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Abstract

This note discusses the relaxation process in an hybrid three-field two-phase flow model. The latter model aims at simulating the flow of a mixture of liquid water and its vapor, together with some non-condensable gas. Since the fast transient flow may involve shock waves, this model is well suited due to its main properties which are recalled in the first section.

Introduction

Some scenarios in nuclear safety studies sometimes require computational models which adequately account for water liquid-vapor two-phase flows including an additional non condensable gas, typically air, which cannot exchange mass with the water component. Among these applications we may at least find RIA or loss of coolant accident (see for instance [11]). More complex situations involving vapor explosion are also at stake ([2], [3] and [4]). Of course the latter applications involve fast transient flows including shock waves, and thus there is a need for meaningful models for such a purpose.

Basically, two types of models are proposed for that aim. The first class considers some instantaneous velocity-equilibrium between phases and components (see for instance [27], [17], and also more recent contributions [18], [25], [31], [30]). The second class relies on the well-known two-fluid approach, where each phase/component has its own velocity field (see [1], [28], [15], [9], [14], [13] among others, for standard gas-particle, gas-liquid or liquid-vapor flows). For some applications involving the break-up of liquid droplets, and the estimation of interfacial areas, models in the second class become almost mandatory. Thus the present work is dedicated to the second class, and more precisely, it gives focus on the hybrid three-field two-phase flow model introduced in [24].

The main concern herein is whether inner processes that are part of the PDE model guarantee the return-to-equilibrium, as it is classically claimed or assumed, and expected. Unlike in [22], which focuses on the **sole** pressure relaxation process, we intend here to investigate and understand the **full** velocity-temperature-pressure coupling in model [24]. This is obviously of interest in order to improve our knowledge of this PDE model. It is also useful for numerical purposes, since some recent computations have clearly exhibited tough situations that easily lead to a blow-up of codes (see for instance [4]).

The paper is organised as follows. We first briefly recall model [24] together with its main properties. Next we discuss and investigate the preservation of admissible states in the convective subset, and in the submodel involving source terms. The latter is then investigated, while decoupling source terms, or keeping them altogether. Some conditions on Equations of State (EoS), and also on initial conditions, will arise from the analysis.

An appendix will also propose some practical algorithms in order to tackle approximate solutions of the whole model, while retaining the standard fractional step approach.

1 The hybrid three-field two-phase flow model

The following set of governing equations is considered, in order to describe two-phase flows involving a mixture of non condensable gas (typically air, with subscript "g") and water in liquid (using "l" subscript) and vapour (with subscript "v") phases. The gas and the vapour are assumed to share the same volume, hence associated statistical fractions are expected to comply with the following constraint:

$$\alpha_v = \alpha_g \tag{1}$$

Thus we have:

$$\alpha_v + \alpha_l = 1 \tag{2}$$

We note W the state variable:

$$W = (\alpha_g, m_g, m_g U_g, \alpha_g E_g, m_v, m_v U_v, \alpha_v E_v, m_l, m_l U_l, \alpha_l E_l)^t$$

In the sequel we will basically use the gas fraction $\alpha_g \in [0,1]$ as a main variable in order to account for statistical fractions. The model reads, for $k \in \{l, g, v\}$:

$$\begin{cases} \dfrac{\partial \alpha_g}{\partial t} + \mathbf{V}_i(\mathbf{W}).\nabla \alpha_g = \phi_g(\mathbf{W}) \\ \dfrac{\partial m_k}{\partial t} + \nabla.(m_k \mathbf{U}_k) = 0 \\ \dfrac{\partial m_k \mathbf{U}_k}{\partial t} + \nabla.(m_k \mathbf{U}_k \otimes \mathbf{U}_k + \alpha_k p_k \mathbf{Id}) + \Pi_k(\mathbf{W}) \nabla \alpha_g = \mathbf{S}_k^U(\mathbf{W}) \\ \dfrac{\partial \alpha_k E_k}{\partial t} + \nabla.(\alpha_k \mathbf{U}_k (E_k + p_k)) - \Pi_k(\mathbf{W}) \dfrac{\partial \alpha_g}{\partial t} = S_k^E(\mathbf{W}) \end{cases} \tag{3}$$

This model was first introduced in [24]. Note that the first equation provides the time-space evolution of the statistical fraction α_g, and the remaining equations correspond to the mass, momentum and energy balance equations for $k = l, g, v$. Variables p_k, ρ_k, $m_k = \alpha_k \rho_k$, $\epsilon_k(p_k, \rho_k)$, $E_k = \rho_k(\epsilon_k(p_k, \rho_k) + U_k^2/2)$ and $\mathbf{U}_k$ respectively denote the mean pressure, the mean density, the partial mass, the internal energy, the total energy and the mean velocity within phase k. The green terms on the right hand side represent the interfacial source terms, which means that:

$$\sum_{k=l,g,v} \mathbf{S}_k^U(\mathbf{W}) = 0 \tag{4}$$

and:

$$\sum_{k=l,g,v} \mathbf{S}_k^E(\mathbf{W}) = 0 \tag{5}$$

whereas the left-hand side of system (3) contains all convective - i.e. all first-order differential- contributions. The latter involve the interfacial velocity $\mathbf{V}_i(\mathbf{W})$, while the so-called interfacial pressure unknowns $\Pi_k(\mathbf{W})$ require some closures.

We will assume from now on that:

$$\mathbf{V}_i(\mathbf{W}) = \mathbf{U}_l \tag{6}$$

which is relevant for our applications. Hence we know (se [24]) that the following closure laws are meaningful for interfacial pressures Π_k:

$$\begin{cases} \Pi_v = -p_v \\ \Pi_g = -p_g \\ \Pi_l = p_v + p_g \end{cases} \tag{7}$$

owing to the entropy inequality of the mixture that is recalled in the sequel. We emphasize that these closures (7) are unique for a given interfacial velocity (6). It also seems worth noting that the latter closure laws enable to comply with the RIP condition (see [22], appendix A). Actually, this model may be viewed as some counterpart of the classical Baer-Nunziato two-phase flow model ([1].

In order to go further on, it remains now to specify the interfacial source terms $\mathbf{S}_k^U(\mathbf{W})$, $\mathbf{S}_k^E(\mathbf{W})$, and also $\phi_g(\mathbf{W})$. The latter contribution reads:

$$\phi_g(\mathbf{W}) = \frac{\alpha_g(1-\alpha_g)}{\Pi_0 \tau^P(\mathbf{W})}(p_v + p_g - p_l) = K(\mathbf{W})(p_v + p_g - p_l) \tag{8}$$

The -positive- pressure relaxation time scale $\tau^P(\mathbf{W})$ is given by formulas detailed in [12], [5] or [6], and the reference pressure Π_0 has to be fixed in agreement. Besides, momentum interfacial terms are given by:

$$S_k^U = \sum_{j \neq k} d_{kj}(W)(U_j - U_k) \tag{9}$$

where the -positive- symmetric scalar functions $d_{kj}(W)$ include velocity relaxation time scales. These correspond to the expected drag effects between fields. Eventually, closure laws for interfacial heat transfers are given by:

$$S_k^E = \sum_{j \neq k} q_{kj}(W)(T_j - T_k) + \sum_{j \neq k} V_{kj} d_{kj}(W)(U_j - U_k) \tag{10}$$

noting: $V_{kj} = \dfrac{U_k + U_j}{2}$. Considering phasic entropies $S_k(p_k, \rho_k)$, phasic temperatures T_k are classically defined as :

$$\frac{1}{T_k} = \left.\frac{\partial S_k(p_k,\rho_k)}{\partial p_k}\right|_{\rho_k} \Big/ \left.\frac{\partial \epsilon_k(p_k,\rho_k)}{\partial p_k}\right|_{\rho_k} \tag{11}$$

The -positive- symmetric scalar functions $q_{kj}(W)$ also involve temperature relaxation time scales. Again, we refer to [26] for further details.

We may now recall some basic properties of the full model in a one-dimensional framework.

Property 1: (Structure of the three-field two-phase flow model)

- *The homogeneous part of the one-dimensional model associated with (3) equiped with (6), (7) is hyperbolic if the non-resonance condition is fulfilled. Introducing phasic celerities $c_k(p_k, \rho_k)$ as:*

$$\rho_k c_k^2 \left.\frac{\partial \epsilon_k(p_k,\rho_k)}{\partial p_k}\right|_{\rho_k} = \frac{p_k}{\rho_k} - \rho_k \left.\frac{\partial \epsilon_k(p_k,\rho_k)}{\partial \rho_k}\right|_{p_k} \tag{12}$$

  Eigenvalues read:

$$\left\{ \begin{array}{lll} \lambda_1 = U_l - c_l & ; & \lambda_2 = \lambda_3 = U_l \quad ; \quad \lambda_4 = U_l + c_l; \\ \lambda_5 = U_v - c_v & ; & \lambda_6 = U_v \quad ; \quad \lambda_7 = U_v + c_v; \\ \lambda_8 = U_g - c_g & ; & \lambda_9 = U_g \quad ; \quad \lambda_{10} = U_g + c_g. \end{array} \right. \tag{13}$$

  Associated right eigenvectors span the whole space of non resonant states. The resonance condition writes : $|U_j - U_l| = c_j$ for $j \in (g, v)$.

- *Fields associated with eigenvalues $\lambda_1, \lambda_4, \lambda_5, \lambda_7, \lambda_8, \lambda_{10}$ are Genuinely Non Linear. Other fields are Linearly Degenerate.*

- *System (3) can be symmetrized away from resonant cases.*

- *Smooth solutions of the full system (3) with closure laws (6), (7), (8) , (9) and (10) comply with the entropy inequality:*

$$\frac{\partial \eta}{\partial t} + \nabla.(F_\eta) \geq 0 \tag{14}$$

  where the entropy-entropy flux pair (η, F_η) is defined by:

$$\eta = m_l S_l(p_l, \rho_l) + m_g S_g(p_g, \rho_g) + m_v S_v(p_v, \rho_v) \tag{15}$$

  and:

$$F_\eta = m_l S_l(p_l, \rho_l) U_l + m_g S_g(p_g, \rho_g) U_g + m_v S_v(p_v, \rho_v) U_v \tag{16}$$

□

The reader is refered to [24] for proofs. In particular the structure of the coupling wave associated with the double eigenvalue $\lambda_{2,3}$ is given in Property 2.3 of the latter reference.

Considering our practical applications in nuclear power plants, where the mean flow velocities are small

compared with the speed of acoustic waves within each phase, the occurence of resonnant cases is very unlikely to happen. Moreover, thanks to Kato theoretical results ([29]), unsteady computations are meaningful for this model of PDEs. We also recall that the structure of the LD coupling wave guarantees that shock solutions are well defined, which is mandatory when aiming at predicting flow configurations involving shock waves (such as vapor explosions, or loss of coolant accident). Actually, jump conditions are uniquely defined field by field, owing to the structure of the interfacial velocity. In practice, it also means that approximate solutions of shocks can be considered in practical applications, since various stable schemes will converge towards the *same* solution when shocks occur. We refer the reader to [16] , figure 8.9, pages 136, which shows some major deficiencies when shocks arise if the coupling wave is no longer LD.

2 A few results on the preservation of admissible states

We focus here on some specific Equations of State (EoS), and we wonder whether model (3) preserves the admissible states in the time-space domain. The following results are not exhaustive of course. We first focus on the convective part, and then on the source terms. Before going further on, we recall that c_k and S_k comply with the identity:

$$c_k^2(p_k,\rho_k)\left.\frac{\partial S_k(p_k,\rho_k)}{\partial p_k}\right|_{\rho_k}+\left.\frac{\partial S_k(p_k,\rho_k)}{\partial \rho_k}\right|_{p_k}=0 \tag{17}$$

for $k\in(l,g,v)$.

2.1 Preservation of admissible states in the convective subset

For a finite time interval $[0,T]$, we introduce some bounded domain Ω. We focus first the homogeneous part of system (3) with closure laws (7) and (6). This writes:

$$\left\{\begin{array}{l}\dfrac{\partial \alpha_g}{\partial t}+\mathbf{U}_l.\nabla\alpha_g=0\\ \dfrac{\partial m_k}{\partial t}+\nabla.(m_k\mathbf{U}_k)=0\\ \dfrac{\partial m_k\mathbf{U}_k}{\partial t}+\nabla.(m_k\mathbf{U}_k\otimes\mathbf{U}_k+\alpha_k p_k\mathbf{Id})+\Pi_k(\mathbf{W})\nabla\alpha_g=0\\ \dfrac{\partial \alpha_k E_k}{\partial t}+\nabla.(\alpha_k\mathbf{U}_k(E_k+p_k))-\Pi_k(\mathbf{W})\dfrac{\partial\alpha_g}{\partial t}=0\end{array}\right. \tag{18}$$

where the blue terms are detailed in (7). We consider smooth solutions of this model, which enables to derive the following governing equations for the pressures P_k, for $k\in(g,v)$:

$$\frac{\partial p_k}{\partial t}+\mathbf{U}_k.\nabla p_k+\rho_k c_k^2\nabla.\mathbf{U}_k+\rho_k c_k^2(\mathbf{U}_k-\mathbf{U}_l).\nabla Log(\alpha_k)=0 \tag{19}$$

and for P_l:

$$\frac{\partial p_l}{\partial t}+\mathbf{U}_l.\nabla p_l+\rho_l c_l^2\nabla.\mathbf{U}_l=0 \tag{20}$$

Let us consider now the following stiffened gas EoS within each phase $k\in(l,g,v)$:

$$p_k+\gamma_k\hat{\Pi}_k=(\gamma_k-1)\rho_k\epsilon_k \tag{21}$$

with: $1<\gamma_k$ and $\hat{\Pi}_k>0$. In that case admissible states of pressure are such that: $p_k+\hat{\Pi}_k>0$. Moreover we recall that: $\rho_k c_k^2=\gamma_k(p_k+\hat{\Pi}_k)$. This enables to state:

Property 2: (Preservation of admissible states in the convective subset)
We consider the above-mentioned stiffened gas EoS (21).

- *Assume that $\boldsymbol{U}_l$ and $\nabla.\boldsymbol{U}_l$ remain bounded in the domain Ω, and also that initial conditions and inlet boundary conditions of the liquid pressure and density are admissible states, then the mean density ρ_l and $p_l+\hat{\Pi}_l$ remain positive in $\Omega\times[0,T]$.*
- *For $k\in(g,v)$, assume that both $\boldsymbol{U}_k$ and $(\nabla.\boldsymbol{U}_k+(\boldsymbol{U}_k-\boldsymbol{U}_l).\nabla Log(\alpha_k))$ remain bounded in the domain Ω, and also that initial conditions and inlet boundary conditions of the pressure p_k and density ρ_k are admissible states, then the mean density ρ_k and $p_k+\hat{\Pi}_k$ remain positive in $\Omega\times[0,T]$.*

□

Proof:
It is classical, considering the governing equations of the densities and pressures (20) and (19), with the convention that inlet boudary conditions in phase k correspond to points on the boundary such that $U_k.n \leq 0$, where the unit normal n points outward. One must simply note that the governing equation for $\psi = p_l + \hat{\Pi}_l$ writes:

$$\frac{\partial p_l + \hat{\Pi}_l}{\partial t} + \mathbf{U}_l.\nabla(p_l + \hat{\Pi}_l) + \gamma_l(p_l + \hat{\Pi}_l)\nabla.\mathbf{U}_l = 0 \tag{22}$$

which enables to conclude. Note that an alternative way to obtain this result consists in using the governing equation for the phasic entropy $S_k(p_k, \rho_k)$, which reads:

$$\frac{\partial S_k(p_k, \rho_k)}{\partial t} + \mathbf{U}_k.\nabla S_k(p_k, \rho_k) = 0 \tag{23}$$

for $k \in (g, v)$. Note that the condition on the boundedness of $(\nabla.\mathbf{U}_k + (\mathbf{U}_k - \mathbf{U}_l).\nabla Log(\alpha_k))$ still remains, due to the governing equation of the density that writes:

$$\frac{\partial \rho_k}{\partial t} + \mathbf{U}_k.\nabla\rho_k + \rho_k\nabla.\mathbf{U}_k + \rho_k(\mathbf{U}_k - \mathbf{U}_l).\nabla Log(\alpha_k) = 0 \tag{24}$$

Actually these results may be extended to other EoS. Consider for instance the case of Nobel-Abel Stiffened Gas (NASG) EoS:

$$(1 - \rho_l b_l)(p_l + \gamma_l\hat{\Pi}_l) = (\gamma_l - 1)\rho_l(\epsilon_l - (\epsilon_l)_0) \tag{25}$$

with $\gamma_l > 1$, $\hat{\Pi}_l > 0$, $b_l > 0$ and $(\epsilon_l)_0 > 0$. In that case equation (20) turns into:

$$\frac{\partial p_l + \hat{\Pi}_l}{\partial t} + \mathbf{U}_l.\nabla(p_l + \hat{\Pi}_l) + \frac{\gamma_l}{1 - \rho_l b_l}(p_l + \hat{\Pi}_l)\nabla.\mathbf{U}_l = 0 \tag{26}$$

This ensures positive values of $p_l + \hat{\Pi}_l$, as soon as the density complies with:

$$0 < \epsilon_0 \leq 1 - \rho_l b_l \tag{27}$$

2.2 Preservation of admissible states in the interfacial transfer

We consider now an homogeneous flow, which is equivalent to investigating solutions of system:

$$\begin{cases} \dfrac{\partial \alpha_g}{\partial t} = \dfrac{\alpha_g(1-\alpha_g)}{\Pi_0 \tau^P(\mathbf{W})}(p_v + p_g - p_l) \\ \dfrac{\partial m_k}{\partial t} = 0 \\ \dfrac{\partial m_k \mathbf{U}_k}{\partial t} = \displaystyle\sum_{j \neq k} d_{kj}(W)(U_j - U_k) \\ \dfrac{\partial \alpha_k E_k}{\partial t} - \Pi_k(\mathbf{W})\dfrac{\partial \alpha_g}{\partial t} = \displaystyle\sum_{j \neq k} q_{kj}(W)(T_j - T_k) + \sum_{j \neq k} V_{kj} d_{kj}(W)(U_j - U_k) \end{cases} \tag{28}$$

Throughout this step, both the total internal energy of the mixture and the entropy of the mixture increase, since:

$$\frac{\partial \sum_k m_k \epsilon_k}{\partial t} = \frac{1}{2}\sum_k \sum_j d_{kj}(W)(\Delta U_{kj})^2 = \sum_{k-j} d_{kj}(W)(\Delta U_{kj})^2 \tag{29}$$

while:

$$\frac{\partial \eta}{\partial t} = \sum_{k-j} \frac{d_{kj}(W)}{T_k}(\Delta U_{kj})^2 + \sum_{k-j} \frac{q_{kj}(W)}{T_k T_j}(\Delta T_{kj})^2 + \frac{\alpha_g(1-\alpha_g)}{T_l \Pi_0 \tau^P(\mathbf{W})}(\Delta P)^2 \tag{30}$$

using the convention:

$$\Delta P = p_l - (p_v + p_g) \tag{31}$$

and also:

$$\Delta\Psi_{kl} = \Psi_k - \Psi_l \tag{32}$$

for: $\Psi = U$, or: $\Psi = T$. Meanwhile, we note that the total momentum remains unchanged:

$$\frac{\partial(\sum_{k=l,g,v} m_k U_k)}{\partial t} = 0 \tag{33}$$

and of course we have:

$$\frac{\partial(\sum_{k=l,g,v} \alpha_k E_k)}{\partial t} = 0 \tag{34}$$

which simply means that the sum of total energies is preserved.

2.2.1 Pressure relaxation terms

Let us consider now the **sole** pressure relaxation terms, that is:

$$\begin{cases} \dfrac{\partial \alpha_g}{\partial t} = \dfrac{\alpha_g(1-\alpha_g)}{\Pi_0 \tau^P(\mathbf{W})}(p_v + p_g - p_l) \\ \dfrac{\partial m_k}{\partial t} = 0 \\ \dfrac{\partial m_k \mathbf{U}_k}{\partial t} = 0 \\ \dfrac{\partial \alpha_k E_k}{\partial t} - \Pi_k(\mathbf{W}) \dfrac{\partial \alpha_g}{\partial t} = 0 \end{cases} \tag{35}$$

Still using (7), the latter system may be rewritten as follows:

$$\begin{cases} \dfrac{\partial \alpha_g}{\partial t} = \dfrac{\alpha_g(1-\alpha_g)}{\Pi_0 \tau^P(\mathbf{W})}(p_v + p_g - p_l) \\ \dfrac{\partial m_k}{\partial t} = 0 \\ \dfrac{\partial m_k \mathbf{U}_k}{\partial t} = 0 \\ \dfrac{\partial S_k}{\partial t} = 0 \qquad (k = g, v) \\ \dfrac{\partial(\sum_{k=l,g,v} m_k \epsilon_k)}{\partial t} = 0 \end{cases} \tag{36}$$

We keep the main scalar variable α_g, and may rewrite all variables as follows:

$$\rho_k(\alpha_g) = \frac{m_k^0}{\alpha_g} \quad (k \in g, v) \qquad ; \qquad \rho_l(\alpha_g) = \frac{m_l^0}{1-\alpha_g} \tag{37}$$

$$P_k(\alpha_g) = p_k(\rho_k(\alpha_g), S_k^0) \qquad ; \qquad e_k(\alpha_g) = \epsilon_k(P_k(\alpha_g), S_k^0) \qquad , with \quad k \in (g, v) \tag{38}$$

and:

$$e_l(\alpha_g) = \left((\sum_{k \in (l,g,v)} m_k \epsilon_k)^0 - m_v^0 e_v(\alpha_g) - m_g^0 e_g(\alpha_g) \right) / m_l^0 \tag{39}$$

but also:

$$P_l(\alpha_g) = p_l(\rho_l(\alpha_g), e_l(\alpha_g)) \tag{40}$$

We consider now some finite time $t \in (0, T)$, and assume that the following integral is defined:

$$H(t) = \int_0^t \frac{(P_g(\alpha_g) + P_v(\alpha_g) - P_l(\alpha_g))(\tau)}{\Pi_0 \tau^P(W(\tau))} d\tau \tag{41}$$

Hence, if $\alpha_g(0) \in]0, 1[$, we get:

$$\frac{\alpha_g(t)}{1-\alpha_g(t)} = \frac{\alpha_g(0)}{1-\alpha_g(0)} exp(H(t)) = R(t) > 0 \tag{42}$$

Thus

$$\alpha_g(t) = \frac{R(t)}{1+R(t)} \tag{43}$$

is defined and lies in $]0,1[$. Phasic densities ρ_k, coming from (37), and gas and vapour pressures $P_{v,g}$ arising from (38), are admissible. Finally, the liquid internal energy arises from (39).

If we turn to (41), and still using (36), we note that straightforward calculations lead to:

$$\Delta P(t) = \Delta P(0) exp\left(- \int_0^t a_{PP}(W(\tau)) d\tau \right) \tag{44}$$

with $a_{PP}(W)$ given by:

$$a_{PP}(W) = \frac{1}{\Pi_0 \tau^P(\mathbf{W})} \left(\alpha_g \rho_l c_l^2 + (1-\alpha_g)(\rho_g c_g^2 + \rho_v c_v^2) - \alpha_g (\rho_l \left. \frac{\partial \epsilon_l}{\partial P_l} \right|_{\rho_l})^{-1} \Delta P \right) \tag{45}$$

.

Property 3: (Pressure relaxation process due to interfacial transfer)
Assume that functions $\frac{1}{\tau^P(\boldsymbol{W})}$ *and* $\rho_k c_k^2$ *remain positive and bounded, for* $k \in (l,g,v)$*, and also that* ΔP *is small enough in the sense that:*

$$a_{PP}(W) > 0 \tag{46}$$

or equivalently :

$$\alpha_g \Delta P < \rho_l \left. \frac{\partial \epsilon_l}{\partial P_l} \right|_{|} \rho_l \left(\alpha_g \rho_l c_l^2 + (1-\alpha_g)(\rho_g c_g^2 + \rho_v c_v^2) \right) \tag{47}$$

Then the sole pressure relaxation process is guaranteed. Statistical fractions remain in $[0,1]$ *and densities are positive. Meanwhile pressures* p_v *and* p_g *are admissible.*
□

Proof:
Actually, the latter boundedness conditions together with: $a_{PP}(W) > 0$ ensure that the integral in (44) is defined and positive. This implies that the pressure relaxation process holds, since (44) guarantees a contraction. Consequently $H(t)$ in (41) is defined. This in turn means that the statistical fraction $\alpha_g(t)$ lies in $]0,1[$, considering (43). Hence densities and pressures $p_{v,g}$ remain in the admissible range (see (37) and (38)).

□
Remark 1
Assume that EoS are such that :

$$p_k(\rho_k, \epsilon_k) + \gamma_k \hat{\Pi}_k = (\gamma_k - 1)\rho_k \epsilon_k \tag{48}$$

with $\gamma_k > 1$, then:

- If EoS are such that: $\hat{\Pi}_l \geq \hat{\Pi}_g + \hat{\Pi}_v$, then the sole pressure relaxation process holds ;
- Otherwise the condition (47) may be violated and the condition must be checked in the computer code at each time step within each cell.

Proof:

For such an EoS we can rewrite condition (47) as follows:

$$\alpha_g(\gamma_l - 1)(\hat{\Pi}_g + \hat{\Pi}_v - \hat{\Pi}_l) < \alpha_g(p_l + \hat{\Pi}_l) + (\alpha_g(\gamma_l - 1) + \alpha_l \gamma_g)(p_g + \hat{\Pi}_g) + (\alpha_g(\gamma_l - 1) + \alpha_l \gamma_v)(p_v + \hat{\Pi}_v)$$

The right-hand side is obviously positive, since $p_k + \hat{\Pi}_k \geq 0$ for $k \in \{l,g,v\}$. Thus the latter inequality is always satisfied if $\hat{\Pi}_g + \hat{\Pi}_v - \hat{\Pi}_l < 0$; otherwise the condition (47) must be checked.

Remark 2
Assuming some specific EoS for gas and vapour quantities, we may improve this result and check that the liquid pressure/internal energy is admissible. If we consider a perfect gas EoS:

$$p_k(\rho_k, \epsilon_k) = (\gamma_k - 1)\rho_k \epsilon_k \tag{49}$$

with $\gamma_k > 1$, for $k \in (v, g)$, we get from (35):

$$\frac{\partial m_k \epsilon_k}{\partial t} + p_k \frac{\partial \alpha_g}{\partial t} = 0 \tag{50}$$

thus:

$$\alpha_k \frac{\partial p_k}{\partial t} + \gamma_k p_k \frac{\partial \alpha_k}{\partial t} = 0 \tag{51}$$

for $k = g, v$, using (49). We must consider two cases:

- If $(p_v + p_g - p_l)(0) > 0$, we know that: $(p_v + p_g - p_l)(t) > 0$, owing to (44). Hence $\alpha_g(t)$ is increasing (see (35) or (36)). Now, using the stationary constraint on the sum of internal energies, we have:

$$[m_l \epsilon_l]_0^t = -\sum_{k \in (g,v)} [m_k \epsilon_k]_0^t = \int_0^t ((\sum_{k=g,v} p_k) \frac{\partial \alpha_g}{\partial t})(\tau) d\tau > 0 \tag{52}$$

  owing to (50). Since: $[m_l \epsilon_l]_0^t = m_l^0 [\epsilon_l]_0^t$ we may conclude that $\epsilon_l(t)$ is increasing, which implies that $\epsilon_l(t)$ is admissible (and thus $p_l(t)$).

- Otherwise, if $(p_v + p_g - p_l)(0) < 0$, (44) guarantees that $(p_v + p_g - p_l)(t) < 0$. Hence $\alpha_g(t)$ is decreasing, and $p_k(t)$ increases for $k = g, v$, due to (51). Considering positive initial conditions $p_v(0)$ and $p_g(0)$, we may conclude that $p_l(t) > (p_v + p_g)(t) > (p_v + p_g)(0) > 0$, which means that $p_l(t)$ lies in the admissible range $\mathscr{R}^+$.

□

We focus now on isolated heat transfer terms.

2.2.2 Temperature relaxation terms

We focus now on the sole temperature relaxation terms, that is:

$$\begin{cases} \dfrac{\partial \alpha_g}{\partial t} = 0 \\ \dfrac{\partial m_k}{\partial t} = 0 \\ \dfrac{\partial m_k \mathbf{U}_k}{\partial t} = 0 \\ \dfrac{\partial \alpha_k E_k}{\partial t} - \Pi_k(\mathbf{W}) \dfrac{\partial \alpha_g}{\partial t} = \displaystyle\sum_{j \neq k} q_{kj}(W)(T_j - T_k) \end{cases} \tag{53}$$

or equivalently:

$$\begin{cases} \dfrac{\partial \alpha_g}{\partial t} = \dfrac{\partial m_k}{\partial t} = \dfrac{\partial m_k \mathbf{U}_k}{\partial t} = 0 \\ \dfrac{\partial (\sum_k m_k \epsilon_k)}{\partial t} = 0 \\ m_k \dfrac{\partial \epsilon_k}{\partial T_k}|_{\rho_k} \dfrac{\partial T_k}{\partial t} = \displaystyle\sum_{j \neq k} q_{kj}(W)(T_j - T_k) \end{cases} \tag{54}$$

Variables α_g, ρ_k, U_k thus remain steady through system (54), and meanwhile temperatures vary. Defining:

$$\underline{\Delta}_T = \begin{pmatrix} \Delta T_{gl} \\ \Delta T_{vl} \end{pmatrix} \tag{55}$$

it remains to solve:

$$\partial_t \underline{\Delta}_T = -\underline{\underline{A}}_{TT}(W)\ \underline{\Delta}_T \tag{56}$$

which gives $\Delta T(t)$, and find $T_l(t)$ solution of the constraint:

$$m_l^0 \epsilon_l(\rho_l^0, T_l(t)) + (\sum_{k=v,g} m_k^0 \epsilon_k(\rho_k^0, T_l(t) + \Delta T_{kl}(t))) = (\sum_{k=l,v,g} m_k \epsilon_k)^0 \tag{57}$$

The matrix $\underline{\underline{A}}_{TT}(W)$ reads:

$$\underline{\underline{A}}_{TT}(W) = \begin{pmatrix} e & f \\ h & i \end{pmatrix} \tag{58}$$

noting:

$$\begin{cases} e = q_{gl}(\dfrac{1}{M_g} + \dfrac{1}{M_l}) + \dfrac{q_{gv}}{M_g} \\ f = \dfrac{q_{lv}}{M_l} - \dfrac{q_{gv}}{M_g} \\ h = \dfrac{q_{lg}}{M_l} - \dfrac{q_{gv}}{M_v} \\ i = q_{vl}(\dfrac{1}{M_v} + \dfrac{1}{M_l}) + \dfrac{q_{gv}}{M_v} \end{cases} \tag{59}$$

with: $M_k = m_k \dfrac{\partial \epsilon_k}{\partial T_k}|_{\rho_k}$. Thus we obtain:

Property 4: (Temperature relaxation process due to interfacial transfer)
Assume that functions $\dfrac{\partial \epsilon_k}{\partial T_k}|_{\rho_k}$ *and* $q_{ij}(W)$ *remain positive and bounded. Then the temperature relaxation process is ensured by* (54). □

Proof:
We first note that $trace(\underline{\underline{A}}_{TT}(W)) = e + i$ is positive, and also that :

$$det(\underline{\underline{A}}_{TT}(W)) = ei - fh > 0 \tag{60}$$

The characteristic polynomial $Q_2(\lambda)$ associated with $\underline{\underline{A}}_{TT}(W)$:

$$Q_2(\lambda) = \lambda^2 - \lambda trace(\underline{\underline{A}}_{TT}(W)) + det(\underline{\underline{A}}_{TT}(W)) \tag{61}$$

has two eigenvalues $\lambda^{\pm}$. Both are real and positive, or complex with a positive real part.
□
Obviously, this also suggests a simple fractional step algorithm in order to account for source terms in (28), considering successively so-called pressure relaxation terms, and then interfacial heat transfer terms associated with ψ_{jk}. In order to clarify ideas, we detail in **Appendix B** such an algorithm. Moreover, a straightforward consequence of the algorithm proposed to deal with pressure relaxation effects is that it gives a discrete counterpart of the proof given in the previous section in property 3 in the continuous framework.

3 Effective relaxation effects

We now define the following vector of unknowns:

$$\underline{\Delta} = \begin{pmatrix} \Delta U_{gl} \\ \Delta U_{vl} \\ \Delta P \\ \Delta T_{gl} \\ \Delta T_{vl} \end{pmatrix} \tag{62}$$

using notations introduced in (31) and (32), and calculate the time evolution of the latter variable $\underline{\Delta}$, using (28). This ends up with:

$$\partial_t \underline{\Delta} = -\underline{\underline{A}}(W)\ \underline{\Delta} \tag{63}$$

with $\underline{\underline{A}}(W) \in \mathbb{R}^5 \times \mathbb{R}^5$ in the specific form:

$$\underline{\underline{A}}(W) = \begin{pmatrix} \underline{\underline{A}}_{UU}(W) & \underline{0} & \underline{\underline{0}} \\ {}^t\underline{a}_{PU}(W) & a_{PP}(W) & {}^t\underline{a}_{PT}(W) \\ \underline{\underline{A}}_{TU}(W) & \underline{a}_{TP}(W) & \underline{\underline{A}}_{TT}(W) \end{pmatrix} \tag{64}$$

$\underline{\underline{A}}_{UU}(W)$, $\underline{\underline{A}}_{TU}(W)$ and $\underline{\underline{A}}_{TT}(W)$ are three matrices in $\mathbb{R}^2 \times \mathbb{R}^2$, and the vectors $\underline{a}_{PU}(W)$, $\underline{a}_{PT}(W)$ and $\underline{a}_{TP}(W)$ lie in $\mathbb{R}^2$. All coefficients are detailed in **appendix A**.

We note that eigenvalues of matrix $\underline{\underline{A}}(W)$ are those of matrices $\underline{\underline{A}}_{UU}(W)$ and :

$$\underline{\underline{A}}_{PT}(W) = \begin{pmatrix} a_{PP}(W) & {}^t\underline{a}_{PT}(W) \\ \underline{a}_{TP}(W) & \underline{\underline{A}}_{TT}(W) \end{pmatrix} \tag{65}$$

It can be simply checked that the two fundamental minors $trace(\underline{\underline{A}}_{UU}(W))$ and $det(\underline{\underline{A}}_{UU}(W))$ of matrix $\underline{\underline{A}}_{UU}(W)$ are positive (see **appendix A**), whatever the state variable W is. This implies that its two eigenvalues are either real positive, or imaginary conjugate with a positive real part. Thus we get:

Property 5: (Velocity relaxation process due to interfacial transfer)
The velocity relaxation process is guaranteed by system (28) for positive values of $d_{kj}(W)$.
□

Moreover, noting:

$$\underline{\underline{A}}_{PT}(W) = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \tag{66}$$

we have:

Property 6: (Pressure-temperature relaxation process due to interfacial transfer)
We still consider positive values of $q_{kj}(W)$ and τ^P. In order to guarantee the pressure-temperature relaxation process through system (28), the following three conditions must be fulfilled:

$$a_{PP}(W) + trace(\underline{\underline{A}}_{TT}(W)) = a + e + i > 0 \tag{67}$$

$$(ae - bd) + (ai - cg) + (ei - fh) > 0 \tag{68}$$

$$det(\underline{\underline{A}}_{PT}(W)) = c(dh - eg) + b(fg - di) + a(ei - fh) > 0 \tag{69}$$

□

Proof: In order to guarantee the relaxation process, eigenvalues of $\underline{\underline{A}}_{PT}(W)$ must be real positive, or complex with a positive real part.

- First note that the three eingenvalues $\lambda_1, \lambda_2, \lambda_3$ of $\underline{\underline{A}}_{PT}(W)$ may be real (case 1), otherwise one is real λ_1, and the other two are complex conjugate $\lambda_2 = \overline{\lambda_3}$ (case 2).

- Define:
$$I_1 = \lambda_1 + \lambda_2 + \lambda_3 \quad ; \quad I_2 = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3 \quad ; \quad I_3 = \lambda_1\lambda_2\lambda_3 \tag{70}$$
Note that these coefficients I_1, I_2, I_3 arise in the characteristic polynomial $Q_3(\lambda)$ associated with $\underline{\underline{A}}_{PT}(W)$:
$$Q_3(\lambda) = (\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3) = \lambda^3 - I_1\lambda^2 + I_2\lambda - I_3 \tag{71}$$
If case 1 is considered, we obviously have:
$$I_1 > 0 \quad ; \quad I_2 > 0 \quad ; \quad I_3 > 0 \tag{72}$$
A similar result holds in (case 2) since:
$$I_1 = \lambda_1 + 2Re(\lambda_2) > 0 \quad ; \quad I_2 = 2\lambda_1 Re(\lambda_2) + \lambda_2\overline{\lambda_2} > 0 \quad ; \quad I_3 = \lambda_1\lambda_2\overline{\lambda_2} > 0 \tag{73}$$

- All coefficients of $\underline{\underline{A}}_{PT}(W)$ are real, thus I_1, I_2, I_3 lie in $\mathbb{R}$. Moreover, the first quantity arising in (67) identifies with I_1, the second one in (68) with I_2, while the third one in (69) is equal to I_3.

□

Remark 3

- Note that when the ratio of relaxation time scales $\frac{\tau^P}{\tau^T}$ tends to zero (with some abuse of notation since we have three temperature time scales τ_{lv}^T, τ_{gv}^T and τ_{lg}^T), the condition (67) degenerates, and one retrieves the sole condition on pressure relaxation (see [22]), which is:

$$\tau^P a_{PP}(W) > 0 \tag{74}$$

(see (47)). Recall that this condition may require that some upper bound on the initial pressure disequilibrium $\Delta P(0)$ holds, for general EoS, as detailed in Property 3 and remark 1.

If $a_{PP}(W) > 0$, and considering standard EoS for which $\left.\frac{\partial \epsilon_k}{\partial T_k}\right|_{\rho_k} = C_{v,k} > 0$, the first condition (67) is always satisfied, whatever the ratio of time scales $\frac{\tau^P}{\tau^T}$ is, since $trace(\underline{\underline{A}}_{TT}(W)) > 0$ (see **appendix A**).

- For practical purposes, when using complex EoS, the three conditions arising in (67), (68), and (69) must be checked in computational codes.
- Eventually, it must noted that the six coefficients arising in $\underline{\underline{A}}_{TU}(W)$ and $\underline{a}_{PU}(W)$ vanish when the two relative velocities ΔU_{gl} and ΔU_{vl} tend to zero (see **appendix A**).

□

Remark 4

- The counterpart of the latter relaxation conditions is given in [20] for a class of non-equilibrium two-phase flow models, with or without mass transfer (see [21] also, which provides some additional details).
- When focusing on immiscible three-phase flow models such as those proposed in [19], a similar analysis may be performed, see [23] . Note that this framework enables to exhibit situations requiring a strong numerical coupling of source terms when one aims at tackling difficult situations such as those occuring in vapor explosion [4].

□

4 Conclusion and perspectives

Focus has been given herein on the three-field flow model introduced in [24]. Actually, an important result is associated with property 6, which provides conditions (67), (68), and (69) arising from the relaxation matrix $\underline{\underline{A}}_{PT}(W)$. These constraints are neccessary to guarantee the whole relaxation process on velocity, pressure and temperature variables.

The latter conditions are also useful for practical purposes, since they may be used with the algorithm detailed below. This one simply consists in solving successively:

$$\left\{\begin{array}{l} \frac{\partial \alpha_g}{\partial t} + \mathbf{V}_i(\mathbf{W}).\nabla \alpha_g = 0 \\ \frac{\partial m_k}{\partial t} + \nabla.(m_k \mathbf{U}_k) = 0 \\ \frac{\partial m_k \mathbf{U}_k}{\partial t} + \nabla.(m_k \mathbf{U}_k \otimes \mathbf{U}_k + \alpha_k p_k \mathbf{Id}) + \Pi_k(\mathbf{W}) \nabla \alpha_g = 0 \\ \frac{\partial \alpha_k E_k}{\partial t} + \nabla.(\alpha_k \mathbf{U}_k (E_k + p_k)) - \Pi_k(\mathbf{W}) \frac{\partial \alpha_g}{\partial t} = 0 \end{array}\right. \tag{75}$$

using **explicit Rusanov scheme**, or some more sophisticated and accurate scheme [7], which is relying on relaxation techniques (see [10] for two-phase flow models with energy, and [32] in the immiscible barotropic

three-phase framework), and then computing approximate **implicit** approximate solutions of :

$$\begin{cases} \dfrac{\partial \alpha_g}{\partial t} = \phi_g(\mathbf{W}) \\ \dfrac{\partial m_k}{\partial t} = 0 \\ \dfrac{\partial m_k \mathbf{U}_k}{\partial t} = \mathbf{S}_k^U(\mathbf{W}) \\ \dfrac{\partial \alpha_k E_k}{\partial t} - \Pi_k(\mathbf{W}) \dfrac{\partial \alpha_g}{\partial t} = S_k^E(\mathbf{W}) \end{cases} \tag{76}$$

The first step involves some constraint on the time step Δt. Depending on the relative values of the relaxation time steps $\tau^P, \tau_{ij}^T, \tau_{ij}^U$, and of Δt, an **implicit** first-order Euler scheme or alternatively higher-order implicit schemes may be considered. Coupled implicit techniques should be priviledged in order to get more stable approximations of (76) , in particular when tackling interactions of shock waves with liquid droplets [8], or vapor explosion ([2]). This will be discussed in a forthcoming paper.

Appendix A

The matrix $\underline{\underline{A}}(W) \in \mathbb{R}^5 \times \mathbb{R}^5$ introduced in (64) is given by:

$$\underline{\underline{A}}(W) = \begin{pmatrix} \underline{\underline{A}}_{UU}(W) & \underline{0} & \underline{\underline{0}} \\ {}^t\underline{a}_{PU}(W) & a_{PP}(W) & {}^t\underline{a}_{PT}(W) \\ \underline{\underline{A}}_{TU}(W) & \underline{a}_{TP}(W) & \underline{\underline{A}}_{TT}(W) \end{pmatrix} \tag{77}$$

- The matrix $\underline{\underline{A}}_{UU}(W)$ arising in (64) reads:

$$\underline{\underline{A}}_{UU}(W) = \begin{pmatrix} d_{gl}(\frac{1}{m_g} + \frac{1}{m_l}) + \frac{d_{gv}}{m_g} & \frac{d_{lv}}{m_l} - \frac{d_{gv}}{m_g} \\ \frac{d_{lg}}{m_l} - \frac{d_{gv}}{m_v} & d_{vl}(\frac{1}{m_v} + \frac{1}{m_l}) + \frac{d_{gv}}{m_v} \end{pmatrix} \tag{78}$$

  This obviously implies that its trace:

$$trace(\underline{\underline{A}}_{UU}(W)) = d_{gl}(\frac{1}{m_g} + \frac{1}{m_l}) + d_{vl}(\frac{1}{m_v} + \frac{1}{m_l}) + d_{gv}(\frac{1}{m_g} + \frac{1}{m_v}) \tag{79}$$

  is positive, and also that :

$$det(\underline{\underline{A}}_{UU}(W)) > 0 \tag{80}$$

  since d_{ij} and partial masses m_k are positive, and:

$$det(\underline{\underline{A}}_{UU}(W)) = (d_{gl}d_{vl} + d_{gl}d_{vg} + d_{gv}d_{vl})(\frac{1}{m_g m_l} + \frac{1}{m_l m_v} + \frac{1}{m_g m_v}) \tag{81}$$

- The diagonal coefficient $a_{PP}(W)$ reads:

$$a_{PP}(W) = a = \frac{1}{\Pi_0 \tau^P(\mathbf{W})} \left(\alpha_g \rho_l c_l^2 + (1-\alpha_g)(\rho_g c_g^2 + \rho_v c_v^2) - \alpha_g (\rho_l \frac{\partial \epsilon_l}{\partial P_l} |\rho_l)^{-1} \Delta P \right) \tag{82}$$

- The matrix $\underline{\underline{A}}_{TT}(W)$ arising in (64) reads:

$$\underline{\underline{A}}_{TT}(W) = \begin{pmatrix} e & f \\ h & i \end{pmatrix} = \begin{pmatrix} q_{gl}(\frac{1}{M_g} + \frac{1}{M_l}) + \frac{q_{gv}}{M_g} & \frac{q_{lv}}{M_l} - \frac{q_{gv}}{M_g} \\ \frac{q_{lg}}{M_l} - \frac{q_{gv}}{M_v} & q_{vl}(\frac{1}{M_v} + \frac{1}{M_l}) + \frac{q_{gv}}{M_v} \end{pmatrix} \tag{83}$$

  noting: $M_k = m_k \left. \frac{\partial \epsilon_k}{\partial T_k} \right|_{\rho_k}$. Its structure is the same as the one of $\underline{\underline{A}}_{UU}(W)$. Thus its trace and determinant are positive, since q_{ij} and M_k are positive.

- Coefficients arising in $\underline{a}_{TP}(W)$ are:

$$\underline{a}_{TP}(W) = \begin{pmatrix} d \\ g \end{pmatrix} = \begin{pmatrix} K(W)(\frac{\Pi_g + N_g}{M_g} - \frac{\Pi_l - N_l}{M_l}) \\ K(W)(\frac{\Pi_v + N_v}{M_v} - \frac{\Pi_l - N_l}{M_l}) \end{pmatrix} \tag{84}$$

  with $N_k = \rho_k^2 \left. \frac{\partial \epsilon_k}{\partial \rho_k} \right|_{T_k}$, $K(\mathbf{W}) = \frac{\alpha_g(1-\alpha_g)}{\Pi_0 \tau^P(\mathbf{W})}$ and Π_k given in (7).

- The matrix $\underline{\underline{A}}_{TU}(W)$ is given by:

$$\underline{\underline{A}}_{TU}(W) = \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix} \tag{85}$$

  noting:

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} d_{lg}(U_l - U_g)(\frac{1}{2M_g} - \frac{1}{2M_l}) + d_{gv}(U_v - U_g)\frac{1}{2M_g} \\ d_{gv}(U_g - U_v)\frac{1}{2M_g} + d_{lv}(U_v - U_l)\frac{1}{2M_l} \\ d_{gv}(U_v - U_g)\frac{1}{2M_v} + d_{lg}(U_g - U_l)\frac{1}{2M_l} \\ d_{lv}(U_l - U_v)(\frac{1}{2M_v} - \frac{1}{2M_l}) + d_{gv}(U_g - U_v)\frac{1}{2M_v} \end{pmatrix} \tag{86}$$

- Eventually we have :

$$\underline{a}_{PT}(W) = \begin{pmatrix} b \\ c \end{pmatrix} = \begin{pmatrix} \frac{q_{gv}}{L_v} - \frac{q_{gl}}{L_l} - \frac{q_{gl}+q_{gv}}{L_g} \\ \frac{q_{gv}}{L_g} - \frac{q_{vl}}{L_l} - \frac{q_{vl}+q_{gv}}{L_v} \end{pmatrix} \tag{87}$$

with $L_k = m_k \left.\frac{\partial \epsilon_k}{\partial P_k}\right|_{\rho_k}$, and:

$$\underline{a}_{PU}(W) = \begin{pmatrix} \frac{1}{2}(d_{lg}(\frac{1}{L_l} - \frac{1}{L_g})(U_l - U_g) + d_{vg}(\frac{1}{L_g} + \frac{1}{L_v})(U_g - U_v)) \\ \frac{1}{2}(d_{lv}(\frac{1}{L_l} - \frac{1}{L_v})(U_l - U_v) + d_{vg}(\frac{1}{L_g} + \frac{1}{L_v})(U_v - U_g)) \end{pmatrix} \tag{88}$$

Appendix B

We propose here a simple fractional step algorithm in order to compute approximate solutions of sources (28).

It consists in solving successively (35) and then (53).

A simple first-order scheme accounting for temperature relaxation terms (53)

In view of section 2.4, the following algorithm arises.

Algorithm A_T

- For a given value of W^n, compute $\underline{\Delta T}^{n+1}$ solution of:

$$\underline{\Delta T}^{n+1} = (\underline{\underline{I}} + \Delta t \underline{\underline{A}}_{TT}(W^n))^{-1} \underline{\Delta T}(W^n) \tag{89}$$

- Find T_l^{n+1} solution of:

$$J(T_l^{n+1}) := m_l^n \epsilon_l(\rho_l^n, T_l^{n+1}) + (\sum_{k=v,g} m_k^n \epsilon_k(\rho_k^n, T_l^{n+1} + \Delta T_{kl}^{n+1})) = (\sum_{k=l,v,g} m_k \epsilon_k)^n \tag{90}$$

- Update E_k^{n+1} in accordance with (54).

□

Remarks on Algorithm A_T

- The first step (89) is defined, and the discrete temperature relaxation process is ensured.
- Asuming that the EoS are such that: $\left.\frac{\partial \epsilon_k(\rho_k, T_k)}{\partial T_k}\right|_{\rho_k} > 0$ for $k \in (l, g, v)$, the fucntion $J(x)$ is increasing, and the equation (90) admits no more than one solution.
- If we assume that EoS are Nobel Abel Stiffened Gas , then:

$$\epsilon_k(\rho_k, T_k) = C_{v,k} T_k + Q_k + \Pi_k (1 - b_k \rho_k)/\rho_k \tag{91}$$

Hence the solution X of (90) exists and is unique. More over it can be obtained explicitly.

□

Proof:
The proof for these three items is simple. First, eigenvalues of $\underline{\underline{I}} + \Delta t \underline{\underline{A}}_{TT}(W^n)$ are $1 + \Delta t \lambda_j$. If λ_j is real positive, $1 + \Delta t \lambda_j$ is greater than 1, whatever $\Delta t > 0$. This guarantees the discrete relaxation process. A similar remark holds when λ_j is complex, when its real part is positive.

Second, equation (90) admits at most one solution since :

$$J'(X) = \sum_{k\in(l,g,v)} m_k^n \left.\frac{\partial \epsilon_k(\rho_k, T_k)}{\partial T_k}\right|_{\rho_k^n} > 0 \tag{92}$$

Eventually, when restricting to NASG EoS, we note that T_l^{n+1} is:

$$T_l^{n+1} = \frac{\sum_{k=l,g,v} m_k^n C_{v,k} T_k^n - \sum_{k=g,v} m_k^n C_{v,k} (\Delta T)_{kl}^{n+1}}{\sum_{k=l,g,v} m_k^n C_{v,k}} \tag{93}$$

□

A simple first-order scheme accounting for pressure relaxation terms (35)

In view of section 2.3, the following algorithm arises.

Algorithm A_P

- Consider some given initial value $X^n = \alpha_g^n \in]0,1[$, and compute $X = \alpha_g^{n+1}$ such that:

$$X - X^n = \frac{\Delta t}{\Pi_0 \tau^P(W^n)} X(1-X)(P_v(X) + P_g(X) - P_l(X)) \tag{94}$$

  using definitions :

$$\rho_k(X) = \frac{m_k^n}{X} \quad (k \in g, v) \qquad ; \qquad \rho_l(X) = \frac{m_l^n}{1-X} \tag{95}$$

$$P_k(X) = p_k(\rho_k(X), S_k^n) \qquad ; \qquad e_k(X) = \epsilon_k(\rho_k(X), S_k^n) \qquad , with \quad k \in (g, v) \tag{96}$$

  and:

$$e_l(X) = \left((\sum_{k\in(l,g,v)} m_k \epsilon_k)^n - m_v^n e_v(X) - m_g^n e_g(X) \right) / m_l^n \tag{97}$$

  but also:

$$P_l(X) = p_l(\rho_l(X), e_l(X)) \tag{98}$$

- Update all variables in agreement with (35).

□

Remarks on Algorithm A_P

- The solution $X \in]0,1[$ of (94) exists and is unique.
- Associated values of updated variables at time t^{n+1} are uniquely defined and in the admissible range.

□

Proof:
If $X^n = 0$ (respectively $X^n = 1$) the obvious solution of (94) is $X = 0$ (respectively $X = 1$). Otherwise, the solution of (94) is also the solution of:

$$f(X) = g(X) \tag{99}$$

where:

$$f(X) = \frac{\Pi_0 \tau^P(W^n)}{\Delta t} \frac{X - X^n}{X(1-X)} \tag{100}$$

and:

$$g(X) = P_v(X) + P_g(X) - P_l(X) \tag{101}$$

The function $f(X)$ is increasing, with $f(X^n) = 0$, and:

$$\begin{cases} \lim\limits_{X \to 1^-} f(X) = \infty \\ \lim\limits_{X \to 0^+} f(X) = -\infty \end{cases} \tag{102}$$

Moreover:

$$P_k'(X) = -c_k^2 \frac{m_k^n}{X^2} \tag{103}$$

for $k \in (g, v)$, and:

$$P_l'(X) = \left.\frac{\partial p_l}{\partial \rho_l}\right|_{\epsilon_l} \frac{m_l^n}{(1-X)^2} + \left.\frac{\partial p_l}{\partial \epsilon_l}\right|_{\rho_l} e_l'(X) \tag{104}$$

with:

$$e_l'(X) = \left.\frac{\partial \epsilon_v}{\partial \rho_v}\right|_{S_v} \frac{(m_v^n)^2}{X^2} + \left.\frac{\partial \epsilon_g}{\partial \rho_g}\right|_{S_g} \frac{(m_g^n)^2}{X^2} \tag{105}$$

Let us choose a triple of EOS, more precisely:

- a perfect gas EoS for $k \in (g, v)$:

$$p_k = (\gamma_k - 1)\rho_k \epsilon_k \qquad with: \quad \gamma_k > 1 \tag{106}$$

- a Nobel Abel Stiffened Gas EoS for the liquid phase, that is:

$$(1 - \rho_l b_l)(p_l + \gamma_l \hat{\Pi}_l) = (\gamma_l - 1)\rho_l(\epsilon_l - \epsilon_0) \tag{107}$$

  with $\gamma_l > 1$, $b_l > 0$, $\hat{\Pi}_l > 0$, and assuming that $1 > \rho_l b_l$.

Hence we have:

- $$\frac{\partial \epsilon_k}{\partial \rho_k}|_{S_k} > 0 \qquad ; \qquad (k \in (g, v)) \tag{108}$$

  thus:

$$e_l'(X) > 0 \tag{109}$$

- $$\left.\frac{\partial p_l}{\partial \epsilon_l}\right|_{\rho_l} = \frac{(\gamma_l - 1)\rho_l}{1 - \rho_l b_l} > 0 \qquad ; \qquad \left.\frac{\partial p_l}{\partial \rho_l}\right|_{\epsilon_l} = \frac{p_l + \gamma_l \hat{\Pi}_l}{\rho_l(1 - \rho_l b_l)} > 0 \tag{110}$$

We may conclude that $P_l'(X) > 0$, which yields:

$$g'(X) = P_v'(X) + P_g'(X) - P_l'(X) < 0 \tag{111}$$

owing to (103). Evenmore, we have:

$$\begin{cases} \lim\limits_{X \to 1^-} g(X) = -\infty \\ \lim\limits_{X \to 0^+} g(X) = +\infty \end{cases} \tag{112}$$

which means that there exists a unique solution $\hat{X} \in]0, 1[$ of (99), or equivalently of (94). Densities and pressures at time t^{n+1} are obtained through (95), (96) and (97).

Eventually, assuming that approximate solutions obtained with this fractional step method converge towards the solution when the mesh size and the time step go to zero, one may conclude that solutions of (28) belong to the space of admissible states.

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