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A three-phase flow model

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Abstract

We present here a three-fluid three-pressure model to describe three-field patterns or three-phase flows. The basic ideas rely on the counterpart of the two-fluid two-pressure model which has been introduced in the DDT (deflagration to detonation theory) framework, and has been more recently extended to liquid-vapour simulations. We first show that the system is hyperbolic without any constraining condition on the flow patterns. This is followed by a detailed investigation of the structure of single waves in the Riemann problem. Smooth solutions of the whole system are shown to be in agreement with physical requirements on void fractions, densities, specific entropies. A simple fractional step method, which handles separately convective patterns and source terms, is used to compute approximations of solutions. A few computational results illustrate the whole approach.

Key words:

Multiphase flows / Finite Volumes / Entropy inequality / Riemann problem .

1 Introduction

Some three-phase flow models are used in the industry, for instance when one aims at computing the motion of gas-oil-water flows in pipes or in porous medium. This particular framework involves incompressible media, and the governing sets of partial differential equations rely on three mass conservation laws. The three (unknowns) saturations b_k should agree with the constraint $b_1 + b_2 + b_3 = 1$. The modelling of velocities within each phase is grounded on Darcy's law, and requires providing mobilities and permeabilities. Pressure differences (or capillary pressures) are assumed to be -given- functions of saturations, and thus the main unknown consists in two independent saturations and one pressure field. For one dimensional flows, using the fact that some velocity field is divergence free enables to eliminate one mass conservation law, and the resulting set of equations governs the variations of two saturations. The reader is referred for instance to [1], [2], [3] and many references therein for a better description of the topic.

In a totally different context, some simulations in the framework of pressurized water reactors in the nuclear energy field require using two-fluid models, and some others ask for a three field description of the whole flow (see [4, 5]). This may happen for instance when predicting the motion of liquid dispersed droplets inside a continuous gas phase, while some gas-liquid interface is moving in the core. Other applications involving a gaseous phase and two distinct liquids (for instance oil and water) also urge for the development of three-field models.

Some models and tools have already been proposed, which basically rely on the two-fluid single-pressure formalism. These either assume that liquid droplets velocities and velocities in the surrounding gas phase are equal, or retain different velocities but assume in any case a local pressure equilibrium between the three components. A straightforward consequence is that these models may suffer from the same deficiencies than standard two-fluid models. More clearly, in some space-time regions, the loss of hyperbolicity of the convective subset implies that computations on sufficiently fine grids rather easily enter "time-elliptic" regions. As a consequence, even the most "stable" upwinding schemes lead to a blow up of the code when refining the mesh, though accounting for stabilizing drag effects (see [6] for instance for such a numerical experience). Though this drawback may be postponed by accounting for suitable added mass effects, an appealing way to tackle multi-phase flows simply consists in retrieving the original approach which does not enforce the local instantaneous pressure equilibrium.

Actually, an alternative way to deal with two-phase flows consists in getting rid of the pressure equilibrium between phases. For two-phase flows, this was first introduced in the framework of the DDT (see [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18], among others), and more recently applied to water-vapour predictions (see [19, 20, 21]). The reader may in particular find many comments on the modelling issues in [9], and on the structure of the solutions of the governing equations. One advantage with the two-fluid two-pressure approach is that it inherits the hyperbolic nature of Navier-Stokes equations -which seems quite reasonable- on the one hand. This is an important feature since users of multiphase codes intend to simulate time dependent flows, while providing initial conditions, which of course implies that one deals with well-posed initial value problems. Moreover, the overall entropy inequality helps providing some better understanding of various interfacial transfer terms.

For all these reasons, it seems compulsory to examine whether one might derive a similar frame-

work to cope with three-phase or three-field flow structures, which is actually the main goal of the present work. For such a purpose, an underlying idea is that the interface between phases remains infinitely thin when submitted to pure convective patterns, which results in the fact that the interface velocity should behave as a contact discontinuity. Another important feature is that non-conservative terms occuring in the whole set should not forbid the derivation of meaningful jump conditions. For sake of clarity, the paper is organised as follows. We will first provide in section 2 the main set of equations of a specific model which includes source terms, viscous terms and convective effects. This model is actually the counterpart of the Baer-Nunziatto model in the framework of two-phase flows. It implicitly assumes that the phase indexed by k=1 corresponds to the dilute phase in the three-phase flow. The main properties of the whole set will be examined in section 3, including a discussion on the solutions of the one dimensional Riemann problem. Smooth solutions of the whole set will guarantee that void fractions, densities and specific entropies will agree with positivity requirements. Though we will focus in this paper on flows with no mass transfer, details pertaining to admissible forms of mass and energy transfer terms can be found in appendix F. In the sequel, section 4 will be devoted to a series of remarks pertaining to the modelling of three-phase flows. More precisely, we will give a class of hyperbolic three-phase flow models, which comply with the same entropy inequality. If one focuses on interface velocities which ensure that the field associated with $\lambda = V_i$ is linearly degenerated, the companion appendix G shows how to derive the unique set of unknowns P_{kl} occurring in the momentum and energy interfacial transfer terms. This section thus allows to investigate the counterpart of the work [20], where focus is given on the specific closure $V_i = (\Sigma_k m_k U_k)/(\Sigma_k m_k)$.

It is clearly beyond the scope of this paper to investigate accurate and optimal schemes to compute approximations of solutions of the governing set of equations. Nonetheless, we wish to present in section 5 some possible way to achieve this. Actually, we will use an entropy-consistant fractional step method to cope with sources and convective terms. The above mentioned properties obviously provide some natural way to compute the convective contributions, using rough schemes (Rusanov scheme for instance) or more accurate approximate Riemann solvers such as those introduced in [22, 23] for instance. A few computational results will illustrate the whole.

2 Governing equations and closure laws

We focus in this paper on the counterpart of the Baer Nunziatto model. hence, we assume that the phase indexed by k=1 is dilute. Actually, a broader class of models may be investigated, but we concentrate now on a particular one and refer the reader to section 4 and its associated *appendix* G for many comments pertaining to its establishment.

2.1 Governing equations

Throughout the paper, the density, velocity, pressure, internal energy and total energy within phase k will be denoted ρ_k , U_k , P_k , $e_k = e_k(P_k, \rho_k)$ and:

$$E_k = 0.5\rho_k U_k U_k + \rho_k e_k (P_k, \rho_k)$$

respectively. The volumetric fraction of phase labelled k is defined as α_k , and the three must comply with the constraint:

$$\alpha_1 + \alpha_2 + \alpha_3 = 1 \tag{1}$$

The governing set of equations is:

$$(I+D(W))\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial G(W)}{\partial x} = S(W) + \frac{\partial}{\partial x}(E(W)\frac{\partial W}{\partial x}) \tag{2}$$

It requires an initial condition $W(x,0) = W_0(x)$ and suitable boundary conditions. The state variable W, the fluxes F(W), G(W) and the source terms S(W) lie in \mathbb{R}^{11} . We set:

$$W^{t} = (\alpha_{2}, \alpha_{3}, \alpha_{1}\rho_{1}, \alpha_{2}\rho_{2}, \alpha_{3}\rho_{3}, \alpha_{1}\rho_{1}U_{1}, \alpha_{2}\rho_{2}U_{2}, \alpha_{3}\rho_{3}U_{3}, \alpha_{1}E_{1}, \alpha_{2}E_{2}, \alpha_{3}E_{3})$$

and, noting $m_k = \alpha_k \rho_k$:

$$\begin{split} F(W)^t &= (0,0,m_1U_1,m_2U_2,m_3U_3,\alpha_1(\rho_1U_1^2+P_1),\alpha_2(\rho_2U_2^2+P_2),\alpha_3(\rho_3U_3^2+P_3),\\ \alpha_1U_1(E_1+P_1),\alpha_2U_2(E_2+P_2),\alpha_3U_3(E_3+P_3)) \end{split}$$

Second rank tensors C(W), D(W), E(W) lie in $\mathbb{R}^{11 \times 11}$. The non-conservative convective terms are :

$$\begin{cases} D(W)\frac{\partial W}{\partial t} = (0,0,0,0,0,0,0,0,0,-P_2\frac{\partial \alpha_2}{\partial t} - P_3\frac{\partial \alpha_3}{\partial t}, P_2\frac{\partial \alpha_2}{\partial t}, P_3\frac{\partial \alpha_3}{\partial t}) \\ C(W)\frac{\partial G(W)}{\partial x} = (U_1\frac{\partial \alpha_2}{\partial x}, U_1\frac{\partial \alpha_3}{\partial x}, 0,0,0,P_2\frac{\partial \alpha_2}{\partial x} + P_3\frac{\partial \alpha_3}{\partial x}, -P_2\frac{\partial \alpha_2}{\partial x}, -P_3\frac{\partial \alpha_3}{\partial x}, 0,0,0) \end{cases}$$
 (3)

Viscous terms should at least account for the following contributions (thermal fluxes might also be included):

$$E(W)\frac{\partial W}{\partial x} = (0,0,0,0,0,\alpha_1\mu_1\frac{\partial U_1}{\partial x},\alpha_2\mu_2\frac{\partial U_2}{\partial x},\alpha_3\mu_3\frac{\partial U_3}{\partial x},\alpha_1\mu_1U_1\frac{\partial U_1}{\partial x},\alpha_2\mu_2U_2\frac{\partial U_2}{\partial x},\alpha_3\mu_3U_3\frac{\partial U_3}{\partial x})$$

Source terms S(W) account for mass transfer terms, drag effects, energy transfer, and other contributions. To simplify our presentation, we only retain here the effect of pressure relaxation and drag effects. Thus:

$$S(W) = (\phi_2, \phi_3, 0, 0, 0, S_{U_1}, S_{U_2}, S_{U_2}, U_1 S_{U_1}, U_1 S_{U_2}, U_1 S_{U_2})$$

$$(5)$$

We also introduce ϕ_1 such that:

$$\phi_1 + \phi_2 + \phi_3 = 0 \tag{6}$$

and we recall that the momentum interfacial transfer terms must comply with:

$$S_{U_1}(W) + S_{U_2}(W) + S_{U_3}(W) = 0 (7)$$

Thus the sum of exchanges between total energies is zero.

2.2 Closure laws

We consider the following closures :

$$\phi_2 = \alpha_2(f_{1-2}(W)\alpha_1(P_2 - P_1) + f_{2-3}(W)\alpha_3(P_2 - P_3))/(|P_1| + |P_2| + |P_3|)$$
(8)

$$\phi_3 = \alpha_3(f_{1-3}(W)\alpha_1(P_3 - P_1) + f_{2-3}(W)\alpha_2(P_3 - P_2))/(|P_1| + |P_2| + |P_3|)$$
(9)

The three positive scalar functions $f_{k-l}(W)$ denote frequencies which should remain bounded over $\Omega \times [0,T]$. These clearly enable to retrieve two-phase closure laws issuing from [7]. Moreover, we will rely on standard closures of the form (see [4] for instance):

$$S_{U_2}(W) = m_2 \psi_2(W)(U_1 - U_2) \tag{10}$$

$$S_{U_3}(W) = m_3 \psi_3(W)(U_1 - U_3) \tag{11}$$

The inverse of the scalar functions $\psi_2(W)$, $\psi_3(W)$ denote the velocity-relaxation time scales, and should remain positive.

Remark 1:

If we set formally $\alpha_3(x,t)=0$ in the above equations (2), we retrieve the Baer-Nunziato model ([7]). Moreover, $\alpha_3(x,t)=0$ is a specific trivial solution of equations ((2)-2), ((2)-5), ((2)-8), ((2)-11). In that case, the constraint $\alpha_1+\alpha_2+\alpha_3=1$ turns into $\alpha_1+\alpha_2=1$. In that sense, we may say that the above three-phase flow model contains the Baer-Nunziato model.

3 Main properties

We focus first on the homogeneous problem associated with the left hand side of (2). We define as usual specific entropies s_k and speeds c_k in terms of the density ρ_k and the internal energy e_k :

$$(c_k)^2 = \frac{\gamma_k P_k}{\rho_k} = \left(\frac{P_k}{(\rho_k)^2} - \frac{\partial e_k(P_k, \rho_k)}{\partial \rho_k}\right) \left(\frac{\partial e_k(P_k, \rho_k)}{\partial P_k}\right)^{-1}$$
$$\gamma_k P_k \frac{\partial s_k(P_k, \rho_k)}{\partial P_k} + \rho_k \frac{\partial s_k(P_k, \rho_k)}{\partial \rho_k} = 0$$

3.1 Structure of fields in the one-dimensional Riemann problem

We first check that the closed set of equations is hyperbolic, without any specific constraint, since:

Property 1:

1.1 The homogeneous system associated with the left hand side of (2) has eigenvalues:

 $\lambda_{1,2,3} = U_1$, $\lambda_4 = U_2$, $\lambda_5 = U_3$, $\lambda_6 = U_1 - c_1$, $\lambda_7 = U_1 + c_1$, $\lambda_8 = U_2 - c_2$, $\lambda_9 = U_2 + c_2$, $\lambda_{10} = U_3 - c_3$, $\lambda_{11} = U_3 + c_3$. Associated right eigenvectors span the whole space \mathbb{R}^{11} unless $U_1 = U_k + c_k$ or $U_1 = U_k - c_k$, for k = 2, 3.

1.2 Fields associated with eigenvalues λ_k with k in (1, 2, 3, 4, 5) are Linearly Degenerated; other fields are Genuinely Non Linear.

Proof

The homogeneous LHS of system (2) may be written for smooth solutions as:

$$\frac{\partial Z}{\partial t} + A(Z)\frac{\partial Z}{\partial x} = 0 \tag{12}$$

The computation of the eigenvalues of the matrix A(Z) and their associated right eigenvectors $r_k(Z)$ is rather easy (see appendix A), when using the non conservative variable:

$$Z^{t} = (\alpha_{2}, \alpha_{3}, s_{1}, s_{2}, s_{3}, U_{1}, U_{2}, U_{3}, P_{1}, P_{2}, P_{3})$$

$$\tag{13}$$

One may also quickly check that:

$$\frac{\partial(\lambda_k(Z))}{\partial Z}.r_k(Z) = 0 \tag{14}$$

if k lies in (1, 2, 3, 4, 5), and $\frac{\partial(\lambda_k(Z))}{\partial Z} r_k(Z) \neq 0$ otherwise.

The list of Riemann invariants through Linearly Degenerated fields associated with k = 4, 5 and Genuinely Non Linear fields (k in (6-11)) may be computed (see *appendix B*), and enables to retrieve the counterpart of sole Euler systems.

Remark 2

We note that this specific variable Z cannot symmetrize the whole convective subset, unless pressure and velocity equilibrium is reached (see appendices A,B,C, and comments in [17]). We also emphasize that these results are indeed close to those detailed in [19, 20].

Remark 3

Of course, celerities involved in the eigenvalues of the homogeneous system should neither be confused with true physical acoustic properties in the real three-phase flow medium (which of course implicitly account for return to equilibrium states), nor with celerities of reduced equations (see [10] for instance).

We may now focus on the Riemann invariants associated with the 1-2-3 wave. This wave fully couples the three phases, in such a way that:

Property 2:

2.1 The latter system admits the following Riemann invariants through the 1-2-3 LD wave:

$$\begin{split} I_1^{1-2-3}(W) &= m_2(U_2-U_1) & I_2^{1-2-3}(W) = m_3(U_3-U_1) \\ I_3^{1-2-3}(W) &= s_2 & I_4^{1-2-3}(W) = s_3 & I_5^{1-2-3}(W) = U_1 \\ I_6^{1-2-3}(W) &= \alpha_1 P_1 + \alpha_2 P_2 + \alpha_3 P_3 + m_2(U_1-U_2)^2 + m_3(U_1-U_3)^2 \\ I_7^{1-2-3}(W) &= 2e_2 + 2\frac{P_2}{\rho_2} + (U_1-U_2)^2 & I_8^{1-2-3}(W) = 2e_3 + 2\frac{P_3}{\rho_3} + (U_1-U_3)^2 \end{split}$$

2.2 We note $\Delta(\psi) = \psi_r - \psi_l$. Apart from the 1-2-3 LD wave, the following exact jump conditions hold for k = 1, 2, 3, through any discontinuity separating states l, r moving with speed σ :

$$\begin{split} &\Delta(\alpha_k) = 0 \\ &\Delta(\rho_k(U_k - \sigma)) = 0 \\ &\Delta(\rho_k U_k(U_k - \sigma) + P_k) = 0 \\ &\Delta(E_k(U_k - \sigma) + P_k U_k) = 0 \end{split}$$

Proof

It is tedious but straightforward. For k = 1 - 3, one only needs to check that :

$$\frac{\partial (I_k^{1-2-3}(Z))}{\partial Z} \cdot r_k(Z) = 0 \tag{15}$$

where $r_k(Z)$ stand for the right eigenvectors of the matrix detailed in appendix A.

Hence, we note the important point that jump conditions are well defined through all fields. This remarkable property is essentially due to the fact that the 1-2-3-wave is Linearly Degenerated, and to the fact that the void fraction remains constant through all fields except for the 1-2-3 fields.

Remark 4

If we formally assume that $(\alpha_k)_L = (\alpha_k)_R = 0$ for k = 2, 3 (and thus $(\alpha_1)_L = (\alpha_1)_R = 1$), the only meaningful Riemann invariants in the 1 - 2 - 3 wave turn out to be $I_5^{1-2-3}(W) = U_1$ and $I_6^{1-2-3}(W) = P_1$ (which correspond to the standard contact discontinuity of Euler equations).

We may now focus on the entropy balance. Actually, we have a result which is indeed similar to the one given in [19, 20].

3.2 Entropy inequality

We now need to define:

$$a_k = (s_k)^{-1} \left(\frac{\partial s_k(P_k, \rho_k)}{\partial P_k}\right) \left(\frac{\partial e_k(P_k, \rho_k)}{\partial P_k}\right)^{-1}$$

and we introduce:

$$\eta_k = Log(s_k) \tag{16}$$

but also the pair (η, F_{η}) such that :

$$\eta = -m_1 \eta_1 - m_2 \eta_2 - m_3 \eta_3 \tag{17}$$

and finally:

$$F_{\eta} = -m_1 \eta_1 U_1 - m_2 \eta_2 U_2 - m_3 \eta_3 U_3 \tag{18}$$

We assume in addition that drag terms $S_{U_k}(W)$ and source terms $\phi_k(W)$ in (2) comply with:

$$0 \le a_2(U_1 - U_2)S_{U_2}(W) + a_3(U_1 - U_3)S_{U_3}(W)$$
(19)

$$0 \le a_1(\phi_1 P_1 + \phi_2 P_2 + \phi_3 P_3) \tag{20}$$

The condition (20) may be written in an alternative form:

$$\phi_2(P_1 - P_2) + \phi_3(P_1 - P_3) \le 0 \tag{21}$$

since $\phi_1 + \phi_2 + \phi_3 = 0$ and $a_1 > 0$ for standard EOS. We now get the following:

Property 3:

Closures in agreement with the above mentionned constraints (19),(20) ensure that the following entropy inequality holds for regular solutions of (2):

$$\frac{\partial \eta}{\partial t} + \frac{\partial F_{\eta}}{\partial x} \le 0 \tag{22}$$

Proof

For regular solutions of system (2), the governing equation for η reads:

$$\frac{\partial \eta}{\partial t} + \frac{\partial F_{\eta}}{\partial x} = -a_1(\phi_1 P_1 + \phi_2 P_2 + \phi_3 P_3) - \sum_k (a_k(U_1 - U_k) S_{U_k}(W))$$
(23)

Now, it obviously follows, on the basis of closure laws (8) detailed above, that (20) holds, since a straightforward calculus provides:

$$\phi_1 P_1 + \phi_2 P_2 + \phi_3 P_3 = (|P_1| + |P_2| + |P_3|)^{-1} \left(\sum_{k \le l} f_{k-l}(W) \alpha_k \alpha_l (P_l - P_k)^2 \right) > 0$$
 (24)

The second sum on the right hand side also agrees with (19), since closure laws (10) provide:

$$0 \le \sum_{k} (a_k(U_1 - U_k)S_{U_k}(W)) = \sum_{k=2}^{3} (m_k \psi_k a_k (U_1 - U_k)^2)$$

which ends the proof.

We emphasize that through the 1-2-3-wave, the entropy balance is ensured since:

$$F_{\eta} - U_{1}\eta = \sum_{k=1}^{3} (m_{k}U_{k}Logs_{k}) - U_{1}\sum_{k=1}^{3} (m_{k}Logs_{k})$$
(25)

and thus:

$$F_{\eta} - U_{1}\eta = \sum_{k=1}^{2} (m_{k}(U_{k} - U_{1})Logs_{k}) = I_{1}^{1-2-3}(W)Log(I_{3}^{1-2-3}(W)) + I_{2}^{1-2-3}(W)Log(I_{4}^{1-2-3}(W))$$
(26)

We emphasize here that the entropy $\eta(W)$ is a (non strictly) convex function of W. We recall that the same occurs in the two-fluid two-pressure approach.

3.3 Physical constraints

3.3.1 Smooth solutions

We may now wonder whether smooth solutions of (2) are physically relevant, assuming admissible initial and boundary conditions.

Property 4:

For k=1,2,3, we assume that the initial conditions satisfy: $0 \le \alpha_k(x,0), \ 0 \le m_k(x,0), \ 0 \le s_k(x,0)$, but also that the boundary conditions fulfill: $0 \le \alpha_k(x_\Gamma,t), \ 0 \le m_k(x_\Gamma,t), \ 0 \le s_k(x_\Gamma,t)$. In addition we assume that $a_k(x,t)$, but also both $U_k(x,t)$ and $\frac{\partial U_k(x,t)}{\partial x}$ remain in $L^{\infty}(\Omega \times [0,T])$. Then regular solutions of the above system agree with the physical requirement:

$$0 \le \alpha_k(x,t)$$
 $0 \le m_k(x,t)$ $0 \le s_k(x,t)$

This is the straightforward counterpart of what happens in two-fluid two-pressure models (see references herein).

Proof

• Actually, for (k, k', k'') in (1, 2, 3) (k, k', k'') all distinct, we have:

$$\frac{\partial \alpha_k}{\partial t} = \alpha_k (f_{k'-k}(W)\alpha_{k'}(P_k - P_{k'}) + f_{k''-k}(W)\alpha_{k''}(P_k - P_{k''}))/(|P_k| + |P_{k'}| + |P_{k''}|) \quad (27)$$

which ensures that $\alpha_k(x,t)$ remains positive, whatever k is. More over, one may check that:

$$\frac{\partial \pi}{\partial t} + U_1 \frac{\partial \pi}{\partial x} = \pi (\sum_{k < l} f_{k-l}(W)(\alpha_k - \alpha_l)(P_l - P_k))(|P_k| + |P_{k'}| + |P_{k''}|)^{-1}$$
 (28)

when defining:

$$\pi = \alpha_1 \alpha_2 \alpha_3 \tag{29}$$

This guarantees that regular solutions $\alpha_k(x,t)$ will remain in the admissible range [0,1] over $\Omega \times [0,T]$, using the constraint $\alpha_1 + \alpha_2 + \alpha_3 = 1$.

• The governing equation of the partial mass m_k simply reads:

$$\frac{\partial m_k}{\partial t} + U_k \frac{\partial m_k}{\partial x} + m_k \frac{\partial U_k}{\partial x} = 0 \tag{30}$$

Hence the expected result $0 \le m_k(x,t)$ also holds.

• When getting rid of source terms, the governing equation for the phasic entropy s_k reads:

$$\frac{\partial s_k}{\partial t} + U_k \frac{\partial s_k}{\partial x} = 0 \tag{31}$$

Once more, we obtain with similar assumptions that $0 \le s_k(x,t)$.

If we account for source mechanism, the latter turns to:

$$\frac{\partial s_k}{\partial t} + U_k \frac{\partial s_k}{\partial x} = r_k s_k \tag{32}$$

noting $r_k = a_k \psi_k(W)(U_1 - U_k)^2$ for k = 2, 3, and : $r_1 = a_1(\phi_2(P_2 - P_1) + \phi_3(P_3 - P_1))/m_1$

Our basic assumptions enable us to conclude that r_k remains bounded over $\Omega \times [0,T]$.

Remark 5

This one concerns the specific case of stiffened gas EOS. For specific thermodynamical laws of the form: $\rho_k e_k(P_k, \rho_k) = \frac{P_k + \gamma_{k,0} P_{k,0}}{\gamma_{k,0} - 1}$, with $\gamma_{k,0} > 1$, the specific entropy is $s_k = (P_k + P_{k,0})(\rho_k)^{-\gamma_{k,0}}$. Vacuum occurence within phase k (that is : $\rho_k = 0$) corresponds to the pressure $P_k = -P_{k,0}$. For these EOS, and unless phase vacuum occurs, the pressure will remain relevant, that is $0 \le P_k(x,t) + P_{k,0}$.

3.3.2 Solutions of the one dimensional Riemann problem

It is however not clear whether the model will ensure that elementary self similar solutions in the one dimensional Riemann problem will remain physically relevant. We focus below on a smaller class of EOS. This enables to prove results by a straightforward construction.

Property 5:

We assume that a perfect gas state law holds within each phase (k = 1, 2, 3). We assume that the initial conditions satisfy: $(\alpha_k)_{L,R}(1 - \alpha_k)_{L,R} \neq 0$, for k = 1, 2, 3. We consider a single wave associated with λ_m , separating two states Z_l, Z_r . The connection of states through this wave ensures that all states are in agreement with:

$$0 \le \alpha_k \qquad 0 \le m_k \qquad 0 \le P_k$$

Proof

The main guidelines are given in appendix E, and are almost the same as in [20]. We denote as usual Z_L and Z_R the initial condition of the one dimensional Riemann problem associated with the left hand side of (2), and we note $\sigma_1 = (U_1)_{1-2-3}$ the speed of the 1-2-3 contact wave. When

focusing on a single field connected with the eigenvalue λ_k where k = 4 to 11, we know that both α_2 and α_3 are Riemann invariants in rarefaction waves, and do not jump through shock waves. Thus, apart from the 1, 2, 3-wave, we may conclude that the solution in terms of void fractions is rather simple. It takes the form:

$$\alpha_k(x < \sigma_1 t, t) = (\alpha_k)_L$$

$$\alpha_k(x > \sigma_1 t, t) = (\alpha_k)_R$$

for k = 1, 2, 3.

Actually, the true coupling of phases occurs through the 1, 2, 3-field. We note Z_l and Z_r the states on each side of this particular wave. In any case, apart from the 1-2-3-wave, the following holds: $(\rho_1)_l > 0$, $(\rho_1)_r > 0$, and also $(P_1)_l > 0$, $(P_1)_r > 0$. This is due to the fact that ρ_1 and P_1 only vary in the 6-wave (respectively the 7-wave) on the left side (resp. the right side) of the 1-2-3-wave.

More precisely, $(P_1, \rho_1)_l$ results from the transformation of $(P_1, \rho_1)_L$ through the 6-wave associated with $U_1 - c_1$. If this 6-wave happens to be a rarefaction wave, the Riemann invariant s_1 is preserved, which guarantees that both $(\rho_1)_l$ and $(P_1)_l$ remain positive when focusing on perfect gas EOS $(s_1(P_1, \rho_1) = P_1(\rho_1)^{-\gamma_1})$. If on the contrary this 6-wave happens to be a shock wave, the jump conditions for a *single phase* perfect gas EOS enforce the positivity of $(\rho_1)_l$ and $(P_1)_l$, since we get: $(\rho_1)_l > (\rho_1)_L$ and $(P_1)_l > (P_1)_L$.

On the other hand, $(P_1, \rho_1)_r$ results from the transformation of $(P_1, \rho_1)_R$ through the 7-wave associated with $U_1 + c_1$. A straightforward counterpart of the above explanation holds. If the 7-wave turns to be a shock wave, we get: $(\rho_1)_r > (\rho_1)_R$ and $(P_1)_r > (P_1)_R$. Otherwise, if it turns to be a rarefaction wave, the condition $(s_1)_r = (s_1)_R$ ensures that both $(P_1)_r$ and $(\rho_1)_r$ remain positive.

In other words, this is almost equivalent to what occurs in a single-phase framework, when focusing on the 1-phase.

We turn to ρ_k , P_k for k=2,3. This requires to distinguish four cases as detailed below.

• Case (i):

We imagine, with no loss of generality, that the contact discontinuities associated with $\lambda_4 = U_2$ and $\lambda_5 = U_3$ are on the right side of $x/t = \sigma_1$. A sketch of the solution is given below, corresponding to this first case (i).

We thus may assume that $(\rho_k)_l > 0$, and $(P_k)_l > 0$ for k = 2, 3. Actually, either: $(P_2)_l = (P_2)_L$ and $(\rho_2)_l = (\rho_2)_L$, or $(P_2, \rho_2)_l$ results from the transformation of $(P_2, \rho_2)_L$ through the 8-wave only (associated with $\lambda_8 = U_2 - c_2$). The above mentionned comments again permit to reach the same conclusions. In a similar way, either: $(P_3)_l = (P_3)_L$ and $(\rho_3)_l = (\rho_3)_L$, or $(P_3, \rho_3)_l$ results from the transformation of $(P_3, \rho_3)_L$ through the 10-wave only (associated with $\lambda_{10} = U_3 - c_3$).

Hence, it remains to check that $(\rho_k)_r > 0$, and $(P_k)_r > 0$ will remain positive when crossing the 1, 2, 3-wave. This is obtained independently.

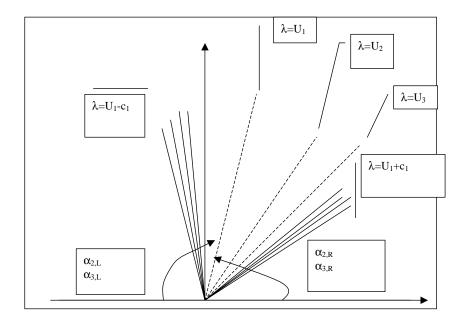


Figure 1: Sketch of the solution of the Riemann problem with IC : Z_L and Z_R . Case (i)

– The computation of $(\rho_2)_r$ issues from :

$$(g_2)_R((\rho_2)_r) = (g_2)_L((\rho_2)_l)$$

see appendix E for notations. It ensures that :

$$\begin{split} I_1^{1-2-3}(W_r) &= I_1^{1-2-3}(W_l) \\ I_3^{1-2-3}(W_r) &= I_3^{1-2-3}(W_l) \\ I_7^{1-2-3}(W_r) &= I_7^{1-2-3}(W_l) \end{split}$$

under the constraint $I_5^{1-2-3}(W_r) = I_5^{1-2-3}(W_l)$, that is: $(U_1)_r = (U_1)_l$. The first two equations enable to express $(U_2)_r$ and $(P_2)_r$ in terms of $(\rho_2)_r$ (see below), and the whole may be injected in the remaining equation $I_7^{1-2-3}(W_r) = I_7^{1-2-3}(W_l)$, which either admits 0 or two positive solutions $(\rho_2)_r$.

Once $(\rho_2)_r$ is computed, the computation of the pressure $(P_2)_r$ will follow from $I_3^{1-2-3}(W-r) = I_3^{1-2-3}(W_l)$, which gives:

$$(P_2)_r = (P_2)_l (\frac{(\rho_2)_r}{(\rho_2)_l})^{\gamma_2}$$

Eventually, the mean velocity within phase 2 is:

$$(U_2)_r = (U_1)_l + \frac{(\alpha_2)_L(\rho_2)_l((U_2)_l - (U_1)_l)}{(\alpha_2)_R(\rho_2)_r}$$

– In a similar way, the computation of $(\rho_3)_r$ issues from :

$$(g_3)_R((\rho_3)_r) = (g_3)_L((\rho_3)_l)$$

which corresponds to the superposition of the three constraints:

$$I_2^{1-2-3}(W_r) = I_2^{1-2-3}(W_l)$$

$$I_4^{1-2-3}(W_r) = I_4^{1-2-3}(W_l)$$

$$I_8^{1-2-3}(W_r) = I_8^{1-2-3}(W_l)$$

with $(U_1)_r = (U_1)_l$. It also admits 0 or two positive solutions $(\rho_3)_r$. The same argument holds for $(P_3)_r$ since:

$$(P_3)_r = (P_3)_l (\frac{(\rho_3)_r}{(\rho_3)_l})^{\gamma_3}$$

Once more, we may deduce the mean velocity within phase 3:

$$(U_3)_r = (U_1)_l + \frac{(\alpha_3)_L(\rho_3)_l((U_3)_l - (U_1)_l)}{(\alpha_3)_R(\rho_3)_r}$$

Of course, there are three other possibilities, with similar conclusions -see $appendix\ E-$; these correspond to :

- (ii) $U_2 < U_1$ and $U_3 < U_1$;
- (iii) $U_2 < U_1$ and $U_3 > U_1$;
- (iv) $U_3 < U_1$ and $U_2 > U_1$).

- Case (ii): $U_2 < U_1$ and $U_3 < U_1$. We may now assume that $(\rho_k)_r > 0$, and $(P_k)_r > 0$ for k = 2, 3. In that case, the unknowns are $(\rho_2)_l$ and $(\rho_3)_l$. The final problem also requires to compute both of these solely, using the same governing equations.
- Case (iii): $U_2 < U_1$ and $U_3 > U_1$. We thus may assume that $(\rho_3)_l > 0$, and $(P_3)_l > 0$, whereas $(\rho_2)_r > 0$, and $(P_2)_r > 0$. The unknowns are $(\rho_2)_l$ and $(\rho_3)_r$ here.
- Case (iv): $U_3 < U_1$ and $U_2 > U_1$. We thus may assume that $(\rho_3)_r > 0$, and $(P_3)_r > 0$, whereas $(\rho_2)_l > 0$, and $(P_2)_l > 0$. In this last case, the unknowns are $(\rho_2)_r$ and $(\rho_3)_l$.

We notice that the sixth Riemann invariant $I_6^{1-2-3}(W)$ has not been used. It is nonetheless the keystone to compute the whole solution of the Riemann problem when connecting states W_L and W_R , which is achieved writing:

$$I_5^{1-2-3}(W_r) = I_5^{1-2-3}(W_l)$$

$$I_6^{1-2-3}(W_r) = I_6^{1-2-3}(W_l)$$

The main problem is that it requires to cope with the possible occurrence of resonance, when $|U_k - U_1| = c_k$ (for k = 2, 3). In that case, the set of eigenvectors no longer spans the whole space, and one needs to find a criteria to select the physically relevant solution (see [24] and [25] for instance which tackle this difficult problem in two distinct frameworks).

4 A few comments on modelling issues

Remark 6

The governing equations for void fractions involve only one interface velocity. Otherwise, the maximum principle for the void fraction may not hold, whenever one considers smooth or discontinuous solutions. One may also note that the source terms ensure that the void fraction within phase k increases when the partial pressure P_k is greater than the one in the other two phases. Actually this is the exact counterpart of what happens in two-fluid two-pressure models. In practical computations, all frequencies f_{k-l} have been taken equal to one another.

Remark 7

The above system takes its grounds on the following class:

$$\begin{split} &\alpha_1 + \alpha_2 + \alpha_3 = 1 \\ &\frac{\partial \alpha_k}{\partial t} + V_i \frac{\partial \alpha_k}{\partial x} = \phi_k \\ &\frac{\partial \alpha_k \rho_k}{\partial t} + \frac{\partial \alpha_k \rho_k U_k}{\partial x} = 0 \\ &\frac{\partial \alpha_k \rho_k U_k}{\partial t} + \frac{\partial \alpha_k (\rho_k U_k^2 + P_k)}{\partial x} + \sum_{l=1, l \neq k}^3 P_{kl}^Q \frac{\partial \alpha_l}{\partial x} = S_{U_k} \\ &\frac{\partial \alpha_k E_k}{\partial t} + \frac{\partial \alpha_k U_k (E_k + P_k)}{\partial x} - \sum_{l=1, l \neq k}^3 P_{kl}^E \frac{\partial \alpha_l}{\partial t} = V_i S_{U_k} \end{split}$$

We have assumed no discrepancy between P_{kl}^E and P_{kl}^Q , that is: $P_{kl}^E = P_{kl}^Q = P_{kl}$.

In order to ensure that the interfacial transfer terms cancel when focusing on the mean flow, the first constraints which arise are:

$$\phi_1 + \phi_2 + \phi_3 = 0$$

$$S_{U_1}(W) + S_{U_2}(W) + S_{U_3}(W) = 0$$

$$P_{12} + P_{32} = P_{13} + P_{23} = P_{21} + P_{31}$$

These ensure that the interfacial transfer terms cancel when focusing on the mean flow. Thus, there exists four independent interface pressure unknowns, owing to the last two constraints.

We have focused on the counterpart of the Baer-Nunziato model, setting $V_i = U_1$. This results in the unique solution in terms of the remaining four unknowns:

$$P_{13} = P_{31} = P_{32} = P_3$$

 $P_{12} = P_{21} = P_{23} = P_2$

Actually, one may derive a unique formulation of the six unknowns P_{kl} , in order to agree with the two constraints $P_{12} + P_{32} = P_{13} + P_{23} = P_{21} + P_{31}$, and to comply with the overall entropy

inequality (22) (see appendix G).

Remark 8

It was shown in [19, 20] that the two-fluid two-pressure formalism admits two distinct classes of interface velocities V_I , when considering (for k = 1, 2):

$$\frac{\partial \alpha_k}{\partial t} + V_I \frac{\partial \alpha_k}{\partial x} = \phi_k \tag{33}$$

with $\phi_1 + \phi_2 = 0$, $\alpha_1 + \alpha_2 = 1$. Both of them ensure that the field associated with the eigenvalue $\lambda = V_I$ will be Linearly Degenerated.

The first one $(V_I = U_k)$ again corresponds to the Baer-Nunziato formulation. It ensures that the field associated with the eigenvalue $\lambda = V_I$ is a LD field. The second admissible choice is $V_I = (m_1U_1 + m_2U_2)/(m_1 + m_2)$. The counterpart of this second branch, that is:

$$V_I = \frac{\sum_{k=1}^{3} (m_k U_k)}{\sum_{k=1}^{3} m_k}$$

has not been investigated till now.

Remark 9

The introduction of mass transfer terms may be achieved, following results of the appendix F for instance. This is a important point for those who aim at predicting the ebulition crisis for instance, or any phenomena involving mass and heat transfer.

5 A simple numerical approach

The objective here is to propose a simple algorithm to compute approximations of the latter set of PDE. It is beyond the scope of the paper to construct an optimal numerical method. Nonetheless, one needs to be careful in order to preserve the overall entropy inequality. Otherwise, it seems difficult to maintain entropy budgets throughout the whole scheme. The following approach, which is the exact counterpart of the one detailed in [20], aims at doing so.

We only provide here a sketch of the numerical method. For further details, one may for instance refer to [20].

5.1 Fractional step method

Actually, the previous properties suggest us to introduce a fractional step approach which is in agreement with the overall entropy inequality. For that purpose, we thus simply compute approximations of the convective subset :

$$(I + D(W))\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial G(W)}{\partial x} = 0$$
(34)

and then account for source terms and viscous terms updating values through the step:

$$(I + D(W))\frac{\partial W}{\partial t} = S(W) + \frac{\partial}{\partial x}(E(W)\frac{\partial W}{\partial x})$$
(35)

When neglecting viscous contributions, the second one turns to an ordinary differential system .

Our basic approach to compute convective terms relies on the Godunov approach [26, 27]. More precisely here, we use the schemes introduced in [20] to compute approximations of the system (34). This is achieved with help of either the Rusanov scheme or the approximate Godunov scheme VFRoe-ncv [22]. In order to cope with the standard step (34) which requires discretizing convective effects, a rather efficient way consists in using the approximate Godunov scheme introduced in [22] with the specific variable:

$$Z^{t} = (\alpha_{2}, \alpha_{3}, s_{1}, s_{2}, s_{3}, U_{1}, U_{2}, U_{3}, P_{1}, P_{2}, P_{3})$$

$$(36)$$

(see [23] which details the main advantages of such a choice). Computations below have been obtained with the former scheme, while fulfilling standard CFL conditions.

Remark~10

This simple numerical approach has another advantage, since it also enables to cope with the instantaneous pressure equilibrium assumption. This may be useful for those who wish to compute models such as those described in [4] for instance. Owing to the entropy structure (see $appendix\ D$), one may actually introduce the pressure relaxation step involved in (35) as a tool to compute the single pressure models detailed in [4]. One must be careful when providing approximations of system (35). Otherwise, the stability of locally equal-pressure regions may be violated. The pressure relaxation scheme discussed in $appendix\ D$ to update pressures and void fractions maintains them positive. We emphasize that the proof given in appendix is only valid when focusing on perfact

gas EOS.

The connection with the relaxation scheme introduced in [28] is obvious. This is also the counterpart of what has been recently achieved in the two-phase framework (see [29, 30] or [6] for instance).

Another important point to be quoted is that numerical experiments confirm that a hudge mesh refinement provide similar results either using the Rusanov scheme or some approximate Godunov scheme such as VFRoe-ncv, though the convective system is not under conservative form. This is due to the fact that non conservative products are uniquely defined, thanks to modelling assumptions on the interface velocity V_i . The reader is referred to [31] for instance, which investigates this specific problem.

5.2 Numerical results

We assume that the perfect gas law holds within each phase: $\rho_k e_k = (\gamma_k - 1)P_k$, setting $\gamma_1 = 7/5$, $\gamma_2 = 1.005$ and $\gamma_3 = 1.001$. The three numerical experiments have been achieved using a time step in agreement with the standard constraint CFL = 0.49. The convective terms have been computed with the non conservative version of the Rusanov scheme. The regular mesh contains ten thousand nodes for the first two tests, and twenty thousand nodes for the third one. The initial conditions for the first test case (fig. (1-3)) are:

```
\begin{array}{l} (\alpha_2)_L=0.4,\ (\alpha_3)_L=0.5,\ (\alpha_2)_R=0.5,\ (\alpha_3)_R=0.4,\\ (U_1)_L=100,\ (\tau_1)_L=1,\ (P_1)_L=10^5,\ (U_1)_R=100,\ (\tau_1)_R=8,\ (P_1)_R=10^5,\\ (U_2)_L=100,\ (\tau_2)_L=1,\ (P_2)_L=10^5,\ (U_2)_R=100,\ (\tau_2)_R=8,\ (P_2)_R=10^5,\\ (U_3)_L=100,\ (\tau_3)_L=1,\ (P_3)_L=10^5,\ (U_3)_R=100,\ (\tau_3)_R=8,\ (P_3)_R=10^5. \end{array}
```

These correspond to the propagation of a contact wave. The initial conditions for the second test case are those of a classical "shock tube apparatus" (fig. (4-6)), and correspond to:

```
\begin{array}{l} (\alpha_2)_L=0.4,\,(\alpha_3)_L=0.5,\,(\alpha_2)_R=0.5,\,(\alpha_3)_R=0.4,\\ (U_1)_L=0,\,(\tau_1)_L=1,\,(P_1)_L=10^5,\,(U_1)_R=0,\,(\tau_1)_R=8,\,(P_1)_R=10^4,\\ (U_2)_L=0,\,(\tau_2)_L=1,\,(P_2)_L=10^5,\,(U_2)_R=0,\,(\tau_2)_R=8,\,(P_2)_R=10^4,\\ (U_3)_L=0,\,(\tau_3)_L=1,\,(P_3)_L=10^5,\,(U_3)_R=0,\,(\tau_3)_R=8,\,(P_3)_R=10^4. \end{array}
```

The initial conditions for the third Riemann problem correspond to an impinging jet on a wall boundary, which results in a propagation of symmetrical shock waves (fig. (7-8)):

```
\begin{array}{l} (\alpha_2)_L=0.4,\,(\alpha_3)_L=0.5,\,(\alpha_2)_R=0.4,\,(\alpha_3)_R=0.5,\\ (U_1)_L=10,\,(\tau_1)_L=1,\,(P_1)_L=10^5,\,(U_1)_R=-10,\,(\tau_1)_R=1,\,(P_1)_R=10^5,\\ (U_2)_L=10,\,(\tau_2)_L=8,\,(P_2)_L=10^5,\,(U_2)_R=-10,\,(\tau_2)_R=8,\,(P_2)_R=10^5,\\ (U_3)_L=10,\,(\tau_3)_L=8,\,(P_3)_L=10^5,\,(U_3)_R=-10,\,(\tau_3)_R=8,\,(P_3)_R=10^5. \end{array}
```

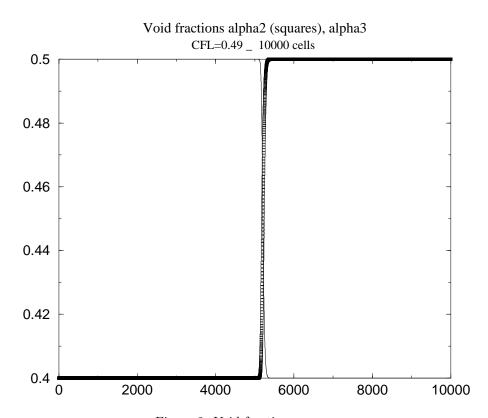


Figure 2: Void fractions α_2 , α_3

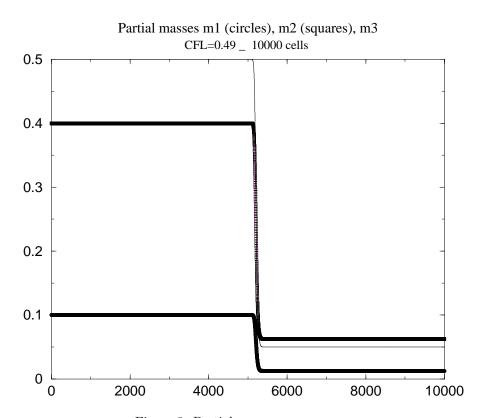


Figure 3: Partial masses m_1, m_2, m_3

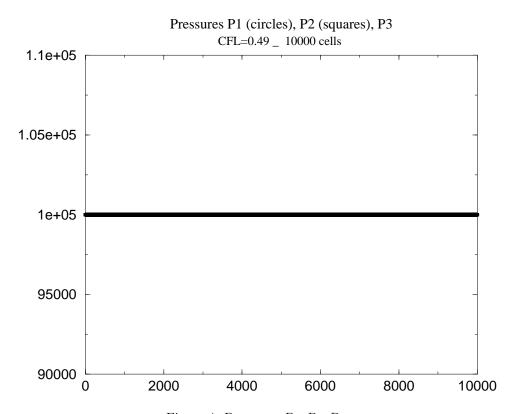


Figure 4: Pressures P_1, P_2, P_3

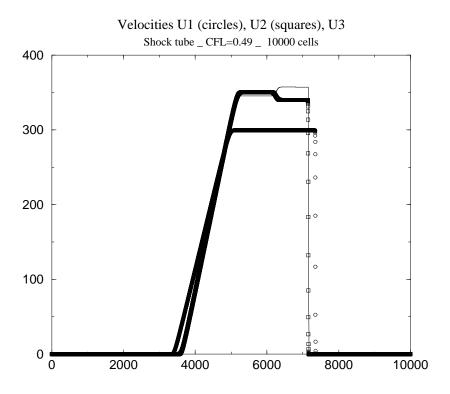


Figure 5: Velocities $U_1,\,U_2,\,U_3$

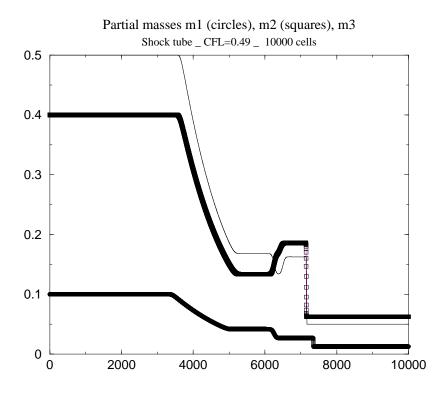


Figure 6: Partial masses m_1, m_2, m_3

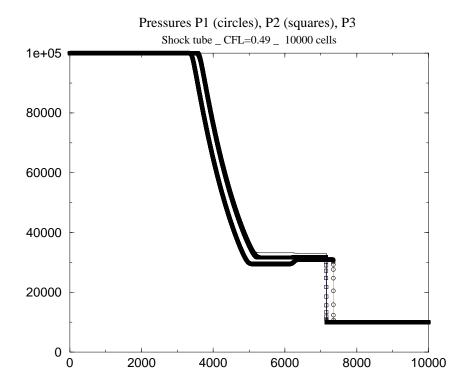


Figure 7: Pressures P_1, P_2, P_3

Symmetrical shock waves Pressure: P1 (dotted), P2 (plain), P3 (dashed) 1.1e+05 1.08e+05 1.06e+05 1.04e+051.02e+051e+05 L 10000

Figure 8: Symmetrical shock waves : mean pressures $P_1,\,P_2,\,P_3.$ The mesh contains 20000 cells.

15000

20000

5000

Symmetrical shock waves

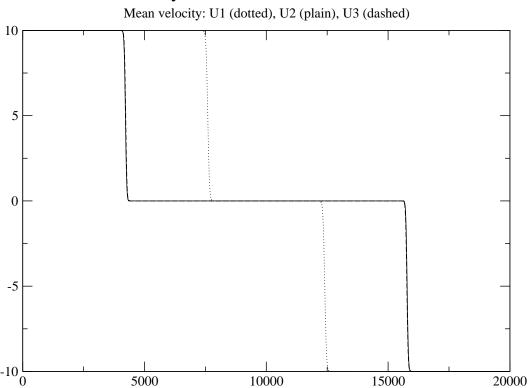


Figure 9: Symmetrical shock waves : mean velocities $U_1,\,U_2,\,U_3.$ The mesh contains 20000 cells.

6 Conclusion

This new model benefits from important properties. From a physical point of view, an interesting point is that it preserves the positivity of (expected) positive quantities: void fractions, mass fractions and internal energies, at least when restricting to sufficiently simple EOS. Its mathematical properties enable us to construct nonlinear stable numerical methods, and thus to explore highly unsteady flow patterns. As happens when focusing on the Baer-Nunziato model, necessary and sufficient conditions to ensure the existence and uniqueness of the exact solution of the one dimensional Riemann problem cannot be obtained easily. A specific difficulty is linked with the possible occurence of the resonance phenomena, and to the great number of possible configurations of waves. We have also briefly discussed a class of hyperbolic models, from which our model issues. This in particular enables to explore the counterpart of the model associated with the interface velocity $V_i = (\Sigma_k m_k U_k)/(\Sigma_k m_k)$, which is discussed in reference [20] for instance.

We emphasize once more that the main objective of the present work consists in deriving a class of meaningful models to describe three-phase flows in such a way that it leads to a well posed initial value problem. Thus the algorithm presented herein is certainly not the ultimate scheme to cope with this kind of model. The improvement of the accuracy is one specific objective of work in progress within this framework. The occurence of three distinct contact discontinuities urges for the development of "high-order" methods; otherwise, the prediction of unsteady patterns will be an illusion.

Part of our current work also concerns the comparison with standard single pressure three-field models, when restricting to coarse meshes of course. This may be achieved using relaxation techniques, following ideas from [29, 30, 32, 28, 33, 34, 35]. An advantage of the latter computational techniques is that they automatically track deficiencies of single pressure models, when occurring (see [6]).

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A Eigenstructure

Restricting to regular solutions, we rewrite the convective system issuing from (1), that is:

$$(Id + D(W))\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial G(W)}{\partial x} = 0$$

in the form:

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

using the specific variable:

$$Z^{t} = (\alpha_{2}, \alpha_{3}, s_{1}, s_{2}, s_{3}, U_{1}, U_{2}, U_{3}, P_{1}, P_{2}, P_{3})$$

The matrix is:

It admits the following right eigenvectors:

$$\begin{split} r_1^t &= (1,0,0,0,0,0,a_7,0,(P_1-P_2)/\alpha_1,a_{10},0) \\ r_2^t &= (0,1,0,0,0,0,0,a_8,(P_1-P_3)/\alpha_1,0,a_{11}) \\ r_3^t &= (0,0,1,0,0,0,0,0,0,0,0) \\ r_4^t &= (0,0,0,1,0,0,0,0,0,0,0) \\ r_5^t &= (0,0,0,0,1,0,0,0,0,0,0,0) \\ r_6^t &= (0,0,0,0,0,\tau_1,0,0,-c_1,0,0) \\ r_7^t &= (0,0,0,0,0,\tau_1,0,0,-c_2,0) \\ r_9^t &= (0,0,0,0,0,\tau_2,0,0,-c_2,0) \\ r_9^t &= (0,0,0,0,0,0,\tau_2,0,0,c_2,0) \\ r_{10}^t &= (0,0,0,0,0,0,0,\tau_3,0,0,-c_3) \\ r_{11}^t &= (0,0,0,0,0,0,0,0,0,0,c_3) \end{split}$$

noting:

$$a_7 = \gamma_2 P_2 \tau_2 (U_2 - U_1) / (\alpha_2 \delta_2) \qquad a_{10} = -\gamma_2 P_2 (U_2 - U_1)^2 / (\alpha_2 \delta_2)$$

$$a_8 = \gamma_3 P_3 \tau_3 (U_3 - U_1) / (\alpha_3 \delta_3) \qquad a_{11} = -\gamma_3 P_3 (U_3 - U_1)^2 / (\alpha_3 \delta_3)$$

$$\delta_k = (U_k - U_1)^2 - (c_k)^2$$

for k = 2, 3. Recall that $c_k = (\gamma_k P_k \tau_k)^{1/2}$.

B Riemann invariants in the k field (k = 4 to k = 11)

Using the above mentionned form of right eigenvectors, one may easily check that $grad_Z\phi(Z).r_k(Z)=0$, for any scalar $\phi(Z)$ chosen among I^k :

$$\begin{split} I^4 &= (\alpha_2,\alpha_3,s_1,s_3,U_1,U_2,U_3,P_1,P_2,P_3) \\ I^5 &= (\alpha_2,\alpha_3,s_1,s_2,U_1,U_2,U_3,P_1,P_2,P_3) \\ I^6 &= (\alpha_2,\alpha_3,s_1,s_2,s_3,U_1+g_1,U_2,U_3,P_2,P_3) \\ I^7 &= (\alpha_2,\alpha_3,s_1,s_2,s_3,U_1-g_1,U_2,U_3,P_2,P_3) \\ I^8 &= (\alpha_2,\alpha_3,s_1,s_2,s_3,U_1,U_2+g_2,U_3,P_1,P_3) \\ I^9 &= (\alpha_2,\alpha_3,s_1,s_2,s_3,U_1,U_2-g_2,U_3,P_1,P_3) \\ I^{10} &= (\alpha_2,\alpha_3,s_1,s_2,s_3,U_1,U_2,U_3+g_3,P_1,P_2) \\ I^{11} &= (\alpha_2,\alpha_3,s_1,s_2,s_3,U_1,U_2,U_3-g_3,P_1,P_2) \end{split}$$

We note here:

$$g_k(\rho_k, s_k) = \int_0^{\rho_k} \frac{c_k(a, s_k)}{a} da$$

C Jump conditions

Whatever the field is, the following jump conditions hold through any discontinuity separating states l, r, and travelling with speed σ (we still note $\Delta(\psi) = \psi_r - \psi_l$):

$$\begin{split} &(\hat{U_1} - \sigma)\Delta(\alpha_k)_{l,r} = 0 \\ &\Delta(m_k(U_k - \sigma))_{l,r} = 0 \\ &\Delta(m_kU_k(U_k - \sigma) + \alpha_k P_k)_{l,r} + \sum_{j=1, j \neq k}^3 \hat{P_{kj}}\Delta(\alpha_j)_{l,r} = 0 \\ &\Delta(\alpha_k E_k(U_k - \sigma) + \alpha_k P_k U_k)_{l,r} + \hat{U_1}\sum_{j=1, j \neq k}^3 \hat{P_{kj}}\Delta(\alpha_j)_{l,r} = 0 \end{split}$$

where : $P_{12} = P_{21} = P_{23} = P_2$ and $P_{13} = P_{31} = P_{32} = P_3$.

These clearly enable to retrieve that the above mentionned scalar quantities remain constant through the 1-2-3 field:

$$\begin{split} \sigma &= (U_1)_l = (U_1)_r \\ I_1^{1-2-3}(W_l) &= I_1^{1-2-3}(W_r) \\ I_2^{1-2-3}(W_l) &= I_2^{1-2-3}(W_r) \\ I_6^{1-2-3}(W_l) &= I_6^{1-2-3}(W_r) \\ I_7^{1-2-3}(W_l) &= I_7^{1-2-3}(W_r) \\ I_8^{1-2-3}(W_l) &= I_8^{1-2-3}(W_r) \end{split}$$

The remaining two constraints $s_k(W_l) = s_k(W_r)$ (for k=2,3) implicitely define the two non-conservative products $P_2 \frac{\partial \alpha_2}{\partial x}$ and $P_3 \frac{\partial \alpha_3}{\partial x}$.

Moreover, they turn to the classical single phase jump conditions for Euler equations apart from the U_1 eigenvalue:

$$\begin{split} &\Delta(\alpha_k)_{l,r}=0\\ &\Delta(\rho_k(U_k-\sigma))_{l,r}=0\\ &\Delta(\rho_kU_k(U_k-\sigma)+P_k)_{l,r}=0\\ &\Delta(E_k(U_k-\sigma)+P_kU_k)_{l,r}=0 \end{split}$$

Thus, for perfect gas EOS, setting $e_k(P_k, \rho_k) = \frac{P_k}{(\gamma_k - 1)\rho_k}$, we get:

$$\begin{split} \beta_k &= \frac{\gamma_k + 1}{\gamma_k - 1} \\ z_k &= \frac{(\rho_k)_r}{(\rho_k)_l} \\ \frac{(P_k)_r}{(P_k)_l} &= \frac{(\beta_k)z_k - 1}{(\beta_k) - z_k} \\ (U_k)_r - (U_k)_l &= - (\frac{((P_k)_l - (P_k)_r)((\rho_k)_l - (\rho_k)_r)}{(\rho_k)_l (\rho_k)_r})^{1/2} \end{split}$$

D Pressure relaxation

In order to simplify the presentation, we set here : $f_{2-3}(W) = 0$.

Part I

We consider here the pressure relaxation step, that is:

$$\begin{split} \frac{\partial \alpha_k}{\partial t} &= \epsilon_k (P_k - P_1) \\ \frac{\partial m_k}{\partial t} &= 0 \\ \frac{\partial m_k U_k}{\partial t} &= 0 \\ \frac{\partial \alpha_k E_k}{\partial t} - \sum_{l=1, l \neq k}^3 P_{kl} \frac{\partial \alpha_l}{\partial t} &= 0 \end{split}$$

with an initial condition in the admissible range $(P_k > 0, \alpha_k > 0)$, and infinite ϵ_k .

We focus on the following scheme (omitting cell subscript i):

$$\begin{split} &(P_k)^{n+1} = (P)^{n+1} \\ &(m_k)^{n+1} = \tilde{m_k} \\ &(m_k U_k)^{n+1} = \tilde{m_k U_k} \\ &(\alpha_k E_k)^{n+1} - (\alpha_k E_k) + (P)^{n+1} ((\alpha_k)^{n+1} - \tilde{\alpha_k}) = 0 \end{split}$$

We notice that the last equation is equivalent to:

$$(m_k e_k)^{n+1} - \tilde{(m_k e_k)} + (P)^{n+1} ((\alpha_k)^{n+1} - \tilde{\alpha_k}) = 0$$

owing to the first three mesh schemes.

If we moreover restrict to perfect gas EOS within each step, setting thus: $(\gamma_k - 1)\rho_k e_k = P_k$, in agreement with condition $\gamma_k > 1$, we immediatly get:

$$\frac{(\alpha_k P_k)^{n+1} - (\alpha_k P_k)}{\gamma_k - 1} + (P)^{n+1} ((\alpha_k)^{n+1} - \tilde{\alpha_k}) = 0$$

Using basic algebra, we hence deduce that:

$$P_k^{n+1} = P^{n+1} = \frac{\tilde{\alpha}_1 \gamma_2 \gamma_3 \tilde{P}_1 + \tilde{\alpha}_2 \gamma_1 \gamma_3 \tilde{P}_2 + \tilde{\alpha}_3 \gamma_1 \gamma_2 \tilde{P}_3}{\tilde{\alpha}_1 \gamma_2 \gamma_3 + \tilde{\alpha}_2 \gamma_1 \gamma_3 + \tilde{\alpha}_3 \gamma_1 \gamma_2}$$

and subsequently:

$$\alpha_k^{n+1} = \tilde{\alpha}_k \left(\frac{\gamma_k - 1}{\gamma_k} + \frac{\tilde{P}_k}{\gamma_k P^{n+1}} \right)$$

One may check that both P^{n+1} and α_k remain positive, assuming relevant initial data.

Morover, the "consistancy condition on pressure" holds; if we assume a perfect balance on initial values of pressures: $\tilde{P}_1 = \tilde{P}_2 = \tilde{P}_3 = \phi$, this will imply that: $P^{n+1} = \phi$, and therefore: $\alpha_k^{n+1} = \tilde{\alpha_k}$ (the relaxation step is a "ghost step" in that particular case).

Part II

Throughout the pressure relaxation step, we note that:

$$\frac{m_k}{s_k} \frac{\partial s_k}{\partial t} = a_k \left(\sum_{l=1, l \neq k}^{3} P_{kl} \frac{\partial \alpha_l}{\partial t} + P_k \frac{\partial \alpha_k}{\partial t} \right)$$

Thus:

$$m_2 \frac{\partial Ln(s_2)}{\partial t} = m_3 \frac{\partial Ln(s_3)}{\partial t} = 0$$

and:

$$\frac{\partial \eta}{\partial t} = -a_1((P_2 - P_1)\phi_2 + (P_3 - P_1)\phi_3)$$

Owing to the expression of ϕ_k for k=2,3, we may get some description of the miminm value obtained in M_0 :

$$\frac{\partial \eta}{\partial t} = 0 \qquad <=> \qquad P_2 - P_1 = P_3 - P_1 = 0$$

Even more, the second derivative around M_0 is:

$$\frac{\partial \eta}{\partial t^2}_{M_0} = a_1((\frac{\gamma_1 P_1}{\alpha_1} + \frac{\gamma_2 P_2}{\alpha_2})X^2 + (\frac{\gamma_1 P_1}{\alpha_1} + \frac{\gamma_3 P_3}{\alpha_3})Y^2 + 2XY\frac{\gamma_1 P_1}{\alpha_1})$$

setting $X = \frac{\partial \alpha_2}{\partial t}$ and $Y = \frac{\partial \alpha_3}{\partial t}$. It is thus positive, and will be null if and only if:

$$\frac{\partial \alpha_k}{\partial t} = 0$$

for k = 2, 3. This ensures that the instantaneous relaxation of pressure minimizes the entropy of the whole system. This result holds true for any EOS.

E Connection through the 1-2-3 wave

We restrict now to perfect gas EOS (results may be extended to the frame of stiffened gas EOS). We set $m_k = \alpha_k \rho_k$ and $s_k = P_k \rho_k^{-\gamma_k}$.

We assume a given state W_l , and also $(\alpha_k)_{L,R}(1-\alpha_k)_{L,R} \neq 0$. Before we connect states through the 1-2-3 wave, we need to recall that both α_2 and α_3 do not vary through fields associated with eigenvalues λ_k (for k=4-11). Thus the left (respectively right) states apart from the triple wave U_1 are $(\alpha_2)_L$, $(\alpha_3)_L$ (respectively $(\alpha_2)_R$, $(\alpha_3)_R$).

Based on the Riemann invariants of the 1-2-3 LD wave, we also know that :

$$(U_1)_r = (U_1)_l$$
 $(s_2)_r = (s_2)_l$ $(s_3)_r = (s_3)_l$ (37)

but also: $(Q_2)_r = (Q_2)_l$ and $(Q_3)_r = (Q_3)_l$. setting:

$$Q_2 = m_2(U_2 - U_1) Q_3 = m_3(U_3 - U_1) (38)$$

The latter two enable to compute $(U_k)_r$ in terms of $(U_k)_l$:

$$(U_k)_r = (U_1)_l + \frac{(Q_k)_l}{(\alpha_k)_R(\rho_k)_r}$$
(39)

for k = 2, 3.

We may parametrize the remaining Riemann invariants in terms of the three main unknowns $(P_1)_r, (\rho_2)_r, (\rho_3)_r$:

$$\begin{split} &(I_1^7)_{L,R}((\rho_2)_r) = \frac{\gamma_2}{\gamma_2 - 1}(s_2)_l(\rho_2)_r^{\gamma_2 - 1} + \frac{(Q_2)_l^2}{2((\alpha_2)_{L,R}(\rho_2)_r)^2} \\ &(I_1^8)_{L,R}((\rho_3)_r) = \frac{\gamma_3}{\gamma_3 - 1}(s_3)_l(\rho_3)_r^{\gamma_3 - 1} + \frac{(Q_3)_l^2}{2((\alpha_3)_{L,R}(\rho_3)_r)^2} \\ &(I_1^6)_{L,R}((P_1)_r, (\rho_2)_r, (\rho_3)_r) = (1 - \alpha_2 - \alpha_3)_{L,R}(P_1)_r + \sum_{k=2}^3 ((\alpha_k)_{L,R}(s_k)_l(\rho_k)_r^{\gamma_k} + \sum_{k=2}^3 (\frac{(Q_k)_l^2}{(\alpha_k)_{L,R}(\rho_k)_r}) \end{split}$$

• Computation of $(\rho_2)_r$ We note:

$$(g_2)_{L,R}(x) = \frac{\gamma_2}{\gamma_2 - 1} (s_2)_l x^{\gamma_2 - 1} + \frac{(Q_2)_l^2}{2((\alpha_2)_{L,R} x)^2}$$

Hence, for given value of $(\rho_2)_l$, the equilibrium $(I_1^7)_R((\rho_2)_r) = (I_1^7)_L((\rho_2)_l)$ implies that:

$$(g_2)_R((\rho_2)_r) = (g_2)_L((\rho_2)_l)$$

The positive function $(g_2)_{L,R}(x)$ is decreasing for $x < (x_2)_{L,R}$, and increasing for $x > (x_2)_{L,R}$, noting:

$$(x_2)_{L,R} = \left(\frac{((Q_2)_l)^2}{\gamma_2(s_2)_l(\alpha_2)_{L,R}^2}\right)^{1/(\gamma_2+1)}$$

The equation $(g_2)_R(x) = (g_2)_L((\rho_2)_l)$ admits two positive solutions if $(g_2)_R((x_2)_R) < (g_2)_L((\rho_2)_l)$ and no solution otherwise.

• Computing $(\rho_3)_r$ Of course, a similar result holds for $(\rho_3)_r$, based on the balance $:(I_1^8)_R((\rho_3)_r)=(I_1^8)_L((\rho_3)_l)$. Defining:

$$(x_3)_{L,R} = \left(\frac{((Q_3)_l)^2}{\gamma_3(s_3)_l(\alpha_3)_{L,R}^2}\right)^{1/(\gamma_3+1)}$$

and:

$$(g_3)_{L,R}(x) = \frac{\gamma_3}{\gamma_3 - 1} (s_3)_l x^{\gamma_3 - 1} + \frac{(Q_3)_l^2}{2((\alpha_3)_{L,R} x)^2}$$

 $(\rho_3)_r$ will be the solution of :

$$(g_3)_R((\rho_3)_r) = (g_3)_L((\rho_3)_l)$$

which exists if : $(g_3)_R((x_3)_R) < (g_3)_L((\rho_3)_l)$.

• We turn now to the last unknown $(P_1)_r$. If we note:

$$K = (I_1^6)_L((P_1)_l, (\rho_2)_l, (\rho_3)_l) - \sum_{k=2}^3 ((\alpha_k)_R(s_k)_l((\rho_k)_r)^{\gamma_k} - \sum_{k=2}^3 (\frac{(Q_k)_l^2}{(\alpha_k)_R(\rho_k)_r})$$

the problem will admit a positive solution if and only if $0 \le K$:

$$(P_1)_r = \frac{K}{(1 - \alpha_2 - \alpha_3)_R}$$

F Influence of mass transfer terms

We still consider system (2) with the full source terms including mass transfer and heat transfer as detailed below:

$$S(W) = (\phi_2, \phi_3, \Gamma_1, \Gamma_2, \Gamma_3, S_{U_1}, S_{U_2}, S_{U_3}, \psi_1 + U_1 S_{U_1}, \psi_2 + U_1 S_{U_2}, \psi_3 + U_1 S_{U_3})$$
(40)

The interfacial mass transfer and heat transfer terms must agree with:

$$\begin{split} \sum_k \Gamma_k &= \sum_k (\sum_{l \neq k} \Gamma_{kl}) = 0 \\ \sum_k \psi_k &= \sum_k (\sum_{l \neq k} \psi_{kl}) + \sum_k (\sum_{l \neq k} \Gamma_{kl} H_{kl}) = 0 \\ \psi_{kl} + \psi_{lk} &= 0 \\ \Gamma_{kl} + \Gamma_{lk} &= 0 \\ H_{kl} &= H_{lk} \end{split}$$

We define:

$$\nu_k = -\frac{1}{2}(U_1)^2 + \frac{1}{2}(U_k - U_1)^2 - \frac{\partial \rho_k e_k}{\partial \rho_k} + \frac{1}{a_k} \frac{\partial \rho_k Ln(s_k)}{\partial \rho_k}$$

If we assume that, for k=2,3:

$$\Gamma_k = \frac{a_k \nu_k - a_1 \nu_1}{\tau_k^{\Gamma}}$$

$$\psi_k = \frac{a_k - a_1}{\tau_k^{\psi}}$$

with $0 \le \tau_k^{\Gamma}$ and $0 \le \tau_k^{\psi}$, then the entropy inequality (22) still holds.

Obviously, it appears that if contributions Γ_k and ψ_k do not act simultaneously, that is if $\frac{1}{\tau_k^{\Gamma}} \frac{1}{\tau_k^{\psi}} = 0$ the two following equilibrium states arise:

$$a_1 = a_2 = a_3$$

 $P_1 = P_2 = P_3$
 $U_1 = U_2 = U_3$

and:

$$a_1\nu_1 = a_2\nu_2 = a_3\nu_3$$

 $P_1 = P_2 = P_3$
 $U_1 = U_2 = U_3$

We recall once more that:

$$a_k = (s_k)^{-1} \left(\frac{\partial s_k(P_k, \rho_k)}{\partial P_k}\right) \left(\frac{\partial e_k(P_k, \rho_k)}{\partial P_k}\right)^{-1}$$

For a perfect gas EOS:

$$\begin{aligned} a_k &= \frac{(\gamma_k - 1)\rho_k}{P_k} \\ \frac{\partial \rho_k Ln(s_k(\rho_k, P_k))}{\partial \rho_k} &= Ln(s_k) - \gamma_k \\ \frac{\partial \rho_k e_k(\rho_k, P_k)}{\partial \rho_k} &= 0 \end{aligned}$$

Actually, any closure should obey the constraint:

$$\begin{split} & \sum_{k} a_{k} \nu_{k} \Gamma_{k} \\ & + \sum_{k} (a_{k} \psi_{k}) \\ & + \sum_{k} (a_{k} S_{U_{k}} (U_{1} - U_{k})) \\ & + \sum_{k} (a_{k} (P_{kl} - P_{k}) \phi_{k}) > 0 \end{split}$$

G Uniqueness of entropy consistent interface pressure terms

We show here that there exists a unique solution for the six unknowns P_{kl} , which is consistent with the entropy inequality.

We start setting:

$$V_i = \beta_1 U_1 + \beta_2 U_2 + \beta_3 U_3 \tag{41}$$

where $0 \le \beta_k$ and $\beta_1 + \beta_2 + \beta_3 = 1$. We still use the same notation for coefficients a_k , and we first note that the entropy inequality (22) implies that:

$$\sum_{k=1}^{3} (U_k - V_i) a_k \left(\sum_{l=1, l \neq k}^{3} (P_k - P_{kl}) \frac{\partial \alpha_l}{\partial x} \right) = 0$$
 (42)

Since both $\frac{\partial \alpha_1}{\partial x}$ and $\frac{\partial \alpha_2}{\partial x}$ are independent, this results in two constraints:

$$a_1(\beta_2(U_1 - U_2) + \beta_3(U_1 - U_3))(P_{13} - P_{12})$$

+ $a_2(\beta_1(U_2 - U_1) + \beta_3(U_2 - U_3))(P_{23} - P_2)$
+ $a_3(\beta_1(U_3 - U_1) + \beta_2(U_3 - U_2))(P_3 - P_{32}) = 0$

and:

$$a_1(\beta_2(U_1 - U_2) + \beta_3(U_1 - U_3))(P_{13} - P_1) + a_2(\beta_1(U_2 - U_1) + \beta_3(U_2 - U_3))(P_{23} - P_{21}) + a_3(\beta_1(U_3 - U_1) + \beta_2(U_3 - U_2))(P_3 - P_{31}) = 0$$

We now note that : $U_1 - U_3 = (U_1 - U_2) + (U_2 - U_3)$. Taking into account the fact that $(U_1 - U_2)$ and $(U_2 - U_3)$ are independent, we may rewrite the latter two constraints as a set of four equations:

$$a_1(\beta_2 + \beta_3)(P_{13} - P_{12}) + a_2\beta_1(P_2 - P_{23}) - a_3\beta_1(P_3 - P_{32}) = 0$$

$$-a_3(\beta_2 + \beta_1)(P_3 - P_{32}) + a_1\beta_3(P_{13} - P_{12}) + a_2\beta_3(P_{23} - P_{2}) = 0$$

$$a_1(\beta_2 + \beta_3)(P_{13} - P_1) + a_2\beta_1(P_{21} - P_{23}) - a_3\beta_1(P_3 - P_{31}) = 0$$

$$-a_3(\beta_2 + \beta_1)(P_3 - P_{31}) + a_1\beta_3(P_{13} - P_1) + a_2\beta_3(P_{23} - P_{21}) = 0$$

We hence may write the previous four equations and the constraints which guarantee the global conservation of momentum and energy:

$$P_{12} + P_{32} - (P_{13} + P_{23}) = 0$$

$$P_{12} + P_{32} - (P_{21} + P_{31}) = 0$$

as a linear system with unknown $Z = (P_{12}, P_{21}, P_{13}, P_{31}, P_{23}, P_{32})$ solution of:

$$BZ = C (43)$$

where B stands for the matrix:

$$B = \begin{pmatrix} a_1(\beta_1 - 1) & 0 & a_1(1 - \beta_1) & 0 & -a_2\beta_1 & a_3\beta_1 \\ -a_1\beta_3 & 0 & a_1\beta_3 & 0 & a_2\beta_3 & a_3(1 - \beta_3) \\ 0 & a_2\beta_1 & a_1(1 - \beta_1) & a_3\beta_1 & -a_2\beta_1 & 0 \\ 0 & -a_2\beta_3 & a_1\beta_3 & a_3(1 - \beta_3) & a_2\beta_3 & 0 \\ 1 & -1 & 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 & -1 & 1 \end{pmatrix}.$$

and the right hand side is:

$$C^{t} = (a_{3}\beta_{1}P_{3} - a_{2}\beta_{1}P_{2}, a_{2}\beta_{3}P_{2} + (1 - \beta_{3})a_{3}P_{3}, a_{3}\beta_{1}P_{3} + (1 - \beta_{1})a_{1}P_{1}, a_{1}\beta_{3}P_{1} + (1 - \beta_{3})a_{3}P_{3}, 0, 0)$$

$$(44)$$

The solution exists and is unique since the determinant reads:

$$det(B) = -(a_1 a_2 \beta_3 + a_1 a_3 \beta_2 + a_2 a_3 \beta_1)^2$$
(45)

In the particular case where $V_I = U_1$, that is $\beta_1 = 1$, and $\beta_2 = \beta_3 = 0$, we retrieve the solution:

$$P_{13} = P_{31} = P_{32} = P_3$$

 $P_{12} = P_{21} = P_{23} = P_2$