Simulation of an Homogeneous Relaxation Model for a three-phase mixture with miscible phases

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Abstract. This paper addresses the numerical approximation of a compressible three-phase flow. The mixture is composed of a liquid, its vapor and an inert gas, with realistic equations of state. Since the liquid is immiscible and the gaseous phases are miscible, it yields constrictive volume and mass constraints. The fluid dynamics is depicted by a one-velocity hyperbolic system with relaxation terms toward the thermodynamical equilibrium of the mixture. The core of the paper is the comparison and the analysis of two possible choices of relaxation terms, accounting for a detailed analysis of mixture entropy and the associated thermodynamical equilibrium. As numerics are concerned, a fractional step approach is proposed, based on a finite volume approximation of the convective part. The complexity of the source term requires an implicit Broyden resolution. Numerical results allow to compare both the performance of the chosen numerical schemes and the impact of the source term choices.

Contents

1. Introduction

The modelling of compressible multiphase flows is of major importance for many industrial applications, notably in the context of safety of nuclear power plants. Loss of coolant accident in pressurized water reactors and vapor explosions are two typical examples of compressible multiphase flows in this framework [11, 12]. The

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literature about immiscible multiphase configurations is huge; the reader may refer to recent publications [16, 13] for the modelling and analysis and to [27, 30] for numerical approximations of such immiscible models. Recently models of compressible flows with miscible phases have been proposed [26, 22, 28, 18, 17], see also [1]. They depict the dynamical and thermodynamical behaviour of a mixture composed of a liquid, its vapor and an inert gas ([17] considers in addition another liquid phase). As the fluid dynamics is concerned, two distinct approaches are available. In [18, 17] the phases evolve with their own velocities, leading to a system of non-conservative evolution equations with so-called interfacial quantities (velocity and pressure terms) with relaxation source terms towards equilibrium. In [26, 22, 28] all the phases evolve with a common velocity, leading to a so-called Homogeneous Relaxation Model (HRM) similar to an Euler system. It is endowed with additional evolution equations on fractions of volume, mass and energy of the phases which contain relaxation source terms towards the thermodynamical equilibrium. The derivation of this model is proposed in [26], based on the preliminar study [1]. The HRM model corresponds to a relaxation of an Homogeneous Equilibrium Model (HEM), namely an Euler system with a complex pressure law which depicts the thermodynamical behaviour of the three-phase mixture. When considering realistic equations of state for each phase, the exact computation of this mixture pressure is out of reach and precludes the use of the HEM model. The relaxation method, used for instance in [9, 23, 15], provides a HRM model with a simpler Euler-type structure with an explicit pressure law, which inherits from the hyperbolic and entropic properties of the HEM model. However it remains to provide relaxation source terms to close the system. These source terms have not only to comply with the second law but also to capture the correct thermodynamical equilibrium of the mixture. Among all possible choices, two sets of source terms have been proposed in [26], namely BGK-like source terms, corresponding to a linearization around the equilibrium state, and source term corresponding to the gradient of the entropy. When considering realistic equations of state for each phase, Quibel and Hurisse propose in [22, 28] numerical simulations of the HRM model with BGK-like source term. The aim of the present paper is, among other things, to compare with the gradient of entropy source term.

The paper is organised as follows.

In a first part, the thermodynamics of the mixture is investigated, when considering that the three phases are depicted by complete equations of state (EoS), focusing on Stiffened Gas (SG) and Noble-Able-Stiffened-Gas-Chemkin (NASG-CK) laws. The mixture entropy is presented in its intensive form (see [26] for an extensive formulation) and its concavity is investigated. The main difficulties of the model are, first, that the gaseous phases are miscible while the liquid is immiscible with them, and second, that the gas is inert, that is it cannot exchange mass with the two remaining phases. This results in constrictive constraints on the volume and mass fractions. Proposition 1 describes the thermodynamical equilibrium as a maximization of the mixture entropy under these constraints and addresses the question of disappearance of phases.

In a second part, the derivation of the evolution equations is proposed, leading to the expected HRM model. Note that this derivation differs from the relaxation method proposed in [26]. A brief study of the hyperbolic structure is given.

Section 2 ends with a comparison of the BGK-like source term and the gradient of entropy one. Properties of the associated dynamical systems are given. If the BGK-like source term can be solved explicitly, it requires the knowledge of the thermodynamical equilibrium for any given state. For realistic EoS, namely NASG-CK or tabulated laws, this is merely out of reach. On the other hand, the gradient of entropy source term cannot be solved explicitly but it enjoys nice properties as well: maximum principle, existence of solutions, asymptotic state in agreement with the expected thermodynamical equilibrium.

Section 3 addresses the numerical approximation of the HRM model by means of a fractional step method. The approximation of the convective part is performed by a finite volume scheme with different numerical schemes. Due to the considered phasic EoS, the computations of internal energy or temperature can be really tedious. For the sake of transparency, we provide in this section detailed algorithms of the computation of internal energy when dealing with either mixture of three SG or with a NASG-CK liquid phase. As the source terms are concerned, their nonlinearity (due to the use of complex phasic EoS) require to use an implicit Broyden algorithm, presented in Section 3.3.

Finally Section 4 contains the numerical results. First validation test cases of the convective part are presented, corresponding to infinitely slow relaxation. Exact Riemann problems are computed for a mixture of three SG and a mixture of a NASG-CK liquid with two SG. In both configurations a low and high pressure test cases are proposed. Convergence results are given which assess the good behaviour of the relaxation and the VFRoe-ncv schemes. However the VFRoe-ncv scheme is shown to be much more CPU time consuming than the relaxation scheme, and has a lack of robustness due to numerous internal energy computations, see Section 4.1.3. To finish a global simulation is proposed, accounting for the relaxation source terms, corresponding to a non-equilibrium test case. Numerical illustrations highlight the impact of the choice of the source terms.

2. The model

This Section presents the modelling of the three-phase mixture. First its thermodynamics is investigated. Compared to [26], complementary results about the mixture entropy concavity and the thermodynamical equilibrium are given. Notably the question of disappearance of phases is addressed. The dynamics of the fluid is depicted by an hyperbolic system with relaxation terms, whose derivation is detailed. The core of the section is the comparison and the analysis of two possible choices of source terms proposed in [26].

2.1. Thermodynamics of the mixture.

The mixture is composed of three *phases*: a liquid (labelled l), its vapor (labelled v) and an inert gas (labelled g). The gas is assumed to be inert in the sense that it cannot exchange mass with the two other phases (hence it is not *stricto sensu* a phase but the terminology is conserved in the sequel). We assume that no vacuum can occur. The main feature of this model relies in the fact that the two gaseous phases are miscible, while the liquid phase is immiscible with them.

In order to describe the thermodynamical behavior of the mixture, we consider a given state (τ, e), with τ the specific volume of the mixture and e its internal energy. The question addressed in the section 2.1.2 is the proper definition of the mixture entropy function which entirely depicts the thermodynamical behaviour of

the mixture. To do so, Section 2.1.1 presents first the complete equation of state for each phase $k \in \{l, g, v\}$. Section 2.1.2 starts by the constraints of mass and energy conservation as well as a volumic constraint which traduces the miscibility of the gaseous phases. It allows to express the mixture entropy as a function of fraction of mass, volume and energy of the phases. According to the second principle of thermodynamics, the thermodynamical equilibrium is reached at the maximum of the mixture entropy. This maximization process is realized under the abovementioned constraints. We present in Section 2.1.3 the associated optimality conditions, that give several constraints on phase disappearance.

2.1.1. *Phasic setting.* Each phase $k = l, g, v$ is depicted by its phasic specific volume $\tau_k > 0$ and its specific energy $e_k > 0$. The thermodynamical behaviour of each phase k is fully described by its intensive entropy function $(\tau_k, e_k) \mapsto s_k(\tau_k, e_k)$ defined on $\Omega_k \subset (\mathbb{R}_*^+)^2$, that is a complete equation of state. By adopting the Gibbs formalism, each entropy function s_k complies with the following differential form:

$$T_k ds_k = de_k + p_k d\tau_k, \tag{1}$$

where the phasic temperature T_k and pressure p_k are defined by:

$$\frac{1}{T_k} = \left.\frac{\partial s_k}{\partial e_k}\right|_{\tau_k}, \qquad p_k = T_k \left.\frac{\partial s_k}{\partial \tau_k}\right|_{e_k}, \tag{2}$$

and the phasic chemical potential by the relation:

$$\mu_k = -T_k s_k + p_k \tau_k + e_k. \tag{3}$$

Following hypotheses that are usually made on the extensive entropies [24], the phasic entropy fonctions are supposed to be:

- strictly concave functions on Ω_k,
- of class $\mathcal{C}^2$ on Ω_k, such that $\forall (\tau_k, e_k) \in \Omega_k$, $T_k(\tau_k, e_k) > 0$.

In practical applications, we focus on two equations of state, namely the Stiffened Gas (SG) and the Noble-Able Chemkin Stiffened Gas (NASG-CK) equations of state (EoS), whose accuracy on a large domain have been studied in [28, chap. 2]. We remind here their definitions.

For a given phasic state $(\tau_k, e_k) \in \Omega_k$, the complete SG reads

$$s_k(\tau_k, e_k) = C_{v,k} \ln\left((e_k - Q_k - \Pi_k \tau_k)\tau_k^{\gamma_k - 1}\right) + s_k^0, \tag{4}$$

where $C_{v,k} > 0$ is the calorific capacity at constant volume, $-\Pi_k$ is the minimal pressure, Q_k is a reference enthalpy, $\gamma_k > 1$ is the adiabatic coefficient and $s_k^0 > 0$ is a reference specific entropy. The case $\Pi_k = Q_k = 0$ corresponds to a perfect gas law [25]. The associated phasic pressure and temperature are

$$p_k(\tau_k, e_k) = (\gamma_k - 1)\frac{e_k - Q_k}{\tau_k} - \gamma_k \Pi_k, \quad T_k = \frac{e_k - Q_k - \Pi_k \tau_k}{C_{v,k}}. \tag{5}$$

In [28, chap. 2] are given sets of parameters for the vapor and liquid phases, which have been fitted with respect to experimental data around a reference point

$(p_{ref} = 80\text{bar}, T_{ref} = 425\text{K})$:

$$
\begin{aligned}
&\gamma_l = 1.39864082368510,\ C_{v,l} = 3.19641035947920 \times 10^3,\\
&Q_l = -1.24606074764184 \times 10^6,\ \Pi_l = 4.79690712132593 \times 10^8,\\
&s_l^0 = -34597.52986978335,\\
&\gamma_v = 1.15442237458290,\ C_{v,v} = 2.91668522329726 \times 10^3,\\
&Q_v = 1.25942536895827 \times 10^6,\ \Pi_v = -3.24993579473092 \times 10^2,\\
&s_v^0 = -33792.18353359583.
\end{aligned} \tag{6}
$$

For further simulations, we will consider a perfect gas law for the inert gas, which corresponds to :

$$\gamma_g = 1.4,\ C_{v,g} = 719,\ Q_g = \Pi_g = 0. \tag{7}$$

The Noble-Able Stiffened Gas Chemkin (NASG-CK) EoS is an extension of the SG where the heat capacity now depends on the temperature. According to [28, chap. 2], the NASG-CK EoS provides a more accurate description of the liquid thermodynamical behaviour on a larger domain than the SG EoS. This accuracy has a cost since its requires nonlinear computations, the NASG-CK law being semi-implicit. Indeed the chemical potential (which is a complete EoS) is classically given in the pressure-temperature plane as follows

$$\mu_l(p_l, T_l) = \mu_l^0(T_l) + b_l p_l + C_l(T_l)\ln(p_l + \Pi_l), \tag{8}$$

where

$$
\begin{aligned}
\mu_l^0(T_l) &= RT_l\left(A_l(1-\ln(T_l)) - \frac{B_l}{2}T_l - \frac{C_l}{6}T_l^2 - \frac{D_l}{12}T_l^3 - \frac{E_l}{20}T_l^4 + \frac{R_l}{T_l} - G_l\right),\\
C_l(T_l) &= C_{v,l}(\gamma_l - 1)T_l,
\end{aligned} \tag{9}
$$

with $R = 0.4615228083134561$ the perfect gas constant for water and b_l a translation of the specific volume coming from the NASG law, see [4]. For further numerical experiments, we focus on parameters given in [28] for the liquid water:

$$
\begin{aligned}
&\gamma_l = 3.27113568773712, \quad C_{v,l} = 7.24509640448929 \times 10^2,\\
&\Pi_l = 1.24425779880749 \times 10^9, \quad b_l = 5.66559849022606 \times 10^{-4},\\
&A_l = 4.69738865636393 \times 10^1, \quad B_l = -4.19269571479452 \times 10^{-1},\\
&C_l = 1.70702143968620 \times 10^{-3}, \quad D_l = -3.04805662517983 \times 10^{-6},\\
&E_l = 2.02814588067819 \times 10^{-9}, \quad F_l = -2.519604765 \times 10^6/R,\\
&G_l = -5.573536947 \times 10^4/R.
\end{aligned} \tag{10}
$$

The computation difficulties come from the implicit calculus of the pressure p_l and the temperature T_l in the (τ_l, e_l) plane. It holds

$$p_l(\tau_l, T_l) = \frac{C_{v,l}(\gamma_l - 1)T_l}{\tau_l - b_l} - \Pi_l, \tag{11}$$

$$
\begin{aligned}
e_l(\tau_l, T_l) = RT_l&\left(A_l + \frac{B_l}{2}T_l + \frac{C_l}{3}T_l^2 + \frac{D_l}{4}T_l^3 + \frac{E_l}{5}T_l^4 + \frac{F_l}{T_l}\right)\\
&- C_{v,l}(\gamma_l - 1)T_l + \Pi_l(\tau_l - b_l).
\end{aligned} \tag{12}
$$

Hence for a given state (τ_l, e_l), first the temperature is computed by solving (12) in a implicit way, and then, the pressure is deduced using (11).

2.1.2. *Intensive constraints and mixture entropy.* We now turn to the description of the thermodynamical behaviour of the mixture. Let $w = (\tau, e)$ be a state vector of the fluid mixture, which is composed of a liquid l, its vapor v and an inert gas g. We denote $y_k \in [0,1]$ the mass fraction of the phase k, $\alpha_k \in [0,1]$ the volume fraction and $z_k \in [0,1]$ the energy fraction. The conservation of total mass and energy provides that

$$\begin{cases} y_l + y_v = 1 - y_g, \\ z_l + z_v + z_g = 1, \end{cases} \tag{13}$$

while the miscibility of the gaseous phases and the immiscible behaviour of the liquid impose that

$$\begin{cases} \alpha_g = \alpha_v, \\ \alpha_l + \alpha_g = 1. \end{cases} \tag{14}$$

Note that the mass fraction y_g of the gas is fixed, since the gas cannot exchange mass with the two remaining phases. The knowledge of the fractions and the mixture state (τ, e) allows to recover the phasic state (τ_k, e_k) since

$$\tau_k = \frac{\alpha_k}{y_k}\tau, \quad e_k = \frac{z_k}{y_k}e. \tag{15}$$

For a given mixture state (τ, e), the mixture entropy is defined as a convex combination of the phasic entropies with weights $y_k \in [0,1]$. Denoting $Y = (y_l, \alpha_l, z_l, z_g)$, it reads

$$\sigma(\tau, e, Y, y_g) = \sum_{k=l,g,v} y_k s_k \left(\frac{\alpha_k}{y_k}\tau, \frac{z_k}{y_k}e \right). \tag{16}$$

The definition domain Ω of the mixture entropy is a convex subset of $(\mathbb{R}_+)^2 \times]0;1[^5$ [24].

Remark 1. *We can show that $(\tau, e) \mapsto \sigma(\tau, e, Y, y_g)$ and $Y \mapsto \sigma(\tau, e, Y, y_g)$ are concave functions [21, 26]. Some comments concerning this strict concavity of the mixture entropy have been provided for instance in [21], in the case of an immiscible mixture. They rely on the study of the concavity of the extensive mixture.*

The idea is to show, for a given extensive state $X = (M, V, E)$ of mass M, volume V and energy E, that the extensive mixture entropy S is a strictly concave function when restricted on the set $\mathcal{H}(M)$ of the states whose total mass is equal to M. If this property is true, then the intensive mixture entropy is strictly concave.

In order to prove the strict concavity of S on $\mathcal{H}(M)$, the idea is to show that the degeneracy manifold of S, that is $\ker \nabla_X^2 S(X)$, coincides with Vect(X) [24]:

$$\forall X, \ \ker \nabla_X^2 S(X) = \mathit{Vect}(X).$$

If so, then the restriction of S on $\mathcal{H}(M)$ is strictly concave since

$$\mathcal{H}(M) \cap \ker \nabla_X^2 S(X) = \{X\}.$$

However, only the inclusion Vect$(X) \subset \ker \nabla_X^2 S(X)$ is shown [24]. One remarks that $\ker \nabla_X^2 S(X)$ is a vectorial subset in the 9-dimensional space in the case of a three-phase flow.

Accounting for the phasic Gibbs relations (1), identities (15) and the definition (3) of the phasic chemical potential μ_k, the differential of the mixture entropy is

$$\mathrm{d}\sigma = \sum_{k=l,g,v} \mu_k \mathrm{d}y_k + \tau \sum_{k=l,g,v} \frac{p_k}{T_k} \mathrm{d}\alpha_k + e \sum_{k=l,g,v} \frac{1}{T_k} \mathrm{d}z_k + \sum_{k=l,g,v} z_k \frac{1}{T_k} \mathrm{d}e + \sum_{k=l,g,v} \alpha_k \frac{p_k}{T_k} \mathrm{d}\tau.$$

Now using the intensive constraints (13) and (14), it holds

$$\begin{aligned} \mathrm{d}\sigma &= (\mu_l - \mu_v)\mathrm{d}y_l + \tau \left(\frac{p_l}{T_l} - \left(\frac{p_v}{T_v} + \frac{p_g}{T_g} \right) \right) \mathrm{d}\alpha_l \\ &+ e \left(\frac{1}{T_l} - \frac{1}{T_g} \right) \mathrm{d}z_l + e \left(\frac{1}{T_v} - \frac{1}{T_g} \right) \mathrm{d}z_v \\ &+ \left(\frac{z_l}{T_l} + \frac{z_v}{T_v} + \frac{z_g}{T_g} \right) \mathrm{d}e + \left(\alpha_l \frac{p_l}{T_l} + (1-\alpha_l) \left(\frac{p_v}{T_v} + \frac{p_g}{T_g} \right) \right) \mathrm{d}\tau. \end{aligned} \tag{17}$$

Hence it follows that the mixture pressure and temperature are defined by:

$$\begin{aligned} \frac{1}{T}(\tau, e, Y, y_g) &= \frac{z_l}{T_l} + \frac{z_v}{T_v} + \frac{z_g}{T_g}, \\ p(\tau, e, Y, y_g) &= \frac{\alpha_l \frac{p_l}{T_l} + (1-\alpha_l)\frac{p_v}{T_v} + (1-\alpha_l)\frac{p_g}{T_g}}{\frac{z_l}{T_l} + \frac{z_v}{T_v} + \frac{z_g}{T_g}}, \end{aligned} \tag{18}$$

where the notations p_k (resp. T_k) stands for $p_k(\tau_k, e_k)$ (resp. $T_k(\tau_k, e_k)$) with relations (15).

2.1.3. *Thermodynamical equilibrium and optimality conditions.* As thermodynamical equilibrium is reached, the mixture entropy achieves its maximum. This maximization process is performed under the constraints (13)-(14). The question addressed here is to characterize the thermodynamical equilibrium and to investigate the possible disappearance of phases. The maximization process can be rewritten in term of the function

$$\Sigma(\tau, e, y_l, y_v, (\tau_k)_k, (e_k)_k) = y_l s_l(\tau_l, e_l) + y_v s_v(\tau_v, e_v) + y_g s_g(\tau_g, e_g), \tag{19}$$

where the fraction of mass $y_g \in]0,1[$ is fixed and the partial quantities τ_k and e_k satisfy the constraints

$$\begin{cases} y_l + y_v = 1 - y_g, \\ y_l \tau_l + y_v \tau_v = \tau, \\ y_v \tau_v = y_g \tau_g, \\ y_l e_l + y_v e_v + y_g e_g = e, \end{cases} \tag{20}$$

which are equivalent to the initial constraints (13)-(14). The second and third relations are consequences of the immiscibility of the liquid and the miscibility of the gaseous phases, coupled with the mass conservation constraint.

The function Σ is C^1 on the space $\mathbb{R}_*^+ \times \mathbb{R}_*^+ \times [0,1]^2 \times (\mathbb{R}_*^+ \times \mathbb{R}_*^+)^3$. The constraints (20) are affine, and thus C^1. We are thus in position to use the Lagrange multipliers characterization of the maximum. Let λ_y, λ_τ, λ_m and λ_e, four reals, corresponding to the four constraints (20).

Using the definitions of the phasic potentials (2), one deduces the following system of optimality conditions

$$
\begin{cases}
s_l(\tau_l, e_l) + \lambda_y + \lambda_\tau \tau_l + \lambda_e e_l = 0, \\
s_v(\tau_v, e_v) + \lambda_y + (\lambda_\tau + \lambda_m)\tau_v + \lambda_e e_v = 0, \\
y_l \left(\dfrac{p_l}{T_l} + \lambda_\tau \right) = 0, \\
y_v \left(\dfrac{p_v}{T_v} + \lambda_\tau + \lambda_m \right) = 0, \\
y_g \left(\dfrac{p_g}{T_g} - \lambda_m \right) = 0, \\
y_l \left(\dfrac{1}{T_l} + \lambda_e \right) = 0, \\
y_v \left(\dfrac{1}{T_v} + \lambda_e \right) = 0, \\
y_g \left(\dfrac{1}{T_g} + \lambda_e \right) = 0.
\end{cases} \tag{21}
$$

Proposition 1. *Consider a mixture state (τ, e). Let $y_g \in]0,1[$. The equilibrium states are*

(1) ***Saturation states****: y_l, y_v belong to $]0,1[$ and $(\tau_k, e_k)_k$ comply with*

$$
\begin{cases}
p_l = p_v + p_g, \\
T_l = T_v = T_g, \\
\mu_l = \mu_v.
\end{cases} \tag{22}
$$

(2) ***Absence of the liquid phase*** *$y_l = 0$. The vapor mass fraction is $y_v = 1 - y_g \in]0,1[$, the gaseous specific volumes are fixed according to*

$$
\tau_v = \tau/(1 - y_g), \quad \tau_g = y_g/(1 - y_g)\tau, \tag{23}
$$

while the gaseous internal energies are fixed with respect to

$$
e = y_v e_v + y_g e_g, \quad T_v = T_g. \tag{24}
$$

The liquid pair (τ_l, e_l) complies with

$$
T_v s_l - (p_v + p_g)\,\tau_l - e_l = -\mu_v, \tag{25}
$$

but remains unfixed.

(3) The case $y_v = 0$, corresponding to the ***absence of the vapor phase****, is not reachable.*

If $y_g = 0$, then only the liquid phase is present with $y_l = 1$, $\tau_l = \tau$ and $e_l = e$. The gaseous pairs (τ_k, e_k), $k = l, g$, are undefined as well as the Lagrange multiplier λ_m.

Proof. Since $y_g \in]0,1[$, the Lagrange multipliers λ_e and λ_m are given by

$$
\lambda_e = -\frac{1}{T_g}, \quad \lambda_m = \frac{p_g}{T_g}.
$$

(1) Saturation case: assume that y_v and y_l belong to $]0,1[$. Thus thermal equilibrium is reached in the sense that

$$
\frac{1}{T_l} = \frac{1}{T_v} = \frac{1}{T_g}.
$$

It follows that the mechanical equilibrium corresponds to the equality of the liquid pressure with the Dalton's law on the gaseous phases

$$-\lambda_\tau = p_l = p_v + p_g.$$

Using now the definitions (3) of the phasic chemical potentials, it holds

$$-\lambda_y = \mu_l = \mu_v.$$

(2) Assume that $y_l = 0$, that is the liquid phase has no mass. The constraint on the mass fractions imposes that $y_v = 1 - y_g \in]0, 1[$. By the mass conservation, it holds

$$\tau_v = \tau/(1 - y_g), \quad \tau_g = y_g/(1 - y_g)\tau.$$

Considering the optimality conditions on the temperature, one deduces the thermal equilibrium of the gaseous phases

$$1/T_v = 1/T_g = -\lambda_e.$$

The mechanical conditions fixes the Lagrange multipliers λ_τ

$$-\lambda_\tau = p_v/T_v + p_g/T_g.$$

Finally the second optimality condition, using the definition (3) of the chemical potential μ_v, fixes the Lagrange multiplier $\lambda_y = \mu_v/T_v$. Note that from the conservation of energy $e = y_v e_v + y_g e_g$ and the thermal equilibrium, one deduces the vapor and gaseous energies e_v and e_g. It remains to fix the liquid quantities, which are *a priori* undefined. Using the first optimality condition, and the gazeous temperatures equality, the pair (τ_l, e_l) has to satisfy

$$T_v s_l - (p_v + p_g)\,\tau_l - e_l = -\mu_v.$$

However an additional constraint is needed to fix the pair.

(3) Assume $y_v = 0$. Hence $y_l = 1 - y_g \in]0, 1[$, such that $\tau_l = \tau/(1 - y_g)$. Note that the miscibility constraint imposes that $\tau_g = 0$, that is the the gaseous phase has a mass but no volume. In particular, the gaseous potential are not defined for $\tau_g = 0$. Hence this case is not reachable.

(4) Assume $y_g = 0$. Then the miscibility condition imposes that $y_v = 0$ since $\tau_v > 0$ and no vacuum is considered. In that case, $y_l = 1$. Observe that the Lagrange multiplier λ_m is not defined, as well as the gaseous pairs (τ_k, e_k), $k = v, g$.

□

The absence of the liquid phase, corresponding to $y_l = 0$, is characterized by Equation (25). Its left hand side is homogeneous to the *liquid* chemical potential. Hence Equation (25) traduces the deviation from the chemical equilibrium between the vapor and the absent liquid phase.

For a given state characterized by relations (22), its counterpart in terms of equilibrium fraction $Y_{eq} = (y_{l,eq}, \alpha_{l,eq}, z_{l,eq}, z_{g,eq})$ maximizes the entropy σ under the constraints (13)-(14). We emphasize that Y_{eq} only depends of (τ, e, y_g), and that its definition requires the strict concavity of $Y \mapsto \sigma(\tau, e, Y, y_g)$, that we

2.2. **Mixture dynamics.** In this section are introduced the evolution equations of the mixture, assuming that each phase evolves with a common velocity field u. Their derivation consists in studying the evolution of an isolated fluid element along a streamline. Note that the resulting set of equations has already been obtained in [26] as a relaxed version of a three-phase equilibrium model.

2.2.1. *Derivation of the evolution equations of the mixture.* The purpose of this section is to derive a simple system of evolution equations of the observable quantities of the mixture in time t and space x, considering that each phase evolves with a common velocity field u. The derivation is performed for $x \in \mathbb{R}^d$, even if we focus in the sequel on the one-dimensional setting. To do so, one considers an isolated fluid element, composed of the three phases, along a streamline. Some standard assumptions have to be stated to perform the derivation, following the formalism depicted in [21]. First, the total mass of the element is conserved along time, as well as the mass fraction of gas y_g. Moreover we assume that the volume variation of the element is solely due to the velocity field divergence. Hence one obtains that

$$\mathrm{d}\tau = \tau \mathrm{div}(u)\mathrm{d}t,$$

where the derivative notation $\mathrm{d}\varphi$ corresponds to the derivative along a streamline of the flow

$$\mathrm{d}\varphi = \partial_t \varphi + u\nabla_x \varphi.$$

Considering now that the only force acting on the fluid element is due to the pressure gradient, the fundamental principle of mechanics states that

$$\mathrm{d}u = -\tau \nabla_x p \mathrm{d}t,$$

where the mixture pressure p corresponds to the mixture pressure (18). The first law of thermodynamics then relates the internal energy to the pressure assuming that the fluid element is not submitted to other heat sources

$$\mathrm{d}e = -p\mathrm{d}\tau.$$

Following [9, 3, 21], we assume that the time-evolution of the phasic quantities are of the form

$$\mathrm{d}Y = \lambda \Gamma(\tau, e, Y, y_g)\mathrm{d}t,$$

where the vector λ corresponds to the time relaxation parameters.

Combining the above equations with the definition of the fluid density $\rho = 1/\tau$, one ends up with a compressible Euler-type system with five additional equations on the fractions with possible relaxation terms. The conservative one-dimensional set of equations reads

$$\begin{cases} \partial_t(\rho Y) + \partial_x(\rho Y u) = \rho\lambda\Gamma(\tau, e, Y, y_g), \\ \partial_t(\rho y_g) + \partial_x(\rho y_g) = 0, \\ \partial_t \rho + \partial_x(\rho u) = 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0, \\ \partial_t(\rho E) + \partial_x\left((\rho E + p)u\right) = 0, \end{cases} \tag{26}$$

where $E = u^2/2 + e$ denotes the total energy of the system and p is the mixture pressure (18).

2.2.2. *Properties of the homogeneous model.* Focusing on the homogeneous part of the model, its hyperbolicity and entropic structure have been studied in [26]. The concavity of σ with respect to (τ, e, Y, y_g) is equivalent to the convexity of $H = -\rho\sigma$ with respect to the conservative variables $W = (\rho Y, \rho, \rho u, \rho E)$. Thus $H = -\rho\sigma$ is a Lax entropy for the system (26) and weak solutions satisfy

$$\partial_t H + \partial_x(Hu) \leq 0.$$

Again hyperbolicity is ensured as soon as the three phases are present and depicted by phasic concave entropies leading to a strictly positive sound speed c defined by

$$\frac{c^2}{\tau^2} = p\partial_e p - \partial_\tau p = -T(p^2\partial_{ee}\sigma - 2p\partial_{\tau e}\sigma + \partial_{\tau\tau}\sigma). \tag{27}$$

The eigenstructure of the system (26) is composed of one linearly degenerate wave, associated to the eigenvalue u, and two genuinely non-linear waves associated to the eigenvalues $u \pm c$, where c is the mixture sound speed defined by (27)

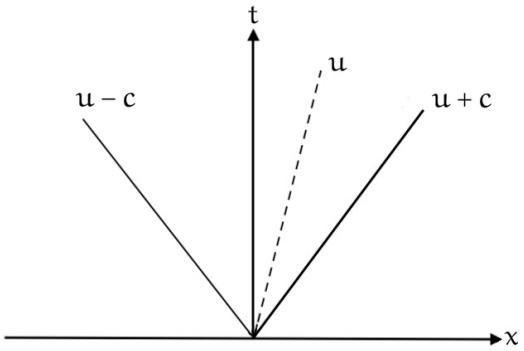


FIGURE 1. Structure: ghost-wave, contact, shock.

Figure 1 represents the wave structure in the (x, t) plane. As the contact wave is conserved (see Figure 1- dashed line), mixture pressure p and velocity u are preserved across it contrary to the fractions Y. For two given states W_L and W_R separated by a genuinely nonlinear wave (plain lines of Figure 1), the jump conditions read

$$\begin{cases} [Y] = 0, \\ J = -\frac{[p]}{[u]}, \\ J^2 = -\frac{[p]}{[\tau]}, \\ [e] + [\tau]\frac{p_L + p_R}{2} = 0, \end{cases} . \tag{28}$$

where $J = \rho u - \sigma$. It means in particular that the fractions are constant through nonlinear waves. In numerical validations, we provide analytical solutions of Riemann problems when the system (26) is endowed with an initial condition $W(0, x) = W_L \mathbf{1}_{x<0} + W_R \mathbf{1}_{x\geq 0}$, see Section 4.1. To do so we make use of the jump relations (28) to compute solutions composed of four constant states separated by a ghost wave, a contact and a shock wave (see also [28] for detailed exact computations).

2.3. **Source terms.** The thermodynamical behaviour of the mixture is not only driven by the mixture pressure p involved in the momentum and total energy conservation laws, but mostly depicted by the relaxation terms acting on the advection equations on the fraction vector Y. Indeed all the thermodynamical disequilibrium is depicted by the dynamical system

$$\frac{\mathrm{d}Y}{\mathrm{d}t} = \lambda\Gamma(\tau, e, Y, y_g). \tag{29}$$

Even if there is no consensus on the choice of relaxation source terms, they have to fullfil some physical requirements. First a thermodynamic evolution of the system must lead to an entropy growth and the equilibrium state corresponds to its maximum. It turns out that the mixture entropy σ verifies the following transport equation:

$$\partial_t\sigma + u\partial_x\sigma = \lambda\Gamma(Y, \tau, e)\nabla_Y\sigma. \tag{30}$$

Hence eligible source terms Γ are such that

$$\lambda\Gamma(Y, \tau, e)\nabla_Y\sigma \geq 0. \tag{31}$$

Moreover the relaxation terms have to preserve the asymptotic states. For a given state (τ, e) of the mixture, the source terms have to capture the correct thermodynamical equilibrium, that is

$$\lim_{t\to+\infty} Y(t) = Y_{eq}.$$

The core of this section is to analyze two possible choices of source terms. The first one, referred in [20] as BGK source term, corresponds to a linearization around the equilibrium vector Y_{eq}. Introduced in [9, 15, 3], it is used in multiphase configurations with complex phasic equations of state [28, 22]. The alternative source terms, proposed in [26], corresponds to the gradient of the mixture entropy which directly satisfies (30).

A similar analysis of these two choices in the immiscible (resp. miscible) diphasic framework is performed in [7]. The advantage of the two-phase case is that the dynamical system admits three (resp. two) equations leading to a convenient vizualisation of the trajectories in the phase plane. For the present problem, the dimension 4 of the system prevents such nice vizualisation.

Remark 2. *Source terms Γ contain time scales $\lambda = (\lambda_1, \lambda_2, \lambda_3, \lambda_4) \in (\mathbb{R}_+)^4$ that model the relaxation speed of the system. We will not consider any time dependence for λ in this paper.*

More precisely, each λ_i is a factor contained by Γ_i, and concerns a specific fraction in system (26). On a physical point of view, λ_1 correspond to the mass transfer, λ_2 to the mechanical, λ_3 and λ_4 to thermal relaxation times.

2.3.1. *BGK-like source terms.* For a given state $(\tau, e, Y, y_g) \in \Omega$, assuming that $Y \mapsto \sigma(\tau, e, Y)$ is *strictly* concave, there exists a unique equilibrium fraction state Y_{eq} which maximises the entropy σ, where Y_{eq} only depends of (τ, e), see Proposition 1.

Definition 1. *For any state $(\tau, e, Y, y_g) \in \Omega$, we define:*

$$\Gamma_1(\tau, e, Y, y_g) = \lambda(Y_{eq}(\tau, e, y_g) - Y), \tag{32}$$

where $\lambda \in (\mathbb{R}_*^+)^4$ is the time scale vector.

Proposition 2. *(Eligibility) Assume that the time scale vector $\lambda > 0$ is such that $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \lambda$, possibly time dependent. For any given state $(\tau, e) \in (\mathbb{R}_*^+)^2$, assume that the entropy function $(\tau, e, Y, y_g) \mapsto \sigma(\tau, e, Y)$ is strictly concave with respect to Y. Then, the source terms Γ_1 complies with the entropy growth criterion (31). Moreover, the stationary states of the dynamical system (29)-(32) coincide with the possible thermodynamical equilibria of Proposition 1.*

Proof. It is obvious that the stationary states of the source term Γ_1 are vector Y_{eq} of Proposition 1. It remains to check the entropy growth. Let $(\tau, e, Y, y_g) \in \Omega$ be a given state. It holds:

$$\begin{aligned}\Gamma_1(\tau, e, Y, y_g)\nabla_Y\sigma(\tau, e, Y, y_g) &= (\lambda(Y_{eq} - Y))\nabla_Y\sigma(\tau, e, Y, y_g)\\ &= \lambda((Y_{eq} - Y)\nabla_Y\sigma(\tau, e, Y, y_g))\\ &\geq \lambda(\sigma(\tau, e, Y_{eq}, y_g) - \sigma(\tau, e, Y, y_g))\\ &\geq 0,\end{aligned}$$

thanks to the concavity of $Y \mapsto \sigma(\tau, e, Y, y_g)$. □

Note that invoking the concavity argument requires to consider a *unique* relaxation parameter λ. Recently a modification of BGK-like source terms which allows distinct time scales has been introduced in [20].

Proposition 3. *Let $(\tau, e, Y_0, y_g) \in \Omega$ be an initial state. The Cauchy problem*

$$\begin{cases}\frac{dY}{dt}(t) = \Gamma_1(\tau, e, Y(t), y_g), \quad t > 0,\\ Y(0) = Y_0,\end{cases}$$

admits a global solution Y given by

$$\forall t \geq 0,\ Y(t) = e^{-\Lambda(t)}(e^{\Lambda(0)}Y_0 + Y_{eq}\int_0^t \lambda(s)e^{\Lambda(s)}\mathrm{d}s), \tag{33}$$

where Λ is a primitive of λ. In the case of a constant in time relaxation parameter λ, it holds

$$\forall t \geq 0,\ Y(t) = e^{-\lambda t}Y(0) + (1 - e^{-\lambda t})Y_{eq}. \tag{34}$$

The proof is direct and this last expression can be interpreted as a barycenter of the initial state $Y(0)$ and the equilibrium state Y_{eq}. Hence it guarantees that $Y(t) \in [0, 1]^4$ for all $t \geq 0$.

One major advantage of the BGK-like source term is that it can be explicitly integrated, since trajectories are exponential towards equilibrium fractions Y_{eq}. However it requires to compute the equilibrium state Y_{eq} for every considered state $(\tau, e, Y, y_g) \in \Omega$, that is to say maximize the mixture entropy (16) under the constraints (13)-(14).

For two-phase mixtures, the maximization can be done explicitly when classical EoS are considered [19]. In our three-phase context, the computations are much more complicated, especially when complex EoS are considered. For sake of illustration, the detailed computation of the equilibrium state Y_{eq} for a mixture of three Stiffened Gases is given in Appendix A.

Figure 2 presents the evolution in time of the fractions $Y(t)$ for a mixture of three SG with parameters (6). One observes the evolution in time of the fractions $Y(t)$ for an initial state $Y(0) = (0.1, 0.1, 0.1, 0.05)$, $y_g = 0.05$, with specific volume $\tau = 5.10^{-3}$ and internal energy $e = 10^8$. The time scale is constant in time and

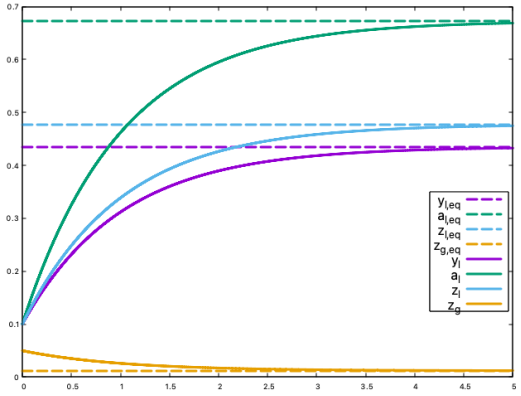


FIGURE 2. BGK-like source term Γ_1. Trajectories toward a three SG mixture equilibrium.

set to $\lambda = 1$. The equilibrium fractions, that can be computed following Appendix A, represented by the dotted lines, are reached at time $t = 5$s. Another important point is that the time when the asymptotic state is reached does not depend on the initial state of the fluid.

When considering a NASG-CK EoS for the liquid, the computation of the equilibrium state vector Y_{eq} requires an implicit solver, for instance using a Broyden algorithm, see [28] for a hint of the method.

2.3.2. *Entropy gradient source terms.* This second type of source terms corresponds to the gradient of the mixture entropy.

Definition 2. *For all $(\tau, e, Y, y_g) \in \Omega$, let Γ_2 be the source terms function defined by*

$$\Gamma_2(Y) = Y(1-Y)\nabla_Y \sigma(\tau, e, Y, y_g) = \begin{pmatrix} y_l(1-y_l)\partial_{y_l}\sigma \\ \alpha(1-\alpha)\partial_\alpha \sigma \\ z_l(1-z_l)\partial_{z_l}\sigma \\ z_g(1-z_g)\partial_{z_g}\sigma \end{pmatrix}.$$

Using intensive potentials (2)-(3), Γ_2 rewrites:

$$\Gamma_2 = \begin{pmatrix} y_l(1-y_l)\left(\frac{\mu_v}{T_v} - \frac{\mu_l}{T_l}\right) \\ \alpha_l(1-\alpha_l)\tau\left(\frac{P_l}{T_l} - \frac{P_v}{T_v} - \frac{P_g}{T_g}\right) \\ z_l(1-z_l)\left(\frac{1}{T_l} - \frac{1}{T_v}\right) \\ z_g(1-z_g)\left(\frac{1}{T_g} - \frac{1}{T_v}\right) \end{pmatrix}. \tag{35}$$

This function corresponds to the entropy gradient times $Y(1-Y)$ understood as a term by term product. Indeed the set of definition of the mixture entropy $Y \mapsto \sigma(\tau, e, Y, y_g)$ is Ω which is included in $]0;1[^4$. Thus a solution Y of the dynamical system $Y'(t) = \nabla_Y \sigma(\tau, e, Y, y_g)$ is such that $Y(t) \in]0;1[^4$, for all $t > 0$. However in numerical applications, this maximum principle is not guaranteed, as illustrated in Figure 3. Trajectories of the fraction vector in time are represented for a mixture of three SG with parameters (6), with initial state $Y(0) = (0.1, 0.1, 0.1, 0.05)$, $y_g = 0.05$, with specific volume $\tau = 5.5.10^{-3}$ and internal energy $e = 10^8$ and

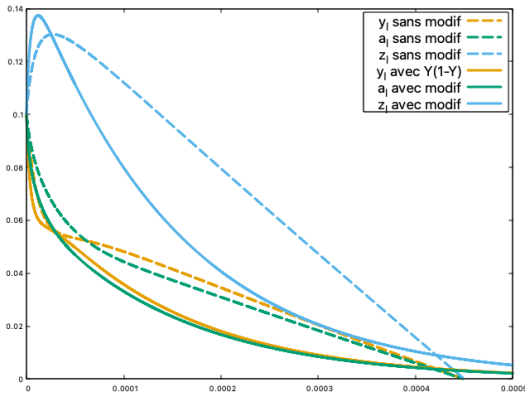


FIGURE 3. Gradient of entropy source term for a three SG mixture. Trajectories of the fractions in time without the correction (dashed lines) and with the correction (plain lines).

$\lambda = (1,1,1,1)^T$. Dashed lines correspond to trajectories when no correction is considered. One observes that the volume fraction becomes nonpositive at time $t < 0.0005$s. The correction term $Y(1-Y)$ ensures the maximum principle as illustrated by the plain lines. Of course, this correction term modifies the trajectories, in particular the return to equilibrium seems to be reached at a longer time. We emphasize that it directly depends on the initial state.

Remark 3. *The source term Γ_2 involves the difference of phasic pressures which acts on the volume fraction equation. Such an expression is rather classical. It can be found in the two-fluid literature, for instance in Baer-Nunziato like model* [2] *and the derivation of such mechanical transfer term is now well understood* [10].

Proposition 4. *(Eligibility) Let $\lambda_0 = \min \lambda_i$ such as $\lambda_0 > 0$. Then, for any state $(\tau, e, Y, y_g) \in \Omega$, the source term Γ_2 satisfies the eligibility criterion* (31) *for all $t > 0$.*

Proof. Let $(\tau, e, Y, y_g) \in \Omega$ a given state. It holds

$$\begin{aligned}
\Gamma_2(\tau,e,Y,y_g)\nabla_Y\sigma(\tau,e,Y,y_g) &= \lambda Y(1-Y)\nabla_Y\sigma(\tau,e,Y,y_g)\nabla_Y\sigma(\tau,e,Y,y_g)\\
&= \sum_{k=l,g,v} \lambda_k y_k(1-y_k)(\partial_{y_k}\sigma)^2(\tau,e,Y,y_g)\\
&\geq \lambda_0 \sum_{k=l,g,v} y_k(1-y_k)(\partial_{y_k}\sigma)^2(\tau,e,Y,y_g)\\
&\geq \lambda_0 \inf_{k=l,g,v} y_k(1-y_k) \sum_{k=l,g,v} (\partial_{y_k}\sigma)^2(\tau,e,Y,y_g)\\
&\geq \lambda_0 \inf_{k=l,g,v} y_k(1-y_k)||\nabla_Y\sigma||^2\\
&\geq 0.
\end{aligned}$$

□

Contrary to the BGK-like source term, the source term Γ_2 does not require conditions on different time scales, thus we can choose distinct ones.

Unlike the Γ_1 source term, solving exactly the ODE system is out of reach. However existence en uniqueness of local solution to Cauchy problem is guaranteed by the Cauchy-Lipschitz theorem.

Proposition 5. *Consider $(\tau, e) \in (\mathbb{R}_*^+)^2$. For all $Y_0 \in (\mathbb{R}_*^+)^4$ such that $(\tau, e, Y_0, y_g) \in \Omega$, there exists an unique maximal solution $(I, Y) \in \mathbb{R}_+ \times]0;1[^4$, with $Y : I \to]0;1[^4$, of the Cauchy problem*

$$\begin{cases} \frac{dY}{dt}(t) = \Gamma_2(\tau, e, Y(t), y_g), \quad t > 0, \\ Y(0) = Y_0. \end{cases} \tag{36}$$

The following purpose is to ensure that the stationary states of the Cauchy problem (36), namely vector $\bar{Y}$ such that $\Gamma_2(\bar{Y}) = 0$, correspond to physically relevant thermodynamical equilibria of the three-phase mixture, in the sense of Proposition 1.

For a given state $(\tau, e) \in (\mathbb{R}_*^+)^2$, if $\bar{Y} \in]0;1[^4$, then $\Gamma_2(\bar{Y}) = 0$ implies that $\nabla_Y \sigma(\tau, e, \bar{Y}, y_g) = 0$. Hence $\bar{Y}$ is such that (22) holds and the thermodynamical equilibrium is a stationary state.

On the other hand, since Γ_2 is not defined on the border of the cube $[0,1]^4$, one cannot determine if single phase states $\bar{Y} = 0_{\mathbb{R}^4}$ or $\bar{Y} = 1_{\mathbb{R}^4}$ are stationary states of the dynamical system and if these states are attractive (using standard arguments like the jacobian linearization). In a similar way, a state $Y = (1 - y_g, 0, 0, 0)$ such that $y_v = 0$ could be a stationary state of the dynamical system. The following result rejects this possibility in the case of a mixture of three Stiffened Gases with parameters (6) and complies with Proposition 1.

Proposition 6 (Exclusion of the border)**.** *Let $(\tau, e) \in (\mathbb{R}_*^+)^2)$ be a given state. For any initial data $Y(0) \in]0,1[^3$, a solution $Y(t)$ of the system (36) cannot converge towards the asymptotic state $Y_0 = (1 - y_g, 0, 0, 0)$.*

Proof. The study of the vector field around $Y_0 = (1 - y_g, 0, 0, 0)$ allows to exclude any possibility of convergence toward this point. Indeed, one can show that $\lim_{Y \to Y_0} \Gamma_{2,1}(Y) = -\infty$, where $\Gamma_{2,1}$ is the first component of Γ_2. We refer to [7] for a detailed proof in the case of a two-phase mixture. □

The high nonlinearity of the source term Γ_2 requires a robust numerical approximation, especially when considering complex EoS such as NASG-CK EoS. The numerical method we consider is depicted in Section 3.3.

3. Numerical approximation by a fractional step method

The fractional step method [31, 3] consists in approximating the convective part and the source terms in two distincts steps. The approximation of the convective part of the model (26) is performed by a Finite Volume method set on regular meshes of size $\Delta x = x_{i+1/2} - x_{i-1/2}$, $i \in \mathbb{Z}$. Time steps are calculated under CFL condition, with the notation $\Delta t^n = t^{n+1} - t^n$. Denoting $W = (\rho Y, \rho, \rho u, \rho E)$ the vector of conserved quantities, the first step of the method corresponds to the approximation of

$$\begin{cases} \partial_t W + \partial_x \mathcal{F}(W) = 0, \\ W(0, x) = W_0(x), \end{cases}$$

where $\mathcal{F}(W) = uW + pD$, with $D = (0, 0, 1, u)^T$ and $W_0(x)$ is a given initial state. Let $W(t^n, w)$ be approximated by

$$W_i^n = \int_{x_{i-1/2}}^{x_{i+1/2}} W(t^n, x)\mathrm{d}x. \tag{37}$$

Integrating the convective part over the space-time domain $[x_{i-1/2}, x_{i+1/2}]\times[t^n, t^{n+1,*})$ gives

$$\int_{x_{i-1/2}}^{x_{i+1/2}} W(t^{n+1,*}, x) - W(t^n, x)\mathrm{d}x + \int_{t^n}^{t^{n+1,*}} \mathcal{F}(W(t, x_{i+1/2})) - \mathcal{F}(W(t, x_{i-1/2}))\mathrm{d}t = 0.$$

Using the notation (37), the Finite Volume formulation reads

$$W_i^{n+1,*} = W_i^n - \frac{\Delta t}{\Delta x}(F_{i+1/2}^n - F_{i-1/2}^n), \tag{38}$$

where the notation $F_{i+1/2}^n$ stands for the two-point approximation of the flux through the interface $x_{i+1/2}$, namely $F_{i+1/2}^n = F(W_i^n, W_{i+1}^n)$. As the second step of the splitting method is concerned, it remains to provide a discretization of the source term with

$$\begin{cases} \dfrac{d}{dt}Y(t) = \Gamma(\tau, e, Y, y_g), \\ \dfrac{d}{dt}\tilde{W}(t) = 0, \end{cases} \tag{39}$$

where $\tilde{W} = (\rho y_g, \rho, \rho u, \rho E)$. Finally the numerical approximation W_i^{n+1} is an approximated solution of (39) at time $t = \Delta t$ with the initial condition $W^{n+1,*}$, deduced from the convection step.

3.1. **Convective part.** Several two-point numerical fluxes have been considered and will be compared in the following section. We focus on standard numerical schemes which are recalled hereafter for the sake of completness.

3.1.1. *Rusanov scheme.* Considering two neighbouring states W_L and W_R, the Rusanov [29] flux reads

$$F(W_L, W_R) = \frac{1}{2}\left(\mathcal{F}(W_L) + \mathcal{F}(W_R)\right) - \frac{\max(\Lambda_R, \Lambda_L)}{2}(W_R - W_L),$$

where $\Lambda_k = \Lambda_k(W_k)$ is the spectral radius of the convection matrix $\nabla_W \mathcal{F}(W_k)$, that is

$$\max(\Lambda_R, \Lambda_L) = \max_{k=L,R}(\mid u_k \pm c_k \mid),$$

where the sound speed c_k is given by (27). Every time step t^n is computed according to the CFL constraint: $\Delta t^n = C\frac{\Delta x}{\max(\Lambda_R, \Lambda_L)}$, with C such as $0 < C < \frac{1}{2}$.

3.1.2. *VFRoe-ncv scheme.* The VFRoe-ncv scheme [6] is an approximation of the Godunov scheme. It consists in considering a linearization of the model. Considering a change of variable for regular solutions

$$W \mapsto V = \Psi^{-1}(W),$$

with Ψ a $\mathcal{C}^1$-diffeomorphism, the system is rewritten under a nonconservative form

$$\partial_t V + A(V)\partial_x V = 0, \tag{40}$$

with $A(V) = (\nabla_V \Psi)^{-1} \nabla_W \mathcal{F}(\nabla_V \Psi)$ the new convection matrix. For two given states V_L and V_R, the linearization is performed around the arithmetic mean $\bar{V} = \frac{V_L+V_R}{2}$.

Thus the numerical flux is defined with the exact solution of the Riemann problem associated to the following linear system

$$\partial_t V + A(\bar{V})\partial_x V = 0.$$

Let $\mathcal{V}(\frac{x}{t} = 0; V_L, V_R)$ be this solution. We get the numerical flux:

$$F(W_L, W_R) = \mathcal{F}(\Psi(\mathcal{V}(x/t = 0, V_L; V_R))),$$

and the linear problem solution is given by

$$\mathcal{V}(x/t = 0, V_L; V_R) = V_L + \sum_{\bar{\beta}_i \leq 0} \bar{\gamma}_i \bar{r}_i,$$

where $(\bar{\beta}_i)_i$ are the eigenvalues of $A(\bar{V})$, $(\bar{r}_i)_i$ its eigenvectors and $(\bar{\gamma}_i)_i$ the coefficients which are solutions of the system $\Delta V = \sum_i \bar{\gamma}_i \bar{r}_i$, with $\Delta V = V_R - V_L$. To avoid the appearance of any non-physical shock, the numerical flux is corrected by an additional diffusive term [14], leading to

$$F(W_L, W_R) = \mathcal{F}(\Psi(\mathcal{V}(x/t = 0, V_L; V_R))) - \frac{\delta}{2}(W_R - W_L), \tag{41}$$

where

$$\delta = \begin{cases} \min(-(u+c)_L, (u+c)_R), & \text{if } (u+c)_L < 0 \text{ and } (u+c)_R > 0, \\ \min(-(u-c)_L, (u-c)_R), & \text{if } (u-c)_L < 0 \text{ and } (u-c)_R > 0, \\ 0, \quad \text{else.} \end{cases} \tag{42}$$

3.1.3. *Relaxation scheme.* The principle of relaxation schemes is to enlarge the system and to relax the nonlinearities (coming from the complex pressure and energy terms), in a way such as all the characteristic fields are linearly degenerate. Doing so, the computations of the solution are explicit and a proper relaxation term allows to recover the initial system solutions. Following for instance [8, Theorem 6], the enlarged system reads

$$\begin{cases} \partial_t(\rho Y) + \partial_x(\rho Y u) = 0, \\ \partial_t(\rho y_g) + \partial_x(\rho y_g u) = 0, \\ \partial_t \rho + \partial_x(\rho u) = 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + \Pi) = 0, \\ \partial_t(\rho \Sigma) + \partial_x(\rho u \Sigma + u \Pi) = 0, \\ \partial_t(\rho \mathcal{T}) + \partial_x(\rho \mathcal{T} u) = \frac{1}{\epsilon}\rho(\tau - \mathcal{T}). \end{cases} \tag{43}$$

Here the quantity $\mathcal{T}$ is such that for all x, $\mathcal{T}(0,x) = \tau(0,x)$ and ϵ is a relaxation parameter. The pressure term is relaxed in the following sense

$$\Pi = p(\mathcal{T}, e, Y, y_g) + a^2(\mathcal{T} - \tau), \tag{44}$$

while the relaxed energy reads

$$\Sigma = e + \frac{u^2}{2} + \frac{\Pi^2 - (p(\mathcal{T}, e, Y, y_g))^2}{2a^2}, \tag{45}$$

with a a parameter chosen such that

$$a > \max\left(\frac{c_l(\tau_l, e_l, Y_l, y_g)}{\tau_l}, \frac{c_r(\tau_r, e_r, Y_r, y_g)}{\tau_r}\right). \tag{46}$$

This above condition, referred as Whitham condition, ensures the hyperbolicity of the relaxed system and well-ordered waves. Finally, considering two states W_L and W_R at a given interface, the two-point numerical flux is

$$F(W_L, W_R) = \left(\frac{Yu}{\tau}, \frac{u}{\tau}, \frac{u^2}{\tau} + \Pi, \frac{u\Sigma}{\tau} + u\Pi \right), \tag{47}$$

where Y, τ, u, Σ are the components of the solution of the enlarged Riemann problem at the considered interface.

3.2. **Computation of the internal energy.** The implementation of the above numerical fluxes requires to handle transits from conservative variables W to observable quantities e.g. pressure and temperature fields and vice versa. Depending on the considered phasic equations of state, these changes of variables can be non explicit and require most of the time an implicit solver. The aim of this section is to provide detailed algorithms for the computation of the internal energy e of the mixture, starting from a mixture state with specific volume $\bar{\tau}$, fraction vector $\bar{Y}$ and pressure $\bar{p}$. Similar algorithms can be adapted when considering an initial temperature $\bar{T}$.

Depending on the phasic equations of state, the algorithms differ. We focus on two configurations: first, all the phases are depicted by Stiffened Gas laws, second, the gaseous phases follow SG laws while the liquid is modeled by a NASG-CK law.

3.2.1. *Computation for a 3 SG mixture.* Let $(\bar{\tau}, \bar{p}, \bar{Y})$ be a given state. The question is to compute the associated internal energy e, which is the root of the function $\mathcal{P}$, defined by

$$\mathcal{P}(e) = p(\bar{\tau}, e, \bar{Y}, y_g) - \bar{p}. \tag{48}$$

Using the mixture pressure definition (18) and and the expressions of the Stiffened Gas pressure and temperature, this function can be written as a third-degree polynomial

$$\mathcal{P}(e) = \bar{A}e^3 + \bar{B}e^2 + \bar{C}e + \bar{D}. \tag{49}$$

We precise here the exact coefficients, for $k, k', k'' \in \{l, g, v\}$ pairwise distinct (note that they sligthly differ from those of [19]):

$$
\begin{aligned}
\bar{A} &= \sum_{k,k',k''} z_k y_k (\gamma_k - 1) \frac{z_{k'}}{C_{k'}} \frac{z_{k''}}{C_{k''}} \frac{1}{\tau}, \\
\bar{B} &= \sum_{k,k',k''} -\alpha_k y_k \frac{1}{C_{k'} C_{k''}} \Bigg(z_{k'} z_{k''} \Big(\Pi_k \gamma_k + \frac{y_k Q_k (\gamma_k - 1)}{\alpha_k \tau} \Big) \\
&\qquad + \frac{z_k (\gamma_k - 1)}{\alpha_k} \frac{1}{\tau} (z_{k'} \omega_{k''} + z_{k''} \omega_{k'}) \Bigg) - z_k y_k \frac{z_{k'} z_{k''}}{C_{k'} C_{k''}}, \\
\bar{C} &= \sum_{k,k',k''} \alpha_k y_k \frac{1}{C_{k'} C_{k''}} \Bigg(\frac{z_k (\gamma_k - 1)}{y_k} \frac{1}{\tau} \omega_{k'} \omega_{k''} \\
&\qquad + \Big(\frac{y_k Q_k (\gamma_k - 1)}{\alpha_k} \frac{1}{\tau} + \Pi_k \gamma_k \Big) \Big(z_{k'} \omega_{k''} + z_{k''} \omega_{k'} \Big) \Bigg) \\
&\qquad + \Big(z_k y_k \frac{1}{C_{k'} C_{k''}} (z_{k'} \omega_{k''} + z_{k''} \omega_{k'}) \Big), \\
\bar{D} &= \sum_{k,k',k''} -\alpha_k y_k \frac{1}{C_{k'} C_{k''}} \Big(\frac{y_k Q_k (\gamma_k - 1)}{\alpha_k} \frac{1}{\tau} + \Pi_k \gamma_k \Big) \omega_{k'} \omega_{k''} \\
&\qquad - y_k z_k \frac{1}{C_{k'} C_{k''}} \omega_{k'} \omega_{k''},
\end{aligned}
\tag{50}
$$

where $\omega_k = y_k Q_k + \alpha_k \Pi_k \tau$. Remark that the coefficients $\bar{A}$ to $\bar{D}$ are explicitly defined by the data $(\bar{\tau}, \bar{p}, \bar{Y})$, the notation $\bar{x}$ being omitted for sake of readability. The algorithm reads as follows.

- For a given state $(\bar{\tau}, \bar{p}, \bar{Y})$, compute the coefficients (50) of $\mathcal{P}$.
- Compute the discrimimant Δ of the derivative of $\mathcal{P}$.

I) If $\Delta \leq 0$, the equation (49) admits an unique solution, which is computed with a Newton's method.

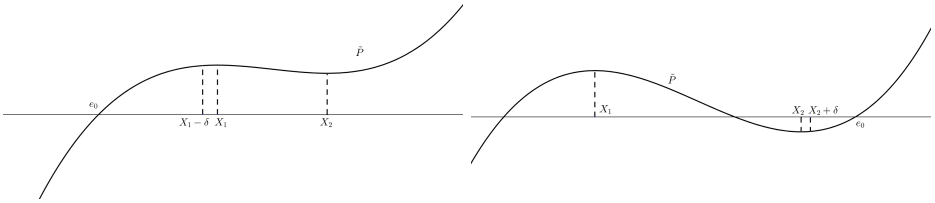
II) If $\Delta > 0$, let X_1, X_2 be the ordered roots of $\mathcal{P}'$, such as $X_1 < X_2$. They correspond to the local extrema of $\mathcal{P}$, see Figure 4.

Let $\delta = 10^9$ and $\gamma = 100$ two parameters.

i) If $\mathcal{P}(X_2)\mathcal{P}(X_2 + \gamma) \leq 0$, there exists a unique root e_0 such as $e_0 > X_2$, see Figure 4-right. We make use of a Newton method with initial condition $X_2 + \delta$ and verify that the solution is greater than X_2. In case of non convergence or if the solution is lower than X_2, a bisection method is launched in the range $[X_2, X_2 + \gamma]$ to ensure to find the correct root.

ii) If $\mathcal{P}(X_2)\mathcal{P}(X_2 + \gamma) > 0$, $\mathcal{P}$ admits only one root e_0 such as $e_0 < X_1$, see Figure 4-left. Indeed, we can't have $X_1 < e_0 < X_2$ because it wouldn't be a unique root. Then we proceed like previously with a Newton method starting from $X_2 - \delta$.

The parameters δ and γ are set arbitrarily and may be modified to optimize the algorithm. Note that the case II)-ii) excludes the possibility of $\mathcal{P}(X_i) = 0$, $i = 1$ or 2. Indeed this situation would correspond to the existence of two roots which have not been encountered in practical simulations.



(A) $\mathcal{P}$ admits one root. (B) $\mathcal{P}$ admits three roots.

FIGURE 4. Computation of the internal energy for a mixture of three SG. Typical graph of $\mathcal{P}$ in the two cases where $\Delta > 0$.

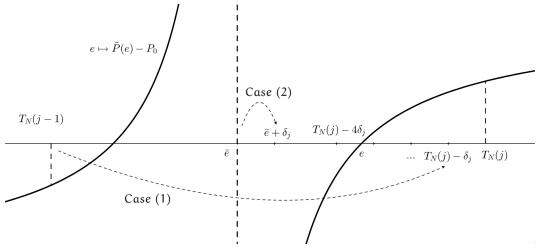


FIGURE 5. Computation of the internal energy for a mixture of two SG and a NASGK-CK liquid. Typical graph of $\mathcal{P}$.

3.2.2. *Computation for a mixture of 2 SG and a NASG-CK liquid phase.* In this configuration, the expression $\mathcal{P}(e) = P(\bar{\tau}, e, \bar{Y}) - \bar{p}$ is no more explicit due to the NASG-CK EoS. Computing the root of $\mathcal{P}(e)$ is tedious because the graph of $\mathcal{P}$ is basically an hyperbola, see Figure 5. To handle this difficulty, a bisection method is preferred (compared to a secant or a Newton method to ensure to find the root in the desired range). The algorithm reads as follows.

- Consider a range of internal energy $[e_{\min}, e_{\max}]$.
- Provide a discretization of $[e_{\min}, e_{\max}]$ with $e_j = e_{\min} + j\Delta e$, $\Delta e = (e_{\max} - e_{\min})/N$.
- Set $\delta_j = \frac{e_j - e_{j-1}}{d}$.
- For $j = N, N-1, ..., 2$, find the first index j_0 such as $\mathcal{P}(e_{j_0-1})\mathcal{P}(e_{j_0}) < 0$.
- Launch a bisection algorithm on $[e_{j_0-1}, e_{j_0}]$.
- If the bisection fails, there must exist a real $\tilde{e} \in [e_{j_0-1}, e_{j_0}]$ where $\mathcal{P}$ is undefined. Hence two cases must be considered.
  (1) If the previous iterations indicate that the root $\bar{e}$ is in the neighbourhood of e_{j_0-1} (resp. e_{j_0}), relaunch the bisection on the ranges $[e_{j_0-1}, e_{j_0-1}+\delta_j]$, $[e_{j_0-1}+\delta_j, e_{j_0-1}+2\delta_j]$,... until convergence is reached (resp. $[e_{j_0}, e_{j_0} - \delta_j]$, $[e_{j_0} - \delta_j, e_{j_0} - 2\delta_j]$,...).
  (2) Else the last iteration e_∞ provides an approximation of $\bar{e}$. If $e_\infty < \bar{e}$ (resp. $e_\infty > \bar{e}$), relaunch the bisection on the range $[e_{j_0-1}, e_\infty]$ (resp. on $[e_\infty, e_{j_0}]$).

In practice we choose $d = 10$ and $N = 10^3$. Higher values of N can be necessary on simulations at high pressure, see Section 4, Figure 4.

Remark 4. *In order to reduce costs of this algorithm, a reminder can be implemented to launch first a bisection method around the solution found on the previous cell if it detects two similar consecutive states. Let e_{old} and e_{new} be the values of the internal energies on consecutive cells. At the beginning of the next computation of the energy, if $|e_{old} - e_{new}| < 1$, we first launch a bisection method on the interval $[e_{new} - 10; e_{new} + 10]$. If the solution is negative or if the bisection algorithm does not converge, it goes back to previous algorithm.*

3.3. **Source term approximation.** The second step of the splitting strategy corresponds to the source term approximation.

As BGK-like source term is concerned, trajectories can be explicitly defined, see Proposition 3, as soon as the equilibrium vector Y_{eq} is determined. Two difficulties arise. First, the uniqueness of this equilibrium is unclear due to Remark 1. Moreover when complex EoS are considered, the maximization process of the mixture entropy (16) under the constraints (13)-(14) has to be performed with an appropriate optimization algorithm. We refer to [28] which proposes a Broyden method to compute the equilibrium for a mixture of two stiffened gases and a NASG-Chemkin law for the liquid phase.

We focus in this section on the the gradient of entropy source term Γ_2.

In order to capture the long-time asymptotic equilibria, an implicit approximation is considered. However the complexity of the source term Γ_2 makes a full implicit discretization out of reach, especially when considering NASG-CK EoS. We propose hereafter a semi-implicit Euler algorithm, based on a Broyden method [5] to evaluate the implicit part.

On the time range $[t^{n+1,*}, t^{n+1}]$, one considers the Cauchy problem (39) with initial condition $W^{n+1,*}$ computed from the convective step. The implicit Euler method boils down to find the root of the nonlinear functional $G : [0,1]^4 \to \mathbb{R}$

$$G(Y) = Y - \Delta t Y(1-Y)\nabla_Y \sigma(\tau_{n+1;*}, e_{n+1;*}, Y, y_g) - Y_{n+1;*}, \tag{51}$$

To do so, we make use of an iterative Broyden algorithm, which requires to compute the Jacobian matrix $J(Y)$ of $G(Y)$ with coefficients

$$\big(J(Y)\big)_{i,j} = \partial_{Y_j} Y_i - \Delta t \lambda_i \partial_{Y_j} \left[Y_i(1-Y_i)\partial_{Y_i}\sigma(\tau_{n+1;*}, e_{n+1;*}, Y, y_g)\right], \quad 1 \le i,j \le 4, \tag{52}$$

where Y_i (resp. λ_i) stands for the $i-$th coefficient of Y (resp. λ). One remarks that only the initialization step requires a jacobian computation. The algorithm consists in computing the sequence $(Y_k)_{k\in\mathbb{N}}$ given by

$$\begin{cases} Y_k = Y_{k-1} - J_{k-1}^{-1} G(Y_{k-1}), \\ J_k^{-1} = J_{k-1}^{-1} + \frac{\Delta Y_k - J_{k-1}^{-1}\Delta G_k}{\Delta Y_k^T J_{k-1} \Delta G_k} (\Delta Y_k)^T J_{k-1}^{-1}, \\ \Delta Y_k = Y_k - Y_{k-1}, \\ \Delta G_k = G(Y_k) - G(Y_{k-1}), \end{cases} \tag{53}$$

until $\|Y_k - Y_{k-1}\| < \eta$, where η is a tolerance ($\eta = 10^{-10}$ in practice). The initialization requires to choose Y_0 to Y_n given by the previous time step computation.

4. Numerical results

This Section provides two types of numerical experiments. First validation test cases assess the good approximation of the convective part of the model (26). They consist the in approximation of exact Riemann problem solutions at low and high

pressure for three-phase mixture with either SG or NASG-CK EoS (for the liquid phase).

A comparison of CPU costs is presented in Section 4.1.3, highlighting the performances of the relaxation scheme compared to the VFRoe-ncv scheme.

Finally a global simulation, accounting for the contribution of the gradient of entropy source term, is presented.

4.1. **Infinitely slow relaxation.** These test cases correspond to the validation of the approximation of the convective part (when the source terms are inactive). For two different sets of phasic EoS, we compare the numerical results of the different numerical fluxes presented in Section 3.1 on Riemann problems at low and high pressure. In both cases, the Riemann problem solutions are built according to Section 2.2.2. Considering a left state W_L, the state W_1 is computed considering that the first nonlinear wave is a ghost wave. Then the contact wave allows to deduce the state W_2, the pressure and velocity being preserved through the contact contrary to Y. Finally a shock wave of velocity ξ separates the state W_2 and W_R while the fractions Y are preserved.

4.1.1. *Mixture of three Stiffened Gases.* Tables 1 and 2 present the exact Riemann data in the low and high pressure case respectively when considering that the three phases are depicted by Stiffened Gas laws with parameters (6). The four constant states are depicted in terms of their primitive variables, namely $Z = (y_l, y_g, \alpha_l, z_l, z_g, \tau, u, p)^T$.

$\xi =$ 708.41563589800251	$Z_L = Z_1$	Z_2	Z_R
y_l	0.91826194646564185	0.89784395822033747	0.89784395822033747
y_g	5.0000000000000003E-002	5.9999999999994613E-002	5.9999999999994613E-002
α_l	1.6767800121816667E-002	1.0000000000001008E-002	1.0000000000001008E-002
z_l	0.41969031490727782	0.30000000000002064	0.30000000000002064
z_g	8.8350466782145878E-002	9.8999999999997021E-002	9.8999999999997021E-002
τ	5.4427805491776261E-002	6.8863503931918257E-002	7.0000000000000007E-002
u	10.0	10.0	-1.5263757834575244
p	1.8668002620104561E5	1.8668002620104561E5	6.9779191756698478E4

TABLE 1. Mixture of three SG. Data for the low-pressure Riemann problem.

The three numerical fluxes are compared with the same CFL parameter set to 0.45, on several test cases that are set on the domain $[0, 1]$. Figures 8-9-12-13 were obtained with 500 cells. The convergence results, obtained for a final time $t = 10^{-3}$s., see Figures 6 and 7, show that the VFRoe-ncv and the relaxation schemes achieve similar convergence rates (of about 1/2).

Figure 8 presents the profiles of density, velocity, pressure and fractions obtained by the relaxation scheme in the low-pressure configuration. One observes the good approximations of the fractions. Some oscillations are present in the pressure and velocity profiles. These spurious oscillations are probably due to the approximation of the ghost wave and mainly due to the nonlinear EoS. These oscillations also

$\xi =$ 578.35007234359045	$Z_L = Z_1$	Z_2	Z_R
y_l	0.39999999999999997	0.37999999999999906	0.37999999999999906
y_g	0.29999999999999999	0.33000000000000052	0.33000000000000052
α_l	8.0000000000000071E-002	6.9999999999999840E-002	6.9999999999999840E-002
z_l	0.25000000000000011	0.21999999999999936	0.21999999999999936
z_g	9.9999999999999978E-002	0.12000000000000005	0.12000000000000005
τ	6.0000000000000010E-003	5.0000000000000062E-003	5.3000000000000000E-003
u	100.0	100.0	71.298995659385199
p	1.4999999999999996E7	1.4999999999999996E7	1.2254174499466641E7

TABLE 2. Mixture of three SG. Data for the high-pressure Riemann problem.

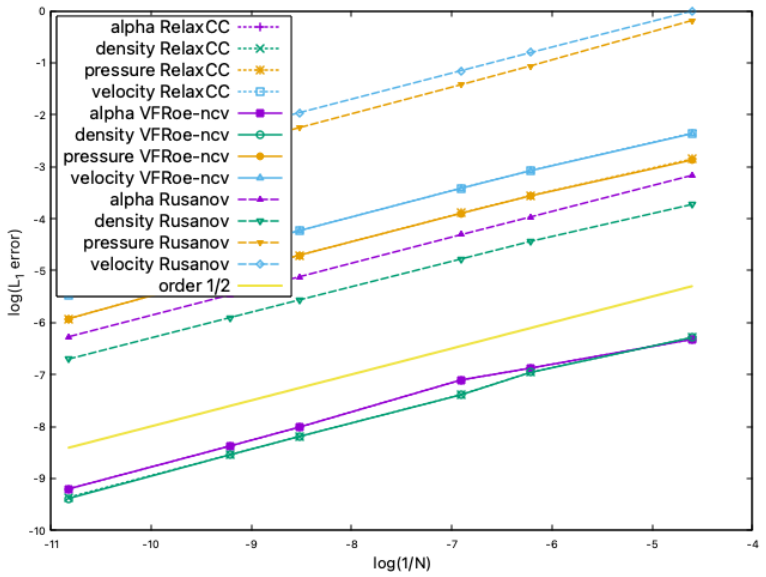


FIGURE 6. Mixture of three Stiffened Gases. L^1-convergence for the low-pressure Riemann problem.

appear in the high-pressure configuration, see Figure 9, while the fraction profiles are still well captured.

4.1.2. *Mixture of two Stiffened Gases with a NASG-CK liquid phase.* Tables 3 and 4 present the exact Riemann data in the low and high pressure cases respectively when considering that the liquid phase is depicted by a NASG-CK law with parameters (10).

The convergence results in Figures 10 and 11 are obtained with the same discretization parameters and CFL condition as in paragraph 4.1.1. One observes that the VFRoe-ncv and the relaxation schemes achieve similar convergence rates.

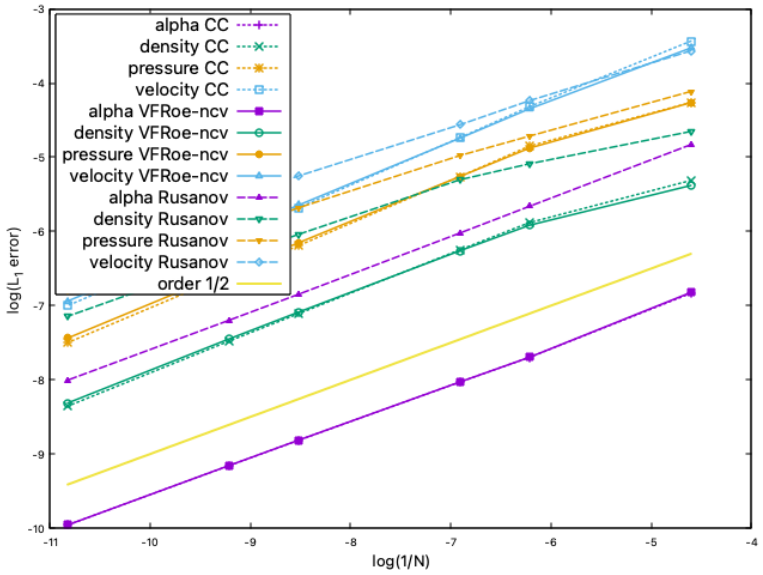


FIGURE 7. Mixture of three Stiffened Gases. L^1-convergence for the high-pressure Riemann problem.

$\xi =$ 1027.3711820835272	$Z_L = Z_1$	Z_2	Z_R
y_l	0.91841879730033971	0.89999999102958528	0.89999999102958528
y_g	5.0000000000000003E-002	5.5000004933728031E-002	5.5000004933728031E-002
α_l	1.6376791114071865E-002	1.4999998527357117E-002	1.4999998527357117E-002
z_l	0.92743215703897408	0.90000000855046036	0.90000000855046036
z_g	1.1475280368993632E-002	9.9999991449539437E-003	9.9999991449539437E-003
τ	0.19492558898696019	0.19500001720076998	0.19700000000000001
u	100.0	100.0	90.488583338128308
p	2.4530790395664933E5	2.4530790395664933E5	2.0007399146972221E5

TABLE 3. Mixture of two Stiffened Gases with a NASG-CK liquid phase. Data for the low-pressure Riemann problem.

The profiles of density, velocity, pressure, temperature and fractions are given in Figure 12 (resp. Figure 13) for the low-pressure (resp. high) configuration with the relaxation scheme. Similar observations can be done. The fractions are well captured whereas oscillations, due to the nonlinearity of the pressure law (with respect to the internal energy), arise. Note that considering the implicit NASG-CK EoS increases the amplitude of the oscillations, at least for the low-pressure test cases.

4.1.3. *Comparison between VFRoe-ncv and the relaxation scheme.* Although the previous section shows that the convergence for the VFRoe-ncv and relaxation schemes are similar, some remarks can be made on their performances.

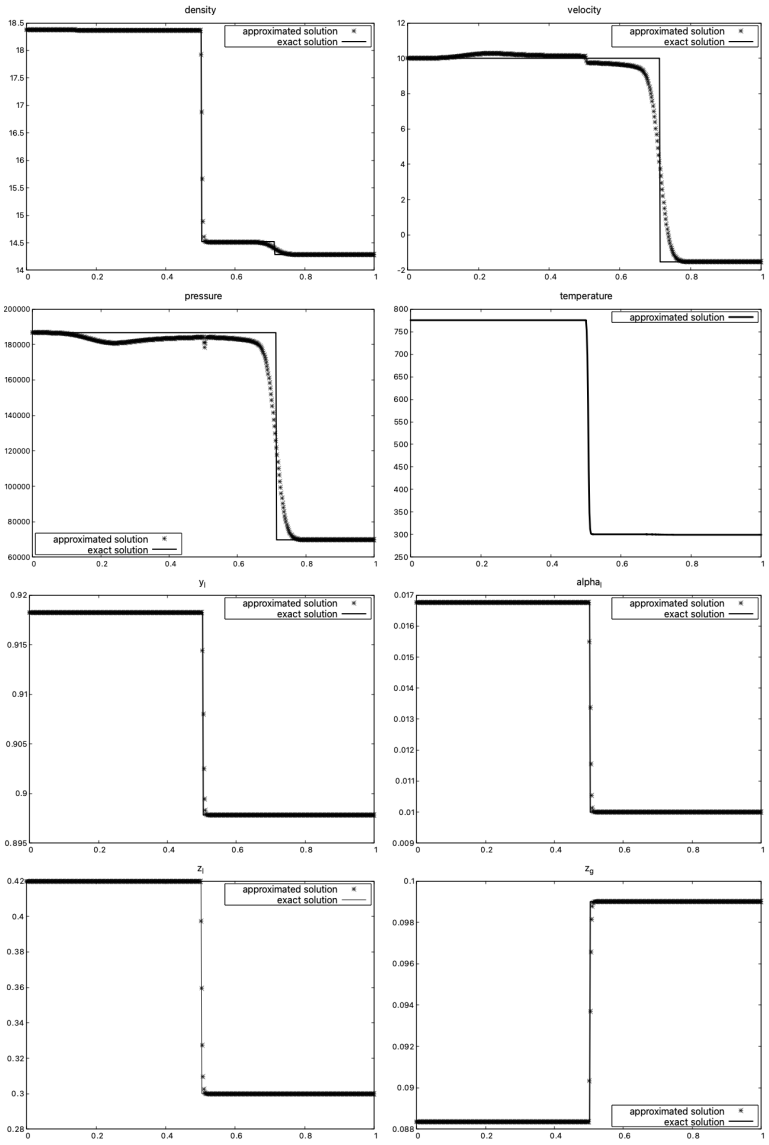


FIGURE 8. Mixture of three Stiffened Gases. Low-pressure test case and comparison with the exact solution. From top left to bottom right, profiles of density, velocity, pressure, temperature, y_l, α_l, z_l and z_g.

As CPU time cost is concerned, a comparison of the two scheme performances is provided in Figures 14 and 15 for the mixture of three SG and a mixture of two SG and a NASG-CK liquid respectively. Obviously the VFRoe-ncv scheme is much more CPU time consuming. This is due to the fact that it requires more internal energy computations. These are done using the algorithms provided in Sections 3.2.1 and 3.2.2. *A contrario* the relaxation scheme only requires two internal energy

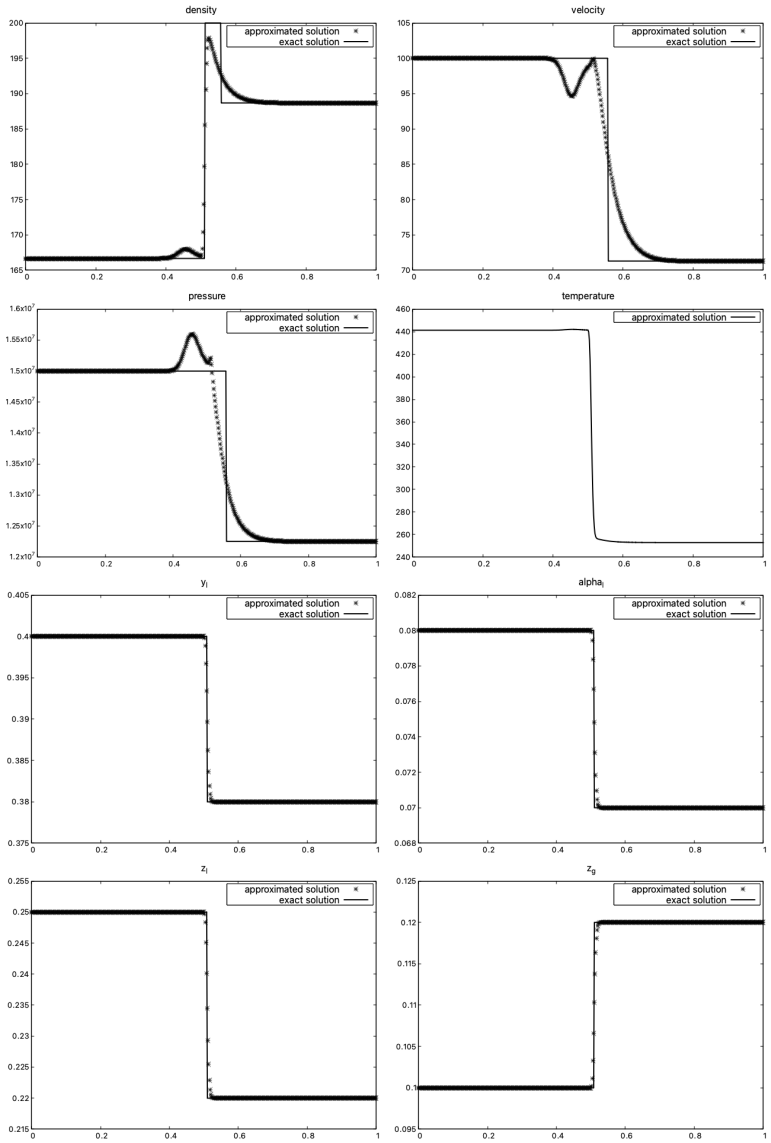


FIGURE 9. Mixture of three Stiffened Gases. High-pressure test case and comparison with the exact solution. From top left to bottom right, profiles of density, velocity, pressure, temperature, y_l, α_l, z_l and z_g.

computations: one at the beginning of each time step to go from conservative to primitive variables, the second at the end, for the inverse change of variables.

Of course, the comparison is even worth when considering a NASG-CK EoS for the liquid phase, since it is not explicit, see Section 3.2.2.

$\xi =$ 1591.8798489453186	$Z_L = Z_1$	Z_2	Z_R
y_l	0.92020382010222246	0.89999998651866320	0.89999998651866320
y_g	5.0000000000000003E-002	5.3000007145108524E-002	5.3000007145108524E-002
α_l	0.68595071360084603	0.59999996404976996	0.59999996404976996
z_l	0.95997763551798010	0.90000000093700905	0.90000000093700905
z_g	6.5876209523389063E-003	7.9999999250392681E-003	7.9999999250392681E-003
τ	4.8078440722228851E-003	5.0000002246889472E-003	5.0699999999999999E-003
u	100.0	100.0	79.113750095130015
p	1.7275285041205704E7	1.7275285041205704E7	1.1043330250633653E7

TABLE 4. Mixture of two Stiffened Gases with a NASG-CK liquid phase. Data for the high-pressure Riemann problem.

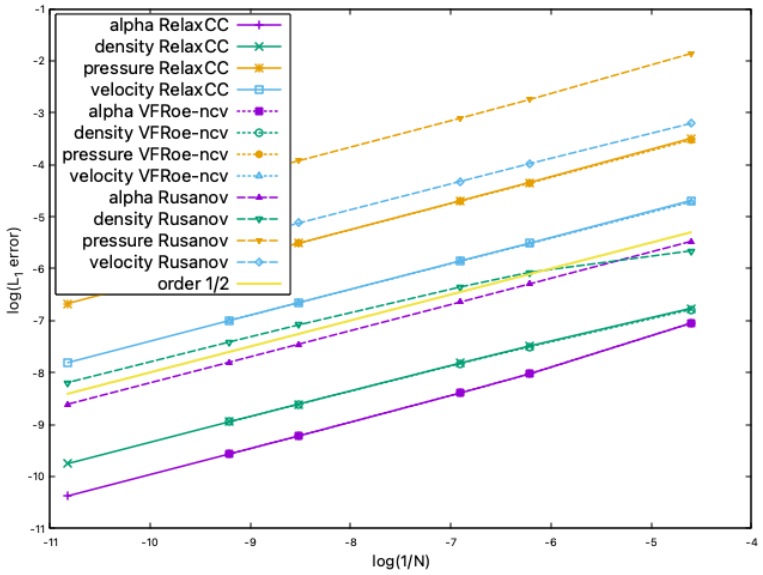


FIGURE 10. Mixture of two Stiffened Gases with a NASG-CK liquid phase. L^1-convergence for the low-pressure Riemann problem.

4.2. **Global out-of-equilibrium simulation.** This final section provides numerical results of the fractional step method, using the relaxation scheme for the convective part and the Broyden algorithm for the source terms. The two source terms of Section 2.3 are compared and several (constant) relaxation time λ as well. We focus on a mixture of three SG in the low-pressure configuration. The initial condition is $Z(0,x) = Z_L \mathbf{1}_{x<0.5} + Z_R \mathbf{1}_{x>0.5}$ with Z_L and Z_R given in Table 1. The computational domain $[0,1]$ contains 1000 cells and the CFL is again 0.45. The final time is $t = 10^{-4}$. The source term Γ_1 requires relaxation time λ between 2.10^3 and 5.10^3 to avoid the appearance of non admissible states. One observes on Figures 16 the impact of the relaxation parameter on the profiles of velocity

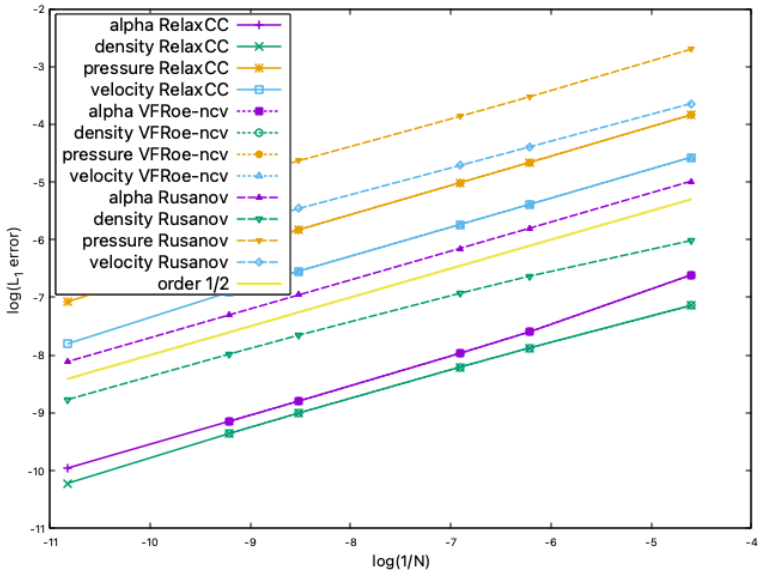


FIGURE 11. Mixture of two Stiffened Gases with a NASG-CK liquid phase. L^1-convergence for the high-pressure Riemann problem.

and pressure mainly. Observe also that the fraction y_l is far from the associated equilibrium Y_{eq}, contrary to the volume fraction α_l. Hence the simulation is clearly out-of-equilibrium.

The source term Γ_2 modifies the density and velocity profiles with a higher sensitivity for larger values of λ. Some intermediate states seem to be well captured, notably in the profiles of the fractions y_l and α_l.

5. Conclusion

This study is focused on the numerical simulation of the so-called homogeneous relaxation model for a three-phase flow with miscible constraints. As the numerical approximation is concerned, the work on the convective part leads to a preference for the relaxation scheme for CPU time and robustness reasons, although convergence results are similar for the relaxation and the VFRoe-ncv schemes. The computation of the internal energy plays a major role in the CPU time cost and robustness, that is why algorithms are detailed since they invlove tricky computations. Secondly, as the thermodynamical modelling is concerned, both the thermodynamical equilibrium of the three-phase mixture and the relaxation towards this equilibrium are analyzed. The good definition of the equilibrium fractions and its constraints are fundamental features. We notably have address the question of disappearance of phases and provide characterizations of the phasic states when one of the phase is absent. When considering the time relaxation towards the thermodynamical equilibrium, two types of source terms have been compared. The BGK type one provides an efficient simulation, as soon as the computation of the equilibrium is reachable, which is a strong constraint. Moreover, it requires that relaxation time scales must be equal, which is again a strong assumption. On the other hand, the gradient type source term is more versatile, despite a far more complex analysis, that leads to

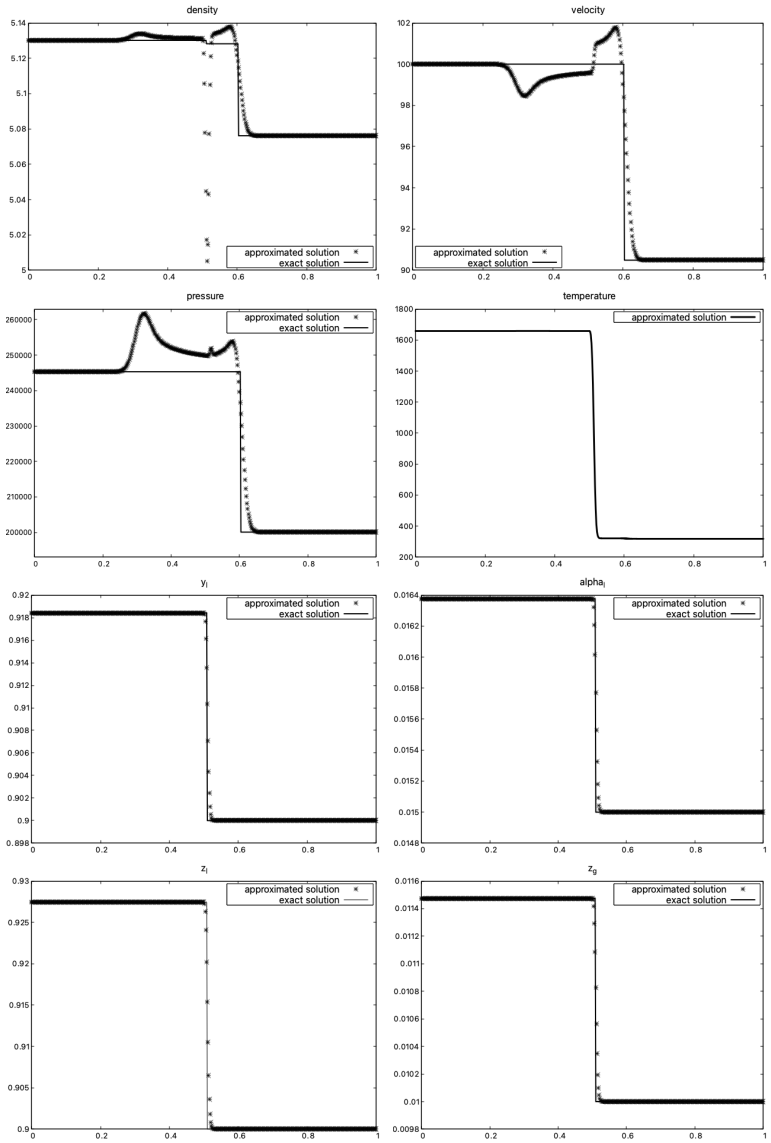


FIGURE 12. Mixture of two Stiffened Gases and a NASG-CK liquid. low-pressure test case and comparison with the exact solution. From top left to bottom right, profiles of density, velocity, pressure, temperature, y_l, α_l, z_l and z_g.

numerical difficulties. These pros and cons are highlighted on a global simulation in the last part.

Acknowledgments

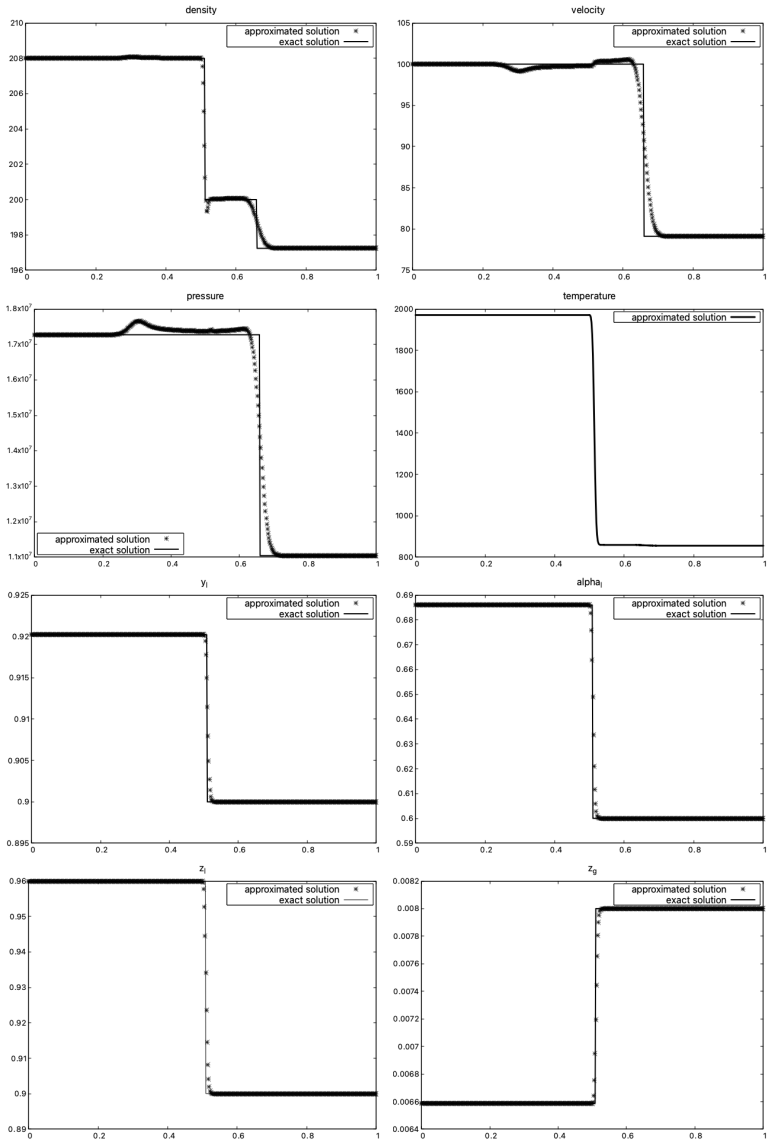


FIGURE 13. Mixture of two Stiffened Gases and a NASG-CK liquid. high-pressure test case and comparison with the exact solution. From top left to bottom right, profiles of density, velocity, pressure, temperature, y_l, α_l, z_l and z_g.

This work has received the financial support from the ANR MoHyCon and the CNRS project Needs M2SIR. Part of the work has benefited from fruitful discussions with Mr Hérard from EDF Lab Chatou.

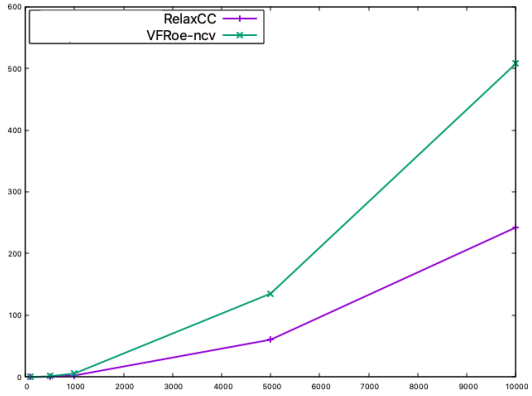


FIGURE 14. Mixture of three Stiffened Gases. Comparison of CPU time costs with respect to the number of cells for the VFRoe-ncv and the relaxation schemes.

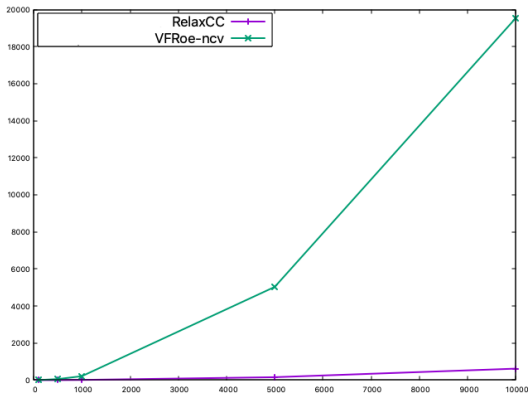


FIGURE 15. Mixture of two Stiffened Gases with a NASG-CK liquid phase. Comparison of CPU time costs with respect to the number of cells for the VFRoe-ncv and the relaxation schemes.

APPENDIX A. EQUILIBRIUM COMPUTATION FOR 3 STIFFENED GAS

Let (τ, e, y_g) be a given state. We assume that the equilibrium Y_{eq} is reached in the interior of $[0,1]^4$, such that it is characterized by (22). Following [1], one characterizes the equilibrium considering first the thermal equilibrium, then the mechanical one and, to finish, the chemical potential equalities. According to the definition (5) of the Stiffened Gas temperature, the sum of the phasic temperatures, weighted by the mass fractions y_k, reads

$$\sum_{k=l,g,v} y_k C_k T_k = e - \sum_k y_k Q_k - \sum_k \alpha_k \Pi_k \tau, \tag{54}$$

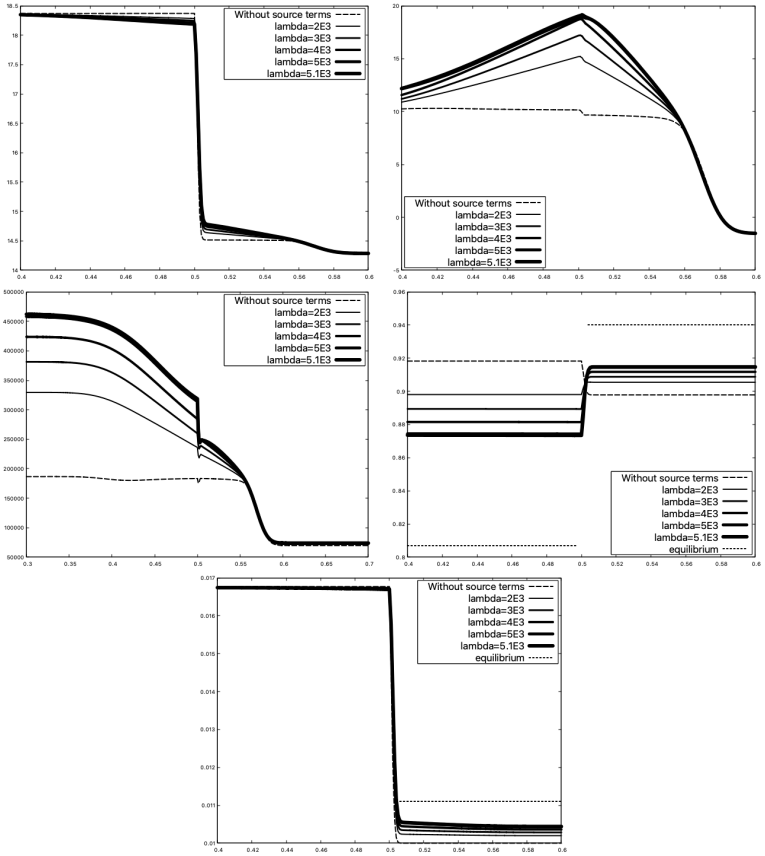


FIGURE 16. Global simulation for a mixture of three SG in the low-pressure configuration with the BGK-like source term Γ_1. Comparison of the impact of the relaxation time. From top left to bottom right, profiles of density, velocity, pressure, y_l, α_l.

where the constraints (20) have been used. The thermal equilibrium $T_l = T_g = T_v = \bar{T}$ gives then

$$\bar{T}(y_v, \alpha_v) = \frac{e - Q(y_v) - \Pi(\alpha_v)\tau}{C(y_v)}, \tag{55}$$

where $C(y_v) = \sum_k y_k C_k$, $Q(y_v) = \sum_k y_k Q_k$ and $\Pi(\alpha_v) = \sum_k \alpha_k \Pi_k$. Using the intensive constraints (13)-(14), one observes that the coefficients $C(y_v)$ and $Q(y_v)$ are solely functions of the vapor mass fraction y_v, while $\Pi(\alpha_v)$ depends only on the volume fraction α_v. Hence the equilibrium temperature $\bar{T}(y_v, \alpha_v)$ does not depend on the energy fractions. This allows to split the computations in two steps: first determine the pair (y_v, α_v) and then, determine the energy fractions (z_l, z_g).

We now turn to the mechanical equilibrium to express α_v as a function of y_v. Indeed the mechanical equilibrium corresponds to $p_l - (p_g + p_v) = 0$ or equivalently to $\alpha_v(1-\alpha_v)[p_l - (p_g + p_v)] = 0$. It turns out that $F_{y_v}(\alpha_v) = \alpha_v(1-\alpha_v)[p_l - (p_g + p_v)]$

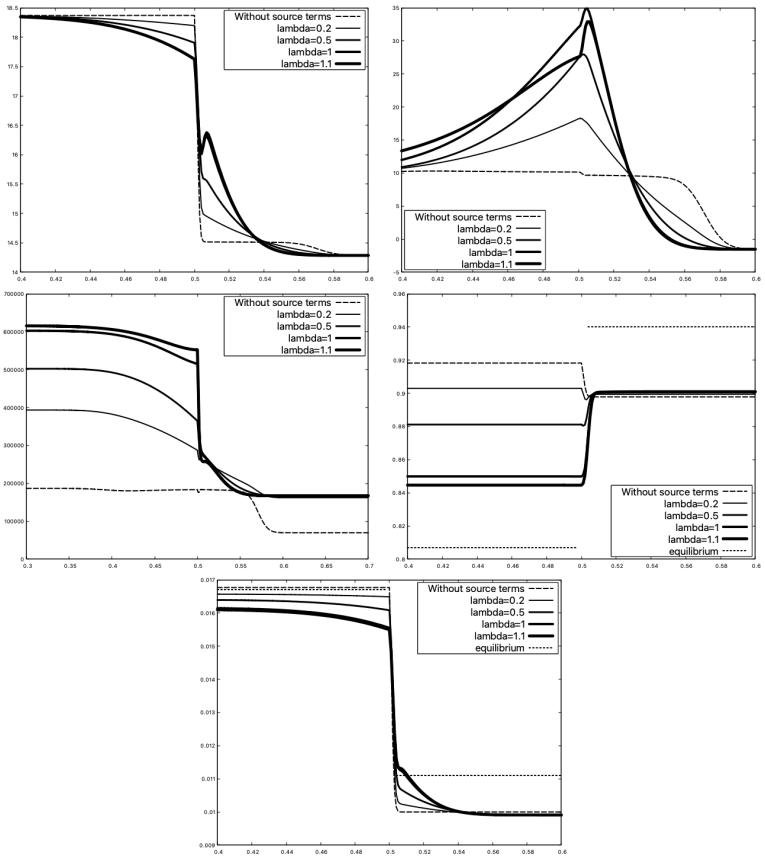


FIGURE 17. Global simulation for a mixture of three SG in the low-pressure configuration with the gradient entropy source term Γ_2. Comparison of the impact of the relaxation time. From top left to bottom right, profiles of density, velocity, pressure, y_l, α_l.

is a second order polynomial is α_v which reads

$$F_{y_v}(\alpha_v) = A_F\alpha_v^2 + B_F\alpha_v + C_F, \tag{56}$$

with coefficients

$$\begin{aligned} A_F &= (\beta+1)\Pi_0, \\ B_F &= -\Pi_0(\beta_v+\beta_g+1) - \beta(\rho(e-Q)-\Pi_l), \\ C_F &= (\beta_v+\beta_g)(\rho(e-Q)-\Pi_l), \\ \Pi_0 &= \Pi_g + \Pi_v - \Pi_l, \\ \beta_k &= (\gamma_k-1)C_k y_k, \\ \beta &= \sum_k \beta_k. \end{aligned} \tag{57}$$

It remains to determine a root α_v of F_{y_v}, which only depends on y_v, according to the coefficient definitions (57). In order to assess the nonnegativity of the mixture temperature $\bar{T}(y_v, \alpha_v)$, this volume fraction α_v should comply with some constraints.

Considering that $\Pi_g = 0$, $\Pi_v < 0$ and $\Pi_v - \Pi_l < 0$ (which is the case for considered data (6)), the temperature positivity is equivalent to $\rho(e - Q(y_v) - \Pi(y_v)) \geq 0$, that is

$$\alpha_v \geq \frac{\rho(e-Q) - \Pi_l}{\Pi_v - \Pi_l} =: \delta(y_v).$$

Hence one must seek for $\alpha_v \in [\alpha_{v,inf}; 1]$, with $\alpha_{v,inf} = \max(0, \min(1, \delta(y_v)) \in [0; 1]$.

Generally, the equation $F_{y_v}(x) = 0$ does not necessarily admit a solution on this interval. If this happens, we must determine which limit case $\alpha_v = \alpha_{v,inf}$ or $\alpha_v = 1$ maximises the entropy.

Thanks to the concavity of $\alpha_v \mapsto \sigma$, one only has to study the sign of $\frac{\partial \sigma}{\partial \alpha_v}$ on the border, and that sign is the same than the sign of $\Delta p = p_v + p_g - p_l$. Thus we have:

- If $\lim\limits_{\alpha_v \to \alpha_{v,inf}} \Delta p(\alpha_v) < 0$, $\alpha_v = \alpha_{v,inf}$ corresponds to a stable state,
- If $\lim\limits_{\alpha_v \to 1} \Delta p(\alpha_v) > 0$, $\alpha_v = 1$ corresponds to a stable state with only gases.

In practical simulations, we choose to solve first $F_{y_v}(x) = 0$, then verify if we have an unique solution α_v in $[0; 1]$ such as $\bar{T}(y_v, \alpha_v) \geq 0$, and if not we consider the limit cases.

At last, the chemical equilibrium $\mu_l = \mu_v$ allows us to determine $(\bar{y}_v, \bar{\alpha}_v)$ in an implicit way, thanks to F_{y_v}. We can already define $y_{v,max} \in [0; 1 - y_g]$ as the the greatest mass fraction of vapor such as the temperature is positive.

Then we must solve the following equation on $[0; y_{v,max}]$:

$$\Delta\mu(y_v) = \Delta\mu(y_v, \alpha_v(y_v)) = \mu_l(y_v, \alpha_v(y_v)) - \mu_v(y_v, \alpha_v(y_v)) = 0, \tag{58}$$

where

$$\begin{cases} \mu_l(y_v, \alpha_v(y_v)) = Q_l + C_l + \bar{T}(y_v, \alpha_v)\Big(\gamma_l - \ln(C_l T) - \frac{s_l^0}{C_l} - (\gamma_l - 1)\ln\big(\frac{(1-\alpha_v)\tau}{1-y_v-y_g}\big)\Big) \\ \mu_v(y_v, \alpha_v(y_v)) = Q_v + C_v + \bar{T}(y_v, \alpha_v)\Big(\gamma_v - \ln(C_v T) - \frac{s_v^0}{C_v} - (\gamma_v - 1)\ln\big(\frac{\alpha_v \tau}{y_v}\big)\Big) \end{cases},$$

and $\alpha_v(y_v)$ is the solution of $F_{y_v}(x) = 0$. As previously, it is possible not to find $y_v \in]0; y_{v,max}[$ and α_v solutions of this equation. This time we use the concavity of $y_v \to \sigma$ and the fact that the sign of $\frac{\partial \sigma}{\partial y_v}$ is the same one as the sign of $\Delta\mu$ to study the limit cases:

- If $\lim\limits_{y_v \to 0} \Delta\mu(y_v) < 0$, $y_v = 0$ corresponds to a stable state, with only liquid and inert gas, *i.e.* $y_l = 1 - y_g$.
- If $\lim\limits_{y_v \to y_{v,max}} \Delta\mu(y_v) > 0$, $y_v = y_{v,max}$ corresponds to a stable state with only gases, *i.e.* $y_l = 0$.

Finally, once $(\bar{y}_v, \bar{\alpha}_v)$ is determined, we can compute $(\bar{z}_v, \bar{z}_g)$ with the following relations:

$$\bar{z}_k = \frac{(\bar{T}(\bar{y}_v, \bar{\alpha}_v)C_k + Q_k)\bar{y}_k + \Pi_k \bar{\alpha}_k \tau}{e}. \tag{59}$$

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