, 2, under the condition $(\alpha_1)_L = (\alpha_1)_R$.

Proof. Since $(\alpha_1)_L = (\alpha_1)_R$, phases evolve independently. Therefore, this proof reduces to the classical theorem of existence and uniqueness for the solution of the Riemann problem associated with the Euler frame 26,50 . \square

We turn now to the connection between W_l and W_r through the 1-wave. Since the interfacial velocity V_i and the interfacial pressure P_i are still undefined, this connection cannot be performed. Let us recall that we restrict our study to interfacial velocities of the form (2.5) and interfacial pressures satisfying (2.6).

2.3.1. Interfacial velocity

As stated in Proposition 1, the type of the field corresponding to the wave V_i is unknown. Two distinct cases immediately appear. In the first one, the function β in (2.5) is such that the 1-field is genuinely non-linear. However, such a choice should give for a class of initial conditions a rarefaction wave for the 1-field. Therefore, a mixture zone would appear inside this rarefaction wave. To avoid this phenomenon, we assume that the 1-field is linearly degenerate, which means that the function β must be such that for all W in Ω we have

$$\nabla V_i(W).r_1(W) = 0,$$

where $r_1(W)$ stands for the right eigenvector associated with the first eigenvalue, namely V_i . Such an assumption ensures that the wave associated with this field remains infinitely thin, whatever initial condition (2.19) is. We have actually the following result:

Proposition 7. Assume that the interface velocity coefficient β takes the form

$$\beta(W) = \beta(\alpha_1, \rho_1, \rho_2, P_1, P_2). \tag{2.21}$$

Therefore, the field associated with the eigenvalue V_i is linearly degenerate if and only if

$$\beta(W) = \frac{\alpha_1 \rho_1}{\alpha_1 \rho_1 + \alpha_2 \rho_2}$$
or $\beta(W) = 1$ or $\beta(W) = 0$, (2.22)

for all W in Ω in the definition (2.5).

Proof. It is quite straightforward to check that any choice of β among the three above provides the required property. The reverse is less obvious. One must first note that, due to the dimensional argument, the form (2.21) may be reduced to

$$\beta(W) = \beta\left(\alpha_1, \frac{\rho_1}{\rho_2}, \frac{P_1}{P_2}\right). \tag{2.23}$$

Tedious calculations are then necessary, which are not exposed here. The form (2.21) satisfies classical requirements such as galilean invariance and objectivity. Nevertheless, one may note that the relative velocity $|U_1 - U_2|$ has not been accounted for in (2.21). Indeed, it seems unfeasable to obtain the most general frame of explicit definitions of β when adding this argument to (2.21). \square

At this stage, the non-conservative product $V_i \partial_x \alpha_1$ is well defined, from a local point of view. Indeed, by definition, V_i is a 1-Riemann invariant. Moreover, α_1 remains unchanged through p-waves (p = 2, 3, ..., 7). Therefore, when one of two factors of the non-conservative product admits a discontinuity, the other one is constant. Therefore, using closure (2.22), one may try to connect state W_l with state W_r . In order to have a parametrisation for the 1-wave, one must find six 1-Riemann invariants $(I_p^1)_{p=1,...,6}$ such that their gradient $(\nabla I_p^1)_{p=1,...,6}$ are linearly independent. Since P_i is not defined, only five 1-Riemann invariants can be provided explicitly:

$$I_1^1(W) = V_i, (2.24)$$

$$I_2^1(W) = \frac{m_1 m_2}{m_1 + m_2} (U_1 - U_2), \tag{2.25}$$

$$I_3^1(W) = \alpha_1 P_1 + \alpha_2 P_2 + I_2^1(W)(U_1 - U_2), \tag{2.26}$$

$$I_5^1(W) = \varepsilon_1 + \frac{P_1}{\rho_1} + \frac{1}{2(m_1)^2} (I_2^1(W))^2,$$
 (2.27)

$$I_6^1(W) = \varepsilon_2 + \frac{P_2}{\rho_2} + \frac{1}{2(m_2)^2} (I_2^1(W))^2.$$
 (2.28)

Now we propose two definitions of the interfacial pressure P_i and derive the last 1-Riemann invariant I_4^1 .

2.3.2. Interfacial pressure

The closure for the interfacial pressure P_i must allow to define the non-conservative product $P_i\partial_x\alpha_1$ and to determine the last 1-Riemann invariant I_4^1 . Here, two ways are investigated. The first one is based on an additional conservation law. This partial differential equation concerns the total entropy and a form of P_i is exhibited in order to ensure the divergence form of this equation. The 1-Riemann invariant I_4^1 is directly derived, which implicitly closes the product $P_i\partial_x\alpha_1$. The related parametrisation is discussed in appendix B. The second closure presented here is directly based on the definition of the product $P_i\partial_x\alpha_1$. Following the behaviour

of the product $V_i \partial_x \alpha_1$, if P_i corresponds to a function which only depends on the 1-Riemann invariants $(I_p^1)_{p=1,\dots,6}$, the product $P_i \partial_x \alpha_1$ is locally well defined. Furthermore, the definition of the 1-Riemann invariant I_4^1 immediately follows. Indeed, replacing locally (in a neighborhood of the 1-wave) $P_i \partial_x \alpha_1$ by $\partial_x (P_i \alpha_1)$ in the equations of partial momentum (2.7d) and (2.7e) provides two conservative equations and thus, an additional 1-Riemann invariant (the second conservation law corresponds to the 1-Riemann invariant I_3^1).

We must emphasize that, though the convective system is non-conservative, 1-Riemann invariants and Rankine-Hugoniot jump relations coincide for the linearly degenerate field associated with V_i , in the sense that they provide the same parametrisation, as stated in appendix A. Therefore, no ambiguity holds in the definition of jump relations and non-conservative products, contrary to the frame studied in Ref ⁴⁴ for instance, where the knowledge of the matrix of diffusion is required.

A conservative equation for the total entropy We restrict ourselves here to interfacial pressures P_i of the form

$$P_i(W) = \mu(W)P_1 + (1 - \mu(W))P_2, \tag{2.29}$$

where the dimensionless function μ is non-negative and bounded by 1. Obviously, definition (2.29) ensures that relation (2.6) is satisfied. Let a_k be the function

$$a_k = \frac{1}{\varsigma_k} \left(\frac{\partial \varsigma_k}{\partial P_k} \right) \left(\frac{\partial \varepsilon_k}{\partial P_k} \right)^{-1}, \quad k = 1, 2.$$
 (2.30)

One may now provide the following result concerning the entropy inequality: **Proposition 8.** Let us define $\eta_k = \text{Log}(s_k) + \psi_k(\alpha_k)$ for k = 1, 2, with $\psi_1(\alpha_1) = \psi_2(1 - \alpha_1)$. If the interfacial pressure P_i is defined by equation (2.29) with (2.30) in

$$\mu = \frac{a_1(1-\beta)}{a_1(1-\beta) + a_2\beta},\tag{2.31}$$

then, defining the entropy-entropy flux pair (η, F_{η}) by

$$\eta = -(\alpha_1 \rho_1 \eta_1 + \alpha_2 \rho_2 \eta_2),
F_{\eta} = -(\alpha_1 \rho_1 \eta_1 U_1 + \alpha_2 \rho_2 \eta_2 U_2),$$

the following entropy inequality holds for smooth solutions of system (2.7) complemented by viscous terms (2.2):

$$\frac{\partial \eta}{\partial t} + \frac{\partial F_{\eta}}{\partial x} \le 0. \tag{2.32}$$

This result is obtained by classical manipulations of the partial differential equations for s_k . Note that $m_1\psi_1 + m_2\psi_2$ stands for an interfacial energy²⁰.

This proposition permits to define the interfacial pressure P_i in function of the interfacial velocity V_i . An advantage of this closure is that entropy inequality (2.32) obviously degenerates to give the expected – single phase – entropy inequality on each side of the 1-contact discontinuity. Herein, system (2.7) is completely closed. Using results of appendix A, equation (2.32) leads to the Rankine-Hugoniot jump relation

$$V_i(\eta(W_r) - \eta(W_l)) = F_{\eta}(W_r) - F_{\eta}(W_l)$$

for the field associated with V_i and alternatively to the last 1-Riemann invariant

$$I_4^1(W) = \frac{\varsigma_1}{\varsigma_2}. (2.33)$$

Now, the parametrisation through the 1-wave which is defined by the 1-Riemann invariants $(I_p^1)_{p=1,\dots,6}$ may be explicitly given (recall that this parametrisation is identical to the parametrisation given by Rankine-Hugoniot jump relations for this linearly degenerate field). This is done is appendix B. The main result in this appendix is that the connection between W_l and W_r through the 1-wave is in agreement with the maximum principle on the volume fraction and the positivity requirements on densities and internal energies. This leads to the following result:

Proposition 9. We assume now that $(\alpha_1)_L \neq (\alpha_1)_R$ and that each phase is governed by a perfect gas equation of state. The connection of constant states through elementary waves in the solution of the Riemann problem (2.7)-(2.19) ensures that all states are in agreement with positivity requirements for volume fraction, mass fractions and partial pressures.

We insist that though the result seems obvious from a physical view point, it may actually not be clear whether solutions of the Riemann problem (2.7)-(2.19) should agree with the positivity requirement. The choice of the above closures a posteriori ensures that physical positivity requirements hold. Unfortunately, the great complexity of the system (2.7) seems to prohibit the exact resolution of the Riemann problem. Indeed, eigenvalues are not arranged in order, which leads to an important number of different cases to investigate. Moreover, the connection through the 1-wave is not totally clear since, for a given state W_l , zero, one or two states W_r may be selected by the parametrisation. Hence, a deeper analysis of the 1-wave may be required, as done in Ref. ⁶ or Ref. ⁴⁸ for rather simple models and Ref. ²⁵.

The interfacial pressure as a function of 1-Riemann invariants Here, the non-conservative product $P_i\partial_x\alpha_1$ is directly closed using a definition of the interfacial pressure such that P_i remains unchanged when α_1 admits a discontinuity. In other words, recalling that the volume fraction α_1 only jumps through the 1-wave, P_i remains constant through this wave if it is a function of the 1-Riemann invariants $(I_p^1)_{p=1,2,\ldots,6}$

$$P_i(W) = \mathcal{F}\big(I_1^1(W), I_2^1(W), ..., I_6^1(W)\big).$$

Note that \mathcal{F} must ensure condition (2.6). Of course, one must provide an explicit form of \mathcal{F} to obtain an explicit form of I_4^1 . Nevertheless, \mathcal{F} and I_4^1 may be linked

 $I_4^1(W) = \frac{P_1 - P_2}{2} + \left(\frac{P_1 + P_2}{2} - P_i\right)(\alpha_1 - \alpha_2) + (U_1 + U_2)I_2^1(W).$

Remark that 1-Riemann invariants I_1^1 and I_4^1 do not satisfy the objectivity requirement (whatever function \mathcal{F} is); furthermore, a dimensionless condition may be invoked, leading to the following list of arguments:

$$P_i(W) = \mathcal{G}(I_3^1(W), I_2^1(W)(I_5^1(W))^{1/2}, I_1^1(W)(I_6^1(W))^{1/2}).$$

Owing to condition (2.6), function \mathcal{G} must satisfy $\mathcal{G}(a,0,0)=a$. Numerous functions \mathcal{G} satisfy all these requirements. Among these, a simple choice could be

$$\mathcal{G}(a,b,c) = a + C_1(C_2|b| + (1 - C_2)|c|), \tag{2.34}$$

with C_1 and C_2 two real constants such that $C_1 > 0$ and $0 \le C_2 \le 1$. In addition to the dimensionless condition, the objectivity requirement and condition (2.6), this choice provides the positivity of the interfacial pressure P_i . Note that the particular choice $\mathcal{G}(a,b,c) = a$ corresponds to the closure retained in Ref. ⁴⁷.

This deserves a few comments about closure laws available in the literature. We note first that proposals by Glimm and co-workers^{23,24} are quite different. Actually, coefficients occuring in their closure play a symmetric role in the interface velocity and interface pressure. Even more, they assume that the interface velocity tends towards the velocity of the vanishing phase $V_i = U_1$ when one phase is no longer present $(\alpha_1 = 0)$. Their proposal looks like $P_i = \alpha_2 P_1 + \alpha_1 P_2$ and $V_i = \alpha_2 U_1 + \alpha_1 U_2$. Note that the closure for V_i implies that the 1-wave corresponds to a genuinely non-linear field. Turning now to the work of Saurel and Abgrall⁴⁵, we note that the usual choice of interface velocity is (2.22). Nonetheless, their closure for the interface pressure is completely different from ours and takes the form: $P_i = \alpha_1 P_1 + \alpha_2 P_2$. Here again, when some phase (phase labelled 1 for instance, which means that $\alpha_1 = 0$) disappears, the couple of interface variables (V_i, P_i) coincides with the velocity-pressure couple in the remaining phase, namely (U_2, P_2) . Furthermore, in Ref. ⁴⁷, the closures are (2.22) and $\mathcal{G}(a,b,c)=a$ in (2.34), but no information is provided about the Riemann problem. In Refs. 2,35,20 , the closures correspond to $P_i = P_1$ (dropping some terms in Ref. ²⁰) and $V_i = U_2$, where subscript 1 refers to the gas phase. As mentioned above, this set of closure satisfies Propositions 7 and 8. Moreover, this choice provides a conservative entropy inequality on each phase.

3. Numerical methods

This section is devoted to the presentation of different Finite Volume methods computed here to approximate the solution of the Cauchy problem (2.1)-(2.3) (note that explicit definitions of interfacial pressure P_i and interfacial velocity V_i are not required to present both following methods). Though the current presentation is in one dimension, the extension to the multidimensional frame is straightforward. In the following of this paper, diffusion terms are omitted. Convective terms and source terms (relaxation terms) are taken into account by a fractional step approach. It is well known the latter is not optimal in terms of accuracy (see Ref. ¹⁸ for instance), but it nonetheless leads to very stable algorithms. Each step aims at approximating the different terms. First, we note δt the time step and δx the length of a cell $(x_{j-1/2}; x_{j+1/2})$ of the regular mesh. Let W^n be the Finite Volume approximation at time $t^n = n\delta t$, $n \in \mathbb{N}$. The approximated solution W^{n+1} (i.e. at time $t^{n+1} = (n+1)\delta t$) of the Cauchy problem

$$\begin{cases} (Id+D(W))\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial W}{\partial x} = S(W), & t \in (t^n, t^{n+1}), x \in \mathbb{R}, \\ W(t^n, x) = W^n(x), & x \in \mathbb{R}, \end{cases}$$

is approximated by splitting the complete problem in two steps. The first one corresponds to the convective part:

$$\begin{cases} (Id + D(W))\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial W}{\partial x} = 0, & t \in (t^n, t^{n+1}), x \in \mathbb{R}, \\ W(t^n, x) = W^n(x), & x \in \mathbb{R}, \end{cases}$$
(3.35)

which provides $W^{n,1}$ (the approximation of $W(t^{n+1},.)$, the solution of (3.35) at time t^{n+1}). The second one corresponds to the relaxation process:

$$\begin{cases} (Id + D(W))\frac{\partial W}{\partial t} = S(W), & t \in (t^n, t^{n+1}), x \in \mathbb{R}, \\ W(t^n, x) = W^{n,1}(x), & x \in \mathbb{R}, \end{cases}$$
(3.36)

which finally gives W^{n+1} (the approximation of $W(t^{n+1},.)$), the solution of (3.36) at time t^{n+1}).

3.1. Computing hyperbolic systems under non-conservative form

Two Finite Volume schemes are presented here. The first one is based on the Rusanov scheme⁴² and the second is an extension of an approximate Godunov scheme, namely the VFRoe-ncv scheme. As usual, the notation

$$W_j^n = \frac{1}{\delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} W(t^n, x) dx, \quad n \ge 0, j \in \mathbb{R},$$

is adopted in the following. Finite Volume schemes are merely designed to hyperbolic systems of conservation laws. Here, the set of partial differential equations (3.35) cannot be written under conservative form. An adaptation is thus required to take into account non-conservative terms in the method. Several techniques have been proposed but numerical difficulties have been pointed out in Ref. ³². Nevertheless, the frame investigated in these references concerns non-conservative products

for genuinely non-linear fields. Here, non-conservative products only arise for linearly degenerate fields and are locally well defined (see appendix A). Therefore, one may expect that both Finite Volume schemes presented below are "consistent" with (3.35), since no additional information to the convective system is required to close non-conservative products.

3.1.1. The Rusanov scheme

We detail herein the Rusanov scheme for the two-fluid two-pressure model (2.7). The equation on the volume fraction α_1 (2.7a) is approximated by

$$\delta x \left((\alpha_1)_j^{n,1} - (\alpha_1)_j^n \right) + \delta t(V_i)_j^n \left((\overline{\alpha_1})_{j+1/2}^n - (\overline{\alpha_1})_{j-1/2}^n \right) - \frac{\delta t}{2} \left(r_{j+1/2} \left((\alpha_1)_{j+1}^n - (\alpha_1)_j^n \right) \right) + \frac{\delta t}{2} \left(r_{j-1/2} \left((\alpha_1)_j^n - (\alpha_1)_{j-1}^n \right) \right) = 0.$$

Equations (2.7b-2.7g) become for k = 1, 2:

$$\delta x \left((Z_k)_j^{n,1} - (Z_k)_j^n \right) + \delta t \left((H_k)_{j+1/2}^n - (H_k)_{j-1/2}^n \right) - \delta t (P_i)_j^n (\phi_k)_j \left((\overline{\alpha_k})_{j+1/2}^n - (\overline{\alpha_k})_{j-1/2}^n \right) = 0.$$

where

$$Z_k = \begin{pmatrix} m_k \\ m_k U_k \\ \alpha_k E_k \end{pmatrix}, \ H_k = \begin{pmatrix} m_k U_k \\ m_k (U_k)^2 + \alpha_k p_k \\ \alpha_k U_k (E_k + p_k) \end{pmatrix}, \ (\phi_k)_j^n = \begin{pmatrix} 0 \\ 1 \\ (V_i)_j^n \end{pmatrix}$$

and

$$r_{j} = \max(|(V_{i})_{j}^{n}|, |(U_{1})_{j}^{n}| + (c_{1})_{j}^{n}, |(U_{2})_{j}^{n}| + (c_{2})_{j}^{n}),$$

$$r_{j+1/2} = \max(r_{j}, r_{j+1}),$$

$$2(H_{k})_{j+1/2}^{n} = (H_{k})_{j}^{n} + (H_{k})_{j+1}^{n} - r_{j+1/2}((Z_{k})_{j+1}^{n} - (Z_{k})_{j}^{n}),$$

$$2(\overline{\alpha_{k}})_{j+1/2}^{n} = (\alpha_{k})_{j}^{n} + (\alpha_{k})_{j+1}^{n}.$$

One may easily prove that the Rusanov scheme preserves the maximum principle for the volume fraction and the positivity of partial masses

$$0 < (\alpha_1)_j^{n,1} < 1$$
 and $(m_k)_j^{n,1} > 0, k = 1, 2$

if W^n in (3.35) belongs to Ω and under the classical C.F.L. condition

$$\frac{\delta t}{\delta x} |\lambda_{MAX}| \le 1,$$

where λ_{MAX} is the maximal speed of wave, computed on each cell of the mesh. These properties can be extended to the multidimensional framework.

$3.1.2.\ The\ VFRoe-nev\ scheme$

The VFRoe-ncv scheme⁴ is an approximate Godunov scheme. This means that it may be written in a similar form to the Godunov scheme²⁷, but the solution at each interface of the mesh is approximated. This approximation is provided by a linearisation of the convective system written with respect to a non-conservative variable (which explains the name of the scheme). Numerous numerical tests¹⁸ show that the VFRoe-ncv scheme provides accurate results, even when focusing on resonant systems⁴⁸. Eventually, results obtained by the VFRoe-ncv scheme are very close to results provided by the Godunov scheme, when dealing with convergence in space (that is when the mesh is refined) as well as with convergence in time (*i.e.* convergence towards steady states when $t \to +\infty$).

Here again, the system which is computed corresponds to system (2.7) instead system of (3.35). Note that these two systems are equivalent, even when focusing on discontinuous solutions. The associated VFRoe-ncv scheme may be written on the cell $j \in \mathbb{Z}$ as

$$\delta x \left(W_j^{n,1} - W_j^n \right) + \delta t \left(F(W_{j+1/2}^*) - F(W_{j-1/2}^*) \right)$$

$$+ \frac{\delta t}{2} \left(G(W_{j-1/2}^*) + G(W_{j+1/2}^*) \right) \left((\alpha_1)_{j+1/2}^* - (\alpha_1)_{j-1/2}^* \right) = 0.$$
(3.37)

where vector G is

$$G(W) = {}^{T}(V_{i}(W), 0, -P_{i}(W), -P_{i}(W)V_{i}(W), 0, P_{i}(W), V_{i}(W)P_{i}(W))$$

The core of the method is the computation of values indexed by $(.)_{j+1/2}^*$, j in \mathbb{Z} . These values are computed from local Riemann problems at each interface of the mesh $x_{j+1/2}, j \in \mathbb{Z}$, as done with the Godunov scheme. Whereas the exact solution of these local Riemann problems is used for the Godunov scheme, the VFRoe-ncv scheme only approximates the solution, allowing a great reduction of the complexity of the solver when dealing with non-linear systems. Moreover, we mentioned above that the complete computation of the exact solution of the Riemann problem (2.7)-(2.19) seems out of reach; nonetheless, the approximate solution of the VFRoe-ncv scheme is obtained by straightforward calculations. Let us provide the main guidelines to compute values $(.)_{j+1/2}^*$, $j \in \mathbb{Z}$. We focus on the local Riemann problem associated with interface $x_{j+1/2}$ at time t^n . It is composed by the set of partial differential equations (2.7) and by the initial condition

$$W(t = 0, x) = \begin{cases} W_i^n & \text{if } x < x_{j+1/2}, \\ W_{i+1}^n & \text{if } x > x_{j+1/2}. \end{cases}$$
 (3.38)

Let Ψ be a regular function from \mathbb{R}^7 to \mathbb{R}^7 and define $Y = \Psi(W)$. Here, we choose the variable $Y = {}^T(\alpha_1, s_1, U_1, P_1, s_2, U_2, P_2)$. The system (2.7) may be written for smooth solutions as

$$\frac{\partial Y}{\partial t} + B(Y)\frac{\partial Y}{\partial x} = 0$$

where $B(\Psi(W)) = \Psi'(W)(Id + D(W))^{-1}(F'(W) + C(W))(\Psi'(W))^{-1}$ and is given by (2.8). This system is linearised, which gives the following local Riemann problem:

$$\begin{cases}
\frac{\partial Y}{\partial t} + B(\hat{Y}) \frac{\partial Y}{\partial x} = 0, \\
Y(t = t^n, x) = \begin{cases} \Psi(W_i^n) & \text{if } x < x_{j+1/2} \\ \Psi(W_{i+1}^n) & \text{if } x > x_{j+1/2} \end{cases},
\end{cases} (3.39)$$

where $\hat{Y} = (\Psi(W_i^n) + \Psi(W_{i+1}^n))/2$. The solution of this system is obvious and its solution yields for all $t > t^n$ and x in \mathbb{R}

$$Y(t,x) = \Psi(W_i^n) + \sum_{\widetilde{\lambda_p} < (x - x_{j+1/2})/(t - t^n)} {T_{\widetilde{l_p}} \cdot (\Psi(W_{i+1}^n) - \Psi(W_i^n)) \hat{r_p}}$$
(3.40a)
$$= \Psi(W_{i+1}^n) - \sum_{\widetilde{\lambda_p} > (x - x_{j+1/2})/(t - t^n)} {T_{\widetilde{l_p}} \cdot (\Psi(W_{i+1}^n) - \Psi(W_i^n)) \hat{r_p}}$$
(3.40b)

$$= \Psi(W_{i+1}^n) - \sum_{\widetilde{\lambda_p} > (x - x_{j+1/2})/(t - t^n)} \left({}^T \widetilde{l_p} \cdot (\Psi(W_{i+1}^n) - \Psi(W_i^n)) \right) \widetilde{r_p}$$
 (3.40b)

where $(\widetilde{l_p})_{p=1,\dots,7}$, $(\widetilde{r_p})_{p=1,\dots,7}$ and $(\widetilde{\lambda_p})_{p=1,\dots,7}$ are the left and right eigenvectors and eigenvalues of the matrix $B(\hat{Y})$ (see (2.9)), respectively. Therefore, since problem (3.39) provides a self-similar solution, we may set

$$W_{i+1/2}^* = \Psi^{-1}(Y(t > t^n, x = x_{j+1/2}))$$

which completes the construction of the VFRoe-ncv scheme. Of course, the properties of this scheme depend on the choice of Y (in general, the function Ψ is nonlinear). Consequently, the behaviour of the VFRoe-ncv scheme is closely related to the definition of Y. Here, $Y = {}^{T}(\alpha_1, s_1, U_1, P_1, s_2, U_2, P_2)$ has been selected in agreement with the analysis of the Riemann problem (2.7)-(2.19) and with numerical tests¹⁷.

We emphasize that both the Rusanov scheme and the VFRoe-ncv scheme may preserve some well-known solutions. Assume first that the equation of state of both phases verifies (2.4). If, for all cell $j \in \mathbb{Z}$, the approximated initial condition agrees with $(U_1)_i^0 = (U_2)_i^0 = U_0$ and $(P_1)_i^0 = (P_2)_i^0 = P_0$, the approximation of the solution computed by both schemes then agrees, at each time step $n \in \mathbb{N}$ and on each cell $j \in \mathbb{Z}$, with

$$(U_1)_j^n = (U_2)_j^n = U_0$$
 and $(P_1)_j^n = (P_2)_j^n = P_0$.

3.2. Numerical treatment of source terms

Source terms of (2.1) are computed using a fractional step method, separating velocity relaxation, pressure relaxation and other contributions. Since $\partial_t \alpha_1$ may be given by the first equation of system (2.1), we have

$$\frac{\partial W}{\partial t} = S_U(W) + S_P(W) + S_O(W)$$

with

$$S_{U}(W) = {}^{T}(0, 0, -K_{U}(U_{1} - U_{2}), -K_{U}V_{i}(U_{1} - U_{2}), 0, +K_{U}(U_{1} - U_{2}), +K_{U}V_{i}(U_{1} - U_{2})),$$

$$S_{P}(W) = {}^{T}(K_{P}(P_{1} - P_{2}), 0, 0, -K_{P}P_{i}(P_{1} - P_{2}), 0, 0, +K_{P}P_{i}(P_{1} - P_{2})),$$

$$S_{O}(W) = {}^{T}(0, \dot{m}, +\dot{m}V_{i}, +\dot{m}E_{i}, -\dot{m}, -\dot{m}V_{i}, -\dot{m}E_{i}),$$

which is split in the three systems (steps 1, 2, 3):

$$\partial_t W = S_U(W)$$
, $\partial_t W = S_P(W)$ and $\partial_t W = S_O(W)$.

According to this decomposition, we introduce some notations. $W^{n,U}$, $W^{n,P}$ and $W^{n,O}$ are the approximations of the solution after respectively: the velocity relaxation by S_U with $W^{n,1}$ as initial condition; the pressure relaxation S_P with $W^{n,U}$ as initial condition; and remaining phenomena S_O with $W^{n,P}$ as initial condition (the initial time corresponds to t^n). We examine below whether α_k , m_k and P_k and their approximations remain positive through these steps assuming that $W^{n,1}$ does lie in Ω and relaxation processes are time continuous.

3.2.1. Step 1: velocity relaxation

Continuous frame The initial condition for this step is $W^{n,1}$, which is supposed to lie in Ω . Note that volume fractions α_k and partial masses m_k remain unchanged during this step. Only the velocities U_k and the energies E_k may vary, which yields the following system:

$$\frac{\partial \alpha_k}{\partial t} = \frac{\partial m_k}{\partial t} = 0,\tag{3.41}$$

$$m_k \frac{\partial U_k}{\partial t} = (-1)^k K_U(W)(U_1 - U_2),$$
 (3.42)

$$m_k \frac{\partial}{\partial t} (e_k + (U_k)^2 / 2) = (-1)^k K_U(W) V_i(U_1 - U_2),$$
 (3.43)

k = 1, 2. We assume of course that $(U_1)^{n,1} \neq (U_2)^{n,1}$. The second ordinary differential equation may be easily replaced by the following equations for the pressures P_k , k = 1, 2:

$$m_k \frac{\partial \varepsilon_k}{\partial P_k} \frac{\partial P_k}{\partial t} = (-1)^k K_U(W)(U_1 - U_2)(V_i - U_k). \tag{3.44}$$

This equation yields the following result:

Lemma 1. If $\partial \varepsilon_k/\partial P_k > 0$, then for all $t \geq t^n$ we have $P_k(t) > 0$ with k = 1, 2. In fact, using the general definition of V_i (2.5), equation (3.44) becomes

$$m_k \frac{\partial \varepsilon_k}{\partial P_k} \frac{\partial P_k}{\partial t} = \beta_{k'}(W) K_U(W) (U_1 - U_2)^2,$$
 (3.45)

with k' = 3 - k, $\beta_1 = \beta$ and $\beta_2 = 1 - \beta$. Recalling that $0 \le \beta \le 1$ (which holds true when using $\beta(W) = m_1/(m_1 + m_2)$, pressures P_1 and P_2 remain positive (since $\partial_t P_k$ is positive for k=1,2) when focusing on simple thermodynamical laws, such as Tammann equation of state or perfect gas equation of state, i.e. equation of state following (2.4). In that case, we simply have $m_k \partial \varepsilon_k / \partial P_k = \alpha_k g_k > 0$.

Let us focus now on the variation of $U_1 - U_2$ during the velocity relaxation step. From equation (3.42), one may deduce the ordinary differential equation

$$\frac{\partial}{\partial t}(U_1 - U_2) = -\frac{m_1 + m_2}{m_1 m_2} K_U(W)(U_1 - U_2).$$

This provides for $t \geq t^n$

$$(U_1 - U_2)(t) = (U_1 - U_2)(t^n) \exp\left(-\int_{t^n}^t K_U(W(\tau)) \left(\frac{m_1 + m_2}{m_1 m_2}\right)(\tau) d\tau\right).$$

It results the lemma:

Lemma 2. The velocity relaxation governed by system (3.41-3.43) satisfies

$$(U_1-U_2)(t)$$
. $(U_1-U_2)(t^n)>0$, for all $t\geq t^n$,
the function $|U_1-U_2|$ is monotone decreasing over $[t^n;+\infty)$
and $\lim_{t\to +\infty} (U_1-U_2)(t)=0$.

Numerical approximation We turn now to the numerical approximation of the system (3.41-3.43). Since $\partial_t \alpha_1 = \partial_t m_k = 0$, k = 1, 2, there simply results

$$(\alpha_1)^{n,U} = (\alpha_1)^{n,1}$$
 and $(m_k)^{n,U} = (m_k)^{n,1}, k = 1, 2$.

The velocities U_k , governed by the ordinary differential equation (3.42), are approximated by

$$\begin{pmatrix} (m_1)^{n,1} + K_U^{n,1} \delta t & -K_U^{n,1} \delta t \\ -K_U^{n,1} \delta t & (m_2)^{n,1} + K_U^{n,1} \delta t \end{pmatrix} \begin{pmatrix} (U_1)^{n,U} \\ (U_2)^{n,U} \end{pmatrix} = \begin{pmatrix} (m_1)^{n,1} (U_1)^{n,1} \\ (m_2)^{n,1} (U_2)^{n,1} \end{pmatrix},$$

(spatial indices are dropped since this scheme is local on each cell and we note $K_U^{n,1} = K_U(W^{n,1})$). We now approximate the solution of (3.45) by

$$(P_k)^{n,U} - (P_k)^{n,1} = \frac{\delta t \beta_{k'}(W^{n,U}) K_U(W^{n,U})}{(\alpha_k)^{n,U} g_k} \Big((U_1)^{n,U} - (U_2)^{n,U} \Big)^2,$$

assuming that the equation of state takes the form (2.4). Finally, using the equation of state and other relations, we obtain $W^{n,U}$. Note that, like in the "continuous" frame, the new pressures $(P_k)^{n,U}$ are positive if $W^{n,1}$ belongs to Ω .

3.2.2. Step 2: pressure relaxation

Continuous frame We study now the following system of ordinary differential equations:

$$\frac{\partial \alpha_1}{\partial t} = K_P(W)(P_1 - P_2),\tag{3.46}$$

$$\frac{\partial m_k}{\partial t} = \frac{\partial m_k U_k}{\partial t} = 0, (3.47)$$

$$m_k \frac{\partial e_k}{\partial t} = (-1)^k K_P(W) P_i (P_1 - P_2),$$
 (3.48)

for k=1,2. The initial condition associated with this system is $W^{n,U}$ (which belongs to Ω). As above, we assume that $(P_1)^{n,U} \neq (P_2)^{n,U}$. This system simply leads to equation

$$\alpha_k \frac{\partial P_k}{\partial t} + \left(\hat{\gamma}_k + (P_i - P_k) \left(\rho_k P_k \frac{\partial \varepsilon_k}{\partial P_k}\right)^{-1}\right) P_k \frac{\partial \alpha_k}{\partial t} = 0. \tag{3.49}$$

Subtracting (3.49) from (3.49) with k = k' gives

$$\frac{\partial (P_k - P_{k'})}{\partial t} + K_P(W) \left(\frac{\hat{\gamma}_{i1} P_1}{\alpha_1} + \frac{\hat{\gamma}_{i2} P_2}{\alpha_2} \right) (P_k - P_{k'}) = 0$$

where k' = 3 - k and

$$\hat{\gamma}_{ik} = \hat{\gamma}_k + (P_i - P_k) \left(\rho_k P_k \frac{\partial \varepsilon_k}{\partial P_k} \right)^{-1}.$$

Therefore, for $t \geq t^n$, we have

$$(P_k - P_{k'})(t) = (P_k - P_{k'})(t^n) \exp\left(-\int_{t^n}^t K_P(W(\tau)) \left(\frac{\hat{\gamma}_{i1} P_1}{\alpha_1} + \frac{\hat{\gamma}_{i2} P_2}{\alpha_2}\right) (\tau) d\tau\right).$$
(3.50)

This provides the following result, which is the counterpart of Lemma 2:

Lemma 3. If $\alpha_2 \hat{\gamma}_{i1} P_1 + \alpha_1 \hat{\gamma}_{i2} P_2 > 0$, then the system (3.46-3.48) yields

$$(P_k - P_{k'})(t) (P_k - P_{k'})(t^n) > 0$$
, for all $t \ge t^n$,

the function $|P_k - P_{k'}|$ is monotone decreasing over $[t^n; +\infty)$

and
$$\lim_{t \to +\infty} (P_k - P_{k'})(t) = 0.$$

Now, we divide equation (3.49) by $\alpha_k P_k$:

$$\frac{\partial}{\partial t}(\operatorname{Log} P_k) + \hat{\gamma}_{ik} \frac{\partial}{\partial t}(\operatorname{Log} \alpha_k) = 0$$

and add it for k = 1 and 2:

$$\frac{\partial}{\partial t} \left(\text{Log}(P_1 P_2) \right) + \hat{\gamma}_{i1} \frac{\partial}{\partial t} (\text{Log} \, \alpha_1) + \hat{\gamma}_{i2} \frac{\partial}{\partial t} (\text{Log} \, \alpha_2) = 0, \tag{3.51}$$

which becomes for $t > t^n$

$$(P_1 P_2)(t) = (P_1 P_2)(t^n) \exp\left(-\int_{t^n}^t \left(\hat{\gamma}_{i1} \frac{\partial}{\partial t} (\operatorname{Log} \alpha_1)\right)(\tau) + \left(\hat{\gamma}_{i2} \frac{\partial}{\partial t} (\operatorname{Log} \alpha_2)\right)(\tau) d\tau\right).$$

Therefore, we have

Lemma 4. For all $t \ge t^n$, $P_k(t) > 0$ holds with k = 1, 2.

We focus now on the preservation of the maximum principle for the volume fraction during this relaxation step. We introduce equation (3.50) in (3.46), which provides

$$\frac{\partial \alpha_1}{\partial t} = K_P(W)(P_1 - P_2)(t^n) \exp\left(-\int_{t^n}^t K_P(W(\tau)) \left(\frac{\hat{\gamma}_{i1} P_1}{\alpha_1} + \frac{\hat{\gamma}_{i2} P_2}{\alpha_2}\right) (\tau) d\tau\right).$$

Furthermore, multiplying by $(1/\alpha_1 + 1/\alpha_2)$ the latter equation, there holds

$$\begin{split} \frac{\partial}{\partial t} \Big(\text{Log} \, \frac{\alpha_1}{\alpha_2} \Big) = & \frac{K_P(W)}{\alpha_1 \alpha_2} (P_1 - P_2)(t^n) \\ & \exp \left(- \int_{t^n}^t K_P(W(\tau)) \left(\frac{\hat{\gamma}_{i1} P_1}{\alpha_1} + \frac{\hat{\gamma}_{i2} P_2}{\alpha_2} \right) (\tau) \, d\tau \right). \end{split}$$

Thus, there follows for $t \geq t^n$

$$\left(\frac{\alpha_1}{\alpha_2}\right)(t) = \left(\frac{\alpha_1}{\alpha_2}\right)(t^n) \exp\left(\int_{t^n}^t \frac{K_P(W(\tau))}{(\alpha_1\alpha_2)(\tau)} (P_1 - P_2)(t^n) \right) \\
\exp\left(-\int_{t^n}^\tau K_P(W(s)) \left(\frac{\hat{\gamma}_{i1}P_1}{\alpha_1} + \frac{\hat{\gamma}_{i2}P_2}{\alpha_2}\right)(s) ds\right) d\tau\right).$$
(3.52)

This gives the following lemma.

Lemma 5. For all $t \ge t^n$, $0 < \alpha_1(t) < 1$ holds.

Numerical approximation Of course, according to (3.47), we have

$$(m_k)^{n,P} = (m_k)^{n,U}$$
 and $(U_k)^{n,P} = (U_k)^{n,U}$. (3.53)

In the following, we use an explicit form of K_P (see equation (2.11)), that is

$$K_P = \frac{1}{\theta} \frac{\alpha_1 (1 - \alpha_1)}{P_1 + P_2}$$

where θ is assumed to be constant. Therefore, multiplying equation (3.46) by $(1/\alpha_1 + 1/\alpha_2)$, we have for $t \geq t^n$

$$\left(\frac{\alpha_1}{1-\alpha_1}\right)(t) = \left(\frac{\alpha_1}{1-\alpha_1}\right)(t^n) \exp\left(\frac{1}{\theta} \int_{t^n}^t \left(\frac{P_1 - P_2}{P_1 + P_2}\right)(\tau) \ d\tau\right).$$

Therefore, we compute $(\alpha_1)^{n,P}$ using

$$\left(\frac{\alpha_1}{1-\alpha_1}\right)^{n,P} = \left(\frac{\alpha_1}{1-\alpha_1}\right)^{n,U} \exp\left(\frac{1}{\theta} \int_{t^n}^{t^{n+1}} \left(\frac{P_1 - P_2}{P_1 + P_2}\right) (\tau) d\tau\right). \tag{3.54}$$

This equation has one and only one solution in (0;1), in agreement with Lemma 5, whatever the approximation of the integral in (3.54) is. In practice, the integral is approximated by $A(t^n)\delta t$ where $A(\tau)$ is the function inside the integral.

The scheme for the computation of pressures is based on a discrete form of equations (3.50) and (3.51). It is

$$(P_k - P_{k'})^{n,P} = (P_k - P_{k'})^{n,U} \exp\left(-\frac{1}{\theta} \int_{t^n}^{t^{n+1}} \left(\frac{\alpha_2 \hat{\gamma}_{i1} P_1 + \alpha_1 \hat{\gamma}_{i2} P_2}{P_1 + P_2}\right) (\tau) d\tau\right),$$

(3.55)

$$(P_1 P_2)^{n,P} = (P_1 P_2)^{n,U} \left(\frac{(\alpha_1)^{n,P}}{(\alpha_1)^{n,U}} \right)^{-\hat{\gamma}_{i1}(W^{n,U})} \left(\frac{(\alpha_2)^{n,P}}{(\alpha_2)^{n,U}} \right)^{-\hat{\gamma}_{i2}(W^{n,U})} .$$
 (3.56)

As above, the integrals in (3.55) and (3.56) are approximated using the value of functions at time t^n . Equations (3.55-3.56) provide two couples (P_1, P_2) of solutions. One consists of both negative pressures and the other of two positive pressures. Of course, the latter is retained, which agrees with Lemma 4. One may easily check that this couple verifies the discrete counterpart of Lemma 3.

Remark 3. To increase the accuracy of the scheme (3.53-3.56), the time step δt may be divided into several local time steps, in particular if θ is much smaller than δt . In such a case, the local time step may be set to θ .

3.2.3. Step 3: other source terms

Other source terms such as the gravity field are accounted for using a centered approximation. No details are given here.

4. Numerical results

In the following, we assume that the equations of state within each phase agrees with

$$\varepsilon_1(P_1, \rho_1) = \frac{P_1}{(\gamma_1 - 1)\rho_1} \quad \text{and} \quad \varepsilon_2(P_2, \rho_2) = \frac{P_2}{(\gamma_2 - 1)\rho_2}.$$
(4.57)

The C.F.L. number N_{CFL} satisfies stability condition

$$\max(|U_k| + c_k)\delta t < N_{CFL}\delta x. \tag{4.58}$$

In the following, N_{CFL} is set to 0.45. Note that for the Rusanov scheme, the maximum is computed using cell values whereas for the VFRoe-ncv scheme, the maximum is computed using interface values.

4.1. Moving contact discontinuity

The length of the domain is $1000 \, m$. the initial datum for the first Riemann problem are given by :

	α_1	$ au_1$	U_1	P_1	$ au_2$	U_2	P_2
Left	0.9	1	100	10^{5}	1	100	10^{5}
Right	0.5	8	100	10^{5}	8	100	10^{5}

We also set $\gamma_1 = \gamma_2 = 1.4$. The resulting flow is rather simple, since $P_1(x,t) =$ $P_2(x,t) = 10^5 Pa$ and $U_1(x,t) = U_2(x,t) = 100 \, m/s$. Thus the mass fractions and the volume fraction are governed by the mass balance equations and the solution is

$$\alpha_1(t,x) = \alpha_1(0, x - 100 t)$$
 and $\alpha_k \rho_k(t,x) = \alpha_k \rho_k(0, x - 100 t), k = 1, 2.$

The results displayed in Figure 1 have been obtained using 1000 cells. The final time is $T_{MAX} = 3 s$.

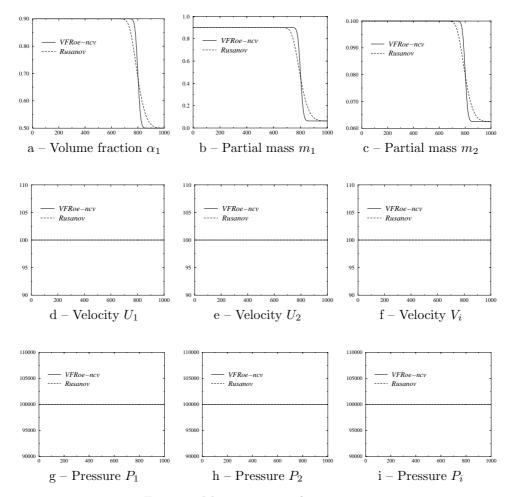


Figure 1: Moving contact discontinuity

One may check in Figure 1 that both schemes exactly preserve constant velocities and pressures. Figures 1.a to 1.c show that the numerical diffusion of the VFRoe-ncv

scheme is less important than the numerical diffusion associated with the Rusanov scheme.

4.2. Shock tube test

In the second test case, we assume a strong desequilibrium between both phases in terms of pressure fields. Initial conditions are

		α_1	$ au_1$	U_1	P_1	$ au_2$	U_2	P_2
I	∠eft	0.9	1	0	10^{5}	0.1	0	10^{4}
R	ight	0.5	8	0	10^{4}	0.8	0	10^{3}

Due to the number of different waves, this test has been performed on a very fine mesh (it contains 50000 cells) in order to obtain good approximation of intermediate states.

All figures are plotted with $T_{MAX}=0.7\,s$. Figures 2.a to 2.c permit to locate different waves. It is worth noting in Figure 2.c that the 7-wave (that is the wave associated with the eigenvalue U_2+c_2) is resonant with the 1-wave. Indeed, the 7-wave is composed by a rarefaction wave followed by a constant state and a shock wave. The jump of m_2 at the end of the rarefaction wave corresponds to the 1-contact discontinuity. Figures 2.d to 2.i represent the six 1-Riemann invariants defined in equations (2.24-2.28) and (2.33), zoomed around the position of the 1-wave. Bold lines correspond to the numerical location of the 1-contact discontinuity expanded due to the numerical diffusion of schemes. Let us emphasize that the scale of the y-axis in Figures 2.d to 2.i is very small with regard to the amplitude of variations of each 1-Riemann invariants (the scale of the y-axis represents around 2% and 10% of the difference between the maximal value and the minimal value of the k-Riemann invariant which is plotted).

4.3. The water faucet problem

This test case is a classical benchmark test in the frame of the numerical simulation of two-phase flow³⁹. This is a one-dimensional configuration, corresponding to a $L=12\,m$ long vertical tube. The initial condition is a uniform column of water (indexed by 1) in the air (indexed by 2), with a volume fraction of the water α_1 equal to 0,8 over the domain. Note that we set $\gamma_1=1,0005$ and $\gamma_2=1,4$ in (4.57). The velocity of the water U_1 is 10 and the velocity of the air U_2 is null. All pressures are set to 10^5 . The initial densities are $\rho_1(t=0,.)=1000$ and $\rho_2(t=0,.)=1$. This initial datum may be interpreted as a flow of water without gravity.

The simulation consists in introducing the gravity field for t > 0. The flow is thus driven by the boundary conditions: $\alpha_1(t,0) = 0, 8$, $U_1(t,0) = 10$, $U_2(t,0) = 0$, $P_1(t,L) = P_2(t,L) = 10^5$, and by the governing equations (2.7) complemented by gravity terms g = 9.8 in (0;L). Moreover, the drag force is not included and the time scale is $\theta = 5.10^{-4} s$ in the pressure relaxation term (2.11). An analytical solution of this test is available for a very simple model, which is actually too simple since the present model (2.7) cannot degenerate to it unless assuming unrealistic

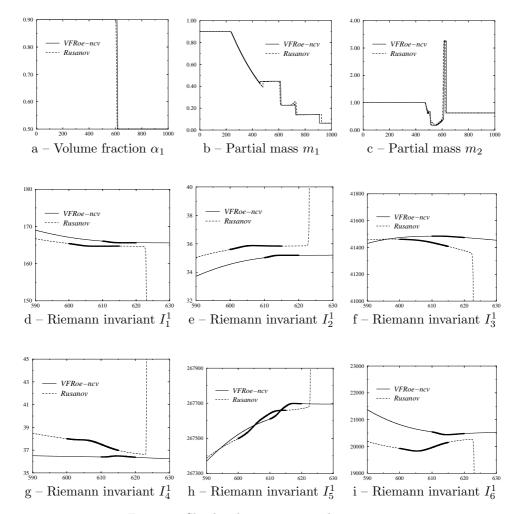


Figure 2: Shock tube test case with resonance

hypotheses³⁰. After some time steps, the volume fraction $(\alpha_1)_0^n$ becomes different from 0,8 and the solution of the associated partial Riemann problem (in the sense of F. Dubois¹²) cannot be solved exactly. Therefore, the previous boundary condition has been changed to $\alpha_1(t,x<0)=0,8,\ \rho_1(t,x<0)=1000,\ \rho_2(t,x<0)=1,\ U_1(t,x<0)=10,\ U_2(t,x<0)=0$ and $P_1(t,x<0)=P_2(t,x<0)=10^5$. This "Dirichlet" boundary condition is solved using the linearisation of the VFRoe-ncv scheme. Concerning the boundary condition at x=L, we may reasonably assume that $V_i>0$ since the velocities U_1 and U_2 are positive all along the simulation. In such a case, the volume fraction $\alpha_1(t,L^-),\ t>t^n$, is equal to $(\alpha_1)_N^n$ (where N is the index of the last cell of the domain) and the partial Riemann problem may be exactly solved by the technique proposed by F. Dubois.

The first results presented here correspond to the profiles plotted at $T_{MAX} = 0.5\,s$. Only the VFRoe-ncv scheme has been tested here for the convective part (3.35). Several meshes have been used. A common problem of the two-fluid one-pressure approach is that, for this test, some complex speeds of waves arise and if the cell number is too large (more than 1000 cells), the volume fraction of the air α_2 becomes negative. Here, computations have been performed over 20000 cells (and may be extended to smaller space steps δx). This is due to the unconditional hyperbolicity of the model. Note that, for the finest mesh presented here, the approximate solution of α_2 in Figure 3 seems smoothed. This is a consequence of the pressure relaxation which is not instantaneous. Furthermore, profiles of velocity U_1 in Figure 4 are in agreement with classical results obtained when focusing on two-fluid one-pressure models, since no pressure relaxation term appears in the governing equations of velocities U_1 and U_2 .

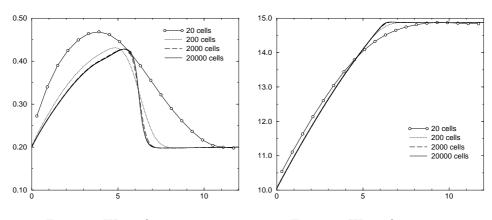
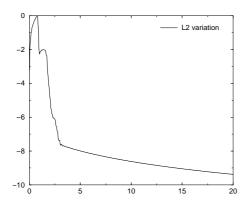


Figure 3: Water faucet Volume fraction α_2

Figure 4: Water faucet Water velocity U_1

We now focus on the convergence of the scheme when $t \to \infty$. In order to evaluate the convergence of the VFRoe-new scheme, the normalised time variations



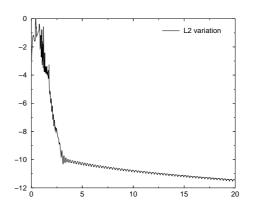


Figure 5: Water faucet Variation of the volume fraction α_2

Figure 6: Water faucet Variation of the water velocity U_2

in the L^2 -norm associated with α_1 and U_1 ,

$$\ln \frac{\left(\sum_{i} \left((\alpha_{1})_{i}^{n+1} - (\alpha_{1})_{i}^{n} \right) \right)^{1/2}}{\max_{\{n; t^{n} \leq T_{MAX}\}} \left(\sum_{i} \left((\alpha_{1})_{i}^{n+1} - (\alpha_{1})_{i}^{n} \right) \right)^{1/2}}$$

and

$$\ln \frac{\left(\sum_{i} \left((U_1)_i^{n+1} - (U_1)_i^n \right) \right)^{1/2}}{\max_{\{n; t^n \le T_{MAX}\}} \left(\sum_{i} \left((U_1)_i^{n+1} - (U_1)_i^n \right) \right)^{1/2}},$$

are plotted in Figures 5-6

4.4. The sedimentation test case

This test case corresponds to a very simple configuration, which is a classical benchmark test for the simulation of two-phase flows^{1,8,9}. A uniform mixture of gas and liquid, $\alpha_1(0,x) = 0, 5, x \in [0,7,5]$, lies in a vertical tube (the subscript 1 corresponds to the water and the subscript 2 corresponds to the air). The initial densities are set to $\rho_1(0,x) = 10^3$ and $\rho_2(0,x) = 1$, both pressures are $P_1(0,x) = P_2(0,x) = 10^5$ and velocities $U_1(0,x)$ and $U_2(0,x)$ are null, $x \in [0,7,5]$. The domain is closed, which means that rigid wall boundary conditions are imposed at x = 0 and x = 7, 5. The equations of state are the same as for the previous test case and $\theta = 5.10^{-4} \, s$ is the pressure relaxation time scale (2.11) (here again, the drag force is not taken into account). The gravity field provides a separation of the phases for t > 0 and the solution at $t = +\infty$ is composed by a distribution at rest of pure air for $x \in [0; 3, 25]$ and by a distribution of pure water for $x \in [3, 25, 7, 5]$. The Figure 7 corresponds to the results obtained by the VFRoe-ncv scheme over 200 cells. This test clearly

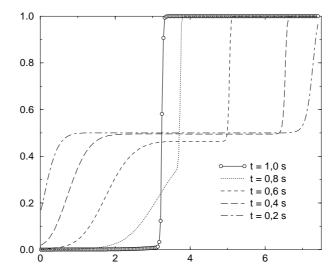


Figure 7: Variation of α_1 for the sedimentation test case (distance $vs \alpha_1$)

shows that the VFRoe-nev scheme reproduces the maximum principle for α_1 .

5. Conclusion

Some new results concerning modeling of two-phase flows with help of the twofluid approach have been presented herein. The main difference with the models issued from the classical literature about the simulation of two-phase flows is that the phase pressures are assumed to be distinct. The system requires giving adequate closures for the interface velocity and the interface pressure, in addition with standard closure laws for drag terms, viscous terms and mass transfer terms. The interfacial velocity has been chosen such that the 1-wave (which corresponds to the transport of the volume fraction) is a contact discontinuity. This implies that this interface remains infinitely thin whatever the initial condition is. Concerning the interfacial pressure, several ways of closure are proposed. The first way of closure aims at defining products of distributions occurring in non-conservative terms. This may be done choosing the interfacial pressure as a function of the 1-Riemann invariants. The other way of closure permits to obtain a meaningful entropy inequality. It enables to check that intermediate states occuring in the solution of the one dimensional Riemann problem are physically releavant, which means that expected positive constraints on some quantities are preserved throughout the connection of states through waves. The system obtained with these closures thus seems adequate to compute two-phase flows. The property of hyperbolicity ensures that for all initial data in Ω the speeds of waves are real. Furthermore, for a class of closure laws for the interfacial pressure and the interfacial velocity, the connection through these waves is in agreement with the maximum principle for the volume fraction and with

the positivity requirements for partial masses and pressures. Note that these important properties are maintained through the relaxation processes. Actually, our study has been led following the theory associated to Riemann problems, such as the one presented in Ref. ⁵⁰ in the frame of gas dynamics for instance. Nonetheless, another way of investigation should be proposed. Indeed, the model presented here may be seen as an extension by a relaxation process of the well-known six equations model⁹, which assumes the pressure equilibrium. Then, one might try to follow the analyses of T.P. Liu³⁸ and G.Q. Chen, C.D. Levermore and T.P. Liu⁵ of hyperbolic systems with relaxation.

Two different Finite Volume methods to compute the convective set have been described, which are based on a non-conservative form of Rusanov scheme and a modified form of VFRoe scheme with non-conservative variables. Source terms have been accounted using a splitting method. Several properties of both methods have been described and emphasized by numerical tests. Evenmore, some computational results enable deeper understanding of the solution of the whole set of partial differential equations, in particular for the resonance phenomenon. A classical benchmark for the simulation of two-phase flows, namely the water faucet problem, has been tested. Very encouraging results have been obtained, since the computations may be performed over very fine meshes without a loss of stability and physical releavance, due to the unconditional hyperbolicity of the model.

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Appendix A. Rankine-Hugoniot jump relations for a linearly degenerate field of a non-conservative system

Let us study the following system:

$$\frac{\partial}{\partial t}W + A(W)\frac{\partial}{\partial x}W = 0, \tag{A.1}$$

with W a function from $\mathbb{R}_+ \times \mathbb{R}$ to Ω (Ω an open subset of \mathbb{R}^p). We suppose that this system is non-conservative and hyperbolic. We focus on the k^{th} field $(1 \le k \le p)$, which is assumed to be *linearly degenerate*, which means that

$$\nabla \lambda_k(W).r_k(W) = 0, \quad W \in \Omega, \tag{A.2}$$

where $\lambda_k(W)$ is the k^{th} eigenvalue of A(W) and $r_k(W)$ the k^{th} right eigenvector of A(W). Let $(I_l^k)_{l=1,\dots,p-1}$ be a family of k-Riemann invariants, i.e. smooth functions from Ω to \mathbb{R} satisfying

$$\nabla I_l^k(W).r_k(W) = 0, \quad W \in \Omega. \tag{A.3}$$

Assume now that the gradients of the k-Riemann invariants $(I_l^k)_{l=1,\ldots,p-1}$ are linearly independent (such a family of k-Riemann invariants exists, see Proposition 17.2 of Ref. ⁵⁰). Using this set of k-Riemann invariants, one may define the curve $C_k(W_L)$, W_L in Ω , by

$$C_k(W_L) = \{ W \in \Omega; I_l^k(W) = I_l^k(W_L), 1 \le l \le p - 1 \}.$$
(A.4)

We suppose that there exists a parametrisation $\Phi_k(W_L, \varepsilon)$ of $\mathcal{C}_k(W_L)$, from $\Omega \times \mathbb{R}$ to Ω , such that $\Phi_k(W_L, 0) = W_L$. One may easily check that

$$\frac{\partial}{\partial \varepsilon} I_l^k(\Phi_k(W_L, \varepsilon)) = 0, \quad \forall 1 \le l \le p - 1.$$
(A.5)

We have the following result:

Proposition 10. The curve $C_k(W_L)$ is the integral curve of the vector field r_k passing through the point W_L .

Proof. Let us define the function V by $V(\varepsilon) = \Phi_k(W_L, \varepsilon)$. Obviously, $V(0) = W_L$ holds. We now aim at verify that vectors $V'(\varepsilon)$ and $r_k(V(\varepsilon))$ are collinear in \mathbb{R}^p . Equation (A.5) becomes

$$\nabla I_l^k(V).V'(\varepsilon) = 0, \quad \forall 1 \le l \le p - 1. \tag{A.6}$$

Therefore, recalling that the right eigenvector r_k satisfies equation (A.3), this proof reduces to check that the family $(\nabla I_l^k(V))_{l=1,\dots,p-1}$ is free, which holds. \square

Let us introduce now two smooth functions u and f from Ω to \mathbb{R} such that

$$u'(W)A(W) = f'(W), \quad W \in \Omega, \tag{A.7}$$

or equivalently such that

$$\frac{\partial}{\partial t}u(W(t,x)) + \frac{\partial}{\partial x}f(W(t,x)) = 0, \quad W \in \Omega.$$
 (A.8)

Note that the partial differential equation (A.8) is a conservation law which is, in general, only available for smooth solutions W of system (A.1). However, focusing on the k^{th} field, the following Rankine-Hugoniot jump relation holds:

Theorem A.1. Let us note $\sigma(W) = \lambda_k(W)$. Then we have

$$\sigma(W)(u(W) - u(W_L)) = f(W) - f(W_L), \quad \forall W \in \mathcal{C}_k(W_L). \tag{A.9}$$

Proof. As above, we define the function V by $V(\varepsilon) = \Phi_k(W_L, \varepsilon)$. Moreover, we set

$$E(\varepsilon) = -\sigma(V(\varepsilon)) (u(V(\varepsilon)) - u(W_L)) + (f(V(\varepsilon)) - f(W_L)). \tag{A.10}$$

Clearly, E(0) = 0. Note that by definition $\lambda_k(W)$ is a k-Riemann invariant, which provides $\sigma(W) = \lambda_k(W_L)$ for all W in $\mathcal{C}_k(W_L)$. Derivating equation (A.10) with respect to ε gives

$$E'(\varepsilon) = -\sigma(V(0))u'(V(\varepsilon)).V'(\varepsilon) + f'(V(\varepsilon)).V'(\varepsilon)$$

= $-\sigma(V(0))u'(V(\varepsilon)).V'(\varepsilon) + u'(V(\varepsilon))A(V(\varepsilon)).V'(\varepsilon).$

Using Proposition 10, it follows

$$E'(\varepsilon) = -\sigma(V(0))u'(V(\varepsilon)).r_k(V(\varepsilon)) + u'(V(\varepsilon))A(V(\varepsilon)).r_k(V(\varepsilon))$$
$$= u'(V(\varepsilon)).(A(V(\varepsilon))r_k(V(\varepsilon)) - \lambda_k(V(\varepsilon))r_k(V(\varepsilon)))$$
$$= 0.$$

Hence, $E(\varepsilon) = 0$ for all ε in \mathbb{R} . \square

As done before for $C_k(W_L)$ with k-Riemann invariants, we define the curve $S_k(W_L)$ from Rankine-Hugoniot jump relations of the form (A.9) associated with system (A.1). A straightforward consequence is that curves $C_k(W_L)$ and $S_k(W_L)$ coincide. So, the k-contact discontinuity propagates at speed $\sigma = \lambda_k$ (which is constant through the discontinuity) and is defined by the curve $S_k(W_L)$ (or equivalently by $\mathcal{C}_k(W_L)$). Finally, the non-conservative frame is identical to the conservative frame when focusing on linearly degenerate fields (note that this result has already been stated 3).

Appendix B. Connection through the 1-wave

The system studied here corresponds to the set of partial differential equations (2.7) with the interfacial velocity V_i defined by (2.5)-(2.22) and the interfacial pressure P_i given by (2.29-2.31), associated with the Riemann initial datum (2.19). Both equations of state follow $P_k = (\gamma_k - 1)\rho_k e_k$, $\gamma_k > 1$, k = 1, 2. We focus here on the parametrisation through the 1-contact discontinuity between W_l and W_r (see notations in the body of the text). Recall that 1-Riemann invariants and Rankine-Hugoniot jump relations lead to the same parametrisation, since this field is linearly degenerate. Therefore, through the 1-wave, the equality

$$I_p^1(W_l) = I_p^1(W_r) (B.1)$$

holds for all $1 \leq p \leq 6$, where the 1-Riemann invariants $(I_p^1)_{p=1,...,6}$ are given in equations (2.24-2.28)-(2.33). Combining I_2^1 , I_3^1 , I_5^1 and I_6^1 leads to

$$I_3^1(W) = (I_2^1(W))^2 \left(\frac{\gamma_1 + 1}{2\gamma_1} \frac{1}{m_1} + \frac{\gamma_2 + 1}{2\gamma_2} \frac{1}{m_2}\right) + I_5^1(W) \frac{\gamma_1 - 1}{\gamma_1} m_1 + I_6^1(W) \frac{\gamma_2 - 1}{\gamma_2} m_2.$$
(B.2)

Inserting the jump relations (B.1) in (B.2) yields

$$I_3^1(W_l) = (I_2^1(W_l))^2 \left(\frac{\gamma_1 + 1}{2\gamma_1} \frac{1}{(m_1)_r} + \frac{\gamma_2 + 1}{2\gamma_2} \frac{1}{(m_2)_r} \right) + I_5^1(W_l) \frac{\gamma_1 - 1}{\gamma_1} (m_1)_r + I_6^1(W_l) \frac{\gamma_2 - 1}{\gamma_2} (m_2)_r,$$
(B.3)

where only $(m_1)_r$ and $(m_2)_r$ are unknown.

We turn now to the jump relation (B.1) with p=4. Since we are dealing with a perfect gas state law within each phase, specific entropies are defined by $s_k = P_k \rho_k^{-\gamma_k}$, k=1,2. One can easily obtain

$$s_k = \frac{\alpha_k^{-\gamma_k + 1}}{m_k^{\gamma_k}} \left(\frac{\gamma_k - 1}{\gamma_k} \right) \left(I_{k+4}^1(W) m_k - \frac{(I_2^1(W))^2}{2m_k} \right).$$
 (B.4)

So, Rankine-Hugoniot jump relations (B.1) and equation (B.4) yield

$$\frac{(1-(\alpha_1)_r)^{-\gamma_2+1}}{(m_2)_r^{\gamma_2}} \left(\frac{\gamma_2-1}{\gamma_2}\right) \left(I_6^1(W_l)(m_2)_r - \frac{(I_2^1(W_l))^2}{2(m_2)_r}\right) \\
= \frac{(s_2)_l}{(s_1)_l} \frac{(\alpha_1)_r^{-\gamma_1+1}}{(m_1)_r^{\gamma_1}} \left(\frac{\gamma_1-1}{\gamma_1}\right) \left(I_5^1(W_l)(m_1)_r - \frac{(I_2^1(W_l))^2}{2(m_1)_r}\right). \quad (B.5)$$

As mentioned above, focusing on the complete Riemann problem, we have $(\alpha_1)_r = (\alpha_1)_R$, where $(\alpha_1)_R$ denotes $\alpha_1(t=0,x>0)$, which means that $(\alpha_1)_r$ is not an unknown. Hence, equations (B.3) and (B.5) compose a non-linear system of two equations with two unknowns $(m_1)_r$ and $(m_2)_r$. Let us describe the solution of this system. First, equation (B.5) is rewritten to provide $(m_2)_r$ as a function of

 $(m_1)_r$. The partial mass $(m_2)_r$ is then replaced in (B.3) by the expression, in order to obtain an equation of the form

$$\mathcal{H}((m_1)_r) = I_3^1(W_l) \tag{B.6}$$

where \mathcal{H} is the suitable function defined from (B.3) and (B.5). Hence, the resolution of the 2×2 system is reduced to the inversion of the function \mathcal{H} . The behaviour of \mathcal{H} may be describe by the following table:

m	0		m_0		$+\infty$
$\mathcal{H}'(m)$	$-\infty$	_	0	+	$+\infty$ $+\infty$
$\mathcal{H}(m)$	+∞		$\mathcal{H}(m_0)$	1	$+\infty$

where

$$m_0 = \left(\frac{(\gamma_1 + 1)(I_2^1(W_l))^2}{2(\gamma_1 - 1)I_5^1(W_l)}\right)^{\frac{1}{2}}.$$

Some constraints on the solution $(m_1)_r$ must be added, in order to ensure that W_r is an admissible state, that is $W_r \in \Omega$. Of course, $(\alpha_1)_r$ belongs to]0,1[since $(\alpha_1)_r = (\alpha_1)_R$. Furthermore, assuming that $(m_1)_r > 0$, positivity of partial mass $(m_2)_r$ is directly ensured by equation (B.3). The internal energy of phase 1 noted $(e_1)_r$ is positive if

$$(m_1)_r^2 > \mu_0 \quad \text{where} \quad \mu_0 = \frac{(I_2^1(W_l))^2}{2I_5^1(W_l)}.$$
 (B.7)

Finally, the internal energy $(e_2)_r$ is positive using the equality $I_4^1(W_l) = I_4^1(W_r)$. Therefore, if a solution $(m_1)_r$ of equation (B.6) verifies inequality (B.7), the whole state W_r calculated from $(m_1)_r$ and jump relations (B.1) is admissible. This allows to state proposition 9.

We discuss now the existence of solutions of equation (B.6) (see Figure B.1 for an illustration). A first condition comes from the value of $I_3^1(W_l)$. If $I_3^1(W_l)$ $\mathcal{H}(m_0)$, then equation (B.6) admits no solution (see Remark 4 for more details). If $I_3^1(W_l) \geq \mathcal{H}(m_0)$, two solutions of equations (B.6) can be constructed (which coincide if the inequality is an equality), referred as $(m_1)_r^-$ and $(m_1)_r^+$ on Figure B.1. We turn now to inequality (B.7). Note that, since $\gamma_1 > 1$, we have $m_0 > \mu_0$. Hence, $(m_1)_r^+$ always verifies (B.7), which means that if $(m_1)_r^+$ exists, this is always an admissible solution of (B.6). Moreover, the root $(m_1)_r^-$ is admissible if and only if $(m_1)_r^- > \mu_0$, which provides two distinct solutions of equation (B.6) (it corresponds to Figure B.1).

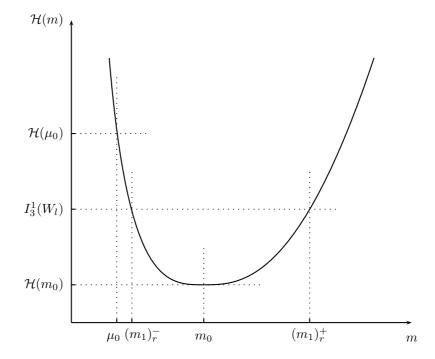


Figure B.1: Resolution of equation (B.6)

Remark 4. As mentioned above, if $I_3^1(W_l) < \mathcal{H}(m_0)$, equation (B.6) admits no solution. It means that no state W_r can be connected to W_l by the 1-contact discontinuity. Therefore, a wave must appear between W_l and the wave V_i to solve the Riemann problem. The same phenomenon occurs when focusing on systems with source terms^{37,6,25} or systems with a flux function involving discontinuous coefficients^{33,48}.

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