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Relaxation process in an immiscible three-phase flow model

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Abstract. This paper deals with the numerical modeling of immiscible three-phase flows. The main focus here is on the numerical treatment of the source terms of the model. A new scheme based on a more coupled approach than the preexisting fractional step strategy is presented. Properties of this scheme are given. Numerical applications highlight the benefits of this scheme in terms of both accuracy and stability.

Keywords: Three-phase flow, Source term, Relaxation, Finite Volume

1 Introduction

Some recent computations of immiscible three-phase flow models have highlighted some weaknesses of existing numerical schemes, for instance when representing vapor explosion [1], and thus have urged the building of robust implicit schemes. This has also motivated to investigate the behavior of solutions of rather complex sets of PDEs, such as those arising in [7], which are used in [1]. Moreover, it is widely admitted by the scientific community that the hyperbolic models at stake here contain inner relaxation processes that guarantee the return-to-equilibrium. The purpose of the current work precisely consists in better understanding the associated (at least expected) relaxation process first, and then taking advantage of the latter in order to stabilize approximate solutions obtained with help of rather classical Finite Volume procedures. In the sequel, we will focus on the model [7], and propose a two-step numerical strategy. This strategy accounts for the expected inner relaxation process in a suitable implicit way, and also uses an explicit Riemann-type solver in order to cope with convective effects.

First, the model presented in [7] is recalled as well as its main properties. We emphasize that the strategy that has been used to derive model [7] is similar to the one that has been used in [2], in the two-phase flow framework. This guarantees a meaningful definition of non-conservative products for these models. Then, the new numerical strategy to compute approximate solutions of [7] is presented. Eventually, numerical cases depict the effectiveness of the new method. This paper is the sequel of a work that is dedicated to two-phase flow models [6].

2 The immiscible three-phase flow model [7]

The system of PDEs governing the time-space evolution of the variables is:

$$\begin{cases} \frac{\partial \alpha_k}{\partial t} + \mathcal{V}_I(W) \cdot \nabla \alpha_k = S_k^\alpha(W) , \\ \frac{\partial m_k}{\partial t} + \nabla \cdot (m_k U_k) = S_k^m(W) , \\ \frac{\partial m_k U_k}{\partial t} + \nabla \cdot (m_k U_k \otimes U_k + \alpha_k P_k \mathcal{I}) + \sum_{l=1, l \neq k}^3 \Pi_{kl}(W) \nabla \alpha_l = S_k^U(W) , \\ \frac{\partial \alpha_k E_k}{\partial t} + \nabla \cdot (\alpha_k E_k U_k + \alpha_k P_k U_k) - \sum_{l=1, l \neq k}^3 \Pi_{kl}(W) \frac{\partial \alpha_l}{\partial t} = S_k^E(W) , \end{cases} \quad (1)$$

where $\forall k \in \llbracket 1, 3 \rrbracket$, $\alpha_k \in]0, 1[$ denote the statistical fractions which satisfy :

$$\alpha_1 + \alpha_2 + \alpha_3 = 1 . \quad (2)$$

ρ_k stand for the densities, $m_k = \alpha_k \rho_k$ are the partial densities, U_k the velocities, P_k the pressures and E_k the total energies which read $E_k = \rho_k(\epsilon_k + U_k^2/2)$. The specific internal energies ϵ_k are obtained through an Equation Of State (EOS): $\epsilon_k = \epsilon_k(\rho_k, P_k)$, and \mathcal{I} stands for the identity. The velocity $\mathcal{V}_I(W)$ is chosen as :

$$\mathcal{V}_I = U_1 , \quad (3)$$

see [7], which leads to the following unique interfacial pressure definition, owing to the entropy inequality (see **Appendix G** of [7]):

$$\begin{cases} \Pi_{12} = \Pi_{21} = \Pi_{23} = P_2 , \\ \Pi_{13} = \Pi_{31} = \Pi_{32} = P_3 . \end{cases} \quad (4)$$

The state variable $W \in \mathbb{R}^{11}$ is defined as:

$$W = (\alpha_2, \alpha_3, m_1, m_1 U_1, \alpha_1 E_1, m_2, m_2 U_2, \alpha_2 E_2, m_3, m_3 U_3, \alpha_3 E_3)^\top . \quad (5)$$

In this work, the phase transitions are neglected, hence:

$$\forall k \in \llbracket 1, 3 \rrbracket, \quad l \neq k \quad S_k^m(W) = 0 . \quad (6)$$

In order to close the source terms, the total entropy $\eta(W)$ paired with its entropy-flux $\mathcal{F}_\eta(W)$, the temperature T_k and the celerity c_k are introduced:

$$\begin{cases} \eta = m_1 s_1(P_1, \rho_1) + m_2 s_2(P_2, \rho_2) + m_3 s_3(P_3, \rho_3) , \\ \mathcal{F}_\eta = m_1 U_1 s_1(P_1, \rho_1) + m_2 U_2 s_2(P_2, \rho_2) + m_3 U_3 s_3(P_3, \rho_3) . \end{cases} \quad (7)$$

$\frac{1}{T_k} = \frac{\partial_{P_k} (s_k(P_k, \rho_k))|_{\rho_k}}{\partial_{P_k} (\epsilon_k(P_k, \rho_k))|_{\rho_k}}$ and $c_k^2 \partial_{P_k} (s_k(P_k, \rho_k))|_{\rho_k} + \partial_{\rho_k} (s_k(P_k, \rho_k))|_{P_k} = 0$.

Functions s_k denote specific entropies. Source terms are written, $\forall k \in \llbracket 1, 3 \rrbracket$, as:

$$\begin{aligned} S_k^\alpha &= \sum_{l=1, l \neq k}^3 K_{kl}(W)(P_k - P_l) \quad ; \quad S_k^U = \sum_{l=1, l \neq k}^3 d_{kl}(W)(U_l - U_k) ; \\ S_k^E &= \sum_{l=1, l \neq k}^3 q_{kl}(W)(T_l - T_k) + \sum_{l=1, l \neq k}^3 d_{kl} V_{kl}(U_l - U_k) , \end{aligned} \quad (8)$$

(see [7, 1]), with the positive parameters $d_{kl}(W) = m_k m_l / (M \tau_{kl}^U(W))$, $K_{kl}(W) = \alpha_k \alpha_l / (\Pi_0 \tau_{kl}^P(W))$ and $q_{kl}(W) = m_k m_l C_{v_k} C_{v_l} / (\tau_{kl}^T(W) (m C_v)_{kl})$. Quantities C_{V_k} denote the specific heat capacities. V_{kl} are phasic mean velocities: $V_{kl} = (U_k + U_l)/2$. Π_0 is a positive pressure of reference, $M = m_1 + m_2 + m_3$ and $(m C_v)_{kl} = m_k C_{v_k} + m_l C_{v_l}$. For each phasic connection $k - l$, $\tau_{kl}^P(W)$, $\tau_{kl}^T(W)$ and $\tau_{kl}^U(W)$ are the positive relaxation time scales related to the return to equilibrium of the associated thermodynamic quantity. Closure laws for the relaxation time scales can be found in the literature, see [4] for the pressure or [9] for the velocity and temperature. Model (1) with closures (3), (4), (6) and (8) is such that:

Property 1: (*three-phase flow model in a 1D framework*)

If $\forall k \in \llbracket 1, 3 \rrbracket$, α_k stay in $]0, 1[$ and $\|U_k - U_1\| \neq c_k$, then:

- The convective part of the model is hyperbolic and the associated eigenvalues are:

$$\begin{aligned} \lambda_{1,2,3}(W) &= U_1 ; \lambda_4(W) = U_2 ; \lambda_5(W) = U_3 ; \\ \lambda_{6,7}(W) &= U_1 \pm c_1 ; \lambda_{8,9}(W) = U_2 \pm c_2 ; \lambda_{10,11}(W) = U_3 \pm c_3 . \end{aligned} \quad (9)$$

- Fields associated with λ_k ($k = 6 - 11$) are **GNL**. Other fields are **LD**.
- Smooth solutions of the model comply with an entropy inequality:

$$\partial_t (\eta(W)) + \nabla \cdot \mathcal{F}_\eta(W) \leq 0 . \quad (10)$$

- The model is symmetrizable.

Proof. The first three items can be found in [7] and the latter is detailed in [8].

3 Numerical scheme

The overall scheme is quite similar to the one detailed in [1]. It is a Finite Volume scheme for unstructured meshes. It consists of two main steps:

- I: First, compute **explicitly** a solution between $t^n \xrightarrow{\Delta t} t^*$ of the convective subsystem:

$$A(W) \partial_t (W) + \nabla \cdot F(W) + C(W) \nabla \cdot W = 0 , \quad (11)$$

using a Rusanov scheme [10] adapted for non-conservative products. Equation (11) exactly corresponds to system (1), while setting all source terms to zero.

- II: Then, compute an approximate solution of the ODE:

$$A(W) \partial_t (W) = S(W) , \quad (12)$$

between $t^* \xrightarrow{\Delta t} t^{n+1}$. Equation (12) corresponds to system (1), when all spatial derivatives are set to zero. This step is solved with an **implicit** scheme.

The discretization of the time derivative is done with a first-order Euler scheme. The time step Δt is determined by the Courant-Friedrich-Levy (CFL) condition of the first step. Details of the convective step are given in [1]. An extension of the scheme proposed in [11] for a barotropic three-phase flow model to the current three-phase flow model (which includes energy equations) would be useful. This would give higher accuracy than the scheme used in the present work. This strategy has already been used in the case of a two-phase flow model in [3].

We focus in the sequel on the numerical treatment of the source terms for this model. A fractional step algorithm, which fully decouples each relaxation effect, is employed in [1]. However, in some cases, this method is not robust enough to compute a solution (see Part 4.4 of [1]). Hereafter, a new method for a better handling of the source terms is presented. Setting for $k \in \llbracket 1, 3 \rrbracket$, $\Phi_k \in \{U_k, P_k, T_k\}$, $\Delta\Phi_{kl} = \Phi_k - \Phi_l$, system (12) reads:

$$\begin{cases} \frac{\partial \alpha_k}{\partial t} = \sum_{l=1, l \neq k}^3 K_{kl}(W) \Delta P_{kl} , \\ \frac{\partial m_k}{\partial t} = 0 , \\ \frac{\partial m_k U_k}{\partial t} = - \sum_{l=1, l \neq k}^3 d_{kl}(W) \Delta U_{kl} , \\ \frac{\partial \alpha_k E_k}{\partial t} - \sum_{l=1, l \neq k}^3 \Pi_{kl}(W) \frac{\partial \alpha_l}{\partial t} = - \sum_{l=1, l \neq k}^3 q_{kl}(W) \Delta T_{kl} - \sum_{l=1, l \neq k}^3 d_{kl}(W) \frac{U_k^2 - U_l^2}{2} . \end{cases} \quad (13)$$

Setting: $\Delta_S \in \mathbb{R}^6$, $\Delta_S = (\Delta U_{12}, \Delta U_{13}, \Delta P_{12}, \Delta P_{13}, \Delta T_{12}, \Delta T_{13})^\top \in \mathbb{R}^6$, it can be derived from (13):

$$\partial_t (\Delta_S) = -R^{relax}(W) \Delta_S , \quad (14)$$

and the five stationary constraints:

$$\forall k \in \llbracket 1, 3 \rrbracket , \quad \partial_t m_k = 0 ; \quad \partial_t \sum_{k=1}^3 m_k U_k = \partial_t \sum_{k=1}^3 \alpha_k E_k = 0 , \quad (15)$$

with R^{relax} a matrix in $\mathcal{M}_6(\mathbb{R})$ of the form:

$$R^{relax}(W) = \begin{pmatrix} R_{UU}(W) & 0 & 0 \\ R_{PU}(W) & R_{PP}(W) & R_{PT}(W) \\ R_{TU}(W) & R_{TP}(W) & R_{TT}(W) \end{pmatrix} , \quad (16)$$

where each sub-matrix $R_{IJ}(W)$, $(I, J) \in \{U, P, T\}^2$ is in $\mathcal{M}_2(\mathbb{R})$. All coefficients of the sub-matrices are given in detail in [5] for a class of three-phase flow models. The counterpart for a similar class of two-phase flow models is given in [6]. From (14) and (16), conditions that guarantee the relaxation process over time can be exhibited, as it has been done in [6] for a two-phase flow model. Because of the block triangular structure of R^{relax} , the overall method to compute an approximate solution of (13) is:

- (i) Estimate the evolution of $\Delta U = (\Delta U_{12}, \Delta U_{13})^\top$ between $t^* \xrightarrow{\Delta t} t^{n+1-}$ according to:

$$\partial_t (\Delta U) = -R_{UU}(W) \Delta U , \quad (17)$$

with $R_{UU}(W) \in \mathcal{M}_2(\mathbb{R})$. Then update the state variable at time t^{n+1-} using the conservation law of the total momentum (see [1] section 3.3.1).

- (ii) Compute the evolution of $\Delta \in \mathbb{R}^4$, $\Delta = (\Delta P_{12}, \Delta P_{13}, \Delta T_{12}, \Delta T_{13})^\top$ between $t^{n+1-} \xrightarrow{\Delta t} t^{n+1}$, solution of:

$$\partial_t (\Delta) = -\mathcal{R}^{PT}(W) \Delta , \quad (18)$$

with $\mathcal{R}^{PT}(W) \in \mathcal{M}_4(\mathbb{R})$ defined as:

$$\mathcal{R}^{PT}(W) = \begin{pmatrix} R_{PP}(W) & R_{PT}(W) \\ R_{TP}(W) & R_{TT}(W) \end{pmatrix} . \quad (19)$$

Moreover, as the velocity relaxation is handled beforehand, the equation of evolution of the sum of the internal energies turns into a conservation law:

$$\partial_t \left(\sum_{k=1}^3 m_k \epsilon_k \right) = 0 , \quad (20)$$

which enables to update W at time t^{n+1} , together with constraint (2).

Hereafter, setting time t^{n+1-} as t^n for clarity, the algorithm in stage (ii) is:

Step 1: Compute the solution of (18) at t^{n+1} with a linear implicit Euler scheme and $\mathcal{R}^{PT}(W)$ frozen at time t^n :

$$\Delta^{n+1} = (\mathcal{I}_4 + \Delta t \mathcal{R}^{PT}(W^n))^{-1} \Delta^n , \quad (21)$$

with \mathcal{I}_4 the identity matrix of size 4.

Step 2: Setting:

$$\begin{cases} \xi_n = m_1 \epsilon_1(P_1^n, T_1^n) + m_2 \epsilon_2(P_2^n, T_2^n) + m_3 \epsilon_3(P_3^n, T_3^n) , \\ T_2^{n+1} = T_1^{n+1} - \Delta T_{12}^{n+1} ; & T_3^{n+1} = T_1^{n+1} - \Delta T_{13}^{n+1} ; \\ P_2^{n+1} = P_1^{n+1} - \Delta P_{12}^{n+1} ; & P_3^{n+1} = P_1^{n+1} - \Delta P_{13}^{n+1} . \end{cases} \quad (22)$$

Compute P_1^{n+1} and T_1^{n+1} , solutions of:

$$\begin{cases} m_1^n \epsilon_1(P_1^{n+1}, T_1^{n+1}) + m_2^n \epsilon_2(P_2^{n+1}, T_2^{n+1}) + m_3^n \epsilon_3(P_3^{n+1}, T_3^{n+1}) = \xi_n , \\ \frac{m_1^n}{\rho_1(P_1^{n+1}, T_1^{n+1})} + \frac{m_2^n}{\rho_2(P_2^{n+1}, T_2^{n+1})} + \frac{m_3^n}{\rho_3(P_3^{n+1}, T_3^{n+1})} = 1 . \end{cases} \quad (23)$$

System (23) comes from (20) and the immiscible constraint (2).

Step 3: Update α_2^{n+1} and α_3^{n+1} :

$$\alpha_2^{n+1} = \frac{m_2^n}{\rho_2(P_2^{n+1}, T_2^{n+1})} \quad ; \quad \alpha_3^{n+1} = \frac{m_3^n}{\rho_3(P_3^{n+1}, T_3^{n+1})} , \quad (24)$$

and the total energies :

$$\begin{cases} (\alpha_1 E_1)^{n+1} = m_1^n \epsilon_1(P_1^{n+1}, T_1^{n+1}) + \frac{1}{2} m_1^n (U_1^n)^2 , \\ (\alpha_2 E_2)^{n+1} = m_2^n \epsilon_2(P_2^{n+1}, T_2^{n+1}) + \frac{1}{2} m_2^n (U_2^n)^2 , \\ (\alpha_3 E_3)^{n+1} = \alpha_1^n E_1^n + \alpha_2^n E_2^n + \alpha_3^n E_3^n - (\alpha_1 E_1)^{n+1} - (\alpha_2 E_2)^{n+1} . \end{cases} \quad (25)$$

Note that system (23) is non linear implicit. Hence we get:

Property 2: (*P-T coupled relaxation algorithm*)

- a) For a mixture of ideal gases, the solution of (23) exists and is unique inside the relevant domain of definition and statistical fractions remain in $[0, 1]$.
- b) If all of the principal minors of $\mathcal{R}^{PT}(W)$ are positive, then (21) ensures the discrete relaxation process over time, whatever the time step Δt is.

Sketch of proof: a) Thanks to the specific structure of the ideal gas EOS, the internal energies are functions of only one thermodynamic variable. Because of that, the conservation of the sum of the internal energies in (23) gives the temperature at time t^{n+1} . The complete proof is similar to the one given in [6] for a two-phase flow model.

b) The proof of the second property is also an extension of the one given in [6].

4 Numerical results

In the sequel, for a quantity $\Psi \in \{P, T\}$, the relaxation time scales are supposed to be identical on each phasic connection: $\tau_{12}^\Psi = \tau_{13}^\Psi = \tau_{23}^\Psi = \tau^\Psi$. For simplicity, they are set as constants: $\tau^P = 10^{-5}s$ and $\tau^T = 10^{-3}s$. Besides, in all of the following numerical test cases, each phase k is given a stiffened gas EOS: $\gamma_1 = 22.84$ ($Jkg^{-1}K^{-1}$), $\Pi_1 = 1.884 \cdot 10^9$ (Pa), $\gamma_2 = 1.615$ ($Jkg^{-1}K^{-1}$), $\Pi_2 = 3.564 \cdot 10^8$ (Pa), $\gamma_3 = 1.086$ ($Jkg^{-1}K^{-1}$), $\Pi_3 = 0$ (Pa). It represents a mixture of hot liquid metal, liquid water and its vapour.

First, let us consider a homogeneous flow. Thus, for each phase k , $U_k = 0$ and for each quantity Ψ_k we have: $\nabla_x \Psi_k = 0$. With this hypothesis, the set of PDEs associated with model (1) is identical to the one approximated by step (ii). At time $t = 0$ s, the pressures are set equal: $P_1 = P_2 = P_3 = 1.0 \times 10^5$ Pa and the temperatures are set as: $T_1 = 2500K$, $T_2 = 363K$ and $T_3 = 1000K$. **Figure 1** highlights the poor behaviour of the fractional step algorithm for the pressure P_1 with coarse time steps. As the time step is given by the convective part of the simulation under a CFL condition, the numerical method used to compute an approximate solution of (13) must be robust. The coupled algorithm obviously better captures the global behaviour of the solution on coarse time steps. **Figure 2** confirms that the two schemes converge to the same solution with order 1.

The second case consists in a liquid water shock tube. For the numerical simulation, two meshes are considered: 50 000 cells and 100 000 cells. The CFL number is set to $1/2$. At time $t = 0s$, the shock tube is set as in **Table 1**. All phasic velocities are set to zero at time $t = 0s$. When the numerical simulation starts, the tube contains three zones: a high pressure chamber filled with liquid water, a low pressure zone full of liquid water, and an interaction zone. In the high pressure chamber, all phasic pressures are set to $15 \times 10^5 Pa$ at time $t = 0s$. Throughout the interaction zone, aluminium droplets of $500\mu m$ diameter are introduced at time $t = 0s$. The droplet temperature is set to $T_1 = 2500K$. Thus, two Riemann problems have to be solved at $x_{I_{12}} = 2.0m$ and $x_{I_{23}} = 2.15m$ in a short transient regime, and then interact with one another. **Figure 3** shows the evolution of the total pressure $P_{mix} = \alpha_1 P_1 + \alpha_2 P_2 + \alpha_3 P_3$ over time at two stations. Station 1 is located at $x_{S_1} = 1.4m$ and Station 2 is positioned at $x_{S_2} = 2.4m$. Focusing first on Station 2, the minor decrease of the total pressure P_{mix} at the beginning of the computation is the counterpart of what happens in the homogeneous case. After that, the small decrease of the total pressure at time $t = 0.4ms$ corresponds to the right-going wave associated with the initial interface located at $x_{I_{23}}$. At time $t = 0.6ms$, the incident right-going shock wave of magnitude $8.5 \times 10^5 Pa$, generated at time $t = 0s$ at $x_{I_{12}}$ arrives at Station 2. Then, the return-to-equilibrium process takes place till $3.8ms$. Afterwards the left-going rarefaction wave reflected from the right-side reaches station 2. Besides, as Station 1 is located inside the initial high pressure chamber, P_{mix} plateaus at $15 \times 10^5 Pa$ till $t = 0.9ms$, which corresponds to the arrival of the left-going rarefaction wave generated at $x_{I_{12}}$.

Abscissa (m)	$x \in [0; 2.0]$	$x \in]2.0; 2.15[$	$x \in [2.15; 3.75]$
α_1	$\epsilon_{lim} = 10^{-8}$	ϵ_{lim}	0.026
α_2	$1 - 2\epsilon_{lim}$	$1 - 2\epsilon_{lim}$	0.884
$P_1 = P_2 = P_3 (Pa)$	$1,5 \times 10^6$	$1,0 \times 10^5$	$1,0 \times 10^5$
$T_1 (K)$	1000	363	2500
$T_2 (K)$	1000	363	363
$T_3 (K)$	1000	363	1000

Table 1. Initial conditions for test case 2. All phasic velocities are set to zero.

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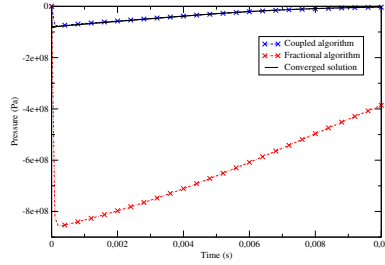


Fig. 1. Evolution of pressure P_1 computed with the coupled and fractional schemes for $\Delta t = 10^{-4} s$. For the converged solution, a time step $\Delta t = 10^{-11} s$ is considered.

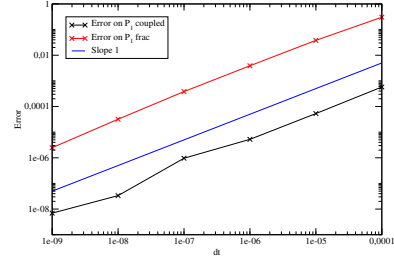


Fig. 2. Convergence curve for the coupled and fractional algorithm ; error on pressure P_1 in L_1 norm.

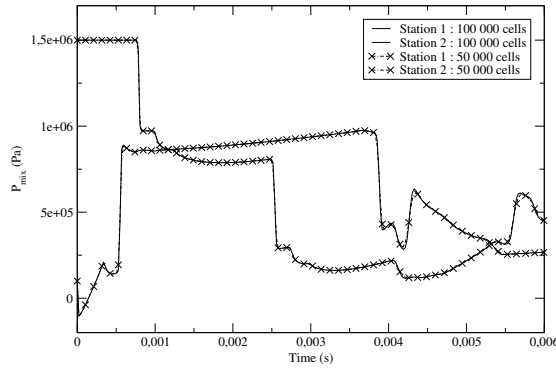


Fig. 3. Evolution of the total pressure $P_{mix} = \alpha_1 P_1 + \alpha_2 P_2 + \alpha_3 P_3$ over time at two different stations and for two different meshes (50 000 cells / 100 000 cells).

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