Pressure relaxation procedures for multiphase compressible flows

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SUMMARY

This paper deals with pressure relaxation procedures for multiphase compressible flow models. Such models have nice mathematical properties (hyperbolicity) and are able to solve a wide range of applications: interface problems, detonation physics, shock waves in mixtures, cavitating flows, etc. The numerical solution of such models involves several ingredients. One of those ingredients is the instantaneous pressure relaxation process and is of particular importance.

In this article, we present and compare existing and new pressure relaxation procedures in terms of both accuracy and computational efficiency. Among these procedures we enhance an exact one in the particular case of fluids governed by the stiffened gas equation of state, and approximate procedures for general equations of state, which are particularly well suited for problems with large pressure variations. We also present some generalizations of these procedures in the context of multiphase flows with an arbitrary number of fluids. Some tests are provided to illustrate these comparisons. Copyright © 2005 John Wiley & Sons, Ltd.

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1. INTRODUCTION

This paper is devoted to the design of efficient pressure relaxation procedures used in hydrocodes and compressible multiphase flows. Multiphase compressible flow models have been proposed in References [1–11].

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Among these models, the multi-velocities models, extended from the work of Baer and Nunziato [3], are of particular interest. Saurel and Abgrall [7] have shown that such a model was able to solve (under a unique formulation) interface problems with a single velocity, as well as multiphase problems involving several velocities [7, 9, 10]. These models use pressure relaxation procedures between phases. They are unconditionally hyperbolic and are able to:

- solve conventional multiphase flows (bubbly flows, flows with droplets, etc.) as well as interface problems. Due to a unique formulation of the whole system, this is realized by solving the full set of equations with the same numerical method at each computational cell. Moreover, this model ensures energy conservation at the interface leading therefore to a proper and accurate solution of the interface conditions;
- solve strong shocks in compressible mixtures (solid alloys, compacted powders) as well as detonation waves in condensed materials [9, 12]. Indeed, conventional models are based on the Euler equations closed by a mixture EOS. But this mixture EOS relies on unphysical equilibrium assumption such as temperature or density equality between phases. The new models allow the determination of all thermodynamic variables of each phase, and consequently make use of pure material EOS without using a mixture EOS. The relaxed pressure is obtained by a relaxation procedure instead of a mixture equation of state;
- deal with situations where interfaces appear dynamically. For instance, gas pockets can be formed during the propagation of rarefaction waves. This is the hydrodynamic part of cavitating flows. Conventional methods need the initial position of these interfaces. The model given in Reference [9] is able to make them appear dynamically.

The numerical solution of this model requires several ingredients. The numerical method involves a non conservative hydrodynamic solver, an instantaneous velocity relaxation procedure (when dealing with a single velocity flow) and an instantaneous pressure relaxation procedure.

Details on the hydrodynamic solver we use in this paper may be found in References [7, 9]. Although perfectable, we use this solver here without modification. Improvements on this solver may be found in References [10–12] but are not used in this article.

The velocity relaxation procedure involves either the resolution of an ODE problem when the velocity relaxation has a finite rate (the phenomenological drag force is known), or an equilibrium procedure (the drag force is infinite). The equilibrium procedure is recalled herein.

The pressure relaxation procedure is much more difficult to solve. It is of paramount importance in interface reconstruction algorithms used in compressible hydrodynamic codes [1, 5, 13] since the pressure equality at the interface is the most difficult condition to fulfill. It is also of major importance for single velocity flow such as detonations, shocks in solid alloys and multiple velocity flows such as cavitation applications and stratified flows. The same type of procedure is necessary to solve in the context of the compressible models presented in References [2, 4, 6, 8, 14–17] as well as in the context of the various models and studies in References [18–20].

The present paper is devoted to the development and assessment of pressure relaxation procedures, as first initiated in Reference [21]. We present a panel of relaxation procedures based on the assumption of either a varying interfacial pressure or a constant pressure. Most of the procedures are presented for multiphase flows (i.e. the number of phases N is such that $N \geqslant 2$), with a special emphasis on both low cost computing and convergence speed.

We first recall that we originally have two existing procedures initially defined for two-phase flows [7]. From the classification *varying interface pressure–constant interface pressure*, we propose here to present the different procedures from the *most restricted* to the *most general*, i.e. from the procedure usable for both two-phase flows only and specific EOS (stiffened gas namely), to the one that can be used for an arbitrary number of phases $N > 2$ and general EOS.

The paper is organized as follows. The 1-D model and its properties are first recalled. Then we detail the different relaxation procedures and at last we perform some representative numerical tests to compare these procedures and give concluding remarks related to the best choice of using these procedures.

2. THE 1-D MULTIPHASE MODEL

We present hereafter the 1-D multiphase model as described in References [7, 9], in which both mass and heat transfer are neglected. Let N be the total number of phases.

2.1. Continuous model

The system related to the jth phase, $j = 1, \dots, N$ reads as

$$\frac{\partial \alpha_j}{\partial t} + V_I \frac{\partial \alpha_j}{\partial x} = \sum_{l=1}^{N} \mu_{jl}(P_j - P_l)$$

$$\frac{\partial}{\partial t}(\alpha_j \rho_j) + \frac{\partial}{\partial x}(\alpha_j \rho_j u_j) = 0$$

$$\frac{\partial}{\partial t}(\alpha_j \rho_j u_j) + \frac{\partial}{\partial x}(\alpha_j \rho_j u_j^2 + \alpha_j P_j) = P_I \frac{\partial \alpha_j}{\partial x} - \sum_{l=1}^{N} \lambda_{jl}(u_j - u_l) \tag{1}$$

$$\frac{\partial}{\partial t}(\alpha_j \rho_j E_j) + \frac{\partial}{\partial x}[u_j(\alpha_j \rho_j E_j + \alpha_j P_j)] = P_I V_I \frac{\partial \alpha_j}{\partial x} + P_I \sum_{j=1}^{N} \mu_{jl}(P_j - P_l) - V_I \sum_{j=1}^{N} \lambda_{jl}(u_j - u_l)$$

The volume fractions α_j verify the saturation constraint

$$\sum_{j=1}^{N} \alpha_j = 1 \tag{2}$$

P_j, u_j and ρ_j denote, respectively, the pressure, velocity and density of the jth phase.

The total energy E_j is related to both the internal (e_j) and kinetic energies by

$$E_j = e_j + \tfrac{1}{2} u_j^2 \tag{3}$$

The averages of interfacial variables are denoted with subscript I.

V_I denotes the interface velocity, that we choose equal to the velocity of the centre of mass. As it will be shown in the following, it also corresponds to the equilibrium velocity:

$$V_I = \left(\sum_{j=1}^{N} m_j u_j \right) \bigg/ \left(\sum_{j=1}^{N} m_j \right) \tag{4}$$

where $m_j \overset{\text{def}}{=} \alpha_j \rho_j$ represents the apparent density. P_I denotes the interface pressure and is estimated equal to the following mixture pressure:

$$P_I = \sum_{j=1}^{N} \alpha_j P_j \tag{5}$$

Other definitions of these interfacial terms are possible (see, e.g. References [12, 22]), but we only use in this paper the interfacial correlations given by (4) and (5). For most pressure relaxation procedures detailed in this paper, a precise definition of P_I is not necessary. Therefore, the proposed procedures are not restricted to the pressure guess given by (5).

The λ_{jl} and μ_{jl} coefficients represent the interactions and relaxation between phases and are functions of the mechanical properties and the topology of the medium. They are, respectively, related to the drag forces and pressure relaxation effects between the phases. Moreover, each jth system is completed by an equation of state relying each pressure P_j to the internal energy e_j of the following form:

$$P_j = P_j(\rho_j, e_j) \tag{6}$$

The most classical EOS used for pure fluids are given below.

1. *Stiffened gas EOS*:

$$P = \frac{(\gamma - 1)\rho e}{1 - \rho b} - \gamma P_\infty \tag{7}$$

where γ, P_∞ and b are constant parameters. When $P_\infty = 0$, we recover the ideal covolume gas EOS. In such a case, γ is the specific heat ratio: $\gamma = C_P/C_V$.

When the covolume $b = 0$, we get the conventional stiffened gas EOS as in Reference [23].

2. *Mie Grüneisen EOS*:

$$P = (\gamma(\rho) - 1)\rho e - \gamma(\rho)P_\infty(\rho) \tag{8}$$

When $\gamma(\rho)$ is constant, we can recover the Jones–Wilkins–Lee (JWL) and Cochran–Chan EOS. This generalization of the previous equations of state is used for solids, liquids as well as gases at very high pressure. The main difficulty consists in determining the functions of ρ, namely $\gamma(\rho)$ and $P_\infty(\rho)$.

These EOS need convexity requirements to get accurate solutions and to ensure that the speed of sound is real [23, 24].

In the context of the multiphase model (1), each phase obeys its own EOS, therefore, a mixture EOS like the Van der Waals EOS is useless.

2.2. Properties of the system

We may rewrite system (1) in terms of primitive variables

$$W = (W_j)_{j=1,\dots,N} \quad \text{with } W_j = (\alpha_j, \rho_j, u_j, P_j)_j^{\mathrm{T}} \quad \text{for } j = 1,\dots,N$$

by

$$\frac{\partial W}{\partial t} + \mathscr{A}(W)\frac{\partial W}{\partial x} = 0$$

where $\mathscr{A}(W)$ is the block diagonal matrix

$$\mathscr{A}(W) = \mathrm{Diag}(\mathbf{A}(W_j)_{j=1,\dots,N})$$

where each 4×4 block matrix $\mathbf{A}(W_j)$ is defined by

$$\mathbf{A}(W_j) = \begin{pmatrix} V_I & 0 & 0 & 0 \\[1.5em] \dfrac{\rho_j}{\alpha_j}(u_j - V_I) & u_j & \rho_j & 0 \\[1.5em] \dfrac{P_j - P_I}{\alpha_j \rho_j} & 0 & u_j & 1/\rho_j \\[1.5em] \dfrac{\rho_j c_{j,I}^2}{\alpha_j}(u_j - V_I) & 0 & \rho_j c_j^2 & u_j \end{pmatrix}$$

and

$$c_j^2 = \frac{\dfrac{P_j}{\rho_j^2} - \dfrac{\partial e_j}{\partial \rho_j}\bigg|_{P_j}}{\dfrac{\partial e_j}{\partial P_j}\bigg|_{\rho_j}}, \quad c_{j,I}^2 = \frac{\dfrac{P_I}{\rho_j^2} - \dfrac{\partial e_j}{\partial \rho_j}\bigg|_{P_j}}{\dfrac{\partial e_j}{\partial P_j}\bigg|_{\rho_j}} \tag{9}$$

represent, respectively, the jth phase speed of sound and the jth phase interfacial speed of sound.

We may easily show that the matrix $\mathscr{A}(W)$ admits $3N + 1$ real eigenvalues λ_I and λ_j^m for $m = +, -, 0$ and $j = 1, \dots, N$

$$\lambda_j^+ = u_j + c_j$$
$$\lambda_I = V_I \quad \text{and} \quad \lambda_j^- = u_j - c_j \tag{10}$$
$$\lambda_j^0 = u_j$$

3. NUMERICAL SOLUTION

The numerical solution of system (1) requires a transport solver $\mathbf{T}$ and two relaxation procedures: $\mathbf{PR}$, for the pressure relaxation, and $\mathbf{VR}$, for the velocity relaxation, used to the solution of the source terms.

The numerical solution may be written by the following splitting scheme, where $\mathscr{U}^n = [(U_j^n)_{j=1,\dots,N}]^{\mathrm{T}}$ stands for the $4N \times 1$ row block vector of the conservative variables for each phase at time t_n and $\mathscr{U}^{n+1}$ for the corresponding updated vector at time $t_{n+1} = t_n + \Delta t$

$$\mathscr{U}^{n+1} = \mathbf{PR}(\mathscr{U})\mathbf{VR}(\mathscr{U})\mathbf{T}(\mathscr{U})(\mathscr{U}^n) \tag{11}$$

U_j is the 4×1 vector of conservative variables for the jth phase

$$U_j = \begin{bmatrix} \alpha_j \\ \alpha_j \rho_j \\ \alpha_j \rho_j u_j \\ \alpha_j \rho_j E_j \end{bmatrix}$$

We first recall the definition of the numerical transport solver as given in Reference [7].

3.1. Transport solver

The transport part of system (1), for the jth phase $(j = 1, \ldots, N)$, reads as

$$\frac{\partial}{\partial t} U_j + \frac{\partial}{\partial x} F(U_j) = H(U_j) \frac{\partial \alpha_j}{\partial x} \tag{12}$$

where

$$F(U_j) = \begin{bmatrix} 0 \\ \alpha_j \rho_j u_j \\ \alpha_j(\rho_j u_j^2 + P_j) \\ \alpha_j(\rho_j E_j + P_j)u_j \end{bmatrix}, \quad H(U_j) = \begin{bmatrix} -V_I \\ 0 \\ P_I \\ P_I V_I \end{bmatrix}$$

Let us drop the j index for each phase and denote now by U_i^k the cell average value of the 4×1 block vector of conservative variables for a given phase, in a given cell indexed by i and at time t_k $(k = n, n+1, n+\frac{1}{2})$; then, the transport solver is composed of a quasi-conservative scheme which reads as (second-order extension of the HLL solver, see Reference [7], p. 443 and replace Φ by F)

$$U_i^{n+1} = U_i^n - \lambda(\Phi_{i+1/2}^{n+1/2} - \Phi_{i-1/2}^{n+1/2}) + \Delta t H(U_i^{n+1/2})\Delta$$

where

- $\lambda = \Delta t/\Delta x$, is the CFL number ($\Delta t$ is the time step and Δx is the mesh size),
- the numerical fluxes

$$\Phi_{i\pm 1/2}^{n+1/2} = \Phi(U_{i\pm 1/2,-}^{n+1/2}, U_{i\pm 1/2,+}^{n+1/2})$$

  are given by the HLL approximate Riemann solver Φ, and
- Δ is the discrete form of $\partial \alpha_j/\partial x$ in cell i, at time t_n, which is also given by the HLL solver.

For more details and a better understanding on the HLL solver, and how Δ is defined accordingly, see Reference [7].

3.2. Velocity relaxation solver

At each time step, once the transport solver is used, we have to apply the velocity relaxation operator **VR** as given in (11). The aim is to give a correction of the different phase velocities resulting from the transport solver by relaxing them towards an equilibrium velocity.

In many situations, and in particular for interface problems or for multiphase condensed matter, instantaneous velocity relaxation is necessary to satisfy the first interface condition corresponding to a normal velocity equality.

The velocity relaxation procedure consists in solving the following ODE system when $\lambda_{jl} \to \infty$ for all $l = 1, \ldots, N$ and for all $j = 1, \ldots, N$

$$\frac{\partial U_j}{\partial t} = \begin{pmatrix} 0 \\ 0 \\ -\sum_{l=1}^{N} \lambda_{jl}(u_j - u_l) \\ -V_I \sum_{l=1}^{N} \lambda_{jl}(u_j - u_l) \end{pmatrix}$$

The solution of this ODE problem in the limit $\lambda_{jl} \to \infty$ is detailed in Reference [7]. Let 0 be the index symbol for the solution obtained after the transport solution of (12) and * be the index symbol for the solution obtained by the velocity relaxation procedure, then we get, for all $j = 1, \ldots, N$ (we set $m_l \stackrel{\text{def}}{=} \alpha_l^0 \rho_l^0$, for all $l = 1, \ldots, N$)

$$\alpha_j^* = \alpha_j^0$$

$$\rho_j^* = \rho_j^0$$

$$u_j^* = V_I^* = V_I^0 = \left(\sum_{l=1}^{N} m_l u_l^0 \right) \Big/ \left(\sum_{l=1}^{N} m_l \right)$$

$$e_j^* = e_j^0 + \tfrac{1}{2}(V_I^* - u_j^0)^2$$

3.3. Pressure relaxation solver

Once the transport solver has been used with possibly the correction brought by the velocity relaxation solver, we end with the pressure relaxation solver **PR** as given in (11).

As a matter of fact, the transport solver by itself does not guarantee that, with or without the velocity correction, the resulting pressures of the different phases are equal and equal to the relaxed interfacial pressure.

The pressure relaxation tends to erase the pressure differences between phases. In most physical situations, the time scale for the pressure relaxation is very small and even negligible compared to other physical relaxation processes such as the velocity drag and thermal relaxation processes.

When dealing with compressible material mixtures, there are situations for which pressure equilibrium is reached so fast that the knowledge of the thermodynamic path of each phase

in concern is useless. Examples are strong shock propagation in solid alloys, detonation in condensed explosives, etc. (see Reference [9]).

Also, as mentioned previously regarding velocity relaxation, when instantaneous velocity relaxation is required (as for interface problems or multiphase condensed matter), instantaneous pressure relaxation is also necessary.

A way to satisfy this condition is to relax instantaneously the pressures between phases towards equilibrium.

There is another reason for which the relaxation procedure is important. There are a lot of situations in which the pressure differences between phases are negligible: almost all situations with liquid and gas mixtures at low velocity. The sound speed in the liquid phase being much greater than the convection velocity, most models assume pressure equilibrium between phases. When such an assumption is made, numerical instabilities occur. Such instabilities are related to a loss of hyperbolicity.

Our strategy is to consider each material as a compressible fluid to let the waves evolve during the transport solution, and then to make the pressures relax towards an equilibrium state. With such a strategy, numerical instabilities are removed and hyperbolicity is guaranteed (10). The aim of this paper is to study the importance of this relaxation step, to improve its accuracy and computational efficiency and try not to be restrictive with respect to both the EOS and two-phase flows.

The instantaneous pressure relaxation procedure consists in solving the following ODE system in the limit $\mu_{jl} \to \infty$, for all $l = 1, \ldots, N$ and $j = 1, \ldots, N$:

$$\frac{\partial U_j}{\partial t} = \begin{pmatrix} \sum_{l=1}^{N} \mu_{jl}(P_j - P_l) \\ 0 \\ 0 \\ -P_I \sum_{l=1}^{N} \mu_{jl}(P_j - P_l) \end{pmatrix} \quad \text{for } j = 1, \ldots, N \tag{13}$$

Each μ_{jl} variable represents an homogenization parameter controlling the rate at which pressures tend towards equilibrium. Its physical meaning has been justified with considerations based on the second law of thermodynamics by Baer and Nunziato [3].

In the general case, these parameters are very complicated functions of all flow variables and micro-structure of the mixture. Since pressure equilibrium is always assumed to happen instantaneously, knowledge of these functions is useless.

Note that during this process, from (13), both partial density $m_j \stackrel{\text{def}}{=} \alpha_j \rho_j$ and velocity u_j remain constant, for all $j = 1, \ldots, N$. Using the first equation of system (13) and replacing it in the last equation lead to the following single energy equation to be solved for the jth phase

$$\frac{\partial}{\partial t}(m_j E_j) + P_I \frac{\partial \alpha_j}{\partial t} = 0 \quad \text{for all } j = 1, \ldots, N \tag{14}$$

If we denote by Δt the time step defined by one iteration of the transport solver (included the solution of the source terms), by T_0 the initialization time of the pressure relaxation process

and by T_* the final time of this process, i.e. the pressure equilibrium final time, for which

$$T_* - T_0 \ll \Delta t$$

and if we integrate Equation (14) in $[T_0, T_*]$, we get, for $j = 1, \ldots, N$

$$m_j(E_g^* - E_j^0) + \int_{T_0}^{T_*} P_I \frac{\partial \alpha_j}{\partial t}\, dt = 0$$

Using the following change of variables $d\alpha = (\partial \alpha_j / \partial t)\, dt$, the equation above rewrites as

$$m_j(E_j^* - E_j^0) + \int_{\alpha_j^0}^{\alpha_j^*} P_I\, d\alpha = 0 \quad \text{for all } j = 1, \ldots, N$$

Using (3) and the fact that u_j is constant during the pressure relaxation process, the expression above is in turn equivalent to

$$m_j(e_j^* - e_j^0) + \int_{\alpha_j^0}^{\alpha_j^*} P_I\, d\alpha = 0 \quad \text{for all } j = 1, \ldots, N \tag{15}$$

This system is supplemented by the saturation constraint

$$\sum_{l=1}^{N} \alpha_l^* = 1$$

The zero index corresponds to the values taken at time $t = T_0$, and the * index stands for the values taken at the final relaxation time $t = T_*$.

4. INSTANTANEOUS PRESSURE RELAXATION PROCEDURES

Before showing the way we solve system (15), let us first give some remarks and general properties we may derive from this system.

4.1. Properties of system (15)

We recall that $m_j = \alpha_j \rho_j$ and u_j remain constant during the pressure relaxation process, for all $j = 1, \ldots, N$. Let us assume that each j-phase has an EOS that may be written by $e_j = e_j(\rho_j, P_j)$, where e_j is continuously differentiable with respect to ρ_j, P_j and also $v_j = 1/\rho_j$. It is also assumed that each EOS fulfills the convexity requirement. Then, Equation (15) may be rewritten, for each $j = 1, \ldots, N$, by the differential form

$$m_j\, de_j = -P_I\, d\alpha_j \tag{16}$$

As a matter of fact, since each variable does not depend on the space variable x anymore but is supposed to be constant on each cell, the equations above have to be understood as local equations considered on a given cell.

Since

$$d\alpha_j = -m_j \frac{d\rho_j}{\rho_j^2} = m_j\, dv_j$$

we may write

$$de_j = -\frac{P_I}{m_j}\,d\alpha_j = \frac{P_I}{\rho_j^2}\,d\rho_j = -P_I\,dv_j \tag{17}$$

Note that these relations look like the first law of thermodynamics applied to each phase for adiabatic transformations. The saturation constraint may be read as

$$\sum_{l=1}^{N}\frac{m_j}{\rho_j} = \sum_{l=1}^{N}m_j v_j = 1$$

Differentiating the j-phase EOS with respect to ρ_j and P_j leads to

$$de_j = \left.\frac{\partial e_j}{\partial \rho_j}\right|_{P_j}\,d\rho_j + \left.\frac{\partial e_j}{\partial P_j}\right|_{\rho_j}\,dP_j$$

$$= -\frac{m_j}{\alpha_j^2}\left.\frac{\partial e_j}{\partial \rho_j}\right|_{P_j}\,d\alpha_j + \left.\frac{\partial e_j}{\partial P_j}\right|_{\rho_j}\,dP_j$$

$$= -\left.\frac{\partial e_j}{\partial \rho_j}\right|_{P_j}\frac{dv_j}{v_j^2} + \left.\frac{\partial e_j}{\partial P_j}\right|_{\rho_j}\,dP_j \tag{18}$$

From (17), (18) and definition of the interfacial speed of sound (9), we can deduce that

$$dP_j = -\frac{m_j}{\alpha_j^2}c_{j,I}^2\,d\alpha_j = c_{j,I}^2\,d\rho_j = c_{j,I}^2\frac{dv_j}{v_j^2} \tag{19}$$

Contrary to the velocity relaxation procedure where the definition of the equilibrium velocity is known, the form of the equilibrium pressure cannot be easily defined. As a matter of fact, it depends on the different EOS of all phases but also on the modellization we take for defining the interface pressure P_I.

In all the procedures presented in this paper, we will say that a procedure is *conservative* (with respect to the total global energy) if

$$\sum_{j=1}^{N}m_j e_j = 0$$

Hereafter, we propose two ways to model that interface pressure P_I during the instantaneous pressure relaxation procedure. Either P_I is assumed to vary during the process, or P_I is assumed to be the final relaxed pressure, i.e. to be the constant external pressure acting on the multiphase medium.

So first, we present procedures based on the first assumption, then we define procedures based on the second assumption.

4.2. Assumption of a varying P_I

In this subsection, the interface pressure P_I is assumed to vary during the relaxation process. The explicit definition of P_I is not used except in the last procedure where we follow for-mulation (5). The procedures presented herein are classified from the most restricted to the

most general. By *most restricted*, we mean procedures usable only for two-phase flows and specific EOS (stiffened gas EOS namely); by *most general*, we mean procedures that can be used for $N > 2$ phases and general EOS.

4.2.1. Procedure 1: stiffened gas EOS and $N = 2$. Definition of this procedure has 'historical' reasons. As a matter of fact, we recall that originally, we had only two iterative procedures restricted to two-phase flows [7]. The major drawbacks of these existing iterative procedures (that will be recalled hereafter), were the arbitrary initial guess for the volume fraction variation and the lack of control concerning both the convergence and convergence rate. Although restricted for two phase flows, the present procedure comes from a deeper insight of how to define an iterative process to reach the equilibrium state for the pressures, therefore, these criteria may be used in a more general context and, in particular, may help in finding a *good* initial guess for the volume fraction variation to start with.

The procedure presented here below is based on a quadrature approximation of the pressure integral (and is, in some sense, a particular case of the procedure 6 for the stiffened gas EOS, as we shall see later on). We first start by showing how we may define this process.

We recall that we initially want to solve the system given by (14). If we integrate these equations in the time interval for two successive iterates $[T_k, T_{k+1}]$, we get, for $j = 1, \ldots, N$

$$m_j[e_j^{k+1} - e_j] = - \int_{\alpha_j}^{\alpha_j^{k+1}} P_I \, \mathrm{d}\alpha_j$$

where the index k is omitted for clarity. Therefore, if we choose the trapezoidal approximation of the pressure integral on $[\alpha_j, \alpha_j^{k+1}]$

$$\int_{\alpha_j}^{\alpha_j^{k+1}} P_I \, \mathrm{d}\alpha_j \simeq \frac{P_I + P_I^{k+1}}{2} \Delta\alpha_j^{k+1} \tag{20}$$

with

$$\Delta\alpha_j^{k+1} \overset{\text{def}}{=} \alpha_j^{k+1} - \alpha_j$$

we get

$$m_j[e_j^{k+1} - e_j] = -\frac{P_I + P_I^{k+1}}{2} \Delta\alpha_j^{k+1} \tag{21}$$

Since, from the stiffened gas EOS, we have, for $m = k, k+1$

$$e_j^{(m)} = \frac{P_j^{(m)} + \gamma_j P_{j,\infty}}{(\gamma_j - 1)\rho_j^{(m)}} = \frac{\alpha_j^{(m)}(P_j^{(m)} + \gamma_j P_{j,\infty})}{m_j(\gamma_j - 1)}$$

we may rewrite (21) by

$$\alpha_j^{k+1} P_j^{k+1} = \alpha_j P_j - \left[\frac{\gamma_j - 1}{2}(P_I + P_I^{k+1}) + \gamma_j P_{j,\infty}\right] \Delta\alpha_j^{k+1} \tag{22}$$

By summing the equations above for $j = 1, \ldots, N$, and following formulation (5) for P_I^{k+1}, we finally get

$$P_I^{k+1} = \frac{1 - \sum_{j=1}^{N} \frac{\gamma_j - 1}{2} \Delta\alpha_j^{k+1}}{1 + \sum_{j=1}^{N} \frac{\gamma_j - 1}{2} \Delta\alpha_j^{k+1}} P_I - \frac{\sum_{j=1}^{N} \gamma_j P_{j,\infty} \Delta\alpha_j^{k+1}}{1 + \sum_{j=1}^{N} \frac{\gamma_j - 1}{2} \Delta\alpha_j^{k+1}} \tag{23}$$

Remark 4.1
Equation (22) may be rewritten by

$$P_j^{k+1} - P_j = -\frac{1}{\alpha_j} \left[\frac{\gamma_j - 1}{2} (P_I + P_I^{k+1}) + P_j^{k+1} + \gamma_j P_{j,\infty} \right] \Delta\alpha_j^{k+1} \tag{24}$$

from which we deduce that the variation $(P_j^{k+1} - P_j)$ and $\Delta\alpha_j^{k+1}$ have opposite signs, and

$$\frac{P_j^{k+1} - P_j}{\Delta\alpha_j^{k+1}} = -\frac{1}{\alpha_j} \left[\frac{\gamma_j - 1}{2} (P_I + P_I^{k+1}) + P_j^{k+1} + \gamma_j P_{j,\infty} \right] < 0$$

which is in agreement with (in the particular case of the stiffened gas EOS concerning the second equality)

$$\frac{\partial P_j}{\partial \alpha_j} = -\frac{m_j}{\alpha_j^2} c_{j,I}^2 = -\frac{\gamma_j - 1}{\alpha_j} \left(P_I + \frac{P_j + \gamma_j P_{j,\infty}}{\gamma_j - 1} \right)$$

and relation (24) is equivalent to

$$\frac{P_j^{k+1} - P_j}{\Delta\alpha_j^{k+1}} = -\frac{\gamma_j - 1}{\alpha_j} \left[\frac{1}{2} (P_I + P_I^{k+1}) + \frac{P_j^{k+1} + \gamma_j P_{j,\infty}}{\gamma_j - 1} \right]$$

i.e. this means that we apply the backward Euler scheme on the partial derivative $\partial P_j / \partial \alpha_j$, a simple average on P_I and we implicit P_j.

Remark 4.2
We might then define other iterative process from the following initial formulation:

$$\int_{\alpha_j}^{\alpha_j^{k+1}} \frac{\partial P_j}{\partial \alpha_j} \, d\alpha_j = -m_j \int_{\alpha_j}^{\alpha_j^{k+1}} \left(\frac{c_{j,I}}{\alpha_j} \right)^2 d\alpha_j$$

by writing

$$\int_{\alpha_j}^{\alpha_j^{k+1}} \frac{\partial P_j}{\partial \alpha_j} \, d\alpha_j = \int_{\alpha_j}^{\alpha_j^{k+1}} dP_j = P_j^{k+1} - P_j$$

and

$$-m_j \int_{\alpha_j}^{\alpha_j^{k+1}} \left(\frac{c_{j,I}}{\alpha_j} \right)^2 d\alpha_j \simeq - \left[\frac{m_j c_{j,I}^2}{\alpha_j^2} \right]_{[\alpha_j, \alpha_j^{k+1}]} \Delta\alpha_j^{k+1}$$

where the term with the brackets in the right-hand side is some average of the term inside the brackets in the interval $[\alpha_j, \alpha_j^{k+1}]$.

In the particular case of the stiffened gas EOS, we get a large choice of averagings since

$$\frac{m_j c_{j,I}^2}{\alpha_j^2} = \frac{1}{\alpha_j}[(\gamma_j - 1)P_I + P_j + \gamma_j P_{j,\infty}]$$

i.e. we may apply averagings either separately or globally on the variables α_j, P_I and P_j.

From (23), we end up with the following expression for P_j^{k+1}, for $j = 1, \ldots, N$

$$\alpha_j^{k+1} P_j^{k+1} = \alpha_j P_j - \left[\frac{\gamma_j - 1}{2} \frac{2P_I - \sum_{m=1}^{N} \gamma_m P_{m,\infty} \Delta\alpha_m^{k+1}}{1 + \sum_{m=1}^{N} \frac{\gamma_m - 1}{2} \Delta\alpha_m^{k+1}} + \gamma_j P_{j,\infty} \right] \Delta\alpha_j^{k+1}$$

i.e. if we know how to get an admissible value for the α_j^{k+1}'s, we may derive values of the interfacial pressure P_I^{k+1}, from which we may deduce the values of the e_j^{k+1}'s following (21). We may easily derive the density values $\rho_j^{k+1} = m_j/\alpha_j^{k+1}$ and therefore the pressures P_j^{k+1} either from its direct previous expression or from the stiffened gas EOS. If the pressures are equal in the sense of some criterion, the process stops, pressures are all relaxed, otherwise, we restart the iteration starting with as initial values those obtained by the previous iteration. There is no obvious way of getting criteria for defining admissible values for $\Delta\alpha_j$, but we are going to give what should be these criteria in the particular case of two-phase flows ($N = 2$), which will define the procedure 1.

So let us suppose now we have two phases $j = 1$ corresponding to the gas phase (g-index) and $j = 2$ corresponding to the liquid phase (l-index). Suppose also that we have

$$\gamma_l > \gamma_g, \quad P_{l,\infty} \gg P_{g,\infty} \tag{25}$$

Since $\Delta\alpha_l = -\Delta\alpha_g$, we have

$$\sum_{m=g,l} \frac{\gamma_m - 1}{2} \Delta\alpha_m^{k+1} = \frac{\gamma_{lg}}{2} \Delta\alpha_g^{k+1}$$

where $\gamma_{lg} \stackrel{\text{def}}{=} \gamma_l - \gamma_g > 0$. The interfacial pressure reads

$$P_I^{k+1} = \frac{1 + \dfrac{\gamma_{lg}}{2} \Delta\alpha_g^{k+1}}{1 - \dfrac{\gamma_{lg}}{2} \Delta\alpha_g^{k+1}} P_I + \frac{\gamma_{lg,\infty} \Delta\alpha_g^{k+1}}{1 - \dfrac{\gamma_{lg}}{2} \Delta\alpha_g^{k+1}} \tag{26}$$

where $\gamma_{lg,\infty} \stackrel{\text{def}}{=} \gamma_l P_{l,\infty} - \gamma_g P_{g,\infty} > 0$. The pressures P_j^{k+1}, for $j = g, l$, have the following expression:

$$\alpha_j^{k+1} P_j^{k+1} = \alpha_j P_j - \left[\frac{\gamma_j - 1}{2} \frac{2P_I + \gamma_{lg,\infty} \Delta\alpha_g^{k+1}}{1 - \dfrac{\gamma_{lg}}{2} \Delta\alpha_g^{k+1}} + \gamma_j P_{j,\infty} \right] \Delta\alpha_j^{k+1} \tag{27}$$

The criteria defining the right value of α_g^{k+1} may be summarized as follows:

1. Admissible value of $\Delta\alpha_g^{k+1}$

$$\alpha_g^{k+1} \in \,]0, 1[$$

2. Positivity of the interfacial pressure

$$P_I^{k+1} > 0$$

3. Convergence of the procedure

$$|P_g^{k+1} - P_I^{k+1}| < |P_g^k - P_I^k|$$

The first item is equivalent to

$$\Delta \alpha_g^{k+1} \in \mathscr{D}_a^{k+1} \overset{\text{def}}{=} \,] - \alpha_g, \alpha_l [$$

The positivity of the interfacial pressure is achieved if $\alpha_g^{k+1} \in \mathscr{D}_I^{k+1} = \{x \in \mathscr{D}_a^{k+1}, f_I(x) > 0\}$, where $x \equiv \Delta \alpha_g^{k+1}$ and

$$P_I^{k+1} = f_I(x) \overset{\text{def}}{=} \frac{1 + \dfrac{\gamma_{lg}}{2} x}{1 - \dfrac{\gamma_{lg}}{2} x} P_I + \frac{\gamma_{lg,\infty} x}{1 - \dfrac{\gamma_{lg}}{2} x}$$

Since $\text{sign}(f_I(x)) = \text{sign}([1 - \frac{\gamma_{lg}}{2} x] Q_I(x))$, where $Q_I(x) = a_{I,0} + a_{I,1} x$, with

$$a_{I,0} = P_I$$

$$a_{I,1} = \frac{\gamma_{lg}}{2} P_I + \gamma_{lg,\infty}$$

the corresponding domain $\mathscr{D}_I^{k+1}$ is therefore

$$\mathscr{D}_I^{k+1} = \,] - \min(\alpha_g, -x_I), \min\left(\alpha_l, \frac{2}{\gamma_{lg}}\right) [$$

where $x_I = -a_I^0/a_I^1 < 0$.

At this stage, the domain in which α_g^{k+1} has an admissible value (i.e. fulfilling items 1 and 2 given above) is therefore defined by $\mathscr{D}_I^{k+1}$.

It remains now to fulfill the item 3 (convergence). It is easy to show that (x stands for $\Delta \alpha_g^{k+1}$, $\Delta P^{k+1} = P_g^{k+1} - P_I^{k+1}$ and $\Delta P = P_g - P_I$),

$$\Delta P^{k+1} = \Delta P - x A^{k+1}(x) \tag{28}$$

where

$$A^{k+1}(x) = \sum_{m \in \{g,l\}} \frac{1}{\alpha_m + x_m^{k+1}} A_m^{k+1}(x)$$

$$A_m^{k+1}(x) = \frac{\gamma_m - 1}{1 - \dfrac{\gamma_{lg}}{2} x} \left(P_I + \frac{\gamma_{lg,\infty}}{2} x\right) + P_m + \gamma_m P_{m,\infty}$$

and $x_m^{k+1} = \Delta \alpha_m^{k+1}$.

Since $\mathrm{sign}(x) = \mathrm{sign}(\Delta P)$, there exists $\mu > 0$ such that $x = \mu \Delta P$. Therefore, from (28), we may write

$$\Delta P^{k+1} = \left(1 - \frac{x}{\Delta P} A^{k+1}(x)\right) \Delta P$$

So, convergence is achieved if we can find $x \in \mathscr{D}_I^{k+1}$ such that

$$\left|1 - \frac{x}{\Delta P} A^{k+1}(x)\right| < 1$$

Suppose we want to bound the convergence rate of the process, i.e. that we are given some parameter $\beta_0 \in \,]0, 1[$, such that

$$\left|1 - \frac{x}{\Delta P} A^{k+1}(x)\right| < 1 - \beta_0$$

then, after some calculations, we can show that this is equivalent to search $x \in \mathscr{D}_I^{k+1}$ such that both following inequalities hold:

$$\begin{aligned}
Q_3(x) &\stackrel{\text{def}}{=} q_0 + q_1 x + q_2 x^2 + q_3 x^3 < 0 \\
R_3(x) &\stackrel{\text{def}}{=} r_0 + r_1 x + r_2 x^2 + r_3 x^3 > 0
\end{aligned} \tag{29}$$

where the coefficients of Q_3 and R_3 are respectively defined by

$$\begin{array}{llll}
q_0 = \beta_0 a_0 & & r_0 = (2 - \beta_0) a_0 \\
q_1 = \beta_0 a_1 - b_0/\Delta P & & r_1 = (2 - \beta_0) a_1 - b_0/\Delta P \\
q_2 = \beta_0 a_2 - b_1/\Delta P & \text{and} & r_2 = (2 - \beta_0) a_2 - b_1/\Delta P \\
q_3 = \beta_0 a_3 - b_2/\Delta P & & r_3 = (2 - \beta_0) a_3 - b_2/\Delta P
\end{array}$$

and the coefficients a_m $(m = 0, \ldots, 3)$ are given by

$$\begin{aligned}
a_0 &= \alpha_g \alpha_l \\
a_1 &= (\alpha_l - \alpha_g) - \frac{\gamma_{lg}}{2} a_0 \\
a_2 &= -\left(1 + \frac{\gamma_{lg}}{2}(\alpha_l - \alpha_g)\right) \\
a_3 &= \frac{\gamma_{lg}}{2}
\end{aligned}$$

and the coefficients b_m $(m = 0, \ldots, 2)$ by

$$\begin{aligned}
b_0 &= \alpha_l \gamma_g (P_I + P_{g,\infty}) + \alpha_g \gamma_l (P_I + P_{l,\infty}) + (\alpha_l - \alpha_g)\Delta P \\
b_1 &= -\left[\frac{\gamma_g + 1}{2}(P_I - \gamma_l P_{l,\infty}) - \frac{\gamma_l + 1}{2}(P_I - \gamma_g P_{g,\infty}) + \left[1 + \frac{\gamma_{lg}}{2}(\alpha_l - \alpha_g)\right]\Delta P\right] \\
b_2 &= \frac{\gamma_{lg}}{2}\Delta P
\end{aligned}$$

After some more manipulations, the coefficients of both Q_3 and R_3 may be written as

$$q_0 = \alpha_g \alpha_l \beta_0$$

$$q_1 = -\left[(\alpha_l - \alpha_g)(1 - \beta_0) + \frac{\gamma_{lg}}{2} q_0 + \frac{1}{\Delta P} [\alpha_l \gamma_g (P_I + P_{g,\infty}) + \alpha_g \gamma_l (P_I + P_{l,\infty})] \right]$$

$$q_2 = (1 - \beta_0)\left(1 + \frac{\gamma_{lg}}{2}(\alpha_l - \alpha_g) \right) + \frac{1}{\Delta P}\left\{ \frac{\gamma_g + 1}{2}(P_I - \gamma_l P_{l,\infty}) - \frac{\gamma_l + 1}{2}(P_I - \gamma_g P_{g,\infty}) \right\}$$

$$q_3 = -(1 - \beta_0)\frac{\gamma_{lg}}{2}$$

and

$$r_0 = \alpha_g \alpha_l (2 - \beta_0)$$

$$r_1 = -\left[(\alpha_l - \alpha_g)(\beta_0 - 1) + \frac{\gamma_{lg}}{2} r_0 + \frac{1}{\Delta P} [\alpha_l \gamma_g (P_I + P_{g,\infty}) + \alpha_g \gamma_l (P_I + P_{l,\infty})] \right]$$

$$r_2 = (\beta_0 - 1)\left(1 + \frac{\gamma_{lg}}{2}(\alpha_l - \alpha_g) \right) + \frac{1}{\Delta P}\left\{ \frac{\gamma_g + 1}{2}(P_I - \gamma_l P_{l,\infty}) - \frac{\gamma_l + 1}{2}(P_I - \gamma_g P_{g,\infty}) \right\}$$

$$r_3 = (1 - \beta_0)\frac{\gamma_{lg}}{2}$$

We may finally define the whole process. For each cell in the interior computational domain for which $\Delta P^0 \neq 0$, we first pre-initialize the volume fraction variation denoted by x^0

[0] Pre-initialization

$$x^0 = \varepsilon_0 \, \text{sign}(\Delta P^0) \min(\alpha_l^0, \alpha_g)$$

where $\varepsilon_0 \in \,]0, 1[$ is a given parameter. Starting with iteration $k = 0$ we proceed as follows:

[1] Computation of the coefficients q_j, r_j, for $j = 1, \ldots, 3$ and x_I from all variables known at iteration k.

[2] Initialization of $x^{k+1} \overset{\text{def}}{=} \Delta \alpha_g^{k+1}$

$$x^{k+1} = \varepsilon_0 \times \begin{cases} \min\left(\alpha_l^k, \dfrac{2}{\gamma_{lg}}, |x^k| \right) & \text{if } \Delta P^k > 0 \\[2mm] -\min(\alpha_g^k, -x_I^k, |x^k|) & \text{if } \Delta P^k < 0 \end{cases}$$

if $\gamma_l \neq \gamma_g$. Otherwise, if $\gamma_g = \gamma_l$ and when $\Delta P^k > 0$, just remove the term $2/\gamma_{lg}$ instead ($\mathscr{D}_I^{k+1}$ reduces to $\,]-\min(\alpha_g, -x_I^k), \alpha_l[$).

[3] Evaluate $Q_3(x^{k+1})$ and $R_3(x^{k+1})$ and perform the test given by (29). If the test does not hold true, modify x^{k+1} by setting

$$x^{k+1} \leftarrow x^{k+1}/2$$

and return to step [3], otherwise define

$$\alpha_g^{k+1} = \alpha_g^k + x^{k+1}$$

and compute the pressure P_j^{k+1} for $j = I, g, l$ using the expressions, respectively, given by (26) and (27). Then test if $|\Delta P^{k+1}| < \varepsilon_P$, where ε_P is a positive arbitrarily small parameter. If the test does not hold, perform a new iteration $k \leftarrow k + 1$ and start from step [1], otherwise, compute e_j^{k+1} from relation (21), $\rho_j^{k+1} = m_j/\alpha_j^{k+1}$ and correct the conservative variables $\alpha_j, \alpha_j \rho_j E_j$, for $j = g, l$.

[4] Inspect a new cell if any, and start from step [0].

This ends the definition of procedure 1 that fully controls the variation of the different quantities leading to the approximated equilibrium state when the pressure variation ΔP^{k+1} is sufficiently small. Note that this process is conservative with respect with the energy and is, by definition, convergent (with a convergence rate bounded above by $(1 - \beta_0)$). Also, as given above, this procedure depends on the stiffened gas EOS, but it can easily be extended to other EOS as far as we may express the energy as a direct function of the pressure and density.

Remark 4.3
The main interest of this procedure lies in the way we define the interval of admissible good starting guess values of the volume fraction variation. Independently to the EOS, we know at this point that we necessarily should start at least in $]0, \alpha_l[$, if the initial pressure variation $P_g - P_l$ is positive, and in $] - \alpha_g, 0[$, otherwise. Final bounds of the intervals that guarantee both decreasing pressure variations and positiveness of the pressures depend on the EOS of each phase. Therefore, a simple dichotomy algorithm may be defined by splitting the initial interval into four equally length intervals and by testing each bound to check which one ensures both positiveness of the updated pressures and decreasing of the absolute value of the pressure variation. Next step will reduce the new test interval of admissible values for the volume fraction variation, the bounds of which are some of the previous interior points of the original interval. The process stops when the interval length or the updated pressure variation are sufficiently small.

4.2.2. Procedure 2: stiffened gas EOS and $N = 2$, an exact procedure. We now describe a procedure that is also related to the stiffened gas EOS as in Procedure 1 and devoted to two-phase flows. In the particular case $N = 2$ where both phases obey a stiffened gas EOS, we have, by differentiation and using the definition (5) of P_I

$$\mathrm{d}P_I = [(\gamma_l - \gamma_g)P_I + \gamma_l P_{l,\infty} - \gamma_g P_{g,\infty}]\,\mathrm{d}\alpha_g$$

Here, we suppose $\gamma_l > \gamma_g$, $P_{l,\infty} > P_{g,\infty}$. Integrating this relation leads to, when $\gamma_l \neq \gamma_g$

$$P_I = \frac{1}{\gamma_{lg}}[-\gamma_{lg,\infty} + (\gamma_{lg}P_I^0 + \gamma_{lg,\infty})g(\Delta\alpha_g)] \tag{30}$$

where $\gamma_{lg} \stackrel{\mathrm{def}}{=} \gamma_l - \gamma_g$, $\gamma_{lg,\infty} \stackrel{\mathrm{def}}{=} \gamma_l P_{l,\infty} - \gamma_g P_{g,\infty}$, $\Delta\alpha_g \stackrel{\mathrm{def}}{=} \alpha_g - \alpha_g^0$ and

$$g(\Delta\alpha_g) \stackrel{\mathrm{def}}{=} \exp(\gamma_{lg}\Delta\alpha_g)$$

i.e. we have an *exact analytic expression* for P_I. Integrating now the relations $m_j\,\mathrm{d}e_j = -P_I\,\mathrm{d}\alpha_j$ for $j=g,l$ and writing $\mathrm{d}\alpha_j = \delta_j\,\mathrm{d}\alpha_g$, with

$$\delta_j = \begin{cases} 1 & \text{if } j=g \\ -1 & \text{if } j=l \end{cases} \tag{31}$$

lead to

$$m_j(e_j^* - e_j^0) = \frac{\delta_j}{\gamma_{lg}} \left\{ \gamma_{lg,\infty}\Delta\alpha_g^* + \left(P_I^0 + \frac{\gamma_{lg,\infty}}{\gamma_{lg}} \right)(1 - g(\Delta\alpha_g^*)) \right\}$$

The stiffened gas EOS gives

$$m_j(e_j^* - e_j^0) = \frac{1}{\gamma_j - 1}[\alpha_j^* P_j^* - \alpha_j^0 P_j^0 + \delta_j\gamma_j P_{j,\infty}\Delta\alpha_g^*]$$

Equalizing the two relations above lead to the following expression for P_j^* ($j=g,l$):

$$P_j^* = \frac{1}{\alpha_j^*} \left[\alpha_j^0 P_j^0 + \delta_j \left(\frac{(\gamma_j - 1)}{\gamma_{lg}}\gamma_{lg,\infty} - \gamma_j P_{j,\infty} \right)\Delta\alpha_g^* + \delta_j \frac{(\gamma_j - 1)}{\gamma_{lg}} \left(P_I^0 + \frac{\gamma_{lg,\infty}}{\gamma_{lg}} \right)(1 - g(\Delta\alpha_g^*)) \right]$$

Since $P_g^* = P_l^*$, we finally end up with the following nonlinear equation for $\Delta\alpha_g^*$ (we drop the index 0 for clarity)

$$\alpha_g\alpha_l\Delta P + [(\alpha_l c_g + \alpha_g c_l) - P_I]\Delta\alpha_g^* + [\alpha_l(\gamma_g - 1) + \alpha_g(\gamma_l - 1) + \gamma_{lg}\Delta\alpha_g^*]c(\Delta\alpha_g^*) = 0$$

where

$$c_j = \frac{\gamma_j - 1}{\gamma_{lg}}\gamma_{lg,\infty} - \gamma_j P_{j,\infty}$$

$$c(\Delta\alpha_g^*) = \frac{1}{\gamma_{lg}} \left(P_I + \frac{\gamma_{lg,\infty}}{\gamma_{lg}} \right)(1 - g(\Delta\alpha_g^*))$$

$$\Delta P = P_g - P_l$$

The equation above may be numerically solved by a Newton type algorithm. Note that with the classical Newton method, we end up with the following solution in one step:

$$\Delta\alpha_g^* = \frac{\Delta P}{a_g + a_l - \dfrac{\alpha_l - \alpha_g}{\alpha_l\alpha_g}\Delta P} \tag{32}$$

where $a_j \overset{\text{def}}{=} (m_j c_{I,j}^2)/\alpha_j^2$, if this value of $\Delta\alpha_g^*$ is admissible (i.e. $\alpha_g^* \in [0,1]$). Otherwise, the procedure becomes iterative with as the initial guess

$$\Delta\alpha_g^{k+1} = \begin{cases} \min\left(\dfrac{\Delta P^k}{a_g^k + a_l^k - \dfrac{\alpha_l^k - \alpha_g^k}{\alpha_l^k \alpha_g^k}\Delta P^k}, B_g, \alpha_l^k \right) & \text{if } \Delta P^k > 0 \\[4mm] -\min\left(\dfrac{-\Delta P^k}{a_g^k + a_l^k - \dfrac{\alpha_l^k - \alpha_g^k}{\alpha_l^k \alpha_g^k}\Delta P^k}, C_l, \alpha_g^k \right) & \text{if } \Delta P^k < 0 \end{cases}$$

where

$$B_g = \frac{1}{\gamma_l - \gamma_g} \log\left(1 + \frac{\alpha_g^k P_g^k}{\dfrac{(\gamma_g - 1)}{(\gamma_l - \gamma_g)}\left(P_I^k + \dfrac{(\gamma_l P_{l,\infty} - \gamma_g P_{g,\infty})}{(\gamma_l - \gamma_g)} \right)} \right)$$

and

$$C_l = \frac{\alpha_l^k P_I^k}{(\gamma_l - 1)P_I^k + \gamma_l P_{l,\infty}}$$

The special case $\gamma_g = \gamma_l$

When $\gamma_g = \gamma_l = \gamma$, the expression of $\mathrm{d}P_I$ reduces to

$$\mathrm{d}P_I = \gamma(P_{l,\infty} - P_{g,\infty})\,\mathrm{d}\alpha_g$$

therefore the exact expression of P_I becomes

$$P_I^* = P_I^0 + \gamma(P_{l,\infty} - P_{g,\infty})\Delta\alpha_g^*$$

Proceeding similarly to the case $\gamma_l \neq \gamma_g$ leads to the following expression for P_j^*, $j = g, l$:

$$P_j^* = \frac{1}{\alpha_j^*}\left[\alpha_j P_j - \delta_j(\gamma - 1)\Delta\alpha_g^*\left(P_I + \frac{\gamma}{\gamma - 1}P_{j,\infty} + \frac{\gamma}{2}(P_{l,\infty} - P_{g,\infty})\Delta\alpha_g^* \right) \right]$$

Using the equilibrium condition $P_g^* = P_l^*$ gives the following second-order equation:

$$c_0 + c_1\Delta\alpha_g^* + c_2(\Delta\alpha_g^*)^2 = 0$$

where the coefficients are defined by

$$c_0 = -\alpha_g\alpha_l\Delta P$$

$$c_1 = \gamma[\alpha_l(P_l + P_{g,\infty}) + \alpha_g(P_g + P_{l,\infty})] > 0$$

$$c_2 = \frac{\gamma(\gamma + 1)}{2}(P_{l,\infty} - P_{g,\infty}) > 0$$

If $\Delta P > 0$, the roots have opposite signs, therefore, we should retain the positive root; if $\Delta P < 0$, the roots have the same sign that should necessarily be negative, therefore, we should retain the root that fulfills the admissibility criteria (positivity of the pressures and resulting volume fraction in $]0, 1[$).

4.2.3. Procedure 3: stiffened gas EOS and $N \geqslant 2$. In the present procedure, we also assume that each phase is governed by a conventional stiffened gas EOS, but, compared to the previous procedures it can be generalized to an arbitrary number $N > 2$ of phases. Moreover, it is a quasi-direct process and, in the particular case when $N = 2$, this procedure reduces to a direct relaxation procedure. It also uses the trapezoidal approximation of the pressure integral as in Procedure 1 and we will indeed see that Procedure 3 is a particular case of Procedure 1 when $N = 2$ and $\beta_0 = 1$.

We recall that the stiffened gas EOS is a good approximation of the behaviour of most pure liquids and that its analytical formulation contains those of ideal gases.

For the present procedure, we therefore use the trapezoidal rule approximation (20), replacing indexes k and $k + 1$ by 0 and $*$, respectively,

$$\int_{\alpha_j^0}^{\alpha_j^*} P_I \, d\alpha_j \simeq \frac{P_I^0 + P_I^*}{2} \Delta \alpha_j^* \quad \text{with } \Delta \alpha_j^* = \alpha_j^* - \alpha_j^0$$

From (17), we get

$$m_j(e_j^* - e_j^0) = -\frac{P_I^0 + P_I^*}{2} \Delta \alpha_j^*$$

Using the stiffened gas EOS

$$e_j = \frac{\alpha_j}{m_j} \frac{P_j + \gamma_j P_{j,\infty}}{(\gamma_j - 1)}$$

lead to

$$\alpha_j^0[P_j^0 + \gamma_j P_{j,\infty}] - \alpha_j^*[P_j^* + \gamma_j P_{j,\infty}] = (\gamma_j - 1)\frac{P_I^0 + P_I^*}{2}\Delta \alpha_j^* \tag{33}$$

Since $P_I^* = P_j^*$ for all $j = 1, \ldots, N$, we get the following expression for P_j^* (provided $a_j d_j - b_j c_j \neq 0$ for all $j = 1, \ldots, N$):

$$P_j^* = \frac{a_j \Delta \alpha_j^* + b_j}{c_j \Delta \alpha_j^* + d_j} \tag{34}$$

where

$$a_j = -\left(\frac{\gamma_j - 1}{2}P_I^0 + \gamma_j P_{j,\infty}\right), \quad b_j = \alpha_j^0 P_j^0$$
$$c_j = \frac{\gamma_j + 1}{2}, \quad d_j = \alpha_j^0 \tag{35}$$

Since all the pressures P_j^* must be equal, we may write, in particular, that

$$P_j^* = P_1^*, \quad \forall j = 2, \ldots, N$$

from which we deduce that

$$\Delta\alpha_j^* = f_j(\Delta\alpha_1^*) = \frac{a_{1j}\Delta\alpha_1^* + b_{1j}}{c_{1j}\Delta\alpha_1^* + d_{1j}}, \quad \forall j = 2, \ldots, N$$

where

$$a_{1j} = a_1 d_j - b_j c_1 = -\alpha_j^0\left[\frac{\gamma_1 - 1}{2}P_I^0 + \frac{\gamma_1 + 1}{2}P_j^0 + \gamma_1 P_{1,\infty}\right]$$

$$b_{1j} = b_1 d_j - b_j d_1 = \alpha_1^0\alpha_j^0(P_1^0 - P_j^0)$$

$$c_{1j} = a_j c_1 - a_1 c_j = \frac{\gamma_1 - \gamma_j}{2}P_I^0 + \frac{\gamma_j + 1}{2}\gamma_1 P_{1,\infty} - \frac{\gamma_1 + 1}{2}\gamma_j P_{j,\infty}$$

$$d_{1j} = a_j d_1 - b_1 c_j = -\alpha_1^0\left[\frac{\gamma_j - 1}{2}P_I^0 + \frac{\gamma_j + 1}{2}P_1^0 + \gamma_j P_{j,\infty}\right]$$

But the α_j^* also verify the saturation constraint (2), therefore

$$\sum_{j=1}^{N} \Delta\alpha_j^* = 0$$

and we may write

$$\Delta\alpha_1^* = -\sum_{j=2}^{N} \Delta\alpha_j^*$$

i.e.

$$\Delta\alpha_1^* = f(\Delta\alpha_1^*)$$

where

$$f(x) = -\sum_{j=2}^{N} f_j(x)$$

This in turn is equivalent to solve the following nonlinear equation:

$$g(x) = 0$$

with $g(x) = x - f(x)$ which can be solved by a Newton type algorithm or a fixed point algorithm $x = f(x)$ since $|f(x)| < 1$.

   If the equation can be solved exactly, the procedure guarantees the conservation of the energy. Otherwise, it is approximately guaranteed with an error proportional to the error introduced in either the Newton type algorithm or the fixed point algorithm.

The particular case when $N = 2$

When $N = 2$, e.g. for two gas (index g) and liquid (index l) phases, equalizing the pressures (34) for $j = g, l$ lead to the following second-order polynomial equation:

$$A_0\Delta P^0 - A_1\Delta\alpha_g^* - A_2(\Delta\alpha_g^*)^2 = 0 \tag{36}$$

where

$$A_0 = \alpha_g^0 \alpha_l^0$$

$$2A_1 = A_0 \left\{ \frac{(\gamma_l + 1)(P_g^0 + P_{l,\infty}) + (\gamma_l - 1)(P_I^0 + P_{l,\infty})}{\alpha_l^0} \right.$$

$$\left. + \frac{(\gamma_g + 1)(P_l^0 + P_{g,\infty}) + (\gamma_g - 1)(P_I^0 + P_{g,\infty})}{\alpha_g^0} \right\} \tag{37}$$

$$2A_2 = \gamma_l(P_I^0 - \gamma_g P_{g,\infty}) - \gamma_g(P_I^0 - \gamma_l P_{l,\infty}) + (\gamma_l P_{l,\infty} - \gamma_g P_{g,\infty})$$

with $\Delta P^0 = P_g^0 - P_l^0$. Since $P_I^* = P_j^*$ for all $j = g, l$, (33) can be rewritten as

$$\alpha_j^0 (P_j^0 - P_j^*) = \left[\frac{\gamma_j - 1}{2}(P_I^0 + P_{j,\infty}) + \frac{\gamma_j + 1}{2}(P_j^* + P_{j,\infty}) \right] \Delta \alpha_j^*$$

we deduce that

$$2\Delta P^0 = \left[\frac{(\gamma_g - 1)(P_I^0 + P_{g,\infty}) + (\gamma_g + 1)(P_g^* + P_{g,\infty})}{\alpha_g^0} \right.$$

$$\left. + \frac{(\gamma_l - 1)(P_I^0 + P_{l,\infty}) + (\gamma_l + 1)(P_l^* + P_{l,\infty})}{\alpha_l^0} \right] \Delta \alpha_g^*$$

and therefore

$$\text{sign}(\Delta \alpha_g^*) = \text{sign}(\Delta P^0)^{\P}$$

On the other hand, under the assumption that $\gamma_l > \gamma_g$, (which is true when the first phase is a gas and the second phase is a liquid), we have $A_2 > 0$, therefore, the root product of Equation (36) has the same sign as $-\Delta P^0$. We conclude that the solution $\Delta \alpha_g^*$ is defined as follows

- if $\Delta P^0 > 0$, the two roots are of opposite signs and we therefore retain the positive root;
- if $\Delta P^0 < 0$, the two roots have the same sign and they are necessarily negative; we must retain the root $\Delta \alpha_g^*$ that satisfies

$$\alpha_g^* = \alpha_g^0 + \Delta \alpha_g^* \in [0, 1]$$

which ends the direct pressure relaxation process for $N = 2$ phases, which is conservative with respect to the energy since the equation is solved exactly.

¶This is in accordance with the fact that $\mathrm{d}(P_g - P_l) = -\left(\frac{m_g c_{g,I}^2}{\alpha_g^2} + \frac{m_l c_{l,I}^2}{\alpha_l^2} \right) \mathrm{d}\alpha_g$ and $\mathrm{d}\alpha_l = -\mathrm{d}\alpha_g$.

Remark 4.4

Note that for the implementation, we should normalize the equation (dividing it by A_2) and use the fact that the resulting new constant coefficient $A_0^{\text{new}} = A_0/A_2$ is the root product. We can therefore use it as a test to get the acceptable root and also to compute them, by first using the usual formula (using the determinant), to get the root having the largest value, then deriving the second one by dividing A_0^{new} by the just computed root. As a matter of fact, if we do not proceed as it, we would get a null value for the admissible root, due to rounding computational errors.

Remark 4.5

This is a particular case of Procedure 1 when $\beta_0 = 1$. As a matter of fact, in Procedure 1, solving $\Delta P^{k+1} = 0$ is equivalent to state

$$Q_3(x) = R_3(x) = 0$$

and we recover the second-order equation stated in Procedure 3 when $N = 2$, since

$$q_0 = r_0 = A_0/\Delta P$$

$$q_1 = r_1 = A_1/\Delta P$$

$$q_2 = r_2 = A_2/\Delta P$$

$$q_3 = r_3 = 0$$

4.2.4. Procedure 4: general EOS and $N = 2$. This procedure was initially proposed in Reference [7]. We recall it in this paragraph and will examine its accuracy and robustness in the results section. The present procedure is valid for only two phases but no assumption is *a priori* made concerning the EOS. As in the previous procedure, it is based on the trapezoidal approximation (20) and may be considered, in some sense, as a variant and iterative version of the direct algorithm deduced from Procedure 3 when $N = 2$ and with stiffened gas EOS.

We suppose that the approximate equilibrium state is reached as soon as either the relative pressure variation between phases

$$\delta P^k \stackrel{\text{def}}{=} \Delta P^k/P_I^0 (= (P_g^k - P_I^k)/P_I^0) \tag{38}$$

or the relative interfacial pressure variation between two iterations

$$\delta_3 P^{k+1} \stackrel{\text{def}}{=} \frac{(P_I^{k+1} - P_I^k)}{P_I^0} \tag{39}$$

is sufficiently small.

At the very first iteration, we start with the following initialization:

$$\alpha_g^{(1)} = \alpha_g^0, \quad P_I^{(1)} = P_I^0$$

$$\Delta \alpha_g^{(1)} = \varepsilon_0 \min(\alpha_g^0, \alpha_l^0), \quad \delta P^0 = C_\delta$$

where ε_0 (resp. C_δ) is a non negative parameter arbitrarily small (resp. large).

For a given iteration k, $(k \geqslant 1)$, we first compute the internal energies for each phase j, $j = g, l$

$$e_j^k = e_j^0 - \frac{P_I^0 + P_I^k}{2m_j} \Delta \alpha_j^k$$

and also the corresponding densities $\rho_j^k = m_j/\alpha_j^k$, from which we may deduce the pressures P_j^k using the EOS related to each j-phase. Let us denote the pressure variation product between two successive iteration by

$$\pi_{\delta_P}^k \overset{\text{def}}{=} \delta P^k \delta P^{(k-1)}$$

and do the following tests:

1. If the absolute value of either (38) or (39) is sufficiently small, then pressures are relaxed and we update the conservative variables, before inspecting the next cell if any

$$\alpha_g = \alpha_g^k$$

$$(m_j E_j) = m_j(e_j^k + \tfrac{1}{2}u_j^2) \quad \text{for } j = g, l$$

2. Otherwise, none of the previous tests done on the relative pressure variations (38) and (39) is satisfied and we proceed as follows:

   (a) if the first test (38) is not satisfied (the relative pressure variation is supposed to be not negligible), and if the variation product $\pi_{\delta_P}^k$ is negative (the relative pressure variation δP^k has the opposite sign of the $(k-1)$-iterate), then we go to the next iteration after setting

   $$\Delta \alpha_g^{k+1} = -\Delta \alpha_g^k/2$$

   $$\alpha_g^{k+1} = \alpha_g^k + \Delta \alpha_g^{k+1}$$

   (b) if the first test related to (38) is not satisfied but if the product $\pi_{\delta P}^k$ is positive then
       • either $|\delta P^k| \leqslant |\delta P^{(k-1)}|$, and in this case we go to the next iteration by first setting

       $$\Delta \alpha_g^{k+1} = \Delta \alpha_g^k, \quad \alpha_g^{k+1} = \alpha_g^k + \Delta \alpha_g^{k+1}$$

       • or

       $$|\delta P^k| > |\delta P^{(k-1)}|$$

       and in this case, we also go to the next iteration but now with the following setting

       $$\Delta \alpha_g^{k+1} = -\Delta \alpha_g^k, \quad \alpha_g^{k+1} = \alpha_g^k + \Delta \alpha_g^{k+1}$$

   (c) If the first test related to (38) is satisfied but if the second test related to (39) is not, then we go to the next iteration with the following setting

   $$\Delta \alpha_g^{k+1} = \Delta \alpha_g^0, \quad \alpha_g^{k+1} = \alpha_g^k$$

In the present procedure, we do not control the monotonicity of the pressure variation at each iteration, but it is again valid for real material EOS and is also conservative. Its generalization for N materials $N > 2$ is not straightforward.

4.2.5. Procedure 5: general EOS and $N \geqslant 2$. The present procedure was also originally proposed and designed for two phases in Reference [7]. It may be used for any EOS and we propose hereafter its generalization for an arbitrary number $N > 2$ of phases. It is again an iterative process in which we compute, at each iteration, the successive estimations of the pressure work until relaxation.

Let us therefore consider the general case where $N > 2$, but not give any assumption on the EOS related to each phase. We recall that we want the solution of the following system:

$$m_j(e_j^* - e_j^0) = -I_j^* \quad \text{for all } j = 1, \ldots, N$$

where

$$I_j^* = \int_{\alpha_j^0}^{\alpha_j^*} P_I \, \mathrm{d}\alpha_j$$

We determine the approximate relaxed pressure P^* by approximating each integral of the right-hand side of $m_j(e_j^{k+1} - e_j^0)$ by

$$I_j^{k+1} = \int_{\alpha_j^0}^{\alpha_j^{k+1}} P_I \, \mathrm{d}\alpha_j = I_j^k + \int_{\alpha_j^k}^{\alpha_j^{k+1}} P_I \, \mathrm{d}\alpha_j$$

until we reach the limit

$$I_j^* = \lim_{k \to \infty} I_j^{k+1}$$

The pressure integral I_j^{k+1} is approximated by the following scheme:

$$I_j^{k+1} \simeq \tilde{I}_j^{k+1} = \sum_{m=0}^{k} P_I^m \Delta\alpha_j^{m+1} = \tilde{I}_j^k + P_I^k \Delta\alpha_j^{k+1}$$

So, the key point is to define the quantities $\Delta\alpha_j^{k+1} = \alpha_j^{k+1} - \alpha_j^k$, at each iteration k and for all $j = 1, \ldots, N$.

In this procedure, we ask the variation $\Delta\alpha_j^{k+1}$, to let the new pressures verify

$$\begin{cases} |\Delta P_{j,1}^{k+1}| < |\Delta P_{j,1}^k| \\ \mathrm{sign}(\Delta P_{j,1}^{k+1}) = \mathrm{sign}(\Delta P_{j,1}^k) \end{cases} \quad \text{for all } j = 1, \ldots, N$$

where $\Delta P_{j,1}^k = P_1^k - P_j^k$, and the iterative process will stop as soon as

$$\max_{j=2,\ldots,N} |\Delta P_{j,1}^{k+1}| \tag{40}$$

is small enough. The conditions given above signify that we want the procedure to be convergent (the pressure variation should decrease) and monotone (the sign of the pressure variation remains the same).

Initially, we know the following quantities:

$$\alpha_m^0, \ \rho_m^0, \ u_m^0, \ e_m^0, \quad m = 1, \ldots, N$$

which correspond to the physical variables of the N phases at the beginning of the pressure relaxation process and computed by the transport solver. The computation is done in each internal cell in which (40) is not sufficiently small.

At the very first initialization of iteration $k+1$, we define a variation guess $\Delta\alpha_j^{k+1}$ for each $j \neq M$, by setting

$$\Delta\alpha_j^{k+1} = \varepsilon_0 \alpha_M \tag{41}$$

where $M \in \{1,\ldots,N\}$ is such that

$$\alpha_M = \min_{j=1,\ldots,N} \alpha_j^k$$

we use $\varepsilon_0 = 1/N$, and define

$$\Delta\alpha_M^{k+1} = -\frac{N-1}{N}\alpha_M$$

in order to fulfill the saturation constraint

$$\sum_{m=1}^{N} \Delta\alpha_m^{k+1} = 0$$

These definitions are valid and lead to admissible values for the corresponding α_j^{k+1}'s, where $\alpha_j^{k+1} = \alpha_j^k + \Delta\alpha_j^{k+1}$.

Once the internal energies e_j^{k+1}'s are computed by the numerical scheme, the densities are given by

$$\rho_j^{k+1} = m_j/\alpha_j^{k+1} \quad \text{for } j = 1,\ldots,N$$

From these quantities, we can derive the corresponding pressures $P_j^{k+1} = P_j(e_j^{k+1}, \rho_j^{k+1})$ using each related EOS.

If the absolute value of the pressure variation given by (40) is sufficiently small, we update the conservative variables as done in the previous procedures and inspect another cell if any. Otherwise, two instances may occur for a given phase $j \neq 1$

1. $\Delta P_{j,1}^{k+1} \Delta P_{j,1}^k < 0$: i.e. the pressure variations are of opposite sign. In this case, we define a new guess value for $\Delta\alpha_j^{k+1}$ by setting

$$\Delta\alpha_j^{k+1,\text{new}} = \Delta\alpha_j^{k+1,\text{old}}/2$$

and must therefore modify accordingly $\Delta\alpha_1^{k+1}$ in order to fulfill the saturation constraint

$$\Delta\alpha_1^{k+1,\text{new}} = \Delta\alpha_1^{k+1,\text{old}} + \Delta\alpha_j^{k+1,\text{old}} - \Delta\alpha_j^{k+1,\text{new}} \tag{42}$$

Then, the corresponding energies $e_1^{k+1,\text{new}}$, $e_j^{k+1,\text{new}}$ and pressures $P_1^{k+1,\text{new}}$ and $P_j^{k+1,\text{new}}$ are updated accordingly. We retest the new pressures as it was done for their previous values and for the same iteration $k+1$.

2. $\Delta P_{j,1}^{k+1} \Delta P_{j,1}^k \geqslant 0$: i.e. the pressure variations have the same sign. In this case, we first check if the absolute value of the pressure variation is decreasing

$$|\Delta P_{j,1}^{k+1}| < |\Delta P_{j,1}^k|$$

if this test is true, we keep on going to the next phase j. If $j = N$, we go to the next iteration $(k + 2)$, otherwise, we must redefine a new guess value for the volume fraction variation $\Delta \alpha_j^{k+1}$ by setting

$$\Delta \alpha_j^{k+1,\text{new}} = -\Delta \alpha_j^{k+1,\text{old}}/2$$

and redefine $\Delta \alpha_1^{k+1}$, as in (42). We proceed as in the first test once the integrals, pressures and energies have been updated accordingly.

For $N > 2$, each k iteration may be costly whenever the initial guess values of the volume fraction variations do not guarantee a monotone decreasing pressure variation, i.e. whenever the pressure variation reaches a local minimum.

The particular case when $N = 2$

When $N = 2$, this process guarantees a monotone variation of the pressure, as long as the pressure is itself monotone, until the equilibrium state is reached.

This procedure does not use any explicit form of the EOS and so is valid for real materials, moreover, it is obviously a conservative process with respect to the energy, and is usable for multiphase flows with $N > 2$.

4.2.6. Procedure 6: general EOS and $N \geqslant 2$. The procedure presented in this section is valid for $N \geqslant 2$ and general EOS. We will see that it is a quasi-direct process, especially in the particular case of two-phase flows and stiffened gas EOS. It is nevertheless also based on the same approximation of the integral used in the previous section

$$I_j = \int_{\alpha_j^0}^{\alpha_j} P_I \, \mathrm{d}\alpha \simeq \frac{P_I + P_I^0}{2} \Delta \alpha_j$$

which leads to the following system of N equations:

$$m_j(e_j - e_j^0) = -\frac{P_I + P_I^0}{2} \Delta \alpha_j \quad \text{for all } j = 1, \ldots, N \qquad (43)$$

with $\Delta \alpha_j = \alpha_j - \alpha_j^0$. We suppose that each EOS may be written by $e_j = e_j(\rho_j, P_j)$ and assume that the pressures are those of the relaxed state

$$P_j^* = P_I^* = P^*$$

System (43) is supplemented by the saturation constraint

$$\sum_{j=1}^{N} \Delta \alpha_j = 0$$

At the end of the relaxation process, we thus have

$$\begin{cases} e_j(\rho_j^*, P_j^*) = e_j(\rho_j^*, P_1^*), & \forall j = 2, \ldots, N \\ P_1^* = P_I^* = P^* \end{cases}$$

adding N equations to system (43) and allowing us to write

$$e_j(\rho_j^*, P_j^*) - e_j^0 = -\frac{P_I^0 + P^*}{2m_j}\Delta\alpha_j^*, \quad \forall j = 1, \ldots, N$$

$$P_j^* = P_1^* = P^*, \quad \forall j = 2, \ldots, N$$

$$\sum_{j=1}^{N}\Delta\alpha_j^* = 0$$

which may be rewritten as

$$P^* = P_j^* = P_I^*$$

$$e_j(\rho_j^*, P_j^*) - e_j^0 + \frac{P_I^0 + P^*}{2m_j}\Delta\alpha_j^* = 0, \quad \forall j = 1, \ldots, N \tag{44}$$

$$\sum_{j=1}^{N}\Delta\alpha_j^* = 0$$

Note that at this stage, if no approximation is used for the energy in the equations above, the solution is obviously conservative. It can also be shown that, when $N = 2$ and with stiffened gas type EOS used for each phase that the resulting procedure is equivalent to Procedure 3.

When we do not know *a priori* the form of the EOS, (44) forms a system of $N+1$ equations with $N+1$ unknowns which are the $\Delta\alpha_j^*$'s, $j = 1, \ldots, N$ and the final relaxed pressure P^*. This system may be rewritten by

$$f_j(\Delta\alpha_j^*, P^*) = 0, \quad j = 1, \ldots, N + 1$$

where

$$f_j(\Delta\alpha_j, P) = e_j(\rho_j, P) - e_j^0 + \frac{P_I^0 + P}{2m_j}\Delta\alpha_j, \quad j = 1, \ldots, N$$

$$f_{N+1}(\Delta\alpha_j, P) = \sum_{m=1,N}\Delta\alpha_m \tag{45}$$

and $\Delta\alpha_j = \alpha_j - \alpha_j^0$. We are thus seeking to find $\mathbf{X} \in \mathbb{R}^N \times \mathbb{R}^{+,*}$, such that

$$\mathbf{F}(\mathbf{X}) = \mathbf{0}_{N+1} \tag{46}$$

where $\mathbf{0}_{N+1}$ is the null $N+1$-row vector of $\mathbb{R}^{N+1}$ and

$$\mathbf{X} = ((\Delta\alpha_j)_{j=1,\ldots,N}, P)^T \in \mathbb{R}^{N+1}$$

$$\mathbf{F}(\mathbf{X}) = (f_j(\Delta\alpha_j, P))_{j=1,\ldots,N+1}^T \in \mathbb{R}^{N+1}$$

The nonlinear equation (46) may be solved by a Newton type algorithm. If $\mathbf{X}^*$ is its solution, then we may write

$$\mathbf{F}(\mathbf{X}^*) = \mathbf{F}(\mathbf{X}^0 + \Delta\mathbf{X}^*) \simeq \mathbf{F}(\mathbf{X}^0) + \mathbf{DF}(\mathbf{X}^0)\Delta\mathbf{X}^*$$

with

$$\mathbf{X}^0 = (\mathbf{0}_N, P_I^0)^{\mathrm{T}}$$

$$\mathbf{X}^* = ((\Delta\alpha_j^*)_{j=1,\ldots,N}, P^*)^{\mathrm{T}}$$

$$\Delta\mathbf{X}^* = \mathbf{X}^* - \mathbf{X}^0 = ((\Delta\alpha_j^*)_{j=1,\ldots,N}, P^* - P_I^0)^{\mathrm{T}}$$

if $\mathbf{X} = (x_j)_{j=1,\ldots,N+1}$ and if $\partial f_j / x_j$ stands for $\partial f_j / x_j(x_j, x_{N+1})$ for $j = 1,\ldots,N$, then

$$\mathbf{DF}(\mathbf{X}) = \begin{pmatrix} \dfrac{\partial f_1}{\partial x_1} & 0 & \cdots & 0 & \dfrac{\partial f_1}{\partial x_{N+1}} \\[2mm] 0 & \dfrac{\partial f_2}{\partial x_2} & \ddots & \vdots & \dfrac{\partial f_2}{\partial x_{N+1}} \\[2mm] \vdots & \ddots & \ddots & 0 & \vdots \\[2mm] 0 & \cdots & 0 & \dfrac{\partial f_N}{\partial x_N} & \dfrac{\partial f_N}{\partial x_{N+1}} \\[2mm] 1 & 1 & \cdots & 1 & 0 \end{pmatrix}$$

and for $j = 1,\ldots,N$

$$\frac{\partial f_j}{\partial x_j} \equiv \frac{\partial f_j}{\partial(\Delta\alpha_j)} = -\frac{m_j}{\alpha_j^2} \left.\frac{\partial e_j}{\partial \rho_j}\right|_P (\rho_j, P) + \frac{P_I^0 + P}{2m_j}$$

$$\frac{\partial f_j}{\partial x_{N+1}} \equiv \frac{\partial f_j}{\partial P} = \left.\frac{\partial e_j}{\partial P}\right|_{\rho_j} (\rho_j, P) + \frac{\Delta\alpha_j}{2m_j}$$

We can notice that $\mathbf{DF}$ has the following structure:

$$\mathbf{DF}(\mathbf{X}) = \begin{pmatrix} \mathbf{D} & \mathbf{b} \\ \mathbf{c}^{\mathrm{T}} & 0 \end{pmatrix}$$

where $\mathbf{D}$ is a $N \times N$ diagonal matrix with diagonal entries d_j, $j = 1,\ldots,N$

$$d_j = -\frac{m_j}{\alpha_j^2} \left.\frac{\partial e_j}{\partial \rho_j}\right|_P (\rho_j, P) + \frac{P_I^0 + P}{2m_j} \tag{47}$$

$\mathbf{b}$ is a N-row vector of $\mathbb{R}^N$, where each component b_j, $j = 1,\ldots,N$ is defined by

$$b_j = \left.\frac{\partial e_j}{\partial P}\right|_{\rho_j} (\rho_j, P) + \frac{\Delta\alpha_j}{2m_j} \tag{48}$$

and $\mathbf{c}^{\mathrm{T}}$ is a N-column constant vector of $\mathbb{R}^N$, where each component is equal to 1

$$\mathbf{c}^{\mathrm{T}} = (1,\ldots,1)^{\mathrm{T}} \tag{49}$$

For $\mathbf{X} = \mathbf{X}^0$, we have

$$\mathbf{F}(\mathbf{X}^0) = (f_j(0, P_I^0))_{j=1,\ldots,N+1}^{\mathrm{T}}$$

where

$$f_j(0, P_I^0) = e_j(\rho_j^0, P_I^0) - e_j^0 \quad \text{for } j = 1, \ldots, N$$

$$f_{N+1}(0, P_I^0) = 0$$

and therefore

$$\mathbf{DF}(\mathbf{X}^0) = \begin{pmatrix} \mathbf{D}_0 & \mathbf{b}_0 \\ \mathbf{c}^\mathrm{T} & 0 \end{pmatrix}$$

where, for $j = 1, \ldots, N$ the diagonal entries of $\mathbf{D}_0$ and the vector components of $\mathbf{b}_0$ are, respectively, defined as

$$\begin{cases} d_{j,0} = -\dfrac{m_j}{(\alpha_j^0)^2} \left. \dfrac{\partial e_j}{\partial \rho_j} \right|_P (\rho_j^0, P_I^0) + \dfrac{P_I^0}{m_j}, & \text{for } j = 1, \ldots, N \\[2ex] b_{j,0} = \left. \dfrac{\partial e_j}{\partial P} \right|_{\rho_j} (\rho_j^0, P_I^0) \end{cases}$$

The first iteration of the standard Newton method reads as

$$\mathbf{DF}(\mathbf{X}^0) \Delta \mathbf{X}^* = -\mathbf{F}(\mathbf{X}^0)$$

i.e. by denoting $\Delta \alpha^* = (\Delta \alpha_j^*)_{j=1,\ldots,N}^\mathrm{T}$

$$\mathbf{D}_0 \Delta \alpha^* + (P^* - P_I^0) b_0 = (e_j^0 - e_j(\rho_j^0, P_I^0))_{j=1,\ldots,N}^\mathrm{T}$$

$$\sum_{j=1}^N \Delta \alpha_j^* = 0$$

i.e.

$$d_{j,0} \Delta \alpha_j^* + b_{j,0}(P_j^* - P_I^0) = e_j^0 - e_j(\rho_j^0, P_I^0), \quad \text{for } j = 1, \ldots, N$$

$$\sum_{j=1}^N \Delta \alpha_j^* = 0 \tag{50}$$

From the first relations of (50) we can deduce the expression of the relaxed pressure for each j-phase

$$P_j^* = P_I^0 + \frac{1}{b_{j,0}}[e_j^0 - e_j(\rho_j^0, P_I^0) - d_{j,0} \Delta \alpha_j^*] \quad \text{for all } j = 1, \ldots, N \tag{51}$$

We may write in particular

$$P_j^* = P_1^*, \quad \forall j = 2, \ldots, N$$

and equalizing the corresponding expressions leads us to the following expression for $\Delta\alpha_j^*$, for all $j = 2, \ldots, N$:

$$\Delta\alpha_j^* = \frac{1}{d_{j,0}} \left[e_j^0 - e_j(\rho_j^0, P_I^0) - \frac{b_{j,0}}{b_{1,0}}(e_1^0 - e_1(\rho_1^0, P_I^0) - d_{1,0}\Delta\alpha_1^*) \right] \tag{52}$$

and, from the last equation of (50), we get

$$\Delta\alpha_1^* = -\sum_{j=2}^{N} \Delta\alpha_j^*$$

Using the expression of $\Delta\alpha_j^*$ in (52) leads us to the following definition of $\Delta\alpha_1^*$:

$$\Delta\alpha_1^* = -\frac{\sum_{j=2}^{N} \dfrac{1}{d_{j,0}} \left[e_j^0 - e_j(\rho_j^0, P_I^0) - \dfrac{b_{j,0}}{b_{1,0}}(e_1^0 - e_1(\rho_1^0, P_I^0)) \right]}{\sum_{j=1}^{N} \dfrac{d_{1,0}b_{j,0}}{d_{j,0}b_{1,0}}} \tag{53}$$

If $\alpha_1^* = \alpha_1^0 + \Delta\alpha_1^* \in]0, 1[$ *and* if $P_1^* > 0$, the definition of $\Delta\alpha_1^*$ is admissible and we may compute α_j^* and P_j^* for all $j = 2, \ldots, N$; otherwise, we may modify the value of $\Delta\alpha_1^*$ as it is done in Procedure 2.

If $\max_{j \neq 1} |P_j^* - P_1^*|$ is small enough, we may stop the procedure and update the conservative variables α_j, $m_j E_j$ for $j = 1, \ldots, N$; otherwise, we restart the procedure with as initial variables α_j^0, e_j^0 and P_j^0 the variables we have defined as α_j^*, e_j^* and P_j^*.

Note that this procedure is *a priori* not conservative with respect to the energy anymore since we have used an approximation for the energy $e_j(\rho_j^*, P^*)$.

Note though that the procedure is valid for real materials and is almost a direct procedure, provided (52) and (53) define admissible values.

The particular case when $N = 2$

As in the particular case of Procedure 1, when using stiffened gas EOS for both phases, we now end up with a quasi-direct process. As a matter of fact, when equalizing the pressures P_g^* and P_l^* (derived from relation (51)), we get the following expression for the volume fraction variation:

$$\Delta\alpha_g^* = \frac{\alpha_g^0 \alpha_l^0 \Delta P^0}{\alpha_g^0 \gamma_l (P_I^0 + P_{l,\infty}) + \alpha_l^0 \gamma_g (P_I^0 + P_{g,\infty})}$$

which can be rewritten as (32) for Procedure 2, except that the associated pressures are different. It can be shown that the expressions given above always define an admissible α_g^* and positive pressures P_j^*. As said previously, the solution is not conservative. As a matter of fact, the expression of the resulting internal energy e_j^* is given by

$$m_j(e_j^* - e_j) = -\delta_j P_I \Delta\alpha_g^* + \frac{(\Delta\alpha_g^*)^2}{\gamma_j - 1}(\gamma_k(P_I + P_{k,\infty}) - \gamma_j(P_I + P_{j,\infty}))$$

where $\delta_j = 1$ and $k = l$ if $j = g$, and $\varepsilon_j = -1$ and $k = g$ if $j = l$, therefore, the corrected energy (leading to conservativity) is defined by

$$e_j^{*,c} = e_j^* + \frac{(\Delta\alpha_g^*)^2}{m_j(\gamma_j - 1)}[\gamma_j(P_I + P_{j,\infty}) - \gamma_k(P_I + P_{k,\infty})]$$

$$= e_j + \delta_j P_I \Delta\alpha_g^*$$

and the corresponding corrected pressures are

$$P_j^{*,c} = P_j^* + \frac{(\Delta\alpha_g^*)^2}{\alpha_j^*}[\gamma_j(P_I + P_{j,\infty}) - \gamma_k(P_I + P_{k,\infty})]$$

$$= P_j - \delta_j \frac{\alpha_j}{\alpha_j^*} a_j \Delta\alpha_g^* \tag{54}$$

where $a_j \overset{\text{def}}{=} m_j c_{I,j}^2/\alpha_j^2$. It can be shown that, with the initial definition of $\Delta\alpha_g^*$, the resulting corrected pressures remain positive and guarantee convergence since we have

$$\Delta P^{*,c} \overset{\text{def}}{=} P_g^{*,c} - P_l^{*,c} = (1 - \beta)\Delta P$$

where

$$\beta = \frac{\dfrac{\alpha_g}{\alpha_g^*}a_g + \dfrac{\alpha_l}{\alpha_l^*}a_l}{a_g + a_l + \dfrac{\alpha_g - \alpha_l}{\alpha_g \alpha_l}\Delta P} \in \;]0, 2[$$

The corrected procedure is now iterative since $P_g^{*,c} \neq P_l^{*,c}$, but is ensured to converge.

4.2.7. Procedure 7: general EOS and $N \geqslant 2$ (new).

In this procedure, we define an iterative process that does not depend on (or that is not restricted to) a given EOS so explicitly as it was done in the three first procedures. It is in fact a particular case of Remark 4.2 and we give hereafter a generalized version for multiphase flows. As in the previous procedure, we will precise the particular case $N = 2$ and see that it is again a quasi-direct process. Although not conservative with respect to the energy, we can propose a correction in the case of stiffened gas EOS.

We recall that we initially aim to solve approximately system (14). This system may be rewritten in terms of the physical variables P_j, P_I, α_j, ρ_j, $c_{j,I}^2$, for $j = 1,\ldots,N$, where $c_{j,I}^2$ stands for the speed of sound at the interface of the fluid j and is defined as in (9). We recall that we have (see (17))

$$\mathrm{d}e_j = -\frac{P_I}{m_j}\,\mathrm{d}\alpha_j$$

from which we deduce (see (19))

$$\mathrm{d}P_j = -\frac{m_j c_{j,I}^2}{\alpha_j^2}\,\mathrm{d}\alpha_j$$

Integrating these equations on the interval $[\alpha_j^0, \alpha_j^*]$, we get

$$P_j^* - P_j^0 = -\int_{\alpha_j^0}^{\alpha_j^*} \frac{m_j c_{j,I}^2}{\alpha_j^2}\, \mathrm{d}\alpha_j$$

It now remains to approximate the integrals of the right-hand sides. Many approximations are available. We choose the following (simplest) one ($j = 1, \ldots, N$):

$$\int_{\alpha_j^0}^{\alpha_j^*} \frac{m_j c_{j,I}^2}{\alpha_j^2}\, \mathrm{d}\alpha_j \simeq \left[\left(\frac{m_j c_{j,I}^2}{\alpha_j^2} \right)^0 \right] \Delta\alpha_j^*$$

This approximation is not the most accurate, but its simple expression allows an easier description of the iterative algorithm. Let us replace now the indexes 0 and $*$ by k and $k+1$, respectively. We then get

$$P_j^{k+1} - P_j^k = -\left(\frac{m_j c_{g,I}^2}{\alpha_j^2} \right)^k \Delta\alpha_j^{k+1} \tag{55}$$

If relaxation is reached at this stage, we necessarily have, for all $j, m = 1, \ldots, N$

$$P_j^{k+1} = P_m^{k+1}$$

and we thus may write in particular the following system (in which we drop the index k for clarity):

$$P_j - a_j \Delta\alpha_j^{k+1} = P_1 - a_1 \Delta\alpha_1^{k+1}, \quad \forall j = 2, \ldots, N$$

where a_j denotes $m_j c_{j,I}/(\alpha_j)^2$. We deduce that

$$\Delta\alpha_j^{k+1} = [(P_j - P_1) + a_1 \Delta\alpha_1^{k+1}]/a_j, \quad \forall j = 2, \ldots, N \tag{56}$$

Since $\sum_{m=1}^{N} \Delta\alpha_m^{k+1} = 0$, we may write

$$\Delta\alpha_1^{k+1} = -\sum_{j=2}^{N} \Delta\alpha_j^{k+1}$$

using the expression of $\Delta\alpha_j^{k+1}$ in (56), we get the expression of $\Delta\alpha_1^{k+1}$

$$\Delta\alpha_1^{k+1} = \frac{\sum_{j=2}^{N}(P_1 - P_j)/a_j}{\sum_{j=1}^{N} a_1/a_j} \tag{57}$$

We must at this stage verify if these definitions lead to admissible values of the volume fractions. Admissibility may be written by

$$-\alpha_j \leqslant \frac{(P_j - P_1) + a_1 \Delta\alpha_1^{k+1}}{a_j} \leqslant 1 - \alpha_j, \quad \forall j = 2, \ldots, N$$

$$-\alpha_1 \leqslant \frac{\sum_{j=1}^{N}(P_1 - P_j)/a_j}{\sum_{j=1}^{N} a_1/a_j} \leqslant 1 - \alpha_1$$

$$\tag{58}$$

which is equivalent to

$$\max_j \left\{ -\frac{(P_j - P_1) + a_j \alpha_j}{a_1} \right\} \leqslant \Delta \alpha_1^{k+1} \leqslant \min_j \left\{ -\frac{(P_j - P_1) - a_j(1 - \alpha_j)}{a_1} \right\}$$

If this inequality is verified for $\Delta \alpha_1^{k+1}$ defined by (57), admissibility holds for all volume fraction variations and we can therefore define the α_j's for $j = 2, \ldots, N$ using (56) that guarantee equality of the pressures (relaxation is reached) and

$$P^* = P_j - a_j \Delta \alpha_j^{k+1}, \quad \forall j = 1, \ldots, N$$

Otherwise, we can define $\varepsilon \in]0, 1[$ such that

$$\Delta \bar{\alpha}_1^{k+1} \overset{\text{def}}{=} \varepsilon \Delta \alpha_1^{k+1}$$

is now admissible (i.e. verifies (58)). We then define the other new volume fraction variations $\Delta \bar{\alpha}_j^{k+1}$ using (56) with $\Delta \alpha_1^{k+1}$ replaced by $\Delta \bar{\alpha}_1^{k+1}$, for $j = 2, \ldots, N$. The corresponding pressures P_m^{k+1} are obtained by (55). If all pressures are equal we end the process and correct the conservative variables as done in all the relaxation procedures described in this paper, otherwise, we reiterate with the data of iteration $k + 1$.

Remark 4.6
As described above, the iterative process is not conservative with respect to the energy. A way to circumvent this problem (if any) is to add a correction step when all pressures are equal. This correction step may be exactly defined in the stiffened gas EOS case, and for $N = 2$. As a matter of fact, it can be shown that

$$\sum_{j=g,l} m_j (e_j^{k+1} - e_j^k) = -\left(\frac{a_g^k}{\gamma_g - 1} + \frac{a_l^k}{\gamma_l - 1} \right) (\Delta \alpha_g^{k+1})^2$$

which obviously cannot be equal to zero for non zero volume fraction variation. The energy e_j^{k+1} may be expressed as

$$e_j^{k+1} = e_j^k - \frac{P_I^k}{m_j} \Delta \alpha_j^{k+1} - \frac{a_j^k}{m_j(\gamma_j - 1)} (\Delta \alpha_j^{k+1})^2$$

from which we derive a natural correction corresponding to the opposite of the third term above. If we denote by $e_j^{k+1,C}$ the energy insuring conservation and d_j^{k+1} the energy correction, then

$$e_j^{k+1,C} = e_j^{k+1} + d_j^{k+1}$$

$$= e_j^k + \frac{P_I^k}{m_j} \Delta \alpha_j^{k+1}$$

with

$$d_j^{k+1} = \frac{1}{m_j} \frac{a_j^k}{\gamma_j - 1} (\Delta \alpha_g^{k+1})^2$$

and the corresponding corrected pressure is written as

$$P_j^{k+1,C} = P_j^{k+1} + \frac{a_j}{\alpha_j^{k+1}}(\Delta\alpha_g^{k+1})^2$$

$$= P_j^k - a_j^k \Delta\alpha_j^{k+1} + a_j^k \frac{(\Delta\alpha_j^{k+1})^2}{\alpha_j^{k+1}}$$

This correction insures that the corrected pressures remain positive. Other corrections may be used but they necessarily are expressed as $d_j^{k+1} + \varepsilon_j^{k+1}/m_j$ where ε_j^{k+1} should satisfy

$$\sum_j \varepsilon_j^{k+1} = 0$$

and the corresponding corrected pressures should remain positive.

The particular case when $N = 2$

In the particular case of $N = 2$, $(j = g, l)$ and if we denote by $\Delta P = P_g - P_l$, we get

$$\Delta\alpha_g^{k+1} = \varepsilon \frac{\Delta P}{a_g + a_l}$$

If $\Delta P > 0$, admissibility is reached if $0 < \Delta\alpha_g^{k+1} < \alpha_l$ and if $\Delta P < 0$ the admissibility becomes $0 < -\Delta\alpha_g^{k+1} < \alpha_g$. Note that these inequalities both ensure that the volume fraction is admissible and that the pressures remain positive. If the admissibility criterion is verified with $\varepsilon = 1$, the method is direct and the relaxed pressure P^* may be expressed as

$$P^* = \frac{a_l}{a_g + a_l}P_g + \frac{a_g}{a_g + a_l}P_l$$

Conservativity may be added as explained in the remark given above.

Remark 4.7
If the stiffened gas EOS is used and when $N = 2$, note that Procedures 2 and 7 are of the same oder of accuracy. As a matter of fact, when $\varepsilon = 1$, and denoting the volume fraction variation by $\Delta\alpha_g^{*,\varphi}$ for Procedure 7 and by $\Delta\alpha_g^{*,E}$ for Procedure 2 and following (32), we have

$$\Delta\alpha_g^{*,E} - \Delta\alpha_g^{*,\varphi} = \frac{\alpha_l - \alpha_g}{\alpha_l\alpha_g}\Delta\alpha_g^{*,E}\Delta\alpha_g^{*,\varphi}$$

i.e. both methods are of the same order of accuracy in the particular case of stiffened gas EOS and two-phase flows.

We thus have defined a simple iterative process which can be used with more general EOS than the stiffened gas EOS. It is moreover almost a direct method due to the definition of the volume fraction variation.

4.3. Procedure based on the assumption of a constant P_I: Procedure 8, stiffened gas EOS and $N \geqslant 2$

The interface pressure is considered as the constant external pressure acting on the multiphase medium. Thus, in this section, no modellization of the interface pressure is needed ($P_I = P^*$).

4.3.1. General case ($N \geqslant 2$, general EOS).
Under the assumption of a constant pressure P^*, we may write that

$$\mathrm{d}e_j = -\frac{P^*}{m_j}\,\mathrm{d}\alpha_j$$

and therefore

$$e_j^* - e_j^o = -\frac{P^*}{m_j}\Delta\alpha_j^*$$

for all $j = 1, \ldots, N$, from which we add each corresponding EOS

$$e_j = e_j(\rho_j, P_j)$$

and supplement them with the saturation constraint

$$\sum_{j=1}^{N} \Delta\alpha_j^* = 0, \quad -\alpha_j^0 \leqslant \Delta\alpha_j^* \leqslant \sum_{m \neq j} \alpha_m^0 \tag{59}$$

We therefore have a system of $2N + 1$ equations with $2N + 1$ unknowns corresponding, respectively, to the e_j^*, $\Delta\alpha_j^*$ and P^*. We mainly have two approaches to solve this system. Either we linearized the e_j^* and solve the resulting nonlinear system, or we start from the original nonlinear system and solve it by a Newton-type algorithm.

(a) *Linearization first*: In this approach, we linearize each energy equation $e_j(\rho_j, P_j)$ from the relaxed state e_j^* considering that both density and pressure (ρ_j, P_j) will evolve using the EOS from the initial state to the final relaxed state ρ_j^*, P_j^*, with $P_j^* = P^*$. We may indeed write that

$$e_j^* \simeq e_j(\rho_j^0, P^*) + \left.\frac{\partial e_j}{\partial \rho_j}\right|_{P_j}(\rho_j^0, P^*)(\rho_j^* - \rho_j^0)$$

and also,

$$e_j(\rho_j^0, P^*) \simeq e_j^0 + \left.\frac{\partial e_j}{\partial P_j}\right|_{\rho_j}(\rho_j^0, P_j^0)(P^* - P_j^0)$$

$$\left.\frac{\partial e_j}{\partial \rho_j}\right|_{P_j}(\rho_j^*, P^*) \simeq \left.\frac{\partial}{\partial P_j}\left(\left.\frac{\partial e_j}{\partial \rho_j}\right|_{P_j}\right)\right|_{\rho_j}(\rho_j^0, P_j^0)(P^* - P_j^0)$$

since $\rho_j^* - \rho_j^0 = -m_j \Delta\alpha_j^* / (\alpha_j^* \alpha_j^0)$), we finally have the following approximation for $\Delta e_j^* \overset{\text{def}}{=} e_j^* - e_j^0$:

$$\Delta e_j^* = -\frac{P^*}{m_j}\Delta\alpha_j^*$$

$$\simeq -\frac{m_j}{\alpha_j^* \alpha_j^0}\frac{\partial e_j^0}{\partial \rho_j}\Delta\alpha_j^* + \left[\frac{\partial e_j^0}{\partial \rho_j} + \frac{\partial}{\partial P_j}\left(\frac{\partial e_j}{\partial \rho_j}\right)^0\right](P^* - P_j^0)$$

where the zero index stands for the initial state (ρ_j^0, P_j^0). Rearranging the expression above leads to the following expression for P^* (we drop the zero index for clarity):

$$P^* = \frac{\dfrac{\partial e_j}{\partial P_j}P_j + \dfrac{m_j}{\alpha_j^* \alpha_j}\left[\dfrac{\partial e_j}{\partial \rho_j} - \dfrac{\partial}{\partial P_j}\left(\dfrac{\partial e_j}{\partial \rho_j}\right)P_j\right]\Delta\alpha_j^*}{\dfrac{\partial e_j}{\partial P_j} + \left[\dfrac{1}{m_j} - \dfrac{m_j}{\alpha_j \alpha_j^*}\dfrac{\partial}{\partial P_j}\left(\dfrac{\partial e_j}{\partial \rho_j}\right)\right]\Delta\alpha_j^*}$$

this expression must hold for all $j = 1, \ldots, N$ with the saturation constraint (59). The resulting system may be solved by a Newton-type algorithm but we will not go forward in this paper.

(b) *Newton first*: In the second approach, we may show that we end up with the following nonlinear system which can be rewritten by

$$f_j((\Delta\alpha_j^*)_j) = 0, \quad j = 1, \ldots, N+1$$

with

$$f_j((\Delta\alpha_j)_j) = e_j(\rho_j, P^*) - e_j^0 + \frac{P^*}{m_j}\Delta\alpha_j, \quad j = 1, \ldots, N$$

$$f_{N+1}((\Delta\alpha_j)_j) = \sum_{j=1}^{N}\Delta\alpha_j$$

If $\Delta\alpha \overset{\text{def}}{=} (\Delta\alpha_j)_j$, note that for all $j \neq N+1$, f_j only depends on $\Delta\alpha_j$, i.e.

$$\forall m \neq j, \quad \frac{\partial f_j}{\partial \alpha_m} = 0$$

Therefore, the classical Newton method applied on this system reads as

$$\frac{\partial f_j}{\partial \alpha_j}(0)\Delta\alpha_j^* = -f_j(0)$$

supplemented by

$$\sum_{j=1}^{N}\Delta\alpha_j^* = 0$$

where

$$f_j(0) = e_j(\rho_j^0, P^*) - e_j^0$$

$$\frac{\partial f_j}{\partial \alpha_j}(0) = \frac{P^*}{m_j} - \frac{m_j}{(\alpha_j^0)^2} \left. \frac{\partial e_j}{\partial \rho_j} \right|_{P_j} (\rho_j^0, P^*)$$

We finally have to solve the following system of $N+1$ equations and $N+1$ unknowns (the $\Delta \alpha_j^*$ and P^*):

$$\left[\frac{P^*}{m_j} - \frac{m_j}{\alpha_j^2} \frac{\partial e_j}{\partial \rho_j}(\rho_j^0, P^*) \right] \Delta \alpha_j^* = e_j^0 - e_j(\rho_j^0, P^*), \quad \forall j = 1, \ldots, N$$

$$\sum_{j=1}^{N} \Delta \alpha_j^* = 0$$

from which we deduce the following expressions for $\Delta \alpha_j^*$ and P^*:

$$\Delta \alpha_j^* = \frac{e_j^0 - e_j(\rho_j^0, P^*)}{\dfrac{P^*}{m_j} - \dfrac{m_j}{\alpha_j^2} \dfrac{\partial e_j}{\partial \rho_j}(\rho_j^0, P^*)}$$

$$P^* = m_j(e_j^0 - e_j^*)/\Delta \alpha_j^*$$

Denoting $\Delta P_j^* = P^* - P_j^0$, we may linearize the previous expression of $\Delta \alpha_j^*$ by using the following approximations:

$$e_j(\rho_j^0, P^*) \simeq e_j^0 + \frac{\partial e_j^0}{\partial P_j} \Delta P_j^*$$

$$\frac{\partial e_j}{\partial \rho_j}(\rho_j^0, P^*) \simeq \frac{\partial e_j^0}{\partial \rho_j} + \frac{\partial}{\partial P_j} \left(\frac{\partial e_j}{\partial \rho_j} \right)^0 \Delta P_j^*$$

leading to the following approximate definition of $\Delta \alpha_j^*$:

$$\Delta \alpha_j^* = \frac{\dfrac{\partial e_j^0}{\partial P_j} \Delta P_j^*}{\dfrac{P^*}{m_j} - \dfrac{m_j}{\alpha_j^2} \dfrac{\partial e_j^0}{\partial \rho_j} - \dfrac{m_j}{\alpha_j^2} \dfrac{\partial}{\partial P_j} \left(\dfrac{\partial e_j}{\partial \rho_j} \right)^0 \Delta P_j^*}$$

and the following expression of P^*:

$$P^* = \frac{\alpha_j^2 \dfrac{\partial e_j^0}{\partial P_j} P_j^0 + m_j \left[\dfrac{\partial e_j^0}{\partial \rho_j} - \dfrac{\partial}{\partial P_j} \left(\dfrac{\partial e_j}{\partial \rho_j} \right)^0 P_j^0 \right] \Delta \alpha_j^*}{\alpha_j^2 \dfrac{\partial e_j^0}{\partial P_j} + \left[\dfrac{\alpha_j^2}{m_j} - m_j \dfrac{\partial}{\partial P_j} \left(\dfrac{\partial e_j}{\partial \rho_j} \right)^0 \right] \Delta \alpha_j^*}$$

Let us drop the zero index and denote

$$C_j = \alpha_j^2 \frac{\partial e_j}{\partial P_j}$$

$$A_j = C_j P_j$$

$$B_j = m_j \left[\frac{\partial e_j}{\partial \rho_j} - \frac{\partial}{\partial P_j} \left(\frac{\partial e_j}{\partial \rho_j} \right) P_j \right]$$

$$D_j = \frac{\alpha_j^2}{m_j} - m_j \frac{\partial}{\partial P_j} \left(\frac{\partial e_j}{\partial \rho_j} \right)$$

for a fixed m in $\{1, \ldots, N\}$, we may show that

$$\Delta \alpha_j^* = \frac{C_j [C_m (P_m - P_j) + (B_m - D_m P_j) \Delta \alpha_m^*]}{(B_j - D_j P_m) C_m + (B_j D_m - B_m D_j) \Delta \alpha_m^*} \tag{60}$$

but, from the saturation constraint we have

$$\Delta \alpha_m^* = -\sum_{j \neq m} \Delta \alpha_j^*$$

so, using expression (60) we end up to the following expression for $\Delta \alpha_m^*$:

$$\Delta \alpha_m^* = g(\Delta \alpha_m^*)$$

with

$$g(\Delta \alpha_m^*) = -\sum_{j \neq m} \frac{C_j [C_m (P_m - P_j) + (B_m - D_m P_j) \Delta \alpha_m^*]}{(B_j - D_j P_m) C_m + (B_j D_m - B_m D_j) \Delta \alpha_m^*}$$

that we can solve using a fixed point algorithm.

4.3.2. Stiffened gas EOS ($N \geqslant 2$). We shall focus on the second approach only. In the case where the different phases obey a stiffened gas EOS, the approximations given above are exact and the expression of the relaxed pressure becomes (we drop the zero index for clarity)

$$P^* = \frac{\alpha_j P_j - \gamma_j P_{j,\infty} \Delta \alpha_j^*}{\alpha_j + \gamma_j \Delta \alpha_j^*}$$

that should be held for $j = 1, \ldots, N$. If we now fix m to be equal to 1, we may derive the following expressions for the volume fraction variations ($j = 2, \ldots, N$):

$$\Delta \alpha_j^* = \frac{\alpha_j}{\gamma_j} \frac{\alpha_1 (P_j - P_1) + \gamma_1 (P_j + P_{1,\infty}) \Delta \alpha_1^*}{\alpha_1 (P_1 + P_{j,\infty}) + \gamma_1 (P_{j,\infty} - P_{1,\infty}) \Delta \alpha_1^*}$$

$$\Delta \alpha_1^* = -\sum_{j \neq 1} \frac{\alpha_j}{\gamma_j} \frac{\alpha_1 (P_j - P_1) + \gamma_1 (P_j + P_{1,\infty}) \Delta \alpha_1^*}{\alpha_1 (P_1 + P_{j,\infty}) + \gamma_1 (P_{j,\infty} - P_{1,\infty}) \Delta \alpha_1^*}$$

Equation for $\Delta\alpha_1^*$ may be solved by a fixed point algorithm as prescribed for general EOS.

The particular case when $N = 2$

When $N = 2$, and with ε_j defined as in (31), we get for P^* and $j = g, l$

$$P^* = \frac{\alpha_j P_j - \varepsilon_j \gamma_j P_{j,\infty} \Delta\alpha_g^*}{\alpha_j + \varepsilon_j \gamma_j \Delta\alpha_g^*}$$

and we end up with the following equation for $\Delta\alpha_g^*$:

$$c_0 + c_1 \Delta\alpha_g^* + c_2 (\Delta\alpha_g^*)^2 = 0$$

where

$$c_0 = -\alpha_g \alpha_g \Delta P$$

$$c_1 = \alpha_l \gamma_g (P_l + P_{g,\infty}) + \alpha_g \gamma_l (P_g + P_{l,\infty})$$

$$c_2 = \gamma_l \gamma_g (P_{l,\infty} - P_{g,\infty})$$

The discriminant $\Delta = c_1^2 - 4c_0 c_2$, if non negative, ensures the existence of at most two solutions. As in the direct procedure 0, it is easy to show that

If $\Delta P > 0$ then $\Delta > 0$ and the roots have opposite signs, therefore we should retain the root having the same sign as ΔP;

If $\Delta P < 0$ and if $\Delta > 0$ still holds, then the roots have the same sign that should necessarily be the sign of ΔP. In this case, we should retain the admissible root (i.e. yielding to $\alpha_g^* \in [0, 1]$ and positive pressures).

Remark 4.8

When all phases obey the perfect gas EOS ($P_{j,\infty} = 0$, $\forall j = 1, \ldots, N$), we get an explicit expression for the relaxed pressure

$$P^* = \frac{\sum_{j=1}^N \dfrac{\alpha_j^0}{\gamma_j} P_j^0}{\sum_{j=1}^N \dfrac{\alpha_j^0}{\gamma_j}}$$

When all phases obey the same perfect gas EOS ($\gamma_j = \gamma$, $\forall j = 1, \ldots, N$), we get another explicit relation for the relaxed pressure which looks like the Dalton law

$$P^* = \sum_{j=1}^N \alpha_j^0 P_j^0$$

5. NUMERICAL TESTS

The various pressure relaxation procedures are tested in terms of performances (mainly and namely efficiency, accuracy and conservativity), over the air/water shock tube test as given

in Reference [7, pp. 448–450]. For this test case, $N = 2$ and both fluids are considered as compressible and governed by the stiffened gas EOS. So we compare the performances of the following algorithms ($N = 2$ version) named as:

1. PR1: Procedure 1 (new iterative procedure, cf. Section 4.2.1);
2. PR2: Procedure 2 (new *exact* quasi-Newton procedure, cf. Section 4.2.2);
3. PR3: Procedure 3 (new direct procedure, cf. Section 4.2.3);
4. PR4: Procedure 4 (old iterative procedure, cf. Section 4.2.4);
5. PR5: Procedure 5 (old iterative procedure, cf. Section 4.2.5);
6. PR6: Procedure 6 (new quasi-direct procedure, cf. Section 4.2.6 with the energy correction proposed in (54));
7. PR7 (NC): Procedure 7 (new quasi-direct procedure, expressed in terms of the acoustic interface variables without energy correction, cf. Section 4.2.7);
8. PR7 (C): Procedure 7 with the energy correction proposed in Remark 4.6;
9. PR8: Procedure 8 (new, based on the assumption that the relaxed pressure is a constant external pressure, direct procedure, cf. Section 4.3).

Let us therefore consider the shock tube of 1 m length, filled on the left by liquid water at high pressure and on the right by air. This problem possesses an analytical solution. The initial data are

$$\rho_l = 10^3 \text{ kg/m}^3, \qquad P_l = 10^9 \text{ Pa}, \qquad u_l = 0 \text{ m/s}$$

$$\gamma_l = 4.4, \qquad P_{l,\infty} = 6 \times 10^8 \text{ Pa}, \quad \alpha_l = 1 - \varepsilon$$

if $x < 0.7$, and

$$\rho_g = 50 \text{ kg/m}^3, \qquad P_g = 10^5 \text{ Pa}, \quad u_g = 0 \text{ m/s}$$

$$\gamma_g = 1.4, \qquad P_{g,\infty} = 0 \text{ Pa}, \qquad \alpha_g = 1 - \varepsilon$$

otherwise. The volume fraction of the fluid in minor concentration in both chamber is set to $\varepsilon = 10^{-8}$. For this test problem, we use the 7 equations model with both velocity and pressure relaxation procedures.

We perform this numerical test with a spacial grid of 301 discretization nodes and compare the results obtained with the different pressure relaxation procedures as given above.

The test parameter used for tolerance for the absolute value of the pressure variation $P_g - P_l$ is the same for all procedures and set to an arbitrarily very small value to show up their performances ($\varepsilon_P = 10^{-10}$).

The numerical approximated solutions at time $t = 229.0 \times 10^{-6}$s are depicted in Figure 1 and compared with the analytical solution. As expected, all the conservative procedures give the same numerical solution, except procedure PR7 (NC) which appears to be more accurate when compared to the analytical solution (Figure 1). The shock position appears better predicted by this non conservative procedure than with the conservative ones. A possible explanation might be that the transport solver used for the numerical test is not accurate enough. We indeed believe that the differences found here would disappear with a more accurate solver. Thanks to a new numerical approach for the building of numerical schemes for mutiphase mixtures, a new hyperbolic solver with improved accuracy, has been proposed in References [11, 22]. We now redo the comparison between the pressure relaxation procedures (conservative and
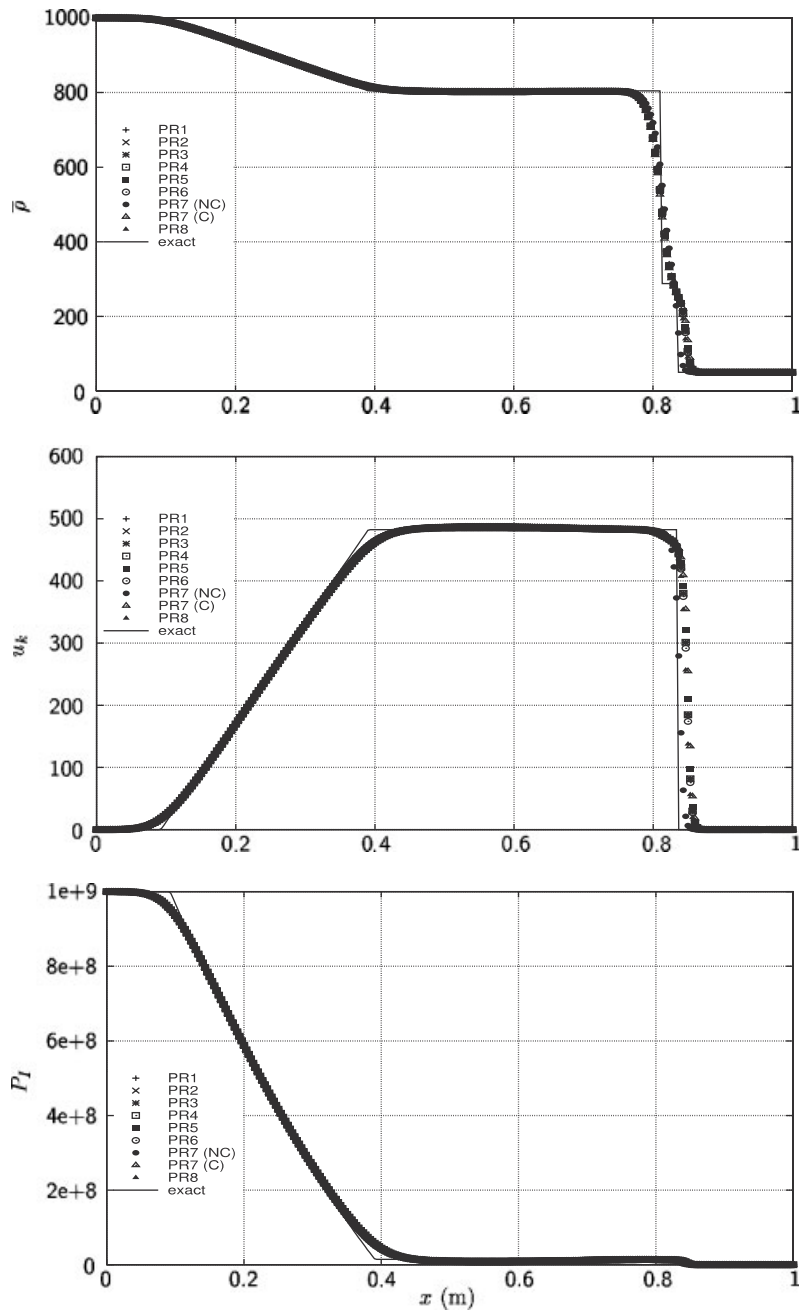
Figure 1. Comparison between the numerical solution obtained with the various pressure relaxation procedures and exact solution for the water/air shock tube problem (301 nodes) at time 229×10^{-6} s. Top: mixture density, middle: mixture velocity, bottom: mixture pressure.
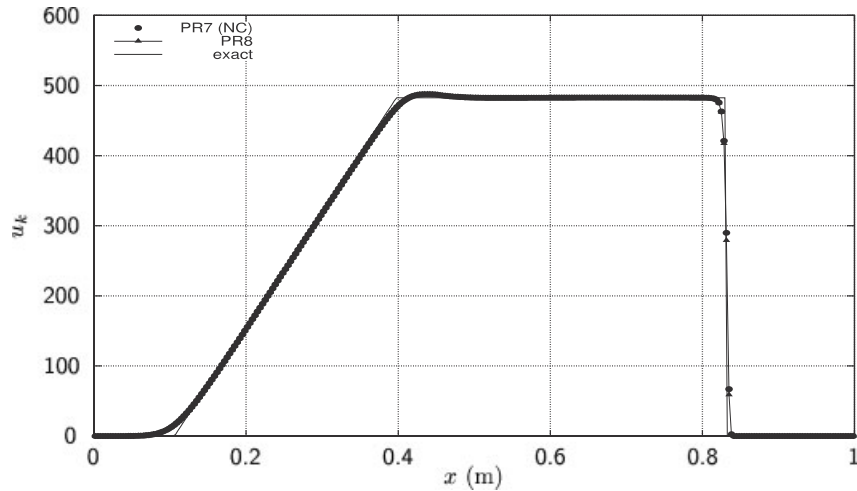
Figure 2. Comparison between the numerical mixture velocity solution obtained by a conservative (PR8) and non conservative (PR7 (NC)) pressure relaxation procedure with the exact solution when using a more accurate transport solver. Air/water shock tube problem (301 nodes) at time 229×10^{-6} s.

non conservative), when employed with this new hyperbolic solver. The computed mixture velocity profiles are compared with the exact solution in Figure 2. It appears clearly that now both the conservative and non conservative pressure relaxation procedures provide the same accuracy, in excellent agreement with the exact solution.

We now exhibit some *qualitative criteria* in order to classify all procedures presented in this paper: efficiency, accuracy and conservativity. For each of the criteria we define a rank number from the best to the worse. For each criterion we summarize these rank numbers in related tables.

The main qualitative criteria are the following ones:

1. *Efficiency*: A procedure is defined as *efficient* if it is both low CPU consuming and convergent. A procedure is defined as *convergent* if it converges up to an arbitrarily small tolerance (or is very close to this tolerance value). A procedure is therefore efficient if it is convergent with a good convergence rate.

   We give in Figure 3 the percentage of CPU spent in each procedure with respect to the total CPU, from the lowest CPU consuming procedure to the highest one. As expected the less CPU consuming procedures are those which are direct (procedures PR3 and PR8) or quasi-direct (procedures PR7 (C), PR7 (NC) and PR2). This figure clearly shows the importance of optimizing the pressure relaxation step.

   To show up the local convergence behaviour of a pressure relaxation procedure, we split the initial space domain into three sub-intervals, namely $[0, 0.5]$, $[0.5, 0.8]$ and $[0.8, 1.0]$. The first sub-interval $[0, 0.5]$ embeds the rarefaction wave location, the second sub-interval $[0.5, 0.8]$ corresponds to a domain in which both mixture velocity and pressure remain uniform and the third sub-interval $[0.8, 1.0]$ embeds the remaining space domain that includes the shock position location. These sub-regions are also used for the *accuracy* criterion below.
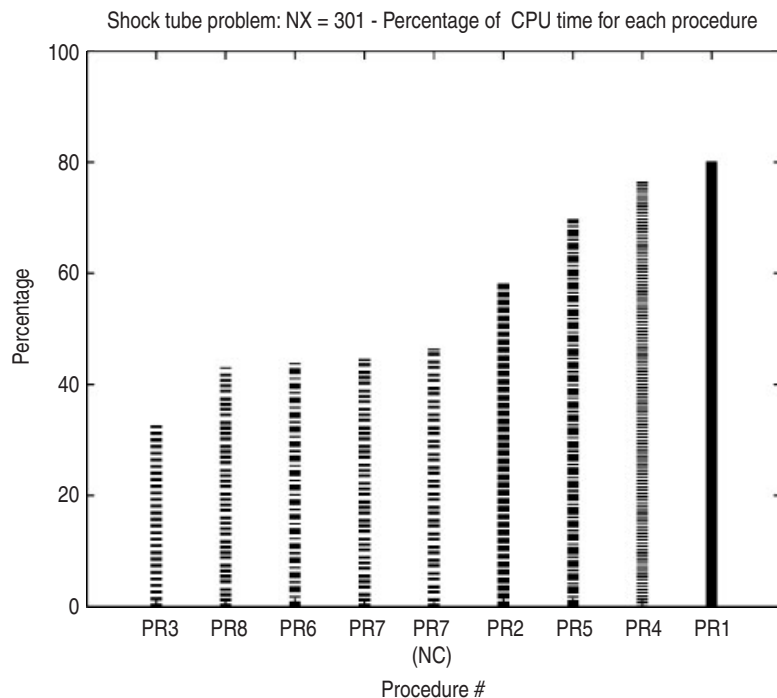
Shock tube problem: NX = 301 - Percentage of CPU time for each procedure

Figure 3. Percentage of CPU taken by each procedure.

Table I. Phase pressure variation extrema.

Proc. #	1	2	3	4	5	6	7 (NC)	7 (C)	8
Min	0.0	0.0	0.0	3.63e−8	0.0	0.0	0.0	0.0	0.0
Max	8.34e−7	10.38	1.07e−6	19.51	29.31	1.19e−7	1.19e−7	1.19e−7	1.58e−3
Cell %	0.0	30.54	0.0	57.42	27.25	0.0	0.0	0.0	7.21e−6

In Figure 7, we have depicted, for each sub-domain defined above, the pressure varia-
tion between phases obtained at the end of the numerical simulation (time 229×10^{-6} s)
for the non conservative procedure PR7 (NC).

Bounds of the pressure variations obtained by all the pressure relaxation procedures
in the whole space domain are summarized in Table I. In this table, the third line
corresponds to the percentage of cells with respect to the total number of cells for
which the tolerance effectively attained by the pressure variation is greater than 10^{-4},
during all the simulation (from time 0 to 229×10^{-6} s). Rank numbers of the various
pressure relaxation procedures related to the convergence criterion are given in Table II:
Procedures PR6 and PR7 (with or without correction) followed by procedure PR1, appear
to be the ones which have the best convergence qualities. Final rank numbers for the
global efficiency criterion (combining both low CPU consuming and good convergence
behaviour) are given in Table III: Procedures PR6, PR7 (with or without correction) and

Table II. Rank of each procedure related to the pressure variation criterion.

Proc. #	1	2	3	4	5	6	7 (NC)	7 (C)	8
Rank	4	7	5	9	8	1	1	1	6

Table III. Rank of each procedure related to the efficiency criterion.

Proc. #	1	2	3	4	5	6	7 (NC)	7 (C)	8
Rank	6	6	3	9	8	1	2	3	5

PR3 followed closely by PR8 are, as expected, the best procedures concerning efficiency.

2. *Accuracy*: A procedure is defined as *accurate* if the relative errors (ε_P, ε_ρ and ε_u) are small enough.

Let us denote by ξ_{ex} the analytical solution and define the relative error ε_ξ by

$$\varepsilon_\xi \stackrel{\text{def}}{=} \frac{\xi_{ex} - \xi_I}{\xi_{ex}}$$

with $\xi = P, \rho, u$ to design the relative pressure, density and velocity errors. P_I, ρ_I and u_I denote the interfacial pressure, the mixture density and the mixture velocity, respectively.

These relative errors are, respectively, depicted in Figure 4 for the mixture pressure, in Figure 5 for the mixture density and finally in Figure 6 for the mixture velocity, for each of the space sub-domains previously defined.

As expected and because of the dissipativity of the transport solver HLL, the amplitude of the error is especially large in the vicinity of the shock and the rarefaction wave region. Note though the importance of the type of relaxation procedure used in this numerical test, especially for procedure PR7 (NC) which appears to be the most accurate except for the mixture velocity for which the improvement is less remarkable.

In Table IV, we summarize, for each procedure and in each sub-domain, the extrema of the relative pressure error together with the percentage of cell numbers for which the local error is greater than half the local maximum error; the last column gives the rank number of each procedure.

Tables V and IX list the corresponding items for the mixture density and velocity errors, respectively. Concerning both mixture pressure and density, the non conservative procedure PR7 confirms to be the most accurate, especially in the third subdomain, where the shock position is the best predicted, since the maximum of the relative error is at least divided by 3 for the pressure error and by 2 for the density error. In addition, the proportion of cells in which the error is large is smaller in this subdomain, compared to all the other conservative procedures. It is followed by procedures PR8 and PR2 for the pressure error and by procedure PR8 for the density error. For the mixture velocity error, procedure PR8 appears to be the best procedure, followed by the non conservative procedure PR7, but procedure PR7 shows that the percentage of cells in which the relative error is large in the shock sub-domain is almost divided by 4.

For the whole space domain, rank numbers of each procedure are summarized in Table VI concerning the total accuracy criterion (i.e. taking into account the qualitative behaviour of the mixture pressure, density and velocity error over the three sub-domains):
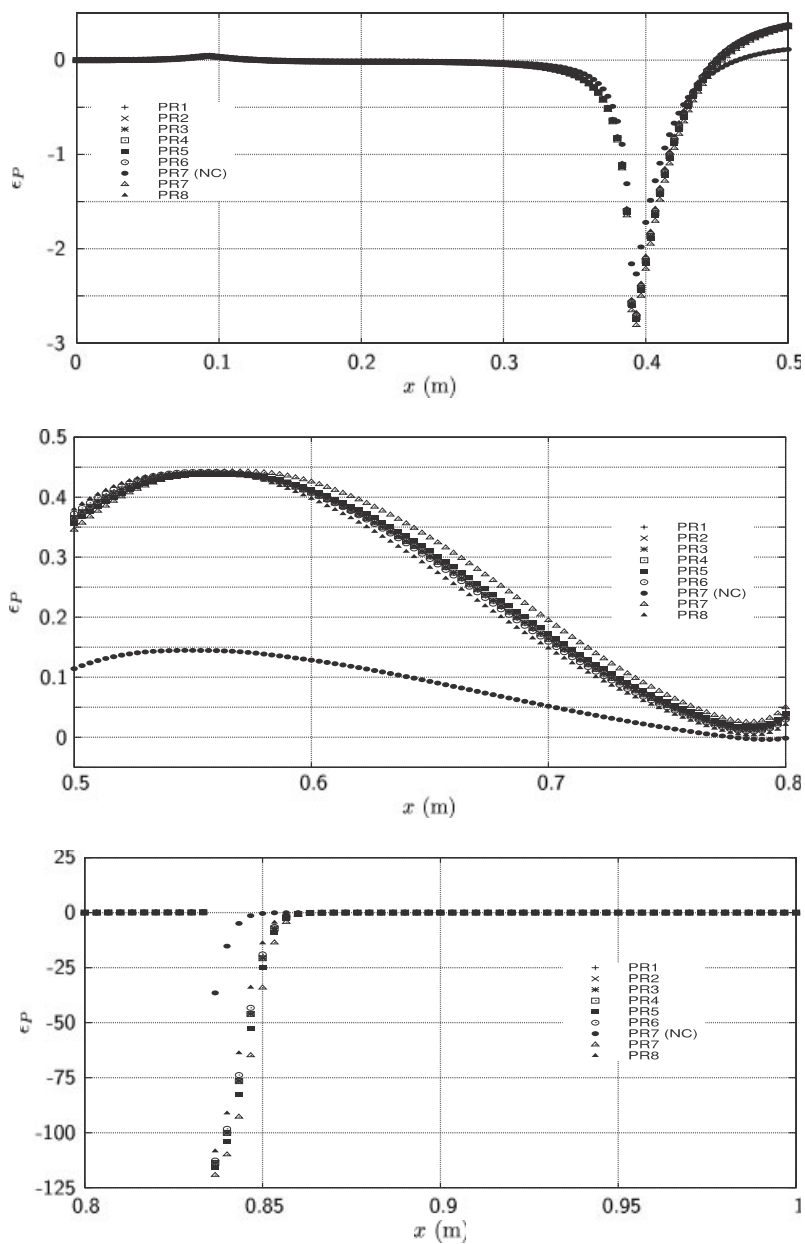
Figure 4. Relative pressure error ε_P.

procedure PR8 appears to be the best globally, followed by the non conservative proce-
dure PR7, together with procedures PR1, PR3 and PR4.

3. *Conservativity*: To verify this criterion, we define the discrete energy conservation mea-
sure over each cell. A procedure is therefore conservative if the maximum over each
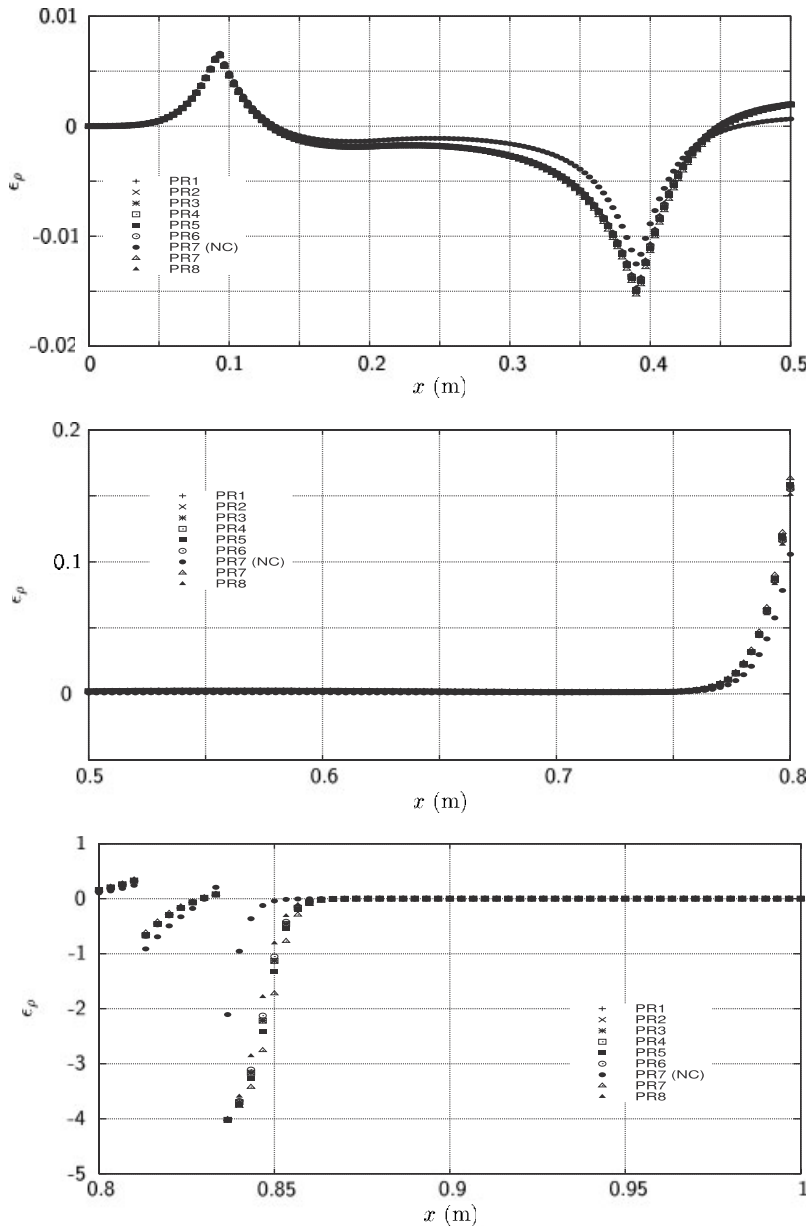
Figure 5. Relative density error ε_ρ.

cell of the energy conservation measure is as small as possible. Table VII gives for each procedure the global extrema (minimum and maximum) together with the average number of cells for which the energy conservation measure is greater than $1.e{-}4$ over all the simulation (third line of this table). Ranks of the procedures concerning this

Figure 6. Relative velocity error ε_u.

conservativity criterion are shown in Table VIII. As expected, the best procedures confirm to be procedures PR4, PR5 and PR3 and the worse to be obviously the non conservative procedure PR7.

Table IV. Relative pressure error.

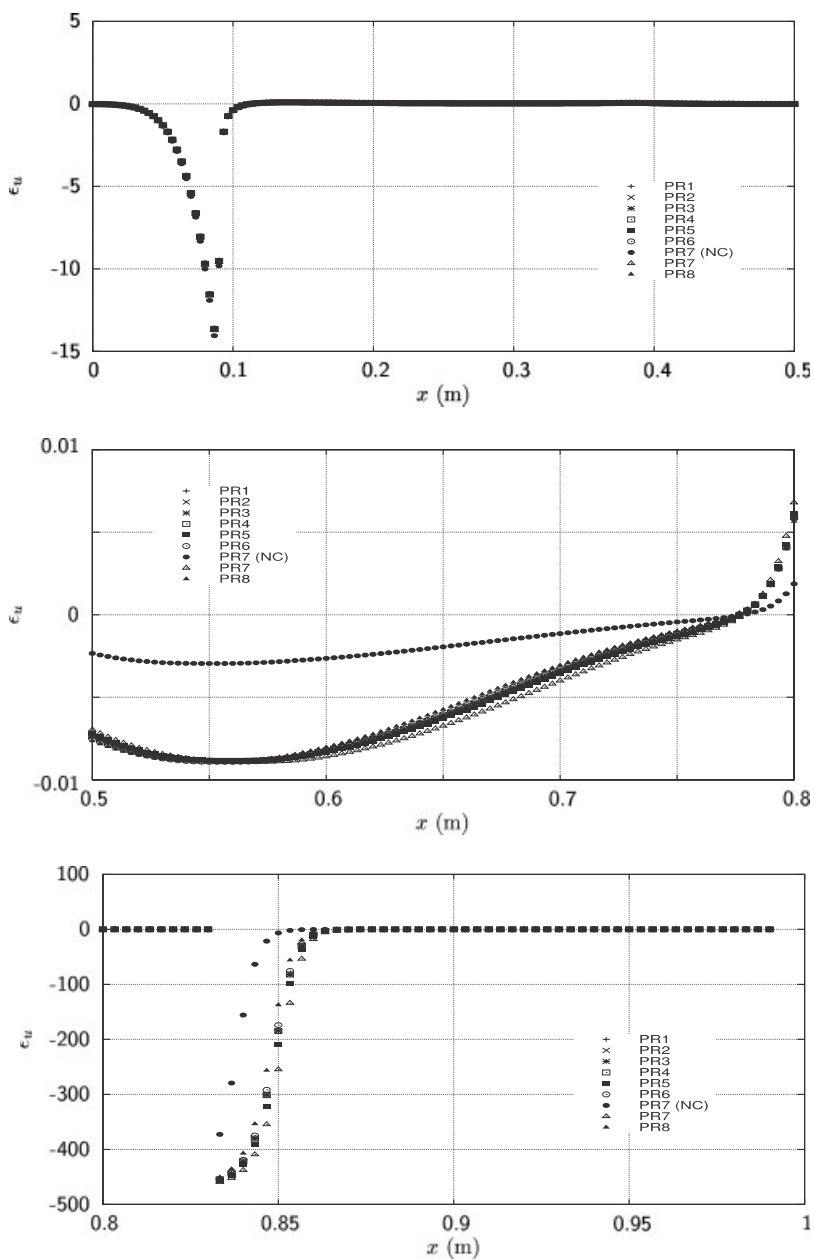| Proc. #	Extrema &	Sub-int. 1	Sub-int. 2	Sub-int. 3	Rank
PR1	Min	3.2e−5	1.28e−2	0.0	4
	Max	2.73	4.40e−1	113.72	
	% cells	5.3	58.89	5.0	
PR2	Min	3.2e−5	1.27e−2	0.0	3
	Max	2.73	4.40e−1	113.69	
	% cells	5.3	58.89	5.0	
PR3	Min	3.2e−5	1.28e−2	0.0	4
	Max	2.73	4.40e−1	113.72	
	% cells	5.3	58.89	5.0	
PR4	Min	3.2e−5	1.28e−2	0.0	4
	Max	2.73	4.40e−1	113.72	
	% cells	5.3	58.89	5.0	
PR5	Min	3.2e−5	1.73e−2	0.0	7
	Max	2.75	4.38e−1	115.95	
	% cells	5.3	61.11	5.0	
PR6	Min	3.2e−5	2.04e−2	0.0	8
	Max	2.77	4.37e−1	117.27	
	% cells	5.3	61.11	5.0	
PR7 (NC)	Min	3.4e−5	4.78e−3	0.0	1
	Max	2.27	1.45e−1	36.47	
	% cells	4.64	57.78	1.67	
PR7 (C)	Min	3.3e−5	2.52e−2	0.0	9
	Max	2.81	4.43e−1	119.30	
	% cells	5.3	63.33	6.67	
PR8	Min	3.2e−5	3.42e−3	0.0	2
	Max	2.68	4.41e−1	108.4	
	% cells	5.3	56.67	5.0	

We finally do an additional test to check the convergence behaviour of all these procedures and the uniqueness of the relaxed solution that we get. The simplest way to check these matters is to start with the same initial state solution and apply each procedure to compare the solutions we get. So we use the same test case described previously (for 101 nodes) and check what we obtain at the very first time iteration (i.e. after one iteration of the same transport solver starting from the same constant initial guess leading therefore to the same starting solution before applying some pressure relaxation process). The tolerance factor is set here to $\varepsilon_P = 10^{-6}$.

In Tables XI and XII, we give, for each procedure, the average convergence factor denoted by $\bar{\mu} = (\Delta P^M / \Delta P^0)^{1/M}$, where M is the total number of iterations needed to reach ε_P (i.e.

Table V. Relative density error.

Proc. #	Extrema &	Sub-int. 1	Sub-int. 2	Sub-int. 3	Rank
PR1	Min	4.27e−6	1.31e−3	2.0e−7	
	Max	1.49e−2	1.56e−1	4.02	3
	% cells	9.27	3.33	6.67	
PR2	Min	4.6e−6	1.31e−3	2.0e−7	
	Max	1.49e−2	1.56e−1	4.02	6
	% cells	9.27	3.33	6.67	
PR3	Min	4.27e−6	1.31e−3	2.0e−7	
	Max	1.49e−2	1.56e−1	4.02	3
	% cells	9.27	3.33	6.67	
PR4	Min	4.27e−6	1.31e−3	2.0e−7	
	Max	1.49e−2	1.56e−1	4.02	3
	% cells	9.27	3.33	6.67	
PR5	Min	4.6e−6	1.35e−3	2.0e−7	
	Max	1.50e−2	1.59e−1	4.02	8
	% cells	9.27	3.33	6.67	
PR6	Min	4.6e−6	1.38e−3	2.0e−7	
	Max	1.51e−2	1.60e−1	4.02	9
	% cells	9.27	3.33	6.67	
PR7 (NC)	Min	4.9e−6	6.89e−4	2.0e−7	
	Max	1.25e−2	1.06e−1	2.11	1
	% cells	8.61	3.33	1.67	
PR7 (C)	Min	4.6e−6	1.45e−3	2.0e−7	
	Max	1.53e−2	1.63e−1	4.01	7
	% cells	9.27	3.33	6.67	
PR8	Min	4.5e−6	1.23e−3	2.0e−7	
	Max	1.47e−2	1.51e−1	4.02	2
	% cells	9.27	3.33	5.0	

Table VI. Global accuracy rank of each procedure.

Proc. #	1	2	3	4	5	6	7 (NC)	7 (C)	8
Rank #	9	6	2	2	7	9	2	9	1

$|\Delta P^M| \leqslant \varepsilon_P$) for cell number 70 and cell number 71 (these are the only cells for which the relaxed pressures have different values and correspond to the position of the shock).

Because of round-off errors due to machine precision, the convergence factor of the direct procedures (namely procedures PR3, PR6 (NC) (which refers to the original version of PR6, without energy correction) and PR8) is not always equal to zero exactly but close to this null value. For the *true* iterative procedures, namely procedures PR1, PR4, PR5, procedure

Table VII. Extrema of the energy conservation measure.

Proc. #	1	2	3	4	5	6	7 (NC)	7 (C)	8
Min	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Max	1.36e−5	4.46e−7	4.44e−7	1.16e−7	2.81e−7	4.76e−7	2.14e+4	4.53e−7	3.73e−6
Cell #	0.0	0.0	0.0	0.0	0.0	0.0	92.61	0.0	0.0

Table VIII. Rank of each procedure related to the energy conservation criterion.

Proc. #	1	2	3	4	5	6	7 (NC)	7 (C)	8
Rank #	8	4	3	1	2	6	9	5	7

Table IX. Relative velocity error.

Proc. #	Extrema &	Sub-int. 1	Sub-int. 2	Sub-int. 3	Rank
PR1	Min	3.96e−1	3.95e−1	4.04e−1	
	Max	1.00	4.04e−1	7.87	2
	% cells	70.86	100	6.67	
PR2	Min	3.96e−1	3.95e−1	4.05e−1	
	Max	1.00	4.04e−1	7.87	6
	% cells	70.86	100	6.67	
PR3	Min	3.96e−1	3.95e−1	4.04e−1	
	Max	1.00	4.04e−1	7.87	2
	% cells	70.86	100	6.67	
PR4	Min	3.96e−1	3.95e−1	4.04e−1	
	Max	1.00	4.04e−1	7.87	2
	% cells	70.86	100	6.67	
PR5	Min	3.96e−1	3.95e−1	2.66e−1	
	Max	1.00	4.04e−1	7.94	5
	% cells	70.86	100	6.67	
PR6	Min	3.96e−1	3.95e−1	1.61e−1	
	Max	1.00	4.04e−1	7.98	8
	% cells	71.52	100	6.67	
PR7 (NC)	Min	3.99e−1	3.98e−1	2.68e−1	
	Max	1.00	4.01e−1	4.59	7
	% cells	70.86	100	1.67	
PR7 (C)	Min	3.96e−1	3.95e−1	7.1e−2	
	Max	1.00	4.04e−1	8.04	9
	% cells	71.52	100	8.33	
PR8	Min	3.96e−1	3.95e−1	1.2e−1	
	Max	1.00	4.03e−1	7.71	1
	% cells	70.86	100	6.67	

Table X. Global rank of each procedure.

Proc. #	1	2	3	4	5	6	7 (NC)	7 (C)	8
Rank #	5	5	1	2	9	5	3	9	3

Table XI. Average convergence factor $\bar{\mu}$ and total iteration number M for cell number 70.

Proc. #	1	2	3	4	5	6 (NC)	6 (C)	7 (NC)	7 (C)	8
$\bar{\mu}$	2.5E−3	6.9E−2	3.6E−16	6.3E−1	2.5E−1	0.0	0.0	0.0	4.6E−2	2.3E−14
M	6	13	1	76	25	1	3	3	6	1

Table XII. Average convergence factor $\bar{\mu}$ and total iteration number M for cell number 71.

Proc. #	1	2	3	4	5	6 (NC)	6 (C)	7 (NC)	7 (C)	8
$\bar{\mu}$	6.1E−3	1.0E−4	9.8E−18	6.3E−1	6.0E−1	3.5E−17	2.7E−8	5.9E−17	1.6E−2	2.0E−17
M	7	3	1	55	51	1	2	1	5	1

PR1 exhibits the best average convergence factor while procedure PR4, due to its oscillating convergence behaviour (the reduction factor at each iteration may be greater than 1) has a relatively poor convergence factor and a rather large total number of iterations M to reach convergence. Among the quasi-direct (Newton-like) procedures, namely procedures PR2, PR6 (C) (i.e. with energy correction), PR7 (with or without energy correction), procedures PR6 (C) together with procedure PR7 (NC), show up the best results in terms of $\bar{\mu}$ and M.

Convergence histories plotting $|\Delta P^k|$, for $k = 0, \ldots, M$ is resumed in Figure 8. We see that the *old* procedures PR4 and PR5 show up either an oscillating convergence behaviour (PR4) or limited convergence (PR5). This also confirms the convergence study concerning each of these procedures in this paper.

In Tables XIII and XIV, we give the resulting approximated relaxed pressures (P_g, P_l and P_I) for cell 70 and 71, respectively, together with the effective absolute precision attained by each of the procedures. As shown in these two tables, this also confirms both existence and uniqueness of the relaxed solution except for the non conservative procedure PR7 (NC) for which the difference is not negligible.

So we may now classify the different procedures as follows: from each of the criteria defined above, we sum up all the rank numbers related to each procedure and classify the different procedures from the one having the lowest rank number to the largest one. Table X gives the final rank of each procedure. The best procedure is PR3 (direct procedure, first position), followed by PR4 (second position) then by the non conservative procedure PR7 together with procedure PR8 (both at the third position). To summarize, we can state the following recommendations: if only efficiency is required, procedures 6 and 7 (with or without correction to get the energy conservation) appear to be robust (i.e. are convergent even if the initial phase pressure variation is large, they can therefore be used when dealing with large pressure variation problems), low CPU consuming and the coding is simple. In addition, they can be used with general EOS. We have seen that the accuracy is more related to the transport solver
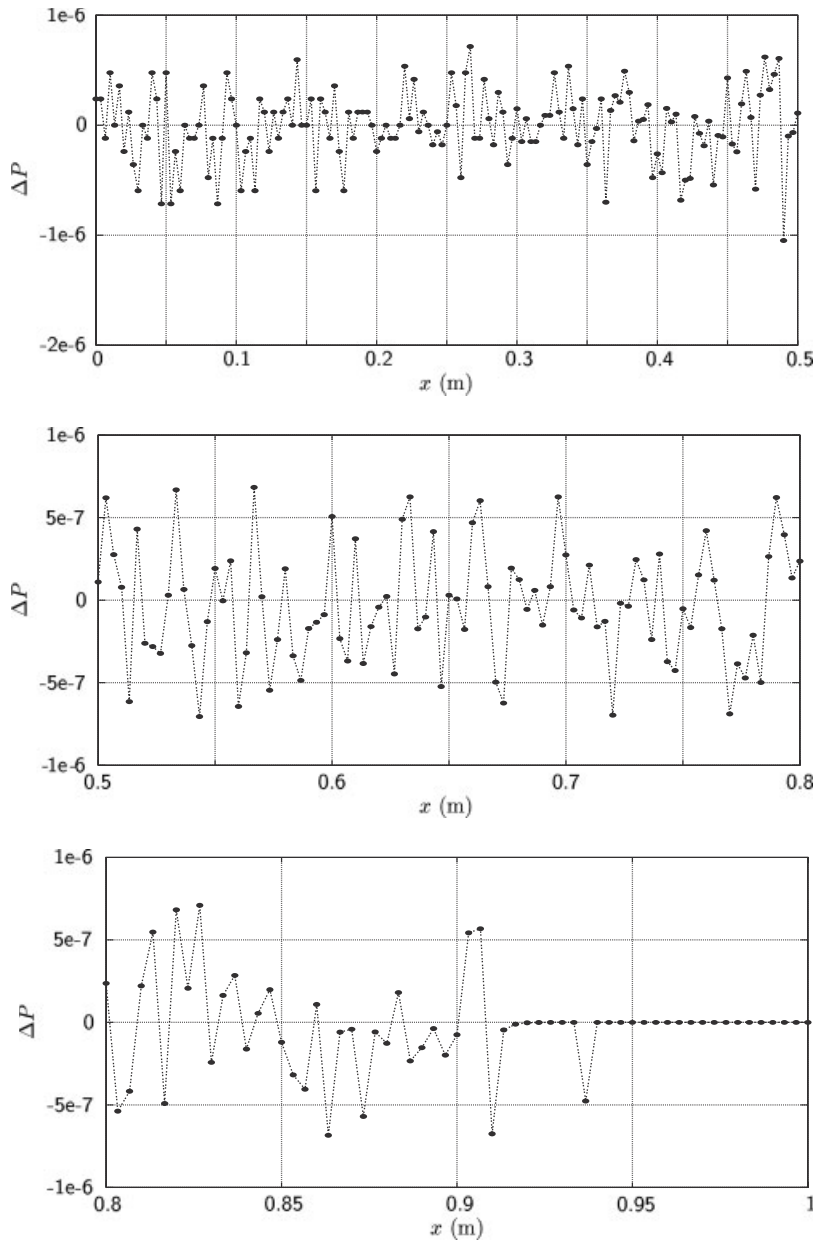
Figure 7. Phase pressure variation—PR7 (NC).

rather than really to the choice of the procedure, even if the non conservative procedure PR7 seems to be the most accurate especially in predicting shock positions. At last, if conservativity is required, the direct procedure 3 is recommended but restricted to stiffened gas EOS.
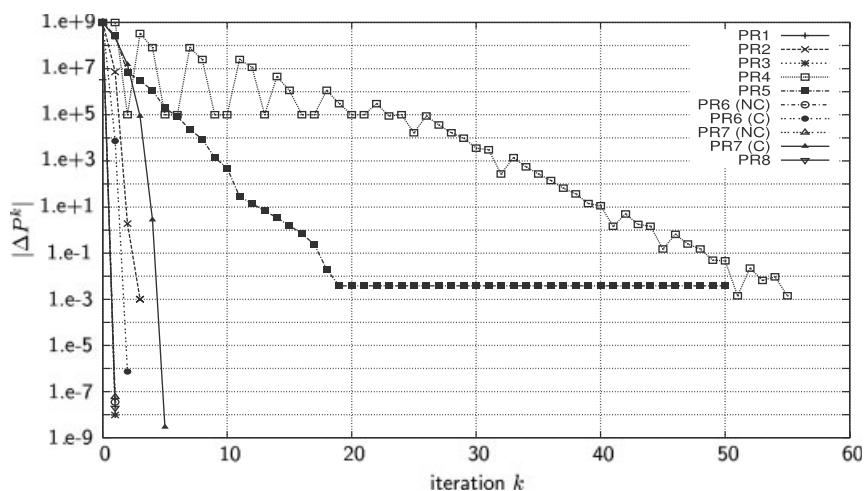
Figure 8. Convergence history of the different procedures for cell number 71.

Table XIII. Approximated relaxed pressures P_g, P_l and P_I and pressure variation
$|\Delta P^M|$ for cell number 70.

Proc. #	P_g	P_l	P_I	$|\Delta P^M|$
1	999866975.935547352	999866975.935547113	999866975.935546994	2.38E−07
2	999866975.935559392	999866975.935560226	999866975.935560226	8.35E−07
3	999866975.935547471	999866975.935547113	999866975.935547113	3.58E−07
4	999866975.935547113	999866975.935547829	999866975.935547829	7.15E−07
5	999866975.538290024	999866975.538308144	999866975.538308144	1.81E−05
6 (NC)	999866982.649324894	999866982.649324894	999866982.649324894	0.0E+00
6 (C)	999866974.537837625	999866974.537837625	999866974.537837625	0.0E+00
7 (NC)	999832511.096870899	999832511.096870899	999832511.096870899	0.0E+00
7 (C)	999866974.828222036	999866974.828221917	999866974.828221917	1.19E−07
8	999866977.333452702	999866977.333475232	999866977.333475232	2.25E−05

This classification does not take into account the possibility of using the procedures with general EOS and/or more than two fluids. To correct this classification for more general EOS and more than two phases, we recall that the procedures which are able to deal with *general EOS* are procedures PR4, PR5, PR6, PR7 (NC) and PR8.

Procedures which may be used for *more than two fluids* are procedures PR3, PR5, PR6, PR7 and PR8; with stiffened gas EOS, we may exhibit the corrections to ensure the conservativity criterion of Procedures PR3, PR6, PR7 and PR8. As a matter of fact, the generalization to more than two fluids necessitates the use of an approximate solver to solve the resulting nonlinear equations in each generalized version of procedures PR3, PR6 and PR8, resulting in a loss of conservativity. Procedure PR5, alone, ensures the conservativity criterion when using general EOS and with an arbitrarily large number of fluids, but may be costly and even inefficient if the interface pressure condition is strictly required, or if the initial phase

Table XIV. Approximated relaxed pressures P_g, P_l and P_I and pressure variation $|\Delta P|$ for cell number 71.

Proc. #	P_g	P_l	P_I	$|\Delta P^M|$
1	100001.455934042897	100001.455933716279	100001.455934042882	3.27E−07
2	100001.455933778852	100001.456946101767	100001.455933815785	1.01E−03
3	100001.455934050682	100001.455934040932	100001.455934050682	9.75E−09
4	100001.455934050682	100001.454513549805	100001.455933705744	1.42E−03
5	100001.84824125699	100001.488646030426	100001.484824265150	3.82E−03
6 (NC)	100001.773916317616	100001.773916282400	100001.773916317616	3.52E−08
6 (C)	100001.508912866921	100001.508913603102	100001.508912866950	7.36E−07
7 (NC)	100001.094652457527	100001.094652398839	100001.094652457527	5.87E−07
7 (C)	100001.487250736129	100001.487250739010	100001.487250736129	2.88E−09
8	100001.402952156088	100001.402952136617	100001.402952156088	1.95E−08

pressure variation is large (arbitrarily small tolerance will not be reached because of a too poor convergence rate).

Procedures PR5, PR6, PR7 and PR8 remain to be used for both general EOS and with an arbitrarily large number of fluids. In terms of both simplicity of coding, convergence concern and robustness, we restrict the choice to PR7, followed by PR6 and PR8.

We end up with two candidates, which are Procedures PR8 and PR7 (with or without the energy correction). In fact, Procedure PR8 is more CPU consuming when $N > 2$ to attain the same convergence tolerance reached by Procedure PR7 as well as in terms of simplicity of coding.

6. CONCLUSION

Several pressure relaxation procedures are developed and compared in terms of accuracy and computational efficiency in the context of a compressible hyperbolic multiphase flow model.

As far as two-phase flows and stiffened gas type EOS are concerned, and according to the numerical tests performed in this paper, Procedures 3, 4, 7 and 8 are recommended to ensure pressure relaxation. The preference to one or the other depending on which criterion is also preferred; the efficiency purpose provides to the choice of the quasi-direct procedure PR6, the additional accuracy criterion leads to the non conservative procedure PR7 and we finally end up with Procedure PR3 when strict conservation is also required.

When dealing with complex EOS, arbitrary number of fluids, the remaining procedures are Procedures PR5, PR6, PR7 and PR8. The simplicity of coding of PR7 (only the convergence condition test is required mainly, since the algorithm ensures automatically admissible pressure and volume fractions) and its robustness (ensurance of its convergence even with initial arbitrarily large pressure variations). The final choice made by the user may depend on the need of strict conservation. If such a feature is mandatory, Procedures 6 or 8 are recommended.

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