Modelling spherical explosions with turbulent mixing and post-detonation

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Abstract

This paper addresses post detonation modelling in spherical explosions. One of the challenges is thus related to compressible turbulent mixing layers modelling. A one-dimensional flow model is derived consisting in a reduced two-phase compressible flow model with velocity drift. To reduce the number of model parameters, the stiff velocity relaxation limit is considered. A semi-discrete analysis is used resulting in a specific artificial viscosity formulation embedded in the diffuse interface model of Kapila et al. \cite{Kapila01}. Thanks to the velocity non-equilibrium model and semi discrete formulation, the model fuls the second law of thermodynamics in the global sense and uses a single parameter. Multidimensional mixing layer effects occurring at gas-gas unstable interfaces are thus summarized as artificial viscosity effects. Model's predictions are compared against experimental measurements of mixing layer growth in shock tubes at moderate initial pressure ratios as well as fireball radius evolutions in air explosions at high initial pressure ratios. Also, pressure signals recorded at various stations are compared, showing excellent agreement for the leading shock wave as well as the secondary one. With the help of various experiments in the low and high initial pressure ratios bounds, estimates for the interpenetration parameter are given.

Key words: Multiphase flows, diffuse interfaces, hyperbolic equations, unstable interfaces, turbulent mixing, detonations, blast waves.
0. Introduction

Post detonation effects that occur during explosion of spherical energetic material charges in air environment result in both enhanced fireball radius and blast effects compared to conventional one-dimensional spherical codes predictions. These conventional codes solve the Euler equations inside the detonation products sphere and the same equations in the air to model the shock wave propagation. The material interface separating the air and the detonation products is usually solved with a front tracking scheme or any method able to fulfil the interface conditions of equal pressure and equal normal velocities (see for example Massoni et al.¹).

Conventional codes predictions of fireball volumes are about 5 times smaller than the ones measured. The reason is that detonation products mix with air through a turbulent layer. As they contain chemical species such as C, CO and H₂, post combustion of detonation products (named ‘post-detonation’ in the rest of the paper) occurs in the mixing layer with air. The energy released by post-detonation can be larger than the energy that supports the detonation wave.

As this post detonation is only possible in the mixing layer, it poses the serious issue of turbulent mixing layers modelling with compressible fluids. A typical explosion situation is shown in the Figure 1 with a TNT charge explosion in air.

![Figure 1. Photograph example of a 1 kg TNT charge explosion in air with post-detonation effects in the mixing layer. The post-detonation energy can be greater than the one supporting the detonation wave. Observed fireball volumes can be one order magnitude larger than conventional codes predictions.](image)

From this picture, it is clear that the mixing zone is highly turbulent. Many Rayleigh-Taylor (RT) type bubbles and spikes are present. Also, it is clear that the flow is multidimensional and multiscale.

A first computational approach could be based on a multi-dimensional computational fluid dynamic code. However, this poses several challenges as:

- The number of RT instabilities is very large and computed results will have sense only if each wave length is spatially and temporally resolved.
- Determination of the initial conditions for the interface perturbations is an issue.
- Even if spatial and temporal resolutions are fine enough, the results may be code dependant. As shown by Liska and Wendroff ², the computation of a single RT type instability is challenging. A meaningful figure issued from that reference is reported in the Figure 2.
Figure 2. Computation of a single RT type instability with various compressible flow solvers, from Liska and Wendroff. The various flow solvers agree with the main flow features, but it is clear that important differences are present in the details. Non negligible differences appear in the growth rates which can be estimated from these pictures. More importantly, the mixing zone between the two fluids, where combustion reaction may occur, presents large differences.

Liska and Wendroff results show that numerical instabilities have serious consequences on physical ones. These differences can be amplified in a context where combustion occurs. The present work deals with a one-dimensional model where multi-D effects occurring in the unstable front result in interpenetration effects. The difficulty is thus to model these effects with an approach that:
- Respects conservation principles and entropy inequality.
- Preserves hyperbolicity of the equations and wave’s dynamics.
- Reproduces the experiments with as few parameters as possible in order to avoid ambiguity in parameters determination.
- Is able to reproduce conventional spherical computations in the limit of vanishing interpenetration effects. In particular, it must be able to fulfil contact interface conditions of equal pressures and equal normal velocities.

The model we are going to develop is aimed to respect these requirements. It contains a single parameter, determined with the help of experimental data.

In the same direction, one-dimensional reduced models have been considered by various approaches. All have been motivated by applications related to inertial confined fusion while the present paper deals with explosions. Three main classes of reduced models are present in the literature:
- \( k-\varepsilon \) type models: Gauthier and Bonnet, Besnard et al. to cite a few. Following the analysis given by Cheng, this class of models uses many parameters.
- Multiphase flow models: Youngs et al., Chen et al., Glimm et al., Scannapieco and Cheng, Saurel et al. Following again the review of Cheng, most models in this class involve many parameters for their calibration too. Some of them do not fulfil the second law of
thermodynamics. The last model in this list deals with wave propagation and turbulent energy production in already created mixing layer. It is not aimed to predict mixing layers growth. It is worth to mention that multi-velocity multiphase flow models have to deal with contradictions when applied to mixing layers creation. Indeed, non-conservative terms \( u \frac{\partial \alpha}{\partial x} \) and \( p \frac{\partial \alpha}{\partial x} \) are present in the equations, with discontinuous variation of the volume fraction \( \alpha \) at interfaces separating fluids. To be in agreement with the second law of thermodynamics, the interfacial variables estimates \( u_1 \) and \( p_1 \) can be:

* \( u_1 = u_1 \), the velocity of the first phase and \( p_1 = p_2 \), the pressure of the second phase, or alternatively,

* \( u_1 = u_2 \), the velocity of the second phase and \( p_1 = p_1 \), the pressure of the first phase (Baer and Nunziato\(^{12}\), or last,

* the estimates given in Saurel et al.\(^{10}\):

\[
\begin{align*}
    u_1 &= \frac{Z_1 u_1 + Z_2 u_2}{Z_1 + Z_2} + \text{sgn} \left( \frac{\partial \alpha}{\partial x} \right) \frac{p_2 - p_1}{Z_1 + Z_2}, \\
    p_1 &= \frac{Z_1 p_1 + Z_2 p_2}{Z_1 + Z_2} + \text{sgn} \left( \frac{\partial \alpha}{\partial x} \right) \frac{Z_2 (u_2 - u_1)}{Z_1 + Z_2}.
\end{align*}
\]

With the first two sets of estimates an issue arises immediately as the predicted mixing layers using the first set are different of those predicted using the second set.

The third set of estimates is symmetric but results in non-permeable interfaces with local fulfilment of the interface conditions \( (u = \text{cst.}, p = \text{cst.}) \) when the volume fraction varies from 0 to 1, forbidding interpenetration. The effects of these terms, when correctly solved in the presence of large volume fraction discontinuities are explained in Abgrall and Saurel\(^{12}\), in the Figures 12 and 13 of that reference.

- Linear perturbations of hyperbolic systems (Olazabal\(^{13}\), Godewski et al.\(^{14}\), Godlewski and Raviart\(^{15}\), Godlewski et al.\(^{16}\), Samtaney\(^{17}\)). These models consist in a set of hyperbolic equations for the mean flow field determination and another set of equations for the perturbations. This second set of partial differential equations corresponds to transport equations with discontinuous coefficients. This approach seems to be the most efficient to predict mixing layers growth in the linear stage, as corresponding models are free of adjustable parameters and reproduce experiments with high fidelity. However, two limitations are present; the first one is obvious and related to the linear character of the perturbations. The second limitation lies in the absence of coupling from the perturbation field to the mean flow field. In particular, there is no mass flux through the interface in the mean flow field.

The reader is referred to the useful and relevant review of reduced models given by Cheng\(^{5}\) giving limitations and number of parameters present in most models mentioned above. There is thus a clear need for models involving as few parameters as possible. A new model is built in the present work and belongs to the class of multiphase flow models. Two key points are considered. The first one is related to the contact interface conditions fulfilment in the limit of vanishing interpenetration effects. This issue is not addressed in existing models, but can be considered in the frame of ‘diffuse interface methods’ (Saurel and Abgrall\(^{18}\), Kapila et al.\(^{19}\)). In this approach, the same equations are solved everywhere, in pure fluids and at interfaces, considered as numerically smeared zones. The second key point lies in the presence of a single parameter in the model we are going to develop to consider interpenetration effects.
In the present work, the Kapila et al. \(^{19}\) model is considered to determine the basic flow solution. Interpenetration effects are added in a thermodynamically consistent way. The corresponding velocity non-equilibrium flow model is then split in two sub systems. On one hand, the Kapila et al. \(^{19}\) model is recovered and on the other hand a new hyperbolic model for interpenetration is obtained.

The interpenetration sub model presents nice features as it is hyperbolic and agrees with the entropy inequality. It contains however several difficulties:
- Non-conservative equations are present, resulting in numerical difficulties.
- Two parameters are present, expressing interpenetration and drag effects.

To reduce the number of parameters the stiff velocity relaxation limit is considered. It results in a single parameter flow model. According to the method used to deal with this reduction, two different limit models are obtained, each one being admissible.

The first one is obtained by conventional asymptotic analysis. It results in an extension of the Kapila et al. \(^{19}\) model where velocity drift effects are modelled by the Darcy law (Guillard and Duval \(^{20}\), Saurel et al. \(^{21}\)). This model is unfortunately unable to correctly predict mixing layer growth. The reason is that during shock interface interaction, fluids inertia is absent, because of the Darcy law. Therefore, the interpenetration stops as soon as pressure gradients vanish, i.e. when pressure waves are far enough of the mixing layer. Typical solutions behaviour with this model are shown in the rest of the paper and compared to experimental data, illustrating this major limitation.

The second limit model is less conventional and is obtained by a semi-discrete analysis. A conventional operator splitting approach is considered to solve the interpenetration model in the stiff velocity relaxation limit. Even if splitting methods are known to induce errors, especially when source or relaxation terms are stiff, they do not violate any fundamental principle, as for example the second law of thermodynamics. The resulting model from this discrete analysis contains diffusion terms for all conservative variables and is reminiscent of artificial viscosity methods, well known as discontinuities capturing methods (von Neumann and Richtmyer \(^{22}\), Lax and Wendroff \(^{23}\), MacCormack \(^{24}\)).

A key point is addressed at this level. With artificial viscosity methods, there is no local fulfilment of the second law of thermodynamics, even when conventional models such as the Euler equations are considered. Thus, these methods seem inappropriate for the modelling of physical effects, such as turbulent mixing. However, the semi discrete analysis of the two-phase flow model with interpenetration in the presence of stiff velocity relaxation shows that global agreement with the second law of thermodynamic is reached. The model is thus admissible and used to deal with turbulent mixing layers, with large ‘artificial viscosity’ or ‘interpenetration parameter’. An implicit diffusion solver is used in this aim while the explicit method of Saurel et al. \(^{25}\) is used to solve the hyperbolic part for the mean flow field. Combination of the two sub models, the Kapila et al. \(^{19}\) one for the mean flow field and the artificial diffusion one for interpenetration, results in a simple and robust approach for turbulent mixing layers.

The ‘interpenetration coefficient’ is estimated with the help of two different sets of experimental data, corresponding to two different facilities. The first one provides mixing layer width records in shock tube experiments while the second one is based on spherical explosions in air. To use the second dataset, post detonation effects occurring in the mixing layer have to be considered. The approach ‘mixed is burnt’ is used, meaning that turbulent mixing controls the rate at which post detonation occurs. Post-detonation effects consequently do not add extra parameters, as no chemical kinetics is needed. The amount of released energy during post detonation is determined with the help of Kamlet and Jacobs \(^{26}\) thermochemical rules.

This dataset, for low initial pressure ratios (shock tube experiments) and high initial ones (air explosions) allows estimation of the interpenetration parameter. Model’s predictions are validated against experimental fireball radius dynamics and pressure gauges signals at various stations, showing excellent agreement.
1. Velocity non-equilibrium model derivation
The model derived in this section is not the final model used for fluids interpenetration but is a necessary step in the building method.
A two-phase mixture of compressible fluids is considered, each one having its own temperature, entropy, density, equation of state and evolving in its own volume. The fluids are assumed to evolve in pressure equilibrium with the centre of mass velocity and some velocity drift.

1.1 Constraints
As the phase are assumed to evolve with velocity fluctuations around the centre of mass velocity, the mass equations read:

\[
\frac{\partial (\alpha \rho)_1}{\partial t} + \frac{\partial (\alpha \rho)_1 u}{\partial x} + \frac{\partial \rho aw}{\partial x} = 0,
\]

\[
\frac{\partial (\alpha \rho)_2}{\partial t} + \frac{\partial (\alpha \rho)_2 u}{\partial x} - \frac{\partial \rho aw}{\partial x} = 0,
\]

(1.1)
where \( w, a, u, \alpha_k \) \((k=1,2)\), \( \rho_k \) and \( \rho \) represent the relative velocity \((w = u_1 - u_2)\), the interpenetration parameter \( (a \text{ positive constant or function}) \), the centre of mass velocity \((u = Y_1 u_1 + Y_2 u_2)\), the volume fractions, the densities and the mixture density \((\rho = (\alpha \rho)_1 + (\alpha \rho)_2)\), respectively. The mass fractions are denoted by \( Y_k = \frac{\alpha_k \rho_k}{\rho} \).

When mass equations (1.1) are compared to those of conventional multiphase flow models,

\[
\frac{\partial (\alpha \rho)_k}{\partial t} + \frac{\partial (\alpha \rho u)_k}{\partial x} = 0,
\]

the corresponding interpenetration parameter is necessarily \( a = Y_1 Y_2 \).

However, this formula for the interpenetration parameter presents a drawback when fluid separation occurs, as the product \( Y_1 Y_2 \) goes to zero. Such situation occurs when a heavy fluid is accelerated into a light one, as there is an ‘inversion phenomenon’ that passes through a separation point. This phenomenon is well known and will be illustrated in Section 4 with the help of shock tube experiments.

We thus prefer to consider that ‘a’ is a parameter and that (1.1) are admissible mass equations, in the sense that,
- mixture mass is preserved,
- weak forms of (1.1) are compatible with weak forms of the conventional mass equations.

Let us mention that the parameter ‘a’ is going to disappear along the derivation. Thus there is no restriction regarding the specific expression of ‘a’.
From conventional multiphase flow models, there is no difficulty to show that momentum equations sum up as,

\[
\frac{\partial p u}{\partial t} + \frac{\partial (p u^2 + p + p_\tau)}{\partial x} = 0,
\]

(1.2)
where a ‘turbulent pressure’ \( p_\tau \) appears as a consequence of relative motion.

The mixture total energy is defined as,

\[
E = Y_1 e_1 + Y_2 e_2 + \frac{1}{2} u^2 + e_t,
\]

(1.3)
where \( e_t \) represents the turbulent energy. Let us speculate that the turbulent kinetic energy is linked to the relative motion as,

\[
e_t = \frac{1}{2} aw^2.
\]

(1.4)
The turbulent energy and turbulent pressure are linked by some kind of equation of state (Saurel et al. 10):

\[ p_t = (\gamma_t - 1)p e_1, \]  \hspace{1cm} (1.5)

where \( \gamma_t = 3 \) for one-dimensional ‘turbulent’ or relative motion.

The derivation assumes that dissipation effects are absent for now. The flow is thus isentropic for both phases in zones where shocks are absent,

\[ \frac{d s_k}{d t} = 0, \quad k=1,2, \]  \hspace{1cm} (1.6)

where \( \frac{d s_k}{d t} = \frac{\partial}{\partial t} + u_k \frac{\partial}{\partial x} \) with,

\[ u_1 = u + \frac{a}{Y_1} w, \]

\[ u_2 = u - \frac{a}{Y_2} w. \]

The assumption regarding isentropic evolution is not restrictive as a quasi-conservative formulation of the flow model will be determined, precisely to handle shocks and discontinuities. For example, Equations (1.1), (1.2) and the mixture energy balance equation (1.7) hereafter are in conservative form, in order to handle discontinuities. Equations (1.6) have to be understood as constraints the model must fulfil in smooth parts of the flow.

Another constraint is given by the total energy conservation:

\[ \frac{\partial}{\partial t} E + \frac{\partial (p E + p + p_1) u}{\partial x} + \frac{\partial p aw (h_1 - h_2)}{\partial x} = 0, \]  \hspace{1cm} (1.7)

where \( h_1 \) and \( h_2 \) denote the specific enthalpies.

This mixture energy balance is a consequence of conventional multiphase flow models too.

The last constraint is given by the pressure equilibrium condition:

\[ p_1 (\rho_1, s_1) = p_2 (\rho_2, s_2) \]  \hspace{1cm} (1.8)

The system made by equations (1.1-1.8) corresponds to a set of constraints the flow model must fulfil. The various functions to determine are: \( a, \alpha_i \) and \( w \). In particular, evolution equations are needed for these last two variables.

1.2 Thermodynamic compatibility – Relative velocity equation

The various equations of System (1.1-1.8) must be compatible. To examine this compatibility, let us present the mass equations (1.1) under the form:

\[ \frac{d Y_1}{d t} = -\frac{1}{\rho} \frac{\partial p aw}{\partial x}, \]  \hspace{1cm} (1.9)

\[ \frac{d Y_2}{d t} = \frac{1}{\rho} \frac{\partial p aw}{\partial x}, \]

with \( \frac{d}{d t} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} \).

After some manipulations, the total energy equation (1.7) becomes:

\[ \rho \frac{d e}{d t} + p u \frac{du}{d t} + \rho \frac{de_t}{d t} + (p + p_1) \frac{\partial u}{\partial x} + u \frac{\partial (p + p_1)}{\partial x} + \frac{\partial p aw (h_1 - h_2)}{\partial x} = 0. \]

The mixture momentum equation (1.2) can be written as:

\[ \rho \frac{du}{d t} + \frac{\partial (p + p_1)}{\partial x} = 0. \]

The energy equation thus becomes,
\[
\frac{de}{dt} + \frac{de_i}{dt} + (p + p_i) \frac{dv}{dt} + \frac{1}{\rho} \frac{\partial p_{aw}(h_1 - h_2)}{\partial x} = 0,
\]

where \( v = \frac{1}{\rho} \) represents the mixture specific volume. In particular, \( v = Y_1 v_1 + Y_2 v_2 \).

Expanding the mixture energy, we have:

\[
Y_1 T_1 \frac{ds_1}{dt} + Y_2 T_2 \frac{ds_2}{dt} + (h_1 - h_2) \frac{dY_1}{dt} + \frac{de_i}{dt} + p_i \frac{dv}{dt} + \frac{1}{\rho} \frac{\partial p_{aw}(h_1 - h_2)}{\partial x} = 0 \tag{1.10}
\]

Using now (1.6) under the form,

\[
\frac{ds_1}{dt} = \frac{a}{Y_1} w \frac{\partial s_1}{\partial x},
\]

\[
\frac{ds_2}{dt} = \frac{a}{Y_2} w \frac{\partial s_2}{\partial x},
\]

and (1.9) we have,

\[
\frac{de_i}{dt} + p_i \frac{dv}{dt} + aw \left( \frac{\partial (h_1 - h_2)}{\partial x} + T_2 \frac{\partial s_2}{\partial x} - T_1 \frac{\partial s_1}{\partial x} \right) = 0.
\]

Using now (1.4), (1.5) and the mixture mass equation, we have:

\[
\frac{dw}{dt} + \frac{daw}{dt} + \frac{\partial (h_1 - h_2)}{\partial x} + T_2 \frac{\partial s_2}{\partial x} - T_1 \frac{\partial s_1}{\partial x} = 0
\]

Thanks to the Gibbs identity it becomes:

\[
\frac{dw}{dt} + \frac{daw}{dt} + (v_1 - v_2) \frac{dp}{\partial x} = 0. \tag{1.11}
\]

This equation expresses relative motion of the phases.

**1.3 Pressure equilibrium condition – Volume fraction equation**

The last equation needed for the system closure is provided by the pressure equilibrium condition (1.8). Under differential form it reads,

\[
c_i^2 \frac{dp_1}{dt} + \rho_i \Gamma_1 T_1 \frac{ds_1}{dt} = c_i^2 \frac{dp_2}{dt} + \rho_2 \Gamma_2 T_2 \frac{ds_2}{dt}, \tag{1.12}
\]

where \( \Gamma_k \) represents the Grüneisen coefficient of the phase \( k \) \( \left( \Gamma_k = \frac{1}{\rho_k} \frac{\partial p_k}{\partial e_k} \right) \).

Expressing the mass equations (1.1) as,

\[
\frac{dp_1}{dt} = \frac{\rho_1}{\alpha_1} \frac{d\alpha_1}{dt} - \rho_1 \frac{\partial u}{\partial x} - \frac{1}{\alpha_1} \frac{\partial p_{aw}}{\partial x},
\]

\[
\frac{dp_2}{dt} = \frac{\rho_2}{\alpha_2} \frac{d\alpha_2}{dt} - \rho_2 \frac{\partial u}{\partial x} + \frac{1}{\alpha_2} \frac{\partial p_{aw}}{\partial x},
\]

and using equations (1.6) the pressure equilibrium condition (1.12) becomes,

\[
\frac{d\alpha_1}{dt} = \frac{1}{\rho_1 c_i^2 + \rho_2 c_i^2} \left[ \left( \rho_2 c_i^2 - \rho_1 c_i^2 \right) \frac{\partial u}{\partial x} - \left( c_i^2 + c_i^2 \right) \frac{\partial p_{aw}}{\partial x} - \rho_{aw} \left( \frac{\Gamma_1 T_1}{\alpha_1} \frac{\partial s_1}{\partial x} + \frac{\Gamma_2 T_2}{\alpha_2} \frac{\partial s_2}{\partial x} \right) \right]. \tag{1.13}
\]

This volume fraction equation agrees with preceding phase transition models (Saurel et al., 27) as \( \frac{\partial p_{aw}}{\partial x} \) represents a differential mass transfer, the last term of the right hand side representing a generalized heat flux.
1.4 Adding dissipative effects
For the present application of interpenetrating fluids, it is important to consider drag relaxation in the relative velocity equation. Equation (1.11) thus becomes:

$$ \frac{\partial w}{\partial t} + \frac{\partial u}{\partial x} + (v_1 - v_2) \frac{\partial p}{\partial x} = -\lambda w, $$

(1.14)

where $\lambda$ represents the velocity relaxation parameter.

We have to check that the model is in agreement with the second law of thermodynamics. To do this, we have to determine the entropy equations. Equations (1.10) and (1.14) imply,

$$ Y_1 T_1 \frac{d s_1}{dt} + Y_2 T_2 \frac{d s_2}{dt} = \lambda a w^2. $$

(1.15)

Equation (1.15) consequently provides a first equation linking the two unknown functions $\frac{d s_1}{dt}$ and $\frac{d s_2}{dt}$. A second equation is provided by the pressure equilibrium condition (1.12) that becomes, with the help of the volume fraction equation (1.13):

$$ \rho_1 T_1 \frac{d s_1}{dt} - \rho_2 T_2 \frac{d s_2}{dt} = 0 $$

(1.16)

Solving System (1.15-1.16) results in,

$$ \alpha_1 \rho_1 \frac{d s_1}{dt} = \rho \Gamma \alpha_1 \frac{\lambda a w^2}{T_1}, $$

$$ \alpha_2 \rho_2 \frac{d s_2}{dt} = \rho \Gamma \alpha_2 \frac{\lambda a w^2}{T_2}, $$

with,

$$ \frac{1}{\Gamma} = \frac{\alpha_1}{T_1} + \frac{\alpha_2}{T_2}. $$

Consequently, the mixture entropy reads,

$$ \frac{\partial \left( \alpha_1 \rho_1 s_1 + \alpha_2 \rho_2 s_2 \right)}{\partial t} + \frac{\partial \left( \alpha_1 \rho_1 u + \alpha_2 \rho_2 u \right)}{\partial x} + \frac{\partial p a w (s_1 - s_2)}{\partial x} = \rho \Gamma \lambda a w^2 \left( \frac{\alpha_1}{T_1} + \frac{\alpha_2}{T_2} \right). $$

(1.17)

This result is in perfect agreement with the second law of thermodynamics.

1.5 Thermodynamic closure
In the present context of turbulent mixing layers, with detonation gas products and air, quite sophisticated equation of state (EOS) is needed for detonation products (DP). The JWL EOS (Lee et al. 28) is used under 'stiffened gas' form, for phase 1 considered as DP,

$$ p_1 (\rho_1, e_1) = (\gamma_1 - 1) \rho_1 (e_1 - \varepsilon_{\text{ref}} (\rho_1)) - \gamma_1 \varepsilon_{\text{ref}} (\rho_1), $$

with,

$$ \varepsilon_{\text{ref}} (\rho_1) = \frac{A}{\rho_{\text{ref}} R_1} e^{-R_1 \rho_{\text{ref}} / \rho_1} + \frac{B}{\rho_{\text{ref}} R_2} e^{-R_2 \rho_{\text{ref}} / \rho_1} + \frac{k}{\rho_{\text{ref}} (\gamma_1 - 1)} \left( \frac{\rho_{\text{ref}}}{\rho_1} \right)^{-(\gamma_1-1)}, $$

$$ p_{\text{ref}} (\rho_1) = \frac{1}{\gamma_1} \left[ A e^{-R_1 \rho_{\text{ref}} / \rho_1} + B e^{-R_2 \rho_{\text{ref}} / \rho_1} + \left( \frac{\rho_{\text{ref}}}{\rho_1} \right)^{-\gamma_1} \right], $$

$$ k = \left[ p_C J - A e^{-R_1 \rho_{\text{ref}} / p_C J} - B e^{-R_2 \rho_{\text{ref}} / p_C J} - \rho_C J (\gamma_1 - 1) C v_{CL} + K \left( \frac{\rho_{\text{ref}}}{p_C J} \right)^{\gamma_1} \right]. $$

Regarding TNT, the various constants are:
\[ p_{\text{ CJ}} = 19.59 \times 10^9 \text{ Pa} \, , \, D_{\text{ CJ}} = 6885.8 \, \text{m/s} \, , \, T_{\text{ CJ}} = 3686 \, \text{K} \, , \, C_{\text{v1}} = 815 \, \text{J/kg/K} \, , \, A = 353.91 \times 10^9 \text{ Pa} \, , \]

\[ B = 3.45 \times 10^9 \text{ Pa} \, , \, R_1 = 4.15 \, , \, R_2 = 0.9 \, , \, \gamma_1 = 1.35 \, . \]

The air is assumed governed by the ideal gas equation of state that can be written as,

\[ p_2 \varepsilon_2 = (\gamma_2 - 1) p_2 (\varepsilon_2 - e_{\infty 2}(p_2)) - \gamma_2 p_{\infty 2}(p_2) \, , \]

with \( \gamma_2 = 1.4 \, , \, e_{\infty 2}(p_2) = 0 \, \) and \( p_{\infty 2}(p_2) = 0 \, . \)

Another explosive (HMX) will be considered, with the following constants:

\[ p_{\text{ CJ}} = 36.59 \times 10^9 \text{ Pa} \, , \, D_{\text{ CJ}} = 9090 \, \text{m/s} \, , \, T_{\text{ CJ}} = 4152 \, \text{K} \, , \, C_{v} = 2750 \, \text{J/kg/K} \, , \, A = 1125.86 \times 10^9 \text{ Pa} \, , \]

\[ B = 11.67 \times 10^9 \text{ Pa} \, , \, R_1 = 4.78 \, , \, R_2 = 1.12 \, , \, \gamma_1 = 1.43 \, . \]

Thanks to the mixture energy definition (1.3) and pressure equilibrium condition (1.8), the mixture equation of state is obtained:

\[ p(\rho, e, \alpha_1, Y_1) = \frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1} \, . \]  \hspace{1cm} (1.18)

1.6 Summary of the velocity non-equilibrium interpenetration model

The flow model corresponds to a velocity and temperature non-equilibrium two-phase flow model with a single pressure. It reads:

\[ \frac{\partial \alpha_1}{\partial t} + \frac{\partial (\alpha_1 \rho \varepsilon_1)}{\partial x} + \frac{\partial \rho \varepsilon_1 \frac{d u}{d x}}{\partial x} = 0 \, , \]

\[ \frac{\partial (\rho u \varepsilon_1)}{\partial t} + \frac{\partial (\rho u^2 + \rho + p)}{\partial x} = 0 \, , \]

\[ \frac{\partial w}{\partial t} + \frac{\partial (v_1 - v_2)}{\partial x} \frac{d \rho}{d x} = -\lambda \rho \, , \]

\[ \frac{\partial p}{\partial t} + \frac{\partial (pE + e_1 u)}{\partial x} + \frac{\partial \rho w (h_1 - h_2)}{\partial x} = 0 \, . \]

With the following definitions,

\[ E = Y_1 e_1 + Y_2 e_2 + \frac{1}{2} u^2 + e_1 \, , \]

\[ Y_1 = \frac{\alpha_1 \rho_1}{\rho} \, , \]

\[ e_1 = \frac{1}{2} \rho w^2 \, , \]

\[ p_1 = 2 \rho e_1 \, , \]

\[ p(\rho, e, \alpha_1, Y_1) = \frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1} \, . \]  \hspace{1cm} (1.18)

The enthalpies, entropies and temperatures are determined from the pure fluids equations of state with the equilibrium pressure given above:

\[ h_k = h_k(p, p_k) \, , \, s_k = s_k(p, p_k) \, , \, T_k = T_k(p, p_k) \, , \, k = 1, 2. \]
This formulation clearly enters in the ‘diffuse interface approach’ of Saurel and Agbrall \textsuperscript{18} and Kapila \textit{et al.} \textsuperscript{19} to cite a few. In particular it extends the model of this last reference to velocity drift effects. The same goal was reached in Guilland and Duval \textsuperscript{20} and Saurel \textit{et al.} \textsuperscript{21} but with velocity drift effects restricted to the Darcy law. In the present model, inertial relative velocity effects are present. It can be shown that this model is hyperbolic for small relative velocities. Nevertheless it is possible to extend the hyperbolicity domain to the entire space by the strategy detailed in the next paragraph.

2. Hyperbolic sub models for the mean flow field and interpenetration

System (1.19) is split in two subsystems:
- A diffuse interface model for the mean flow field, in particular mean interface transport.
- An ‘interpenetration system’.

2.1 Hyperbolic subsystem for the mean flow field

The mean flow field system, including mean interface transport, is now considered:

\[
\begin{align*}
\frac{\partial \alpha_1}{\partial t} + u \frac{\partial \alpha_1}{\partial x} &= \frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\rho_1 c_1^2 + \rho_2 c_2^2} \frac{\partial u}{\partial x} \\
\frac{\partial (\alpha p)_1}{\partial t} + \frac{\partial (\alpha p)_1}{\partial x} u &= 0 \\
\frac{\partial (\alpha p)_2}{\partial t} + \frac{\partial (\alpha p)_2}{\partial x} u &= 0 \\
\frac{\partial w}{\partial t} + \frac{\partial w}{\partial x} u &= 0 \\
\frac{\partial p u}{\partial t} + \frac{\partial p u^2 + p + p_1}{\partial x} &= 0 \\
\frac{\partial p E}{\partial t} + \frac{\partial (p E + p + p_1) u}{\partial x} &= 0
\end{align*}
\]

(2.1)

with,

\[
E = Y_1 e_1 + Y_2 e_2 + \frac{1}{2} u^2 + e_1, \\
e_1 = \frac{1}{2} aw^2, \\
p_1 = 2pe_1.
\]

System (2.1) is a slight variant of the Kapila \textit{et al.} \textsuperscript{19} model. It is hyperbolic with wave speeds,

\[
\begin{align*}
u, u + \sqrt{c_w^2 + 3 \frac{p_1}{\rho}} \quad \text{and} \quad u - \sqrt{c_w^2 + 3 \frac{p_1}{\rho}},
\end{align*}
\]

where the sound speed is defined by (Wood \textsuperscript{29}),

\[
\frac{1}{\rho c_w^2} = \frac{\alpha_1}{\rho_1 c_1^2 + \rho_2 c_2^2}.
\]

(2.2)

2.2 Hyperbolic interpenetration subsystems

The subsystem dealing with fluid interpenetration effects through the interface is obtained by removing the space derivative terms of System (2.1) in (1.19):

\[
\begin{align*}
\frac{\partial \alpha_1}{\partial t} + \frac{c_1^2}{\alpha_1} \frac{\partial p}{\partial x} &= \frac{\rho aw}{\rho_1 c_1^2 + \rho_2 c_2^2} \left( \frac{\Gamma_1}{\alpha_1} \frac{\partial s_1}{\partial x} + \frac{\Gamma_2}{\alpha_2} \frac{\partial s_2}{\partial x} \right),
\end{align*}
\]
\[
\frac{\partial (\alpha \rho)}{\partial t} + \frac{\partial \rho w}{\partial x} = 0, \\
\frac{\partial (\alpha \rho)}{\partial t} + \frac{\partial \rho w}{\partial x} = 0, \\
\frac{\partial \rho u}{\partial t} = 0, \\
\frac{\partial w}{\partial t} + (v_1 - v_2) \frac{\partial p}{\partial x} = -\lambda w, \\
\frac{\partial \rho E}{\partial t} + \frac{\partial \rho w (h_1 - h_2)}{\partial x} = 0,
\]

with \( E = Y_1 e_1 + Y_2 e_2 + \frac{1}{2} u^2 + e_i \).

This system is completed by the following entropy equations:

\[
\frac{\partial \alpha \rho s_1}{\partial t} + \frac{\partial \rho w s_1}{\partial x} = \rho \Gamma_1 \frac{\alpha_1}{\Gamma_1} \lambda a w^2, \\
\frac{\partial \alpha_2 \rho s_2}{\partial t} - \frac{\partial \rho w s_2}{\partial x} = \rho \Gamma_2 \frac{\alpha_2}{\Gamma_2} \lambda a w^2.
\]

In the absence of velocity relaxation, System (2.3) can be expressed under the following form:

\[
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & aw & 0 & 0 & 0 \\
0 & 0 & 0 & -aw & 0 & 0 \\
aw & 0 & 0 & 0 & 0 & a \\
v_1 - v_2 cn_1^2 & 0 & \frac{\alpha_1}{\rho cn_1^2} (v_1 - v_2) pc_n^2 \frac{\partial p_1}{\partial s_1} \rho_1 & \frac{\alpha_2}{\rho_2 cn_2^2} (v_1 - v_2) pc_n^2 \frac{\partial p_2}{\partial s_2} \rho_2 & (v_1 - v_2) \rho^2 c_n^2 & 0
\end{pmatrix}
\begin{pmatrix}
\rho \\
u \\
s_1 \\
s_2 \\
w \\
Y_1 \\
w
\end{pmatrix}
= 0
\]

Therefore, the wave speeds are,

\[
\lambda_0 = 0 \text{ two times fold,}
\]

\[
\lambda_1 = \frac{aw}{Y_1},
\]

\[
\lambda_2 = -\frac{aw}{Y_2},
\]

\[
\lambda_3 = -|v_1 - v_2| pc_n \sqrt{\alpha},
\]

\[
\lambda_4 = |v_1 - v_2| pc_n \sqrt{\alpha}.
\]

System (2.3) is consequently hyperbolic. It is worth to mention that, in the single phase limit, the wave speeds \( \lambda_1 \) and \( \lambda_2 \) are singular if ‘a’ or ‘w’ are finite. However, in this limit, the relative velocity does not make sense anymore, as the fluid becomes single phase. At the computational level, the mass fractions may be arbitrarily small and difficulties may appear if ‘a’ or ‘w’ do not tend fast enough to zero. An option to overcome this difficulty is to choose a function for ‘a’ linked to the product \( Y_1 Y_2 \) when it tends to zero, in order to have a smooth transition.

However, System (2.2) contains difficulties related to the various non-conservative terms appearing in the volume fraction and relative velocity equations. In particular, positivity issues
may result from the various non-conservative terms present in the volume fraction equation. Following Saurel et al. a pressure non-equilibrium formulation may help to preserve volume fraction positivity and improve mathematical properties.

2.3 Pressure non-equilibrium interpenetration model
Let's consider the following sub-system:

\[
\begin{align*}
\frac{\partial \alpha_1}{\partial t} &= \mu (p_1 - p_2), \\
\frac{\partial (\alpha p)_1}{\partial t} + \frac{\partial p_{aw}}{\partial x} &= 0, \\
\frac{\partial (\alpha p)_2}{\partial t} - \frac{\partial p_{aw}}{\partial x} &= 0, \\
\frac{\partial p_u}{\partial t} &= 0, \\
\frac{\partial w}{\partial t} &= v_1 \frac{\partial p_1}{\partial x} - v_2 \frac{\partial p_2}{\partial x} = -\lambda w, \\
\frac{\partial \alpha_1 p_{aw_1}}{\partial t} + \frac{\partial p_{aw_1}}{\partial x} &= \rho \Gamma_1 \frac{\alpha_1}{T_1} \lambda w^2 + \theta \frac{\mu (p_1 - p_2)^2}{T_1}, \\
\frac{\partial \alpha_2 p_{aw_2}}{\partial t} - \frac{\partial p_{aw_2}}{\partial x} &= \rho \Gamma_2 \frac{\alpha_2}{T_2} \lambda w^2 + (1 - \theta) \frac{\mu (p_1 - p_2)^2}{T_2}, \\
\frac{\partial pE}{\partial t} + \frac{\partial p_{aw} (h_1 - h_2)}{\partial x} &= 0,
\end{align*}
\]

with the same total energy definition as previously. The parameter \( \theta \) in the entropy equations varies between zero and one. There is no need to determine precisely its expression as a stiff pressure relaxation method will be used. It is shown in Appendix A that the stiff pressure relaxation limit of System (2.4) corresponds to System (2.3). This model is thus an interesting alternative for the resolution of System (2.3).

The entropy equations structure ensures mixture entropy positive production. However, it is important to check thermodynamic compatibility of the equations as well as system's hyperbolicity. These properties are examined in the Appendix B. The main result is that System (2.4) is unconditionally hyperbolic with wave speeds:

\[
\begin{align*}
\lambda_0 &= 0 \quad \text{three times fold,} \\
\lambda_1 &= -\frac{aw}{Y_1}, \\
\lambda_2 &= \frac{aw}{Y_2}, \\
\lambda_3 &= \sqrt{a \left( \frac{c_{11}^2}{Y_1} + \frac{c_{22}^2}{Y_2} \right)}, \\
\lambda_4 &= -\sqrt{a \left( \frac{c_{11}^2}{Y_1} + \frac{c_{22}^2}{Y_2} \right)}.
\end{align*}
\]

As System (2.4) is hyperbolic, it is an excellent candidate to solve the interpenetration System (2.3). Some comments are due regarding these systems.

As mentioned in Section 1, the correct formulation for the interpenetration parameter is \( a = Y_1 Y_2 \) when the flow under interest contains bubbles, droplets or grains. In such situation, the
flow model involves a single parameter, or more precisely a single drag correlation function, $\lambda$
like all existing multiphase flow models when heat and mass transfers are omitted.
The main difficulty lies into the numerical solver that has to be designed carefully (Huber 30).
To be more precise, a non trivial Godunov type solver has been derived in this reference, and nice
agreement was obtained for the mixing layer configuration of Section 4.1. However, it failed for
the reverse situation of heavy/light fluid studied in Section 4.2.
In the present context of mixing layer modelling, both parameters ‘$a$’ and $\lambda$ are unknown, as the
assumption $a = Y_2^1 Y_3^1$ fails. As both ‘$a$’ and $\lambda$ are related to relative motion a single parameter
should summarize their effects. Extra reduction is therefore addressed.
Two different reduction methods are considered. The first one is based on conventional
asymptotic analysis and results in a Darcy type model. The second one is based on semi-discrete
considerations in the frame of splitting methods and results in an artificial viscosity type model.
These limit models are derived and discussed hereafter.

3. Stiff velocity relaxation limit models
To determine an interpenetration flow model with as few parameters as possible the stiff velocity
relaxation limit is examined. This limit is addressed with two different methods as detailed
hereafter.

3.1 Conventional stiff velocity relaxation
The unsplit velocity non-equilibrium flow model (1.19) is considered. The stiff velocity relaxation
limit ($\lambda \rightarrow +\infty$) is assumed and focus is done on the relative velocity equation:
$$\frac{\partial w}{\partial t} + \frac{\partial w u}{\partial x} + (v_1 - v_2) \frac{\partial p}{\partial x} = -\lambda w$$
By denoting,
$$\lambda = \frac{1}{\varepsilon} \text{ and } w = w_0 + \varepsilon w^1,$$
with $\varepsilon \rightarrow 0^-$ we obtain:
$$\frac{\partial (w_0 + \varepsilon w^1)}{\partial t} + \frac{\partial (w_0 + \varepsilon w^1) u}{\partial x} + (v_1 - v_2) \frac{\partial p}{\partial x} = -\frac{1}{\varepsilon} (w_0 + \varepsilon w^1).$$
This equation results in three new equations:
- At the order $\frac{1}{\varepsilon}$ : $w_0 = 0$.
- At the order $\varepsilon$ : $\frac{\partial w^1}{\partial t} + \frac{\partial w^1 u}{\partial x} = 0$.
- At zero order : $(v_1 - v_2) \frac{\partial p}{\partial x} = -w^1$.

Thus, $w = w_0 + \varepsilon w^1 = -\varepsilon (v_1 - v_2) \frac{\partial p}{\partial x}.$

The stiff velocity relaxation limit thus results in the following Darcy type flow model:
$$\frac{\partial (\rho c^2 \alpha)}{\partial t} + \frac{\partial (\rho c^2 \alpha u)}{\partial x} = 0,$$
$$\frac{\partial (\rho e \alpha)}{\partial t} + \frac{\partial (\rho e \alpha u)}{\partial x} = 0,$$
$$\frac{\partial (\rho e \alpha)}{\partial t} + \frac{\partial (\rho e \alpha u)}{\partial x} = 0.$$
With the following definition for total energy,
\[ E = Y_e e_0 + Y_e e_2 + \frac{1}{2} u^2. \]

The absence of turbulent energy is due to the presence of a quadratic \( \varepsilon \) term that becomes negligible. For the same reason, the turbulent pressure disappears.

The limit model (3.1) now contains a single parameter, corresponding to the product \( \varepsilon a \). System (3.1) is close to the models of Guillard and Duval, Ambroso et al., and Saurel et al. This model is interesting but inappropriate for the application of unstable interfaces and interpenetrating fluids. Indeed, the interpenetration effect, present in the relative mass flux,
\[ \rho \varepsilon a (v_i - v_j) \frac{\partial p}{\partial x}, \]

is non-zero only when pressure gradients are present. For example, during shock – interface interaction, this term is non zero only during the shock propagation inside the mixing layer. Relative motion interrupts immediately after. This is incorrect as the inertia stored in the fluids during shock acceleration is responsible for the mixing zone growth at later times. This incorrect behaviour will be illustrated in the Section 4.

3.2 Semi-discrete stiff velocity relaxation

The second method used to determine another stiff velocity relaxation limit model considers the velocity non-equilibrium System (1.19) under its split form, with Subsystem (2.1) for the mean flow field and Subsystem (2.4) for interpenetration.

As this second method is dealing with semi-discrete analysis, it is necessary to introduce some numerical considerations.

Mean flowfield solver

The mean flow field solver for System (2.1) is very important when building a computational code with material interfaces. A simple and efficient strategy has already been developed in Saurel et al. For the present analysis where interpenetration effects are under focus, these numerical method details are useless. Therefore, the method given in that reference is summarized in the Appendix C.

Interpenetration solver

Numerical resolution of System (2.3) is addressed with the help of the extended System (2.4) with the same philosophy as in the one summarized in Appendix C: An extended hyperbolic system is used to solve another system of lower dimension.

Let’s consider part of the System (2.4) with the following set of variables:
\[ \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \] (3.2)

with \( U = (\alpha_0, (\alpha \rho)_0, (\alpha \rho)_2, \rho u, \rho E)^T \) and \( F = (0, \rho aw, -\rho aw, \rho aw (h_i - h_j))^T \).

Let’s consider the Godunov scheme,
\[ U_i^{n+1} = U_i^n - \Delta t \frac{\Delta x}{\Delta x} (F_{i+1/2}^n - F_{i-1/2}^n), \]
with the Rusanov flux at each cell boundary separating a left state \((L)\) and a right one \((R)\),

\[
F^* = \frac{F_R + F_L}{2} + \frac{S}{2} (U_L - U_R),
\]

where \(S\) represents the maximum wave speed: \(S = \text{Max} \left( \left| \frac{\lambda_{Lj}}{\lambda_{Rk}} \right|, \ j = 0,...,4 \right)\).

These ingredients are very conventional and possibly the simplest when dealing with numerical integration of hyperbolic systems. Let’s now imagine that a numerical scheme is used to solve the non-conservative relative velocity equation and the entropies (or equivalent energies) phases equations. Whatever the numerical scheme is for these equations, the evolution step ends with a relative velocity and pressure relaxation step, where the asymptotic state solution of the following system is determined:

\[
\begin{align*}
\frac{\partial \alpha_1}{\partial t} &= \mu (p_1 - p_2), \\
\frac{\partial (\alpha p)_1}{\partial t} &= 0, \\
\frac{\partial (\alpha p)_2}{\partial t} &= 0, \\
\frac{\partial p u}{\partial t} &= 0, \\
\frac{\partial w}{\partial t} &= -\lambda w, \\
\frac{\partial \alpha_{i} p s_{1}}{\partial t} &= \rho \Gamma \frac{\alpha_1}{\Gamma_1} \lambda aw^2 + \theta \frac{\mu (p_1 - p_2)^2}{T_1}, \\
\frac{\partial \alpha_{2} p s_{2}}{\partial t} &= \rho \Gamma \frac{\alpha_2}{\Gamma_2} \lambda aw^2 + (1 - \theta) \frac{\mu (p_1 - p_2)^2}{T_2}, \\
\frac{\partial p E}{\partial t} &= 0,
\end{align*}
\]

with \(\lambda \to +\infty\) and \(\mu \to +\infty\).

Two important remarks follow:
- This relaxation step is entropy preserving.
- It obviously implies, \(w = 0\) at any time and in any computational cell.

Therefore, there is no need to know precisely the numerical scheme for the relative velocity equation, as \(w = 0\). Moreover, as a consequence of (3.5), the Godunov scheme reduces to:

\[
U_{i+1} = U_i - \Delta t \left( \frac{S_{i+1/2}}{2} \left( U_i - U_{i+1} \right) - \frac{S_{i-1/2}}{2} \left( U_{i-1} - U_i \right) \right)
\]

Indeed, all flux vectors \(F_R\) and \(F_L\) are zero in (3.3) thanks to (3.5). It means that the artificial viscosity terms only remain present for the solution evolution.

The wave speeds appearing in (3.6) are linked to the eigenvalues \(\lambda_i = -\frac{aw}{Y_1}, \lambda_2 = \frac{aw}{Y_2}\),

\[
\lambda_i = \sqrt{\frac{a}{Y_1} \left( \frac{c_i^2}{Y_1} + \frac{c_j^2}{Y_2} \right)} \quad \text{and} \quad \lambda_4 = -\sqrt{\frac{a}{Y_1} \left( \frac{c_i^2}{Y_1} + \frac{c_j^2}{Y_2} \right)},
\]

every one of them involving the interpenetration parameter ‘a’. Thus, setting the parameter ‘a’ sets the wave speeds \(S_{i+1/2}\) and \(S_{i-1/2}\). Expressing (3.6) as,
the following continuous limit system appears,

\[ \frac{\partial U}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial U}{\partial x} \right), \]

with \( U = (\alpha_i, (\alpha \rho)_1, (\alpha \rho)_2, \rho u, \rho E)^T \) and \( \nu = \frac{S \Delta x}{2} \).

It is thus equivalent to consider interpenetration through the parameter ‘a’ or through the artificial viscosity coefficient \( \nu \).

In System (2.4) and (3.4), the pressures are out of equilibrium. Before going to pressure equilibrium, it is necessary to determine the energy or entropy equations for the phases.

When the entropy equations of System (2.4) are considered, System (3.7) is completed by entropy equations having the same type of diffusive term as the other equations. But, the corresponding entropy equations are not compatible with the mixture momentum and mixture energy equations of System (3.7). To preserve compatibility of the equations, the following formulation is retained:

\[ \frac{\partial (\alpha \rho E)_1}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial (\alpha \rho E)_1}{\partial x} \right), \]

\[ \frac{\partial (\alpha \rho E)_2}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial (\alpha \rho E)_2}{\partial x} \right), \]

where \( E_k = e_k + \frac{1}{2} u^2 \).

The solution is thus updated with (3.7-3.8). An implicit scheme is detailed in Appendix D in this aim.

The diffusion step is followed by a pressure relaxation step. This means that the pressure relaxation terms of System (2.4), omitted during the diffusion step (3.7-3.8) are now considered with a stiff pressure relaxation solver. It corresponds to the algebraic System (C.2) solution.

The pressure is then recomputed with the help of the mixture equation of state (1.18), based on the mixture energy. Phase’s energies are then reset with this corrected pressure.

System (3.8) is thus only used to predict the energies and pressures before pressure relaxation. It plays the same role as the internal energy equations of System (C.1). To preserve consistence with the total mixture energy, formulation (3.8) is used.

### 3.3 Effective diffusion-interpenetration model

Thanks to the preceding discrete analysis, the overall solution is obtained with the help of two subsystems:

- A hyperbolic flow model for the mean flow field and interface dynamics (Kapila et al. 19).
- A diffusive flow model (3.7-3.8) with relaxation.

When these two sub models are merged in a single one, the following continuous analogue is obtained, as detailed in the Appendix E:
\[ \frac{\partial \alpha_1}{\partial t} + u \cdot \frac{\partial \alpha_1}{\partial x} - \frac{\partial}{\partial x} \left( \nu \frac{\partial \alpha_1}{\partial x} \right) = \frac{1}{\alpha_1} \left( \rho_1 c_1^2 + \rho_2 c_2^2 \right) \]

\[ \frac{\partial \alpha_2}{\partial t} + u \cdot \frac{\partial \alpha_2}{\partial x} - \frac{\partial}{\partial x} \left( \nu \frac{\partial \alpha_2}{\partial x} \right) = 0, \]

\[ \frac{\partial (\alpha p_1)_1}{\partial t} + \frac{\partial}{\partial x} \left( (\alpha p_1)_1 u - \nu \frac{\partial (\alpha p_1)_1}{\partial x} \right) = 0, \]

\[ \frac{\partial (\alpha p)_2}{\partial t} + \frac{\partial}{\partial x} \left( (\alpha p)_2 u - \nu \frac{\partial (\alpha p)_2}{\partial x} \right) = 0, \]

\[ \frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x} \left( \rho u^2 + p - \nu \frac{\partial \rho u}{\partial x} \right) = 0, \]

\[ \frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x} \left( (\rho E + p) u - \nu \frac{\partial \rho E}{\partial x} \right) = 0, \]

where \( H_k = E_k + \frac{p}{\rho_k} \).

From the model's structure, it is clear that the desired mixed hyperbolic – elliptic character is obtained. The volume fraction equation is clearly complicated, but it poses no difficulty at the numerical level as extended systems out of pressure equilibrium are considered, with quite simple structures.

The thermodynamic compatibility of this system with respect to the second law of thermodynamics poses an extra issue. There is no guarantee that the entropy inequality be \emph{locally} fulfilled. However, it is worth to mention that this issue is even present for the Euler equations with artificial viscosity of Lax-Wendroff type methods, such as MacCormack scheme. This is even true with Riemann problem based methods that contain artificial viscosity too. Indeed, the continuous limit of theses scheme for the Euler equations is:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left( \rho u - \nu \frac{\partial \rho}{\partial x} \right) = 0, \]

\[ \frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x} \left( \rho u^2 + p - \nu \frac{\partial \rho u}{\partial x} \right) = 0, \]
The associated entropy equation reads,
\[ \frac{\partial s}{\partial t} + \frac{\partial s u}{\partial x} = \frac{1}{T} \left[ \frac{\partial}{\partial x} \left( \frac{\partial E}{\partial x} \right) - \left( \frac{E + P}{\rho} - u^2 \right) \frac{\partial}{\partial x} \left( \frac{\partial p}{\partial x} \right) - \frac{u}{\partial x} \left( \frac{\partial p u}{\partial x} \right) \right]. \]

It clearly shows a production term with undefined sign. However, artificial viscosity methods are efficient to capture discontinuities as they fulfill the entropy inequality in the global sense.

In the present work, we have shown that the extended hyperbolic system with relaxation (System (2.4)) was in local agreement with the entropy inequality. When solved in the stiff velocity relaxation limit, the entropy inequality is necessarily fulfilled too. Thus, System (3.9) is physically admissible.

System (3.9) presents similarities with the flow model of Liu et al. developed for the same goal as the present study, i.e. turbulent mixing layers modelling with reduced models. There are however important differences:
- Dissipative terms have different structures.
- The present approach deals with two-phase diffuse interfaces while the Liu et al. model is single phase.
System (3.9) can be used for turbulent mixing layers computation in shock tubes as shown in the next section with fluids governed by different equations of state. Post-detonation modelling and spherical explosions will be addressed later.

4. Mixing layers in shock tube experiments
Richtmyer-Meshkov instabilities (RMI) appear when a perturbed interface separating two gases of different densities grows due to impulsive acceleration. We use, in the present work, results issued from shock tube experiments undertaken in our laboratory. Experiments were performed in a horizontal shock tube of 7 m length and 20x20 cm² square cross section. It was coupled to a high speed laser sheet device (1 frame = 100 µs) which allowed a 2D visualization of the interface. The imaging technique is based on the Mie scattering of a copper vapour laser light source (532 nm) by small smoke incense particles seeded in one of the two test gases (air). To achieve experimentally the materialization of the initial interface, a thin nitrocellulosic membrane (0.5 µm thick) was deposited on a stereo lithographed grid support, computer-aided designed and constructed with chosen shape and dimensions. Generally, sinusoidal shape is adopted in order to have well defined initial conditions. The experimental device is described in more details in Houas et al. and Mariani et al.

Questions may arise regarding reliability of the experiments with respect to membrane effects and incense particles as fluid markers. In all existing horizontal (with membrane) or vertical (without membrane but diffusive interface) shock tube facilities, the initial conditions involve uncertainties. Regarding the incense smoke, the particles size is small enough to consider nearly instantaneous velocity relaxation. Indeed, typical incense particle radius is about 0.1 µm. By considering drag effects modelled by the Stokes law and maximum slip velocity of the order of 100 m/s, the corresponding maximum relaxation time is roughly 10 µs. This delay time is negligible compared to the characteristic times under interest, typically of the order of 1 ms.

4.1. Light/heavy fluid configuration
In the present configuration, a shock tube containing a light fluid (air) on the left and a heavy one (sulphur hexafluoride - SF₆) on the right, separated by a sinusoidal perturbed interface as shown in the Figure 3 is considered.
Figure 3. A shock tube containing a light fluid on the left and a heavy one on the right is considered. The two fluids are separated by a perturbed interface having a sinusoidal shape. The corresponding wave diagram is shown on top.

The light gas (air seeded with smoke of incense) and the heavy gas (SF\textsubscript{6}) are introduced on each side of the membrane by a constant circulation. The initial perturbation imposed by the grid is a sine line of wavelength 80 mm and amplitude 3 mm. RMI are produced by the interaction of a weak shock wave (M=1.15 in air) with the air/SF\textsubscript{6} interface. When the shock wave interacts with the interface, a mixing zone appears, as shown in the Figure 4. In this figure, only four pictures, taken during the incident phase, before the interaction with the reflected shock wave (about 3 ms after the initial acceleration) are shown. All the images were digitally processed in order to extract the perturbation amplitude, i.e. the mixture layer thickness.

Figure 4. Laser sheet pictures showing the interaction of a shock wave (M=1.15), moving from left to right, with a stereolithographed sinusoidal interface (\( \lambda_0 = 80\text{mm} \) and \( \eta_0 = 3\text{mm} \)) in the light/heavy configuration (air on the left and SF\textsubscript{6} on the right).
The experimental configuration consists in a shock tube with a high pressure chamber filled with air at the pressure of 4.78 atm and density $5.69 \text{kg/m}^3$. The low pressure chamber is divided into two parts separated by the sinusoidal membrane. The left part is filled with air ($\gamma = 1.4$) at the pressure of 1 atm and at density $1.19 \text{kg/m}^3$. The right part is filled with SF$_6$ ($\gamma = 1.09$) at the same pressure and at density $5.99 \text{kg/m}^3$. The sinusoidal membrane is located at 48 cm from the tube end. The shock-interface interaction sets in motion the interface which thickens.

In the present air/SF$_6$ case, the interface perturbations grow monotonously in the shock wave propagation direction until interaction with the reflected shock wave occurs. The interface thickness is recorded and compared to the models prediction. First, the Darcy type model, corresponding to System (3.1) is considered. The diffusive one (System 3.9) is then considered.

**Darcy type model**

System (3.1) treats interpenetration across the interface with a Darcy type formulation, the mean flow being solved by the Kapila et al. model. A numerical scheme to solve the Darcy part is given in Saurel et al. This scheme is used in the present computations. The interface thickness is reported in the Figure 5 with several interpenetration parameters and compared to experimental records in symbols.

![Figure 5](image)

*Figure 5.* Experimental (symbols) and numerical interface thickness (dashed lines) versus time. Experimental mixing layer is measured with the extreme points of the interface contour. The parameter $\xi a$ is set equal to $1.01 \times 10^{-2}$, $1.2510^{-2}$, and $1.510^{-2}$ s. The results without drift ($\xi = 0$) are shown with solid line on bottom. This curve shows the interface numerical diffusion. A mesh with 1000 cells is used with higher order extension of the method. Poor agreement is obtained whatever the $\xi a$ parameter is.

We observe that the mixture zone thickness increases with increasing permeation coefficient $\xi a$. But the numerical and experimental dynamics are very different. Indeed, in the experiments the interfacial thickness grows almost linearly, whereas the numerical growth rate is very high at first and then decreases dramatically. Indeed, the slow growth stage that appears during the second stage matches the numerical diffusion one. Thus, drift effects are zero during the second stage. Examining the relative velocity definition of System (3.1) it is clear that interpenetration occurs only when pressure gradients are non zero. The relative velocity definition does not consider the fluids inertia, resulting in poor agreement, as shown in the Figure 5.
**Diffusion type model**

We now consider System (3.9) to model interpenetration. The mean interface dynamics is still predicted by the Kapila *et al.* model, solved by the method of Appendix C, while diffusion effects are solved by the method of Appendix D. The interpenetration parameter is modelled as:

\[ v = Y_1 Y_2 v_0 \]  

(4.1)

The product \( Y_1 Y_2 \) is necessary to prevent excessive artificial viscosity effects at shocks and expansion waves. With (4.1), extra diffusion appears at interfaces only. The parameter \( v_0 \) is set equal to \( 0.1 \text{m}^2/\text{s} \) and the corresponding numerical results are compared to the experiments in the Figure 6.

![Figure 6. Mixing layer width evolution for the air-SF₆ shock tube configuration. The experimental records, the computed results with and without interpenetration are shown, respectively, with square symbols, cross symbols and dash lines. Good agreement is observed.](image)

The results shown in the Figure 6 are obtained with the same mesh resolution as previously and show a quite good agreement.

Let us mention that the present model is compared only for the incident phase of the instability before the reflected shock wave interaction. This is not a limitation for spherical explosions in air. Also, it is worth to mention that the parameter \( v_0 \) has been estimated to obtain qualitative agreement, as shock tube experiment conditions are far from those of high explosive conditions which constitute in the main interest of this study.

**4.2. Heavy/light fluid configuration**

The shock tube now contains a heavy fluid (air) on the left and a light one (helium-He) on the right, separated by a perturbed interface as previously. The same initial perturbation imposed by the grid is used with a sine line of wavelength 80 mm and amplitude 3 mm. RMI are produced by the interaction of a weak shock wave (M=1.15 in air) with the air/He interface. When the shock wave interacts with the interface, a mixing zone appears, as shown in the Figure 7. As we can see in the present configuration, the heavy/light interface overturns immediately following the incident shock acceleration. The ‘inversion phenomenon’ mentioned in the Section 1 is clearly visible. Later, a distortion of the interface to mushroom type structures is observed before the reflected shock wave interaction occurs at approximately time 0.9 ms. Before this time, the good quality of the frames allows to extract clear contours of the interface. On each picture, the perturbation amplitude (i.e. the mixture layer thickness) is measured between the extreme points of the interface contour.
The experimental configuration uses the same initial data as those of the preceding test case of Figure 4, except the shock tube right part, now filled with He ($\gamma = 1.67$) at atmospheric pressure and at density 0.164 kg/m$^3$. The shock-interface interaction sets in motion the interface that first sharpens and then thickens.

The Darcy type model (3.1) has been tested first. Starting from the initial condition where the interface has a 3mm thickness, a sharp profile was obtained during shock interaction, corresponding to the ‘inversion phenomenon’ stage. When the interface was captured in one or zero point, a code failure occurred as the volume fractions on both side of the interface tended to 0 and 1, corresponding to pure fluids. It was thus impossible to obtain interface thickening.

The results of the diffusion model only are reported in the Figure 8, with the same interpenetration parameter as previously ($\nu_0 = 0.1$ m$^2$/s ).

The interpenetration effects appear again clearly the Figure 8 results with quite good agreement with the experiments. The same mesh resolution with 1000 cells for a domain of 0.5 m was used as in the previous air/SF$_6$ test. It is interesting to note that the same interpenetration coefficient is used, while the growth rates in the two experiments (air/SF$_6$ and air/He) vary by a factor of two.

We now address experiments in another range of initial pressure ratios with spherical explosions. To this end, post detonation modelling has to be addressed.
5. Post detonation modelling

The turbulent mixing of detonation products with air yields a post detonation reaction. In this process the detonation products become reactive species that burn with air. The first issue is to determine the energy and air consumption for the post detonation reaction. The energetic test materials considered in the present study are TNT and HMX. Some basic thermochemical data are given in the Table 1.

<table>
<thead>
<tr>
<th>Species</th>
<th>$M_{mol}$ (g / mol)</th>
<th>$\Delta H_i$ (kJ / mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2O_{(g)}$</td>
<td>18</td>
<td>-241.8</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>44</td>
<td>-393.5</td>
</tr>
<tr>
<td>$N_2$</td>
<td>28</td>
<td>0</td>
</tr>
<tr>
<td>$O_2$</td>
<td>32</td>
<td>0</td>
</tr>
<tr>
<td>$C$</td>
<td>12</td>
<td>0</td>
</tr>
<tr>
<td>TNT</td>
<td>227</td>
<td>-59.2</td>
</tr>
<tr>
<td>$C_7H_5N_3O_6$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HMX</td>
<td>296</td>
<td>74.6</td>
</tr>
<tr>
<td>$C_4H_8N_8O_8$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Air</td>
<td>28.97</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 1. Thermochemical data of TNT and HMX and related detonation products.

Prior to the post detonation energy release, it is first needed to determine the detonation energy and the chemical composition of the detonation products. Following Kamlet and Jacobs, conventional chemical reaction equilibration provides enough accuracy for both detonation products composition and energy release determination. This method is adopted hereafter and yields for TNT detonation reaction:

$$C_7H_5N_3O_6 \rightarrow \frac{7}{4}CO_2 + \frac{5}{2}H_2O + \frac{3}{2}N_2 + \frac{21}{4}C$$

$$\Delta H_R = -1233.9 \text{kJ / mol} = -5.435 \text{MJ / kg}$$

The accuracy of this simplified method has been checked for example in Heuze and Bauer, where the corresponding Chapman Jouguet (CJ) detonation velocity is compared to measurements, with less than 5% error for 34 different explosives. When the detonation products, appearing in the right hand side of this equation react with air, the following post detonation reaction occurs:

$$\frac{7}{4}CO_2 + \frac{5}{2}H_2O + \frac{3}{2}N_2 + \frac{21}{4}C + \frac{21}{4}(O_2 + 3.76N_2) \rightarrow \frac{7}{4}CO_2 + \frac{5}{2}H_2O + \frac{3}{2}N_2 + \frac{21}{4}CO_2 + 19.74N_2$$

$$\Delta H_R = -2065.9 \text{kJ / mol} = -9.100 \text{MJ / kg}_{\text{TNT}}$$

The sum of the two energies (detonation and post detonation) has been compared to experimental measurements done in micro calorimeters and has shown very good agreement (Munier). It is now possible to express this post-detonation reaction in terms of unit mass reactant:

$$1 \text{kg TNT detonation products} + 3.17 \text{kg Air} \rightarrow 4.17 \text{kg final products} \quad (5.1)$$

From this reaction it is clear that detonation products need a fair amount of air for the post detonation process. Also, it is clear that the post-detonation energy is comparable to the detonation reaction energy.
The same calculations are considered for HMX detonation and post-detonation reactions. Following again Kamlet and Jacobs \(^{25}\) the HMX detonation reaction reads:

\[
C_4H_{8}N_8O_8 \rightarrow 2CO_2 + 4H_2O + 4N_2 + 2C
\]

\[
\Delta H_R = -1828.8 \text{kJ/mol} = -6.175 \text{MJ/kg}
\]

The post-detonation reaction thus reads:

\[
2CO_2 + 4H_2O + 4N_2 + 2C + 2(O_2 + 3.76N_2) \rightarrow 2CO_2 + 4H_2O + 4N_2 + 2CO_2 + 7.52N_2
\]

\[
\Delta H_R = -787 \text{kJ/mol} = -2.657 \text{MJ/kg}
\]

In terms of unit mass reactant, the air mass consumption is given by:

1 kg HMX detonation products + 0.927 kg Air $\rightarrow$ 1.927 kg final products

The post-detonation energy and air consumption are consequently lower than those of TNT but cannot be neglected as will be shown later.

The aim is now to insert these effects in the interpenetration two-phase flow model. Let us denote by:

1 = the detonation products, corresponding now to the reactive gas,

2 = the gas mixture containing the air and final combustion products.

After the hyperbolic, interpenetration and pressure relaxation steps, the following system has to be considered, as the post-detonation transforms phase 1 to gas mixture 2:

\[
\frac{\partial \alpha_1}{\partial t} = -\frac{c_1^2 + c_2^2}{\rho_1c_1^2 + \rho_2c_2^2} \dot{m}_1
\]

\[
\frac{\partial (\alpha \rho)_1}{\partial t} = -\dot{m}_1
\]

\[
\frac{\partial (\alpha \rho)_2}{\partial t} = \dot{m}_1
\]

\[
\frac{\partial \rho u}{\partial t} = 0,
\]

\[
\frac{\partial \rho E}{\partial t} = 0.
\]

The coefficient appearing in the right hand side of the volume fraction equation is derived in Saurel et al. \(^{25}\), Petitpas et al. \(^{33}\). However, phase 2 contains now several species and the reaction is only possible if the air and detonation products (DP) are in correct proportions. Thus, three mass species equations are needed to describe the concentrations evolution in this phase. Let us denote by \(y_k\) the mass fraction of species k in phase 2. The evolution equations read:

\[
\frac{\partial (\alpha \rho)_2 y_{\text{air}}}{\partial t} = -\phi \omega,
\]

\[
\frac{\partial (\alpha \rho)_2 y_{\text{DP}}}{\partial t} = \dot{m}_1 - \omega,
\]

\[
\frac{\partial (\alpha \rho)_2 y_{\text{final products}}}{\partial t} = (\phi + 1)\omega,
\]

where \(\phi\) represents the air consumption coefficient and is given by the appropriate post detonation reaction. For TNT, \(\phi = 3.17\) as given by (5.1) while for HMX, \(\phi = 0.927\).
In the mass transfer system given by (5.2)-(5.3) DP, which represent the reactive species, are first transferred to the gas mixture. Then a post detonation reaction occurs with the depletion rate $\dot{\omega}$. Assuming this depletion reaction as infinitely fast, DP in the phase 2 gas mixture are always absent: $y_{DP} = 0$. Thus,

\[ \dot{\omega} = \dot{m}_1. \]

Two species concentrations are thus enough to characterise the gas mixture:

\[ \frac{\partial (\alpha \rho)_{2 \, \text{air}}}{\partial t} = -\varphi \dot{m}_1 \]

\[ \frac{\partial (\alpha \rho)_{2 \, \text{final products}}}{\partial t} = (\varphi + 1)\dot{m}_1 \]

Summing these equations, the phase 2 mass equation is obviously recovered.

The post-detonation model thus reduces to:

\[ \frac{\partial \alpha_1}{\partial t} = -\frac{c_1^2 + c_2^2}{\alpha_1 \alpha_2} \dot{m}_1 \]

\[ \frac{\partial (\alpha \rho)_{1}}{\partial t} = -\dot{m}_1 \]

\[ \frac{\partial (\alpha \rho)_{2}}{\partial t} = \dot{m}_1 \]

\[ \frac{\partial (\alpha \rho)_{2 \, \text{air}}}{\partial t} = -\varphi \dot{m}_1 \]

\[ \frac{\partial \rho u}{\partial t} = 0 \]

\[ \frac{\partial \rho E}{\partial t} = 0 \]

It remains to adopt a mass transfer model between the two phases. One option is to consider the reaction as instantaneous between the reactant and the air. To do this, the reactant and air masses are compared:

if $(\alpha \rho)_{1} > (\alpha \rho)_{2 \, \text{air}} / \varphi$ then $dm = (\alpha \rho)_{2 \, \text{air}} / \varphi$, otherwise, $dm = (\alpha \rho)_{1}$. The masses thus evolve as:

$(\alpha \rho)_{1}^{\text{new}} = (\alpha \rho)_{1}^{\text{old}} - dm$

$(\alpha \rho)_{2}^{\text{new}} = (\alpha \rho)_{2}^{\text{old}} + dm$

\[ \left( (\alpha \rho)_{2 \, \text{air}} \right)^{\text{new}} = \left( (\alpha \rho)_{2 \, \text{air}} \right)^{\text{old}} - \varphi dm \]

This mass transfer step is followed by a pressure relaxation step to determine the new volume fractions as done previously with the hyperbolic and the interpenetration ones. The pressure is then computed with the mixture equation of state (1.18).

To account for the post-detonation energy release, a constant has to be added in functions $e_{\text{onk}}$ of the equations of state: $e_{\text{onk}} = e_{\text{onk}}(\rho_k) + q_k$. 

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For TNT post detonation: \( q_1 = 9.1 \text{MJ} / \text{kg} \), \( q_2 = 0 \). For HMX post detonation: \( q_1 = 2.657 \text{MJ} / \text{kg} \), \( q_2 = 0 \). The present post-detonation model does not add any new parameter to the overall reacting-mixing flow model. The only model parameter is still the interpenetration one (\( v \)) that controls the rate at which the two phases mix and burn.

This procedure is simple, efficient and accurate when each fluid is governed by an equation of state having a consistent fundamental basis. This is the case of the ideal gas EOS, but not for JWL. In this last case, corrections have to be done as detailed in the Appendix F.

6. Comparison with explosion experiments

Explosions in air have been achieved at CEA Gramat, France, with the help of spherical charges suspended in air, as schematized in the Figure 9.

The test facility shown in the Figure 9 is used to assess blast and fireball effects from spherical charges with central ignition. Pressure gauges (PCB piezoelectric gauges with specific holder design) are pointed towards the charge centre at different distances. The charge is suspended to a support in order to avoid early reflections from the ground surface. The pressure gauges are PCB piezoelectric gauges with integrated amplifier. The signals are recorded by a Nicolet acquisition card system. The pressure gauges are located respectively at \( R_1 = 13.58 R_0 \), \( R_2 = 27.16 R_0 \) and \( R_3 = 40.75 R_0 \) where \( R_0 \) represents the initial charge radius (7.36 cm) for the TNT shot. They are located at \( R_1 = 21.78 R_0 \), \( R_2 = 35.33 R_0 \) and \( R_3 = 44.44 R_0 \) for the HMX shot, with \( R_0 = 45 \text{ mm} \). High-speed video cameras (30 000 frames/s) are used to record the fireball evolution and blast wave. In all tests, an initiation probe at the explosive surface gives the emergence time of the detonation wave.

6.1 Initial conditions

When dealing with explosions in air with near field pressure measurements (less than 40 initial charge \( R_0 \) radii) it is important to account for the pressure, velocity and density radial profiles in the detonation products. The detonation is initiated at the charge centre and a spherical detonation wave emerges. The instant when the detonation interacts with the air interface corresponds to the initial time in the present computations.

As the flow in the detonation products are governed by non ideal equation of state (JWL), there is no analytical solution for the flow variables profiles. A detonation tracking method in spherical geometry has been developed in Massoni et al. \(^1\) to determine corresponding initial conditions. These profiles are shown in the Figure 10 for a 7.36 cm radius TNT charge, corresponding to an initial mass of 2.8 kg.
Figure 10. Detonation products profiles for TNT spherical detonation at time corresponding to the wave emergence from the centre to the explosive – air interface. The JWL EOS is used.

With the help of these initial conditions, it is now possible to solve shock wave transmission through the interface, interface motion and expansion of the detonation products sphere.

6.2 TNT results without interpenetration

For a first run, interpenetration effects as well as post-detonation ones are omitted. The computation thus consists in solving the Kapila et al. 19 model in spherical symmetry with one of the phases governed by the JWL EOS. The computed and experimental pressure signals are compared at three different spatial stations in the Figure 11.

Figure 11. Comparison between computed and measured pressure signals at three spatial locations. There is no difficulty to distinct theoretical and experimental signals that are noisier. The agreement is excellent for the first two pressure signals and quite good for the third one.
Figure 11 clearly shows that the model without interpenetration provides results of very good accuracy, at least regarding blast effects. The slight discrepancy that is reported for the third pressure gauge is certainly due to the lack of accuracy of the JWL EOS at low densities and low pressures. The mesh involves 7000 cells in all presented explosion computations. A typical run is about 20 mn on a laptop.

We now compare computed and experimental interface trajectories in the Figure 12.

![Figure 12. Computed interface trajectory on left (mass fraction contours) versus experimental one on right (red curve). The maximum dimensionless radius reached by the computed interface is 17. After that point, the detonation products bubble collapses. The experimental interface trajectory increases monotonously and reaches the dimensionless radius of 24 (red curve of the right graph). The computed (dark line) and experimental (red line) trajectories are shown in the right graph on the same scale.](image)

Figure 12 shows serious discrepancies between the computed interface trajectory and the experimental one. The contraction effect that occurs in the bubble radius computation is well known and is due to inertial effects. In the experiments, these effects are balanced by turbulent mixing and an overall radius expansion is observed. It is clear that interpenetration effects have to be considered.

The same computed results are obtained when a front tracking scheme (Massoni et al. 1) is used instead of the diffuse interface formulation. The interface smearing observed on the computed results in the same figure (left graph) are due to conventional numerical diffusion effects. The present diffuse interface model is solved everywhere and doesn’t need any front tracking scheme.

### 6.3 TNT results with interpenetration

Interpenetration and post-detonation effects are now considered. Let us recall that a single parameter is used in the model when interpenetration and post detonation are considered. The parameter \( \nu_c \) is taken as a constant and equal to 50 m²/s in the following test. It is adjusted to obtain an interface trajectory close to the experimental one. In the Figure 13, the computed interface trajectories, with and without interpenetration/post detonation are compared.

![Figure 13. Computed interface trajectories (mass fraction contours) with and without interpenetration/post-detonation effects. The interpenetration effects are clearly visible.](image)

Computed (with interpenetration) and experimental trajectories are compared in the Figure 14.
The agreement shown in the Figure 14 with the computed and experimental interface trajectories is quite good. The agreement could be improved with a better adjustment of the \( \nu_0 \) parameter, but the aim is more to determine its order of magnitude yielding clear results improvement. We now check in the Figure 15 that the pressure signals are still in correct agreement.

The new model is thus able to predict correctly both blast effects and fireball dynamics. Pressure gauges results with and without interpenetration are very close, which means that only using the shock wave time arrival and peak pressures is not selective enough. This fact is well known in the blast community, since even very simple empirical / analytical models are able to give relatively correct overpressure / distance curves. However, the additional measure of fireball radius versus time clearly shows that the model without interpenetration is unable to reproduce the fireball dynamics. We now consider another explosive (HMX).

### 6.4 HMX results with interpenetration

A spherical HMX charge of 708 g mass, corresponding to an initial radius of 45 mm is considered. Same computations as previously are addressed considering both interpenetration and post-combustion. The interpenetration parameter \( \nu_0 \) is set equal to 15 m²/s. The computed mixing layer trajectory is shown in the Figure 16 with mass fraction contours on left. The mixing layer external boundary trajectory is compared to the experimental one on the right graph of the same figure. The fireball radius reaches 25 R₀.
Figure 16. Computed mixing layer trajectory (mass fraction contours) with both interpenetration and post-detonation effects is shown on the left graph. Comparison with experimental fireball radius is shown on right, the experimental trajectory being in red lines and the computed one in dark lines.

The interpenetration parameter $\nu_0$ used in these computations is slightly smaller than the one used for TNT (15 m²/s instead of 50 m²/s) but keeps the same magnitude order. We now examine pressure signals in the Figure 17 that show interesting features.

Figure 17. Comparison between computed pressure signals at three stations with experimental pressure records. The computations consider both interpenetration and post-detonation effects. The agreement is excellent for the leading shock wave and very good for the secondary shock.

The leading shock wave dynamics is perfectly predicted. The shock peaks are in perfect agreement as well as the expansion wave. Compared to the preceding set of results with TNT, new features appear. As the experimental pressure signal is recorded on a longer period-of time, a secondary shock wave appears. This shock is a result of the expansion wave created at early times in the detonation products sphere which was focused to the centre and reflected as a shock wave. Obviously, this shock wave is of low amplitude, as the media has been expanded. When this shock propagates in the mixture layer, its speed tends to acoustic waves speed, with the mechanical equilibrium sound speed (2.2). As the sound speed is strongly dependant on fluids concentration, sound and weak shock waves cannot have the correct kinematics if the mixture is badly described. The presence of this secondary shock with correct kinematics is thus a way to check accuracy of the gas mixture proportions predicted by the model. In the Figure 17, the
experimental pressure signal for the first pressure gauge is in red lines. The reflected shock wave appears at time 0.002 s approximately. The computed pressure signal is shown in purple lines. It perfectly fits the leading wave. The computed reflected shock is difficult to observe, but it appears (still in purple lines) at time 0.0019 s. The second pressure gauge corresponds to the green lines for the experimental pressure record and light blue lines for the computed one. Both curves are superimposed for leading and secondary waves, the secondary one appearing at 0.003 s. For the last pressure gauge, the experimental signal is shown in deep blue lines and the computed one in brown lines. These curves are in very good agreement too.

These results give extra validation of the present modelling work, in particular regarding the mixing layer concentration field.

7. Concluding remarks
The flow model developed in the present work deals with interfaces of simple contact when interpenetration is absent and considers interpenetration effects when non-zero interpenetration coefficient is used. It works in the presence or absence of the ‘inversion phenomenon’ mentioned in Section 4 and accounts for post detonation effects. From TNT and HMX comparisons with experiments, some observations appear:
- Mixing and post-detonation is fundamental to predict fireball dimensions.
- Oppositely, their influence is negligible for the leading shock dynamics.
- It becomes again fundamental for the secondary shock wave prediction.

Regarding shock tube experiments dealing with initial pressure ratios of the order of 4-5, the interpenetration coefficient has been set equal to 0.1 m²/s. For spherical explosions, the initial pressure ratio is of the order of 100 000 and the interpenetration coefficient varies in the range 10-100 m²/s. These large coefficient variations between shock tube and spherical explosions observations may be explained as follows:
- In the fireball fast expansion stage (say for t/R0 less than 0.01s/m) the interpenetration is certainly present but with negligible effects. During this stage, interpenetration possibly occurs at the same rate as in the shock tube experiments, i.e., with interpenetration coefficient of the order of 0.1 m²/s.
- Then, bubble contraction occurs as a result of inertial effects. The acceleration changes sign and the mixing layer grows dramatically. It occurs with an interpenetration coefficient of the order of 10-100 m²/s.
- The interpenetration coefficient for TNT is about 3.3 times greater than the one of HMX. This is precisely the same ratio as post detonation air coefficients defined in (5.1):

\[
\frac{\phi_{\text{TNT}}}{\phi_{\text{HMX}}} = \frac{3.17}{0.927} = 3.42.
\]

A possible physical interpretation appears: The mixing between detonation products and air is enhanced by the post detonation reaction proportionally to the air consumption, resulting in the following estimate for the interpenetration coefficient:

\[
\nu_0 = 15\phi \text{ m}^2/\text{s}.
\]

Experiments with explosions in pure nitrogen and pure oxygen may be used to precise this last relation.

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**Appendix A. Asymptotic reduction of the pressure non-equilibrium interpenetration subsystem**

The aim is to show that System (2.4) admits System (2.3) as asymptotic limit when stiff pressure relaxation is considered.

Masses and mixture momentum equations are unchanged during the asymptotic analysis:

\[
\frac{\partial (\alpha p_1)}{\partial t} + \frac{\partial (\rho_1 u)}{\partial x} = 0
\]

\[
\frac{\partial (\alpha p_2)}{\partial t} - \frac{\partial (\rho_1 u)}{\partial x} = 0
\]

\[
\frac{\partial \rho u}{\partial t} = 0
\]

Volume fraction and entropy equations have to be considered:

\[
\frac{\partial \alpha}{\partial t} = \mu (p_1 - p_2)
\]

\[
\frac{\partial (\alpha s_1)}{\partial t} + \frac{\partial (\rho s_1 u_1)}{\partial x} = \frac{\theta \mu (p_1 - p_2)^2}{T_1}
\]
\[ \frac{\partial (\alpha s)}{\partial t} + \frac{\partial p_{aw}}{\partial x} = (1-\theta) \frac{\mu (p_1 - p_2)^2}{T} \]

The velocity relaxation entropy production terms have been omitted for the sake of simplicity, as they have no importance in the present analysis. The entropy equations are transformed to pressure equations with the help of the mass and volume fraction equations:

\[ \frac{\partial p_1}{\partial t} + \frac{aw \partial p_1}{\partial x} + \rho_1 c_1^2 \frac{\partial \alpha_{aw}}{\partial x} = \theta \frac{\mu (p_1 - p_2)^2}{\alpha_1} - \frac{\rho_1 c_1^2}{\alpha_1} \mu (p_1 - p_2). \]

A symmetric result is obtained for the second phase. Taking the difference of the two pressure equations reads,

\[ \frac{\partial p_1 - p_2}{\partial t} + \frac{aw \partial p_1}{\partial x} + \frac{aw \partial p_2}{\partial x} + \frac{\rho_1 c_1^2}{\alpha_1} \frac{\partial \alpha_{aw}}{\partial x} + \frac{\rho_2 c_2^2}{\alpha_2} \frac{\partial \alpha_{aw}}{\partial x} = 0. \]

The asymptotic limit of this equation in the presence of stiff pressure relaxation provides the pressure fluctuation difference,

\[ p_1' - p_2' = \frac{\rho_{aw} \left( \frac{c_1^2}{\alpha_1} \frac{\partial p_1}{\partial x} - \frac{c_1^2}{\alpha_1} \frac{\partial p_1}{\partial x} \right) + \frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2} \frac{\partial p_{aw}}{\partial x}}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}. \]

With the help of the Gibbs identity under the form,

\[ \frac{\partial p_k}{\partial x} = c_k^2 \frac{\partial p_k}{\partial x} + \rho_k \Gamma_k \frac{\partial s_k}{\partial x}, \]

the pressure fluctuation difference becomes,

\[ p_1' - p_2' = \frac{\rho_{aw} \left( \frac{\Gamma_1 T_1}{\alpha_1} \frac{\partial s_1}{\partial x} + \frac{\Gamma_2 T_2}{\alpha_2} \frac{\partial s_2}{\partial x} \right) + \frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2} \frac{\partial p_{aw}}{\partial x}}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}. \]

As the volume fraction equation becomes at leading order,

\[ \frac{\partial \alpha_1}{\partial t} = p_1' - p_2', \]

the first equation of System (2.3) is recovered.

**Appendix B. Thermodynamic compatibility and hyperbolicity of the pressure non-equilibrium interpenetration model**

The thermodynamic compatibility of System (2.4) is examined. With the help of the mixture mass and mixture momentum equations, the total energy equation can be written as,

\[ \rho \left( Y_1 \frac{\partial e_1}{\partial t} + Y_2 \frac{\partial e_2}{\partial t} \right) + \rho \left( e_1 - e_2 \right) \frac{\partial Y_1}{\partial t} + \rho \frac{\partial e_1}{\partial t} + \rho \frac{\partial e_2}{\partial t} + \rho \left( h_1 - h_2 \right) \frac{\partial p_{aw}}{\partial x} + \rho_{aw} \frac{\partial (h_1 - h_2)}{\partial x} = 0. \]

With the help of the mass equation for phase 1 under the form,
and the turbulent energy definition it becomes,
\[ \rho \left( Y_1 \frac{\partial e_1}{\partial t} + Y_2 \frac{\partial e_2}{\partial t} \right) + \rho \frac{\partial w}{\partial t} + \rho \left( p_1 v_1 - p_2 v_2 \right) \frac{\partial p_{aw}}{\partial x} + \rho \frac{\partial (h_1 - h_2)}{\partial x} = 0. \]

The relative velocity equation,
\[ \frac{\partial w}{\partial t} = -v_1 \frac{\partial p_1}{\partial x} + v_2 \frac{\partial p_2}{\partial x} - \lambda w, \]
is now inserted,
\[ \rho \left( \frac{d_1 c_1}{dt} + \frac{d_2 c_2}{dt} \right) + \rho a w \left( \frac{\partial v_1}{\partial x} - \frac{\partial v_2}{\partial x} \right) + \left( p_1 v_1 - p_2 v_2 \right) \frac{\partial p_{aw}}{\partial x} = \lambda p_{aw}^2, \]
with
\[ \frac{d_1}{dt} = \frac{\partial}{\partial t} + \frac{aw}{Y_1} \frac{\partial}{\partial x} \quad \text{and} \quad \frac{d_2}{dt} = \frac{\partial}{\partial t} - \frac{aw}{Y_2} \frac{\partial}{\partial x}. \]

Using the Gibbs identity for each phase we have:
\[ \rho \left( Y_1 \frac{\partial v_1}{\partial t} - v_1 \frac{\partial p_{aw}}{\partial x} \right) - p_2 \left( \frac{\partial Y_2}{\partial t} + v_2 \frac{\partial p_{aw}}{\partial x} \right) = -\mu (p_1 - p_2)^2. \]

With the help of the entropy equations of System (2.4) and expanding the specific volumes time derivatives it becomes:
\[ -p_1 \rho Y_1 \frac{\partial v_1}{\partial t} - p_2 \rho Y_2 \frac{\partial v_2}{\partial t} = -\mu (p_1 - p_2)^2. \]

With the help of the two mass and the volume fraction equations it finally becomes:
\[ -p_1 \mu (p_1 - p_2) + p_2 \mu (p_1 - p_2) = -\mu (p_1 - p_2)^2. \]
This result being obviously true, System (2.4) is thermodynamically compatible.

**Hyperbolicity**
System (2.4) hyperbolicity is examined in the absence of relaxation terms. This system can be expressed as:
\[
\begin{bmatrix}
\frac{\partial}{\partial t} & \frac{u}{\alpha_1} & \frac{\alpha_1}{s_1} & \frac{s_2}{\rho_1} & \frac{\rho_2}{w} \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{aw}{Y_1} & 0 & 0 \\
0 & 0 & 0 & -\frac{aw}{Y_2} & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{\partial p_1}{\partial s_1} & -\frac{\partial p_2}{\partial s_2} & 0 \\
\frac{\partial p_1}{\alpha_1} & 0 & 0 & -\frac{\alpha_1}{\alpha_2} & 0 \\
\frac{\partial p_2}{\alpha_2} & 0 & 0 & -\frac{\alpha_2}{\alpha_1} & 0 \\
\end{bmatrix}
= 0
\]

The wave’s speeds are:
\[ \lambda_0 = 0 \text{ three times fold, } \lambda_1 = -\frac{aw}{Y_1}, \lambda_2 = \frac{aw}{Y_2}, \lambda_3 = \sqrt{a \left( \frac{c_1^2}{Y_1} + \frac{c_2^2}{Y_2} \right)} \text{ and } \lambda_4 = -\sqrt{a \left( \frac{c_1^2}{Y_1} + \frac{c_2^2}{Y_2} \right)}. \]

System (2.4) is thus hyperbolic.
Appendix C. Summary of the mean flow field solver

The method to solve the mean flow field is presented in the frame of the Kapila et al. 19 model as it replaces System (2.1) after stiff velocity relaxation. In other words, the final model with interpenetration uses the Kapila et al. 19 model for the mean flow field and a diffusion model for interpenetration.

A method to solve the Kapila et al. 19 model is detailed in Saurel et al. 25. It uses an extended system with 7 equations instead of the 5 equations model of Kapila. After several successive steps, solutions of the 5 equations model are reached in a robust and accurate way. The method proceeds with three successive steps.

Step 1. Extended hyperbolic system

The following pressure non-equilibrium system is considered instead of (2.1):

\[
\begin{align*}
\frac{\partial \alpha_i}{\partial t} + u \frac{\partial \alpha_i}{\partial x} &= \mu (p_1 - p_2), \\
\frac{\partial (\alpha p)_{1,k}}{\partial t} + \frac{\partial (\alpha p)_{1,k} u}{\partial x} &= 0, \quad k=1,2, \\
\frac{\partial (\alpha p)_{1,k} e_{1} + \partial (\alpha p)_{1,k} e_{u} u + (\alpha p)_{1} u}{\partial x} &= -p_i \mu (p_1 - p_2), \\
\frac{\partial (\alpha p)_{2,k} e_{2} + \partial (\alpha p)_{2,k} e_{u} u + (\alpha p)_{2} u}{\partial x} &= p_i \mu (p_1 - p_2), \\
\frac{\partial p_i u + \partial p_i u^2 + (\alpha p)_{1} + (\alpha p)_{2}}{\partial x} &= 0, \\
\frac{\partial p E + \partial (p E + (\alpha p_1 + \alpha p_2) u)}{\partial x} &= 0,
\end{align*}
\]

(C.1)

with \( E = Y_1 e_1 + Y_2 e_2 + \frac{1}{2} u^2 \).

There is no need to detail the interfacial pressure \( p_i \) as the stiff mechanical relaxation limit is to be considered (\( \mu \rightarrow +\infty \)). Indeed the asymptotic limit of System (B.1) is precisely the Kapila et al. 19 system. A proof is given in Saurel et al. 25.

During the hyperbolic step System (C.1) is solved with a Godunov type scheme in the absence of relaxation terms.

This system is over-determined by one of the energy equations. However, this over determination is used during Step 3 to correct inaccuracies linked to the non-conservative internal energy equations.

Step 2. Pressure relaxation

Instead of solving a stiff ODE system, an algebraic one is solved to determine the asymptotic relaxed pressure and corresponding volume fractions. The algebraic system to solve is composed of the saturation constraint (\( \sum_k \alpha_k = 1 \)) under the form:

\[
\begin{align*}
\sum_k (\alpha p)_{k} v_{k} (p) &= 1, \\
v_{k} (p) &= \frac{\left( p_{k}^0 + Y_k p_{p} + (Y_k - 1)p \right) \nu_k^0}{Y_k (p + p_{p})},
\end{align*}
\]

(C.2)

The second relation provides the phase’s specific volumes. The Newton method is used to solve this non-linear system. See Saurel et al. 25 for the details.

Step 3. Pressure computation with the mixture EOS
Once the volume fractions are determined from (C.2), the mixture EOS (1.18) is used to correct the pressure computation. The mixture EOS uses the mixture energy that is unambiguously determined from the associated conservation law. Thus, if some inaccuracies have been done during the numerical integration of the non-conservative internal energies, their effect is lowered by the pressure computation based on the mixture total energy and mixture EOS.

With the new computed pressure, the phases' internal energies are reset with the help of their equations of state before going to the next time step. Robustness, efficiency and accuracy of the three steps method has been demonstrated in various papers, dealing with various theoretical models of diffuse interfaces:

- Multiphase detonation with material interfaces: Petitpas et al. 38.
- Phase transition fronts: Saurel et al. 27, Petitpas et al. 39, Petitpas et al. 40.
- Powders compaction: Saurel et al. 21.

Appendix D. Implicit scheme for the interpenetration effective sub model

The interpenetration effective sub model reads:

\[
\frac{\partial U}{\partial t} = \frac{\partial}{\partial x} \left( \nu(U) \frac{\partial U}{\partial x} \right) \tag{D.1}
\]

where \( \nu(U) \) represents the interpenetration coefficient. This coefficient is taken under the form,

\[
\nu = \nu_0 Y_1 Y_2, \tag{D.2}
\]

where \( Y_i \) represent the mass fractions and \( \nu_0 \) is a pure constant.

This non-linear coefficient is necessary to avoid artificial shock waves damping, as the product \( Y_1 Y_2 \) tends to zero far from interfaces. Oppositely, this product being non-zero at interfaces, interpenetration will occur.

Let’s consider a cell boundary \( i+1/2 \) separating two computational cell centers \( i \) and \( i+1 \). Solution and flux continuity expressed at the cell boundary imply:

\[
\frac{U_{i+1/2} - U_i}{\Delta x} = \frac{U_{i+1} - U_{i+1/2}}{\Delta x}.
\]

Thus,

\[
U_{i+1/2} = \frac{\nu_i U_i + \nu_{i+1} U_{i+1}}{\nu_i + \nu_{i+1}}.
\]

Consequently the flux reads,

\[
q_{i+1/2} = a_{i+1/2} \frac{U_{i+1} - U_i}{\Delta x},
\]

with \( a_{i+1/2} = 2 \frac{\nu_{i+1} \nu_i}{\nu_i + \nu_{i+1}} \).

Equation (D.1) can be approximated as:

\[
\frac{U_{i+1}^{n+1} - U_i^n}{\Delta t} = \frac{q_{i+1/2}^{n+1} - q_{i-1/2}^{n+1}}{\Delta x} \tag{D.3}
\]

When the fluxes are expressed with variables \( U \) taken at time level \( n \), the following explicit numerical scheme is obtained:

\[
U_{i+1}^{n+1} = U_i^n + \frac{\Delta t}{\Delta x^2} \left( a_{i+1/2}^{n} \left(U_{i+1}^{n} - U_i^n\right) - a_{i-1/2}^{n} \left(U_{i}^{n} - U_{i-1}^{n}\right) \right).
\]

Its stability restriction is: \( \Delta t \leq \frac{\Delta x^2}{\nu} \).

To overcome this limit, a Taylor expansion of the numerical flux is done,
\[ q_{i+1/2}^{n+1} = q_{i+1/2}^n + \frac{\partial q_{i+1/2}}{\partial U_i} (U_{i+1}^n - U_i^n) + \frac{\partial q_{i+1/2}}{\partial U_{i+1}} (U_{i+1}^n - U_{i+1}^n), \]

i.e.,
\[ q_{i+1/2}^{n+1} = q_{i+1/2}^n - \frac{a_{i+1/2}}{\Delta x} \Delta U_i + \frac{a_{i+1/2}}{\Delta x} \Delta U_{i+1}, \]

with, \( \Delta U_i = U_{i+1}^{n+1} - U_i^n \).

These last relations are now inserted in (D.3),
\[
\frac{U_i^{n+1} - U_i^n}{\Delta t} = \left( q_{i+1/2}^n - \frac{a_{i+1/2}}{\Delta x} \Delta U_i + \frac{a_{i+1/2}}{\Delta x} \Delta U_{i+1} \right) - \left( q_{i-1/2}^n - \frac{a_{i-1/2}}{\Delta x} \Delta U_{i-1} + \frac{a_{i-1/2}}{\Delta x} \Delta U_i \right).
\]

Rearranging this expression, the following formula is obtained:
\[
- \frac{\Delta t}{\Delta x^2} a_{i+1/2} \Delta U_i + \left( I + \frac{\Delta t}{\Delta x^2} (a_{i+1/2} + a_{i-1/2}) \right) \Delta U_i - \frac{\Delta t}{\Delta x^2} a_{i-1/2} \Delta U_{i-1} = \frac{\Delta t}{\Delta x} \left( q_{i+1/2}^n - q_{i-1/2}^n \right) \]

Formulation (D.4) results in a tridiagonal system. The solution is reached with the Gauss method for each variable of the U vector.

When the increments \( \Delta U_i \) are determined, the solution is updated by:
\[ U_i^{n+1} = U_i^n + \Delta U_i. \]

We now examine the spherical 1D method extension, useful for the spherical explosion tests. Formula (D.3) becomes,
\[ \Delta U_i = \frac{\Delta t}{V_i} \left( (S q)_{i+1/2}^n - (S q)_{i-1/2}^n \right), \]

where \( V_i \) represents the computational cell volume and \( S q_{i+1/2} \) the cell boundary surfaces.

Inserting the Taylor flux expansion in this formula results in the following tridiagonal system,
\[
- \frac{\Delta t}{V_i} \frac{(S a)_{i-1/2}^n}{\Delta x} \Delta U_{i-1} + \left( I + \frac{\Delta t}{V_i} \left( \frac{(S a)_{i+1/2}^n}{\Delta x} + \frac{(S a)_{i-1/2}^n}{\Delta x} \right) \right) \Delta U_i - \frac{\Delta t}{V_i} \frac{(S a)_{i+1/2}^n}{\Delta x} \Delta U_{i+1} = \frac{\Delta t}{V_i} \left( (S q)_{i+1/2}^n - (S q)_{i-1/2}^n \right)
\]

**Appendix E. Effective diffusion-interpenetration limit model derivation**

The diffusion-interpenetration submodel (3.7-3.8) is solved in conjunction with a pressure relaxation procedure. The diffusion submodel is expressed in terms of total energies while the pressure relaxation solver is expressed in terms of entropies. To determine the effective diffusion-interpenetration sub model, it is first needed to express the overall subsystem with the same set of variables. The second step consists in inserting the interpenetration submodel in the mean flow field model to determine the effective one.

The pressure relaxation step solution corresponds to the asymptotic solution of the following ODE system, corresponding to System (3.4) in the absence of relative motion:
\[
\frac{\partial \alpha_i}{\partial t} = \mu(p_1 - p_2),
\]
\[
\frac{\partial (\alpha \rho)}{\partial t} = 0,
\]
\[
\frac{\partial (\alpha \rho u)}{\partial t} = 0,
\]
\[
\frac{\partial \rho u}{\partial t} = 0,
\]

(E.1)
The phase 1 entropy equation can be written as:
\[
\alpha_1 \rho_1 \left( \frac{\partial \alpha_1}{\partial t} + p_1 \frac{\partial v_1}{\partial t} \right) = \theta \mu (p_1 - p_2)^2
\]
Or alternatively,
\[
\frac{\partial \alpha_1 \rho_1 E_1}{\partial t} = -\mu (p_1 - p_2) ((1 - \theta)p_1 + \theta p_2).
\]
For the second phase, a symmetric result is obtained:
\[
\frac{\partial \alpha_2 \rho_2 E_2}{\partial t} = \mu (p_1 - p_2) ((1 - \theta)p_1 + \theta p_2)
\]
The pressure non-equilibrium diffusion subsystem thus reads:
\[
\frac{\partial \alpha_1}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial \alpha_1}{\partial x} \right) + \mu (p_1 - p_2)
\]
\[
\frac{\partial \alpha_1 \rho_1}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial \alpha_1 \rho_1}{\partial x} \right)
\]
\[
\frac{\partial \alpha_2 \rho_2}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial \alpha_2 \rho_2}{\partial x} \right)
\]
\[
\frac{\partial p u}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial p u}{\partial x} \right)
\]
\[
\frac{\partial (\alpha_1 E_1)}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial (\alpha_1 E_1)}{\partial x} \right) - \mu (p_1 - p_2) ((1 - \theta)p_1 + \theta p_2)
\]
\[
\frac{\partial (\alpha_2 E_2)}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial (\alpha_2 E_2)}{\partial x} \right) + \mu (p_1 - p_2) ((1 - \theta)p_1 + \theta p_2)
\]
This system is obviously compatible with the mixture energy conservation:
\[
\frac{\partial p E}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial p E}{\partial x} \right).
\]
The interpenetration subsystem (E.2) is out of pressure equilibrium. To insert interpenetration effects in the Kapila et al. \(^{19}\) mean flow field model the pressure equilibrium limit model of (E.2) has to be determined. From (E.2) the pressure evolution equation of phase 1 is,
\[ \frac{\partial p_i}{\partial t} = \frac{\Gamma_i}{\alpha_i} \left\{ -Y_i u \frac{\partial}{\partial x} \left( \nu \frac{\partial pu}{\partial x} \right) + \left( \alpha_i \frac{\partial}{\partial x} \left( \nu \frac{\partial \alpha_i}{\partial x} \right) \right) \right\} + \mu \left( p_1 - p_2 \right) \left\{ \left( p_1 - \frac{\rho_1 c_i^2}{\Gamma_i} \right) - \left( (1-\theta)p_1 + \theta p_2 \right) \right\}, \]

where \( H_k = E_k + \frac{p_k}{\rho_k}, k=1,2. \)

A symmetric result is obtained for the second phase. Taking the difference of the two pressure equations and considering the stiff pressure relaxation limit (\( \mu \to +\infty \)) of the corresponding equation provides the pressure fluctuation difference:

\[ (p_1' - p_2') = \frac{1}{\rho_1 c_1^2 + \rho_2 c_2^2} \left\{ \frac{\rho_1}{\alpha_1} + \frac{\rho_2}{\alpha_2} \right\} \]

Consequently the pressure equilibrium interpenetration sub model resulting of (E.2) reads:

\[ \frac{\partial \alpha_i}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial \alpha_i}{\partial x} \right) + (p_1' - p_2') \]

\[ \frac{\partial \alpha_{i_1} \rho_1}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial \alpha_{i_1} \rho_1}{\partial x} \right) \]

\[ \frac{\partial \alpha_{i_2} \rho_2}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial \alpha_{i_2} \rho_2}{\partial x} \right) \]

\[ \frac{\partial \rho u}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial \rho u}{\partial x} \right), \]

\[ \frac{\partial \rho E}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial \rho E}{\partial x} \right). \]

Thus, the overall flow model including mean interface dynamics and interpenetration corresponds to System (3.9). The volume fraction equation is clearly complicated, as \( (p_1' - p_1) \) is given by the formula above, but is never considered under this form at the numerical level. Indeed, the numerical strategy is based on augmented systems with separate pressure relaxation.

**Appendix F. Post-detonation model with JWL EOS**

The JWL EOS is fitted to reproduce the expansion curve of detonation products from the CJ point. It can be expressed as,
\[ e(p, \rho) = \frac{p + \gamma \rho \rho_m(\rho)}{(\gamma - 1) \rho} + \rho e(\rho). \]

If mass transfer is considered with (5.4), the densities of the phases are going to vary, resulting in strong variations of the non-linear functions \( p_m(\rho) \) and \( e_m(\rho) \). When they are used in the mixture EOS (1.18), a pressure decrease is observed even if the reaction is exothermic. To overcome this incorrect behaviour, the mass transfer System (5.4) is modified as follows:

\[
\begin{align*}
\frac{\partial \alpha_1}{\partial t} &= 0 \\
\frac{\partial (\alpha \rho)}{\partial t} &= 0 \\
\frac{\partial (\alpha \rho)_1}{\partial t} &= 0 \\
\frac{\partial (\alpha \rho)_2 y_{\text{air}}}{\partial t} &= -\varphi \dot{m}_1 \\
\frac{\partial p}{\partial t} &= 0 \\
\frac{\partial \rho E}{\partial t} &= \dot{m}_1 q_1
\end{align*}
\]

It means that the two-phase mixture composition is unchanged, only the mixture products composition changes with a decrease of the air content. When the air is consumed by the post-detonation reaction, extra energy is released to the system. This extra energy is not present in the constants of the JWL EOS as this post detonation reaction is absent of the fitting process used to determine the JWL coefficients. Adding a constant to \( e_m(\rho) \) is not enough to correct the non-linear effects related to density variations.