Diffuse interfaces and capturing methods in compressible two-phase flows

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Abstract
Simulation of compressible gas dynamics flows became routinely with the appearance of capturing methods. These methods have the capability to compute routinely all waves and in particular discontinuous ones. However, additional difficulties may appear in two-phase and multimaterial flows since each phase or material is governed by its own equation of state with discontinuous thermodynamic representation at interfaces. To overcome this difficulty, augmented systems of governing equations have been developed to extend the shock-discontinuity capturing strategy. These extended systems are ‘diffuse interfaces’ models in the sense that they are designed to compute flow variables correctly in numerically diffused zones surrounding interfaces. In particular, they couple correctly the dynamics of the two fluids evolving on both sides of the (diffuse) interface and tend to the proper fluid governing equations far from said interfaces.
Such strategy is now efficient for contact interfaces separating fluids governed by different equations of state, in the presence or absence of capillary effects, with or without phase transition. More sophisticated materials than fluids (elastic-plastic materials for example) have been considered as well.
In this article a review of two-phase flow modeling for compressible flows with diffuse interfaces is presented.
1. INTRODUCTION

In this review, we concentrate on recent advances in the methodology for the simulation of compressible flow with material interfaces. The focus here is on advances in the formulation, their efficient numerical implementation in modern computing architectures, and finally we highlight selected recent applications to complex flows. While we have tried to be exhaustive, we have given precedence to writing a coherent, self-contained, description of the state of the art in the field and to discuss certain problems that, in our opinion, deserve immediate consideration. Unintended omissions of contributions to this field are unavoidable and we apologize beforehand.

A new discontinuity, in addition to the well-known discontinuous waves that arise in single-phase gas dynamics, appears as soon as the flow involves two distinct fluids (or materials). This discontinuity is usually named a contact wave and corresponds to the interface that separates the two fluids, e.g., air and water. The interface may have additional thermodynamic properties from those of the two separate phases, which may obey the same type of governing equations or not, e.g., ideal gas and stiffened equation of state. Interface motion has been addressed by several classes of computational methods that can be classified as follows. In the first class, the interface is preserved as a resolved surface as grid deforms following the kinematics of the interface. Prominent examples are the Lagrangian [von Neumann and Richtmyer 1950] and Arbitrary-Lagrangian-Eulerian (ALE) methods [Hirt et al. 1974]. These methods can be very accurate if the deformation of the interface is not too large but they become limited by mesh distortions at large deformations. In the second class, the front tracking method [Glimm et al. 1998] attempts to reduce these distortions by considering fixed meshes for the bulk flow and tracking the moving interface by Lagrangian markers. The approach requires the management of at least two flow solvers and it becomes geometrically challenging as the interface distortion grows. In the third class, progress in the direction of simplicity and generality was achieved by the development of the Level Set Method [Dervieux and Thomasset 1980], which was adapted to compressible fluids [Aslam et al. 1996] and the more modern Ghost Fluid Method (GFM) [Fedkiw et al.].
1999] used to compute the pressure in mixture cells. To avoid the complexity related to mesh management with previous methods, the interface was tracked implicitly through an Eulerian function and two sets of Euler equations were used to store and evolve the fluid variables when needed, in particular in mixture cells. The GFM is used to transfer the boundary conditions at interfaces from one set of Euler equations to the other. Although apparently simple, this method still requires careful considerations to ensure robustness and conservation.

In this review, we are concerned with computational methods that artificially let the two fluids develop a small amount of mixing at the otherwise resolved interface, and this justify the terminology of *diffuse interface methods* (DIM). This presents its own problems because the thermodynamic state of the mixture needs to be defined as the interface evolves. The bulk fluids typically have density and internal energy that are significantly different from that of the mixture and in general it is not straightforward to compute the mixture thermodynamics and in particular the pressure across the diffused interface without additional closures. Two subclasses of DIM are present in the literature. The first one considers physically diffuse interfaces, having a well-defined visco-capillary structure [Cahn and Hilliard 1958]. In order for these methods to work correctly, the spatial resolution must be sufficiently fine to accurately resolve the interface width, *i.e.*, up to a few nanometers. In addition, the equation of state is aimed to describe phase transition between a liquid and its vapor through a cubic type equation of state (EOS). In this approach, thermodynamics and capillarity are coupled. In the author's knowledge, this approach has never shown its capability to compute interfaces between immiscible fluids (water and air for example). This approach is well-suited to the simulation of phase transition in very small systems. The second subclasses of DIM addresses mixture cells having computational origins instead of physical ones. Pioneer work in this direction was done with VOF methods [Hirt and Nichols 1981] in the frame of incompressible fluids. Here, an extra evolution equation is added to the flow model representing the volume fraction of a given phase. At this level, the model adopts a two-phase description of the flow, with sub-volumes occupied by the phases and several mass balance equations. Extension of this approach to compressible fluids was done in [Saurel and Abgrall 1999a] and [Kapila et al. 2001].

The success of two-phase compressible flow simulations is certainly a consequence of the formidable growth in computational power, readily available to scientists and engineers, combined with the availability of advanced and efficient numerical methods for the simulation of flows possessing discontinuities (a hallmark of compressible flow). These advances have made complex two-phase flow simulations a routine practice in recent years. The great advantage of these methods is the use of a single set of equations to describe the two-phase nature of the flow at all the computational cells; avoiding the explicit tracking of the interface separating different phases. This progress has been made possible thanks to the tremendous advances in the development of methods for single-phase compressible flow simulation that took place in the last century. It was realized early that shocks and contact discontinuities could be captured (instead of resolved) easily by the use of enlarged artificial diffusivity without causing too damaging errors outside the inner region of the discontinuity, see [von Neumann and Richtmyer 1950]. This is certainly true for simple shock waves and it allows the prediction of shock propagation in complex situations by using just a few mesh points across the wave inner region. Later, Godunov [Godunov 1959] developed an improved method where cell boundary fluxes were determined using the fundamental Riemann problem structure, which accounts for all types of wave interactions.
Many researchers have improved and simplified the wave capturing method [Harten et al. 1983, Osher and Solomon 1982, Roe 1981, Toro et al. 1994, van Leer 1979]. Research is still in active progress to improve accuracy; e.g., essentially non-oscillatory schemes (ENO, WENO) [Harten et al. 1987, Shu and Osher 1988], Discontinuous Galerkin methods [Cockburn and Shu 1989], ADER schemes [Titarev and Toro 2002]; and robustness for strong shocks or contact interfaces [Zhang and Shu 2012].

Contrarily to shock-capturing schemes, the computation of interfaces separating two immiscible phases with different thermodynamics has no physical viscous regularization. Consequently, the approaches of von Neumann-Richtmyer-Godunov [Godunov 1959, von Neumann and Richtmyer 1950] are not as effective as they are for shocks. Traditional shock-capturing methods generally result in excessive and artificial diffusion of as well as a loss of mechanical equilibrium at the interface; appearance of spurious velocity and pressure fluctuations resulting in computational failure. Removing the latter spurious mechanical phenomena requires a well-behaved relaxation of the mixture thermodynamics as one traverses from one phase to the other [Kapila et al. 2001, Lund 2012, Saurel and Abgrall 1999a]. Furthermore, since the pure phases are governed by hyperbolic systems of equations (super-sets of Euler equations), the mixture thermodynamics and governing equations must be compatible with this level of description. In this context, [Abgrall 1996] considered interface formulations separating two ideal gases. [Shyue 1998] and [Saurel and Abgrall 1999b] considered liquid-gas interfaces and added evolution equations for the stiffened gas EOS parameters to compute mixture cells thermodynamics. These methods were generalized and rationalized with the help of multiphase flow modeling [Allaire et al. 2002, Kapila et al. 2001, Massoni et al. 2002, Murrone and Guillard 2005, Saurel and Abgrall 1999a, Saurel et al. 2009]. In all these formulations the aim is to solve interfaces with a unique set of partial differential equations (an extended flow model) and a unique hyperbolic solver. Because interface deformations in most compressible flows are arbitrarily complex, one retains the philosophy of shock-capturing methods and abandons the tracking or reconstruction of the interfaces.

Finally, it is possible to alleviate the smearing or artificial diffusion introduced by capturing methods by purely numerical techniques that attempt to sharpen the interfaces [Chiapolino et al. 2017b, Shukla et al. 2010, Shyue and Xiao 2014, Tiwari et al. 2013] as well as to increase the order of approximation and global accuracy [Loubere et al. 2014]. Additional, physical extensions have been addressed as well: chemical reactions [Petitpas et al. 2009], phase change [Saurel et al. 2016], surface tension [Perigaud and Saurel 2005], solid-fluid [Favrie et al. 2009], and plastic transformation [Ndanou et al. 2015], to cite a few.

The review is organized as follows. In Section 2 several flow models of diffuse interfaces are presented and the link between them are explained. Section 3 presents the main ingredients for the numerical resolution of some of these models. Section 4 showcase results to illustrate the methods’ capabilities. Section 5 discusses future research directions.

2. THEORETICAL FORMULATIONS

The various diffuse interface models for compressible flows mentioned in the introduction are based on reductions or enhancements of the non-equilibrium model of Baer and Nunziato [Baer and Nunziato 1986], which we refer to as the BN model for short. The BN model is based on the incompressible Euler equations of a two-phase mixture, while the core of a compressible phase is based on the compressible Euler equations. The interface would be a sharp one, allowing the phases to be described separately. An interfacial thickness is introduced to avoid the need to track the interface explicitly, at the cost of some numerical diffusion. This approach is an example of a diffuse interface model. It also illustrates the need to balance the level of diffusion with the need to model the phase change at the interface.
laws can be considered as well to model a given media. The differences between models arise owing to changes of space and time scales, when reducing the computational cost, usually by decreasing the required number of fields, or to improve their physical accuracy in different scenarios. Figure 1 highlights the two typical scenarios considered in this review. The sketch to the left indicates a two-phase flow composed of a phase that is finely dispersed but otherwise embedded in a carried phase. The typical size of the fine phase is too small for any reasonable computational grid to resolve its fluid and thermochemical details and therefore one relays on an homogenized or average description of the flow; termed average mixture in the figure. Such typical situation of mixture in disequilibrium is in general considered through systems of Baer and Nunziato [1986] type. In the second scenario, the size of both phase volumes can be resolved by the available computational mesh and the interface separating the two phases is accurately captured; termed resolved interface in the figure. Such typical situation of resolved interface is considered in the present work through diffuse interface formulations. The conventional notation in two-phase flow literature is used below, where $\alpha_k$, $\rho_k$, $u_k$, $p_k$, $E_k = e_k + \frac{1}{2} u_k \cdot u_k$, $e_k$, denote, respectively, the volume fraction, density, velocity, pressure, total energy and internal energy of phase $k = 1$ or $2$.

A rational method to deduce diffuse-interface two-phase flow models from the total non-equilibrium BN model is given in Lund [2012] on the basis of asymptotic analysis. Furthermore, it is possible to insert additional physics, such as solid mechanics with elastic plastic flows in similar formulations. We refer to Favrie et al. [2009] and Ndanou et al. [2015] for further detailed documentation and analytical convergence results.
2.1. Non-equilibrium model

In this model, the balance equations of phase $k$ are,

\[
\frac{\partial \alpha_k}{\partial t} + \mathbf{u}_I \cdot \nabla \alpha_k = \mu (p_k - p_{k^*}),
\]

\[
\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = 0,
\]

\[
\frac{\partial \alpha_k \rho_k \mathbf{u}_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \otimes \mathbf{u}_k) + \nabla (\alpha_k \rho_k) - p_I \nabla \alpha_k = \lambda (\mathbf{u}_{k^*} - \mathbf{u}_k),
\]

\[
\frac{\partial \alpha_k \rho_k E_k}{\partial t} + \nabla \left[ \alpha_k (\rho_k E_k + p_k) \mathbf{u}_k \right] - p_I \mathbf{u}_I \cdot \nabla \alpha_k = -\mu p'_{I} (p_k - p_{k^*}) + \lambda (\mathbf{u}_{k^*} - \mathbf{u}_k) \mathbf{u}'_I,
\]

(1)

From this point onwards, we will refer right-hand side terms as interaction ones among the phases. Index $k^*$ denotes the conjugate phase to $k$; i.e., $k = 1$ implies $k^* = 2$, and vice versa.

Relaxation parameters $\mu$ and $\lambda$ denote the rate at which pressures and velocities tend to equilibrium respectively. The quantities $p_I$ and $\mathbf{u}_I$ denote the pressure and velocity of the interfaces, respectively. The ensemble of coefficients, interfacial pressures, and velocities are modeling elements, some introduced by Baer and Nunziato [1986], to produce a flow model whose dynamics approximates those of immiscible two-phase flows.

The first equation of System (1) represents the $k$-phase volume fraction, $\alpha_k$, transported at velocity $\mathbf{u}_I$, defined as

\[
\mathbf{u}_I = \mathbf{u}'_I + \text{sgn}(\nabla \alpha_k) \frac{p_{k^*} - p_k}{Z_1 + Z_2},
\]

(2)

where $Z_k = \rho_k c_k$ denotes the acoustic impedance and $c_k$ denotes the sound speed of phase $k$, respectively, and the interfacial velocity existing inside a droplet or bubble cloud is defined by,

\[
\mathbf{u}'_I = \frac{Z_1 \mathbf{u}_1 + Z_2 \mathbf{u}_2}{Z_1 + Z_2}.
\]

(3)

During advection, volume variations due to pressure differential among the phases are considered through the relaxation term $\mu (p_{k^*} - p_k)$ with $\mu$ controlling the rate at which pressure equilibrium is reached, is defined as

\[
\mu = \frac{A_I}{Z_1 + Z_2},
\]

where $A_I$ represents the specific interfacial area of the mixture. The second and third equations of System (1) express the mass and momentum balance of phase $k$, respectively. The velocity relaxation term in the right-hand side of the momentum equation is $\lambda (\mathbf{u}_{k^*} - \mathbf{u}_k)$, where $\lambda$ is the product of the specific interfacial area with the pressure drag coefficient,

\[
\lambda = Z_1 Z_2 \mu.
\]

Viscous drag effects can be considered as well through correlations based on the Reynolds number. The non-conservative term $p_I \nabla \alpha_k$ represents the pressure force acting at the droplet cloud boundaries. The interfacial pressure at this level is approximated as,

\[
p_I = p'_I + \frac{Z_1 Z_2}{Z_1 + Z_2} \text{sgn}(\nabla \alpha_k) \cdot (\mathbf{u}_2 - \mathbf{u}_1),
\]

(4)

where the interfacial pressure acting inside the droplet or bubble cloud is defined by,

\[
p'_I = \frac{Z_1 p_2 + Z_2 p_1}{Z_1 + Z_2}.
\]

(5)
The expressions above were obtained in Saurel et al. [2003b]. Finally, the fourth equation in System (1) expresses the energy balance of phase $k$, which is non-conservative due to the $p_1 u_1 \cdot \nabla \alpha_k$ and relaxation terms in the right-hand side of that equation. These terms appear in the correct form to ensure thermodynamic and mechanical consistency. Eqs. (2)-(5) are derived from the local Riemann-problem solution that obviously provide correct local interfacial variables, but these linearized solutions should be replaced by non-linear solutions when dealing with strong shocks.

System (1) is hyperbolic with wave speeds $u_1, u_k, u_k \pm c_k$, where $c_k$ denotes the sound speed of phase $k$. Therefore, 7 wave speeds are present, instead of 6 in the original BNM, because of the interfacial velocity given by Eq. (2). The system admits the following entropy equation

$$ \frac{\partial \alpha_k \rho_k s_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k s_k u_k) = \frac{1}{T_k(Z_k + Z_k^*)} \times $$

$$ \left\{ Z_k(Z_k + Z_k^*)^{-1} [(p_k^* - p_k) + \text{sgn}(\nabla \alpha_k) \cdot (u_k^* - u_k) Z_k^*] | \nabla \alpha_k | + \right.$$ 

$$ \left. \mu Z_k^* (p_k^* - p_k)^2 + \lambda Z_k (u_k^* - u_k) \cdot (u_k^* - u_k) \right\}. $$

Note that the right-hand side of Eq. (6) is non-negative for all $k$ and this ensures that the mixture entropy, $s = \sum_k \rho_k \alpha_k s_k$, necessarily agrees with the second law of thermodynamics.

System (1) is a two-phase model for mixture flows evolving in velocity and temperature non-equilibrium, such as clouds of drops, bubbles, or granular beds; additional physical effects are needed in the latter [Bdzil et al. 1999]. To close the system of equations, an estimate is needed for the specific interfacial area $A_I$. The most convenient method is to supplement System (1) with evolution equations for the specific number density of drops (or grains) $n_k$ per unit mass of phase $k$, obeying the equation

$$ \frac{\partial \alpha_k \rho_k n_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k n_k u_k) = \alpha_k \rho_k \dot{n}_k,$$

where the production rate of number of drops or bubbles, $\dot{n}_k$, is modeled by known correlations that depend on the Weber and Reynolds numbers; see for example [Furfaro and Saurel 2016]. Knowledge of number density $n_k$ and volume fraction $\alpha_k$ enables the calculation of the time and space dependent drops radius and associated interfacial area.

Alternative formulations of the volume fraction transport equation have been proposed recently [Saurel et al. 2017] with the aim of improving the acoustic properties of the BN model, in particular when one of the phases is discontinuous and unable to propagate sound. It occurs for dispersed liquid suspensions, as the sound can propagate in the liquid at drop scale with the liquid sound speed, but not between drops with the same sound speed as there is no material support to propagate such sound disturbance. For liquid drops suspended in a gas, the volume fraction of System 1 is replaced by the following one:

$$ \frac{\partial \alpha_1}{\partial t} + \nabla \cdot (\alpha_1 u_1) = \mu(p_1 - p_2) $$

For gas bubbles suspended in a liquid, the following volume fraction equation is recommended,

$$ \frac{\partial \alpha_2}{\partial t} + \nabla \cdot (\alpha_2 u_2) = \mu(p_2 - p_1) $$

These two options (7, 8) can be combined with the balance equations of mass, momentum and energy of System 1. They result in the volume fraction equation provided.
that the pressure relaxation coefficient is stiff \( (\mu \rightarrow +\infty) \). They both yield hyperbolic two-phase flow models with more realistic acoustic properties. The first option (7) results in wave’s speeds \( u_1, u_2, u_2 + c_2 \) and \( u_2 - c_2 \) while the second option (8) results in different wave speeds, \( u_2, u_1, u_1 + c_1 \) and \( u_1 - c_1 \). Moreover, these alternative formulations remain compatible with the reduced models examined later. In particular, the [Kapila et al. 2001] model can be derived from the formulations given in [Saurel et al. 2017].

The above formulation with the described closures is applicable to two-phase mixtures with velocity non-equilibrium as well as resolved interface separating two pure fluids. In the latter situation, volume fractions evolve from 0 to 1 in short distances while the interfacial area \( A_I \) has no meaning. Interface conditions are respected thanks to the various terms appearing in the right-hand side of the system and the associated interfacial variables. System (1) is able to fulfill the expected interface condition of mechanical equilibrium, continuity of pressure and normal velocities, under either one of the two possibilities: \( \lambda = \mu = 0 \), or \( \lambda = \mu \rightarrow +\infty \).

In the first possibility, the interface conditions are ensured by the non-conservative terms since the symmetric interfacial variables Eqs. (2)-(4) model contact interface conditions as general solutions of local Riemann problems. This possibility has been used for example in [Layes and Le Metayer 2007] for the study of shock interaction with a gas bubble. It is also able to deal with permeable interfaces: boundaries of bubbles or droplets clouds. It has been used for permeable granular interfaces in [Saurel et al. 2014] where an extension of System (1) is provided to account for granular effects. This capability is not possible with the original BN model, where the interfacial variables are estimated as \( p_I = p_2 \) and \( u_I = u_1 \), which turn out to be too crude approximations of the local interfacial pressure and velocity.

The second possibility relies on stiff mechanical relaxation. In this limit the mixture evolves with a single pressure and single velocity. This approach was proposed in [Saurel and Abgrall 1999a] in a splitting formulation where the hyperbolic System (1) was solved during a time step in the absence of source terms, followed by pressure and velocity relaxation steps [Lallemand and Saurel 2000, Lallemand et al. 2005] that account for the sources \( \mu(p_k - p_k^*) \), \( \lambda(u_k^* - u_k) \) with both \( \lambda = \mu \rightarrow +\infty \). Rather than solving stiff systems of ODE’s, pressure and velocity relaxation solvers are built, resulting in non-linear algebraic systems free of relaxation parameters. These systems sometimes admit exact solutions, when the phase’s EOS are simple enough, but are often solved with the Newton’s method. The second approach, based on stiff relaxation solvers is very robust, more than the first possibility based on non-conservative terms, that has less entropy production. However, the first possibility enables consideration of permeable and impermeable interfaces [Saurel et al. 2003a, 2014] as well as velocity disequilibrium two-phase mixtures. When considering situations with resolved interfaces only (the aim of the present review), as schematized in Figure 1, the method based on stiff relaxation can be simplified to a two-phase mixture model where the phases evolve in both pressure and velocity equilibrium. Such reduction is addressed hereafter.

2.2. Reduced model of Kapila et al.

An asymptotic expansion of System (1) in the limit of stiff mechanical relaxation (\( \lambda = \mu \rightarrow +\infty \)) and asymptotically close to the following model due to Kapila et al. [2001], a formal
to as the Kapila model for short from now onwards, and given by

\[ \frac{\partial \alpha_k}{\partial t} + \mathbf{u} \cdot \nabla \alpha_k = \beta_k \nabla \cdot \mathbf{u}, \]

\[ \frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}) = 0, \]

\[ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = 0, \]

\[ \frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + p) \mathbf{u}] = 0, \]

where the same notations as before are employed and the mixture density is defined by

\[ \rho = \sum_k \alpha_k \rho_k \]

while the mixture total energy is given by \( \rho E = \sum_k \alpha_k \rho_k E_k \) and the coefficient \( \beta_k \) is given by

\[ \beta_k = \frac{\rho_k c_k^2 - \rho_k^* c_k^*}{\rho_k^2 \alpha_k^{-1} + \rho_k^* c_k^* \alpha_k^*}. \]

The internal energy \( e_k = e_k(p, \rho_k) \) is given by the (convex) caloric equations of state, as well as the sound speed, \( c_k = c_k(p, \rho_k) \) of the phases \( k = 1, 2 \), respectively. Since the pressure is in equilibrium for this model, each phase is allowed to possess different temperatures \( T_k \); which can be determined with the help of the thermal equation of state \( e_k(\rho_k, T_k) \) which is not necessary to integrate System (9).

The first equation of System (9) expresses a non-conservative volume fraction transport. The right-hand side term in this equation is precisely the limit of the relaxation term \( \mu(p_1 - p_2) \) in the first equation of System (1). The pressure that appears in the momentum and energy equations is given by the mixture equation of state. It is derived from the mixture energy definition given above and the pressure equilibrium condition \( p_1 = p_2 \). Furthermore, System (9) admits the following entropy equations,

\[ \frac{\partial \alpha_k \rho_k s_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k s_k \mathbf{u}) = 0, \]

which are thermodynamically consistent. Also, System (9) is hyperbolic with wave speeds \( u, u \pm c_w \), where \( c_w \) denotes the mechanical equilibrium sound speed [Wood 1930], given by

\[ \frac{1}{\rho c_w^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2}. \]

System (9) describes mixtures of compressible fluids in mechanical equilibrium but out of thermal equilibrium. It was derived to model granular mixtures of reactive materials but is perfectly suitable for the computation of interfaces separating pure fluids. The contact interface conditions of System (9) have equal pressures and equal normal velocities. In addition, since it involves two temperatures, the absence of temperature relaxation in numerically diffuse interfaces produces pressure-oscillation-free solutions. This property is absent in the reactive Euler equations, widely used in combustion, that assume temperature equilibrium among the constituents and tend to produce spurious (artificial) pressure oscillations [Abgrall 1996].

### 2.3. Pressure non-equilibrium model

The Kapila model involves however a specific numerical issue related to the non-conservative term in the right-hand side of the volume fraction equation of System (9). To overcome this...
difficulty a homokinetic model in pressure non-equilibrium (PNE) was derived in [Saurel et al. 2009]. It consists of a hyperbolic over-determined system of 7 partial differential equations, given by

\[ \frac{\partial \alpha_k}{\partial t} + \mathbf{u} \cdot \nabla \alpha_k = \mu(p_k - p_k^*), \]
\[ \frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}) = 0, \]
\[ \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = 0, \]
\[ \frac{\partial \alpha_k \rho_k e_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k e_k \mathbf{u}) + \alpha_k p_k \nabla \cdot \mathbf{u} = -\mu p'_1(p_k - p_k^*), \]
\[ \frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + p) \mathbf{u}] = 0, \]  

where
\[ p = \sum_k \alpha_k p_k. \]  

The interfacial pressure is defined by Eq. (5), and the entropy equations are given by
\[ \frac{\partial \alpha_k \rho_k s_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k s_k \mathbf{u}) = \mu(p_k - p_k^*) \frac{Z_k}{Z_k + Z_k^*}. \]  

In this formulation, the volume fraction corresponds to a simple transport equation with relaxation, for which there is no difficulty to preserve volume fraction positivity. Another advantage of this model is that it exhibits a mixture sound speed, \( c_f \), defined as,
\[ \rho c_f^2 = \sum_k \rho_k c_k^2, \]
that is monotonic with respect to the volume fraction, contrarily to the previous model. This monotonic behavior simplifies the construction of numerical methods and respects better wave propagation in diffuse interfaces.

With this method, the internal energies are just used to determine the volume fractions at the end of the pressure relaxation process. The difficulties related to the presence of non-conservative terms in these equations are of minor importance. Indeed, the slight deviations a given numerical approximation of these non-conservative terms can produce compared to another one results in little change in the volume fraction computation at pressure equilibrium. This volume fraction is then used in the mixture equation of state \( p = p(\rho, e, \alpha_k) \) that uses the mixture internal energy as argument, and not those of the phases. The mixture internal energy is deduced from the (conservative) total energy equation. Then, from this mixture pressure \( p \), the phase’s internal energies are reset with they equations of state \( e_k = e_k(p, \rho_k) \), removing possible skid effect related to non-conservative terms. Thanks to these successive corrections numerical computations even in extreme conditions have shown perfect convergence to exact solutions for interface computations, separating (nearly pure) fluids.

2.4. Inclusion of additional physics

The previous formulations can be enhanced to include several important physical effects, such as surface tension and phase change.
2.4.1. Surface tension. Following Brackbill et al. [1992], the surface tension can be modeled as a body force, defined by

\[ F_\sigma = -\sigma \kappa \nabla Y_k \]

where \( Y_k = \frac{\alpha_k \rho_k}{\rho} \) denotes the mass fraction of one of the phases (liquid or gas), \([Y_k]\) is the mass fraction jump across the interface, \(\kappa\) represents (twice the mean) curvature of the interface, and \(\sigma\) is the surface tension coefficient, which is assumed constant here. Thanks to this formulation of capillary effects, the Kapila model can be extended [Perigaud and Saurel 2005] by adding to the momentum and energy equations the capillary force and power, respectively, and by attaching one equation for the mass fraction of one of the phases, giving

\[ \frac{\partial \alpha_k}{\partial t} + \mathbf{u} \cdot \nabla \alpha_k = \beta_k \nabla \cdot \mathbf{u}, \]

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \]

\[ \frac{\partial \rho Y_j}{\partial t} + \nabla \cdot (\rho Y_j \mathbf{u}) = 0, \]

\[ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = -\sigma \kappa \nabla Y_j, \]

\[ \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E + p) \mathbf{u} = -\sigma \kappa \mathbf{u} \cdot \nabla Y_j, \]

where \(j = 1\) or \(2\) (but not both since \(\sum_k Y_k = 1\)) and \(\kappa = \nabla \cdot \frac{\nabla Y_j}{|\nabla Y_j|}\). Eq. (16) can also be rewritten in conservation form, according to

\[ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \nabla \cdot (\sigma \mathbf{W}), \]

\[ \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E + p) \mathbf{u} = \nabla \cdot (\sigma \mathbf{W} \cdot \mathbf{u}), \]

where

\[ \mathbf{W} = |\nabla Y_j| \mathbf{I} - \frac{\nabla Y_j \otimes \nabla Y_j}{|\nabla Y_j|}, \quad \rho \tilde{E} = \rho E + \sigma |\nabla Y_j|. \]

Above, the total energy \(E\) is still given by the definition used in the Kapila model.

It worth remarking that there are some differences between the present formulation and the second-gradient formulation of Cahn and Hilliard [1958]. First, the current thermodynamics is independent of capillary effects, by construction. Second, the conservative formulation in momentum and energy guarantees correct pressure jumps at interfaces, independently of mesh resolution.

2.4.2. Phase change. Phase transition can be considered as well by adding Gibbs free energy relaxation effects to the mass and volume fraction equations, according to

\[ \frac{\partial \alpha_k}{\partial t} + \mathbf{u} \cdot \nabla \alpha_k = \beta_k \nabla \cdot \mathbf{u} + \frac{\rho}{\rho^*} \nu (g_k^* - g_k), \]

\[ \frac{\partial \rho Y_j}{\partial t} + \nabla \cdot (\rho Y_j \mathbf{u}) = \rho \nu (g_j^* - g_j), \]

where \(g_k = h_k - T_k s_k\) denotes the Gibbs free energy of phase \(k\) and \(\nu\) denotes the evaporation/condensation kinetic rate. To close the system of equations, appropriate convex EOS are used for each phase, and their variation in space and time. The interface density

\( \rho I \) is

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that appears in the volume fraction equation has been determined in [Saurel et al. 2008], and it is given by

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

To complete the formulation the relaxation parameter \( \nu \) has to be specified. When dealing with two-phase mixtures, bubbly and droplet flows for example, the specific interfacial area must be known and a subscale model, based on local saturation condition, and both heat and mass diffusion enables determination of the parameter \( \nu \); details can be found in Abramzon and Sirignano [1989] and Furfaro and Saurel [2016]. The local saturation condition, \( p = p_{\text{sat}}(T) \) consequence of \( g_1(T,p) = g_2(T,p) \) is anyway valid in almost all situations of liquid-vapor interfaces. Therefore, when dealing with resolved interfaces, local thermodynamic equilibrium is enforced taking \( \nu \to \infty \). Such treatment is simple and accurate enough to determine the amount of liquid and vapor at saturation when the energy needed for phase change is already present in the liquid. This is the case of cavitating and flashing flows, as discussed for example in [Saurel et al. 2016]. A method to deal with stiff phase transition \( (\nu \to \infty) \) will be summarized in the numerical section.

2.4.3. Boiling flows. When dealing with boiling flows, extra physics is needed as the energy responsible for phase change is not present initially in the liquid but comes from external boundaries. Adding heat diffusion and buoyancy renders the model appropriate for the computation of boiling flows. However, when heat diffusion is considered, temperature becomes continuous at interfaces, contrarily to interfaces with simple mechanical contact. The previous formulations, involving two temperatures may be reduced to a single temperature model, which is easier to solve since the non-conservative volume fraction equation vanishes. The formulation uses Eq. (20) and considers gravity and heat conduction effects in the momentum and energy equations [Le Martelot et al. 2014], resulting in

\[ \begin{align*}
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u) + \nabla p - \nabla \cdot (\sigma W) &= \rho g, \\
\frac{\partial \rho \tilde{E}}{\partial t} + \nabla \cdot [(\rho \tilde{E} + p) u] - \nabla \cdot (\sigma W \cdot u + \lambda_c \nabla T) &= \rho g \cdot u,
\end{align*} \]

where \( g \) denotes the gravity acceleration vector and \( \lambda_c = \alpha_1 \lambda_1 + \alpha_2 \lambda_2 \) represents the mixture thermal conductivity. This system is closed by the mixture EOS

\[ p(\rho, e, Y_1) = \frac{A_1 + A_2 - (P_{\infty,1} + P_{\infty,2})}{2} + \sqrt{\frac{1}{4} (A_2 - A_1 - (P_{\infty,2} - P_{\infty,1}))^2 + A_1 A_2} \]  

(22)

where \( A_k = \frac{Y_k (\gamma_k - 1) C_v, k}{Y_{1,C_v,1} + Y_{2,C_v,2}} [\rho(e - q) - P_{\infty,k}] \) and \( q = Y_1 q_1 + Y_2 q_2 \). This EOS is derived from mixture density and internal energy definitions under the constraints of equal pressures and equal temperatures. One can verify that System (20) is hyperbolic and it posses the entropy equation,

\[ \frac{\partial \rho s}{\partial t} + \nabla \cdot \left( \rho s u - \lambda_c \frac{1}{T} \nabla T \right) = \frac{\rho \nu (g_2 - g_1)^2}{T} + \lambda_c \frac{(\nabla T)^2}{T^2}, \]

(23)

which is in agreement with the second law of thermodynamics.
3. NUMERICAL METHODS

The mathematical structure of the previous formulations can be described according to the following generic representation,

\[
\frac{\partial Q}{\partial t} + \nabla \cdot F(Q) + B(Q) \cdot \nabla Q = S(Q),
\]  

(24)

where \(Q\) denotes the vector of evolution variables (conserved and not conserved), \(F\) is a flux function, \(B\) denotes the advection matrix of all differential terms that cannot be written in conservation form; i.e., not in \(F\); and \(S\) is a source. In some of the previous formulations \(B\) or \(S\) may be identically zero. It is assumed here that all intermediate quantities, such as \(u_I, u_I', p_I, p_I', \lambda, \mu\), etc., are expressed as functions of \(Q\) and eliminated from the list of dependent variables, in order for us to retain only the evolution fields.

The most accepted method to solve Eq. (24) for compressible two-phase flows is the finite volume method (FVM). The FVM has proven to be a robust and reliable numerical approach for the simulation of compressible flows in the presence of shock wave interactions. The basis of the finite volume method is discussed in detail in standard references [LeVeque 2002, Toro 2009]. The starting point is a decomposition of the computational domain \(\Omega\) into disjoint cells \(C_i\), which may be associated with a structured or unstructured grid, and to perform integration of Eq. (24) along each cell and over the interval of time advancement, \(\Delta t = t^{n+1} - t^n\), where \(t^n\) denotes the times at which the solution is calculated, resulting in

\[
Q_i^{n+1} = Q_i^n - \frac{1}{V(C_i)} \int_{t^n}^{t^{n+1}} \int_{\partial C_i} F(Q) \cdot n \, dS dt - \frac{1}{V(C_i)} \int_{t^n}^{t^{n+1}} \int_{C_i} B(Q) \cdot \nabla Q \, dx dt + \frac{1}{V(C_i)} \int_{t^n}^{t^{n+1}} \int_{C_i} S(Q) \, dx dt.
\]  

(25)

where

\[
Q_i^n = \frac{1}{V(C_i)} \int_{C_i} Q(x, t^n) \, dx,
\]  

(26)

with \(V(C_i)\) denoting the volume and \(\partial C_i\) the surface of cell \(C_i\), respectively. The solution strategy usually employed to completely define Eq. (25) uses operator splitting techniques [Glowinski et al. 2010] according to which the flux, the non-conservative, and the source integrals are determined sequentially, independently of each other (care must be used if higher than first-order in time accuracy is desired). The flux term, second in the right-hand side of Eq. (25), can be obtained by the Godunov (flux difference splitting) or the Boltzmann (flux vector splitting) method. The details of each of these approaches are beyond this review since they can be found in standard books on FVM [LeVeque 2002, Toro 2009]. The general strategy is typically:

i. Use \(\bar{Q}_i^n\) to reconstruct \(Q(x, t^n)\) in each cell.

ii. Solve exact or approximate Riemann problems at the faces of the computational cells (ignore sources), often with the HLLC solver [Toro et al. 1994] since Eq. (13) involves only 3 waves.

iii. Determine fluxes and non-conservative product contributions, perform the integrals in Eq. (25), and advance to \(Q_i^n\) by a Godunov-type method (or higher order variant).

iv. Explicit integration of the source contribution (when present) from \(Q_i^n\) to \(Q_i^{n+1}\).
typically assuming

\[
\frac{1}{V(C_i)} \int_{t^n}^{t^{n+1}} \int_{C_i} S(Q) \, dx \, dt \approx \int_{t^n}^{t^{n+1}} S(\bar{Q}(t)) \, dt.
\] (27)

A difficult challenge in the simulation of compressible two-phase flows in the presence of shocks or discontinuities is the non-conservative term, third term in the right-hand side of Eq. (25). For Godunov-type methods based on Riemann problem solutions, the structure of the solution is determined by both \( F \) and \( B \); i.e., operator splitting cannot be used safely. The non-conservative structure precludes the unique determination of wave speeds and additional kinematic conditions must be attached to the formulation, see DalMaso et al. [1995]. Only when shocks are not present one can resort to the operator splitting method and discretize the non-conservative integral directly. Next, we describe the general computational aspects that are pertinent to the different models.

### 3.1. Methods for BN-type models

BN-type models are perhaps the most delicate systems to solve among those presented above; addressing interface motion is not simple. They are of particular interest when velocity and temperature disequilibrium are present. The Riemann problem has up to 6 or 7 wave speeds, depending on the variants of the formulation, rendering its solution intricate. In addition, many non-conservative terms are present and the evolution of the non-conservative volume fraction cell average has no physical sense in the presence of discontinuities. Several approaches have been developed and improved over the years to address these difficulties. Saurel and Abgrall [1999a] constructed a Godunov-type method for these equations, in conjunction with a treatment of non-conservative terms, that preserves mechanical equilibrium at interfaces. Stiff pressure and velocity relaxation solvers were developed in the same reference to ensure interface conditions of equal pressures and normal velocities, allowing the model to deal with diffuse interfaces. Abgrall and Saurel [2003] introduced two improvements. First, the 7 waves present in the flow model are considered through a composite two-phase Riemann solver, made of several Riemann solvers for the Euler equations. Second, the non-conservative terms are solved accurately by enforcing that a local diffraction occurs each time a non-linear wave (shock or expansion) interacts with an interface, rendering both pressure and velocity locally constant, precisely at the location where the volume fraction is discontinuous. Thanks to this diffraction process, computed with the help of a Riemann solver for the Euler equations, the various non-conservative products are computed unambiguously. The only remaining issue is the interpretation of the volume fraction cell average at shocks. Saurel et al. [2007a] and Petitpas et al. [2007] studied this problem further but a general solution is still lacking. Tokareva and Toro [2010] and Furfaro and Saurel [2015] have proposed methods that use the HLLC-type Riemann solver including non-conservative products while Dumbser et al. [2010] and Franquet and Perrier [2012] developed discontinuous Galerkin methods for the BN model. The methods that follow consider flow models with a single velocity, more specific to interface computations.

### 3.2. Methods for the Kapila model and its variants

The flow model of Kapila is particularly interesting to compute interfaces separating fluids. It also has the ability to create interfaces dynamically. This capability is...
of the non-conservative term in the right-hand side of the volume fraction equation. The velocity divergence term, when positive, results in subscale bubble growth, resulting in the appearance of macroscopic interfaces (gas cavities for example). However, this model has two important numerical difficulties. First, under some conditions, the non-conservative divergence terms just mentioned may produce negative volume fractions, resulting in immediate simulation failure. Second, the manner by which shock energy is partition among various interfaces may be ambiguous. The first issue has been addressed in Saurel et al. [2009] with the pressure non-equilibrium formulation that replaces the non-conservative term in the volume fraction equation by a relaxation one. This is achieved at the price of the insertion of extra energy equations, to compute pressure imbalance. The method of this last reference fits in the frame of Eq. (25) where a specific HLLC-type Riemann solver is built based on the sound speed reported with the PNE model. The hyperbolic step is followed by a pressure relaxation to reach the equilibrium pressure of the mixture. The method is simple and very robust, even in extreme flow conditions. Another issue is related to shock relations for the Kapila model. Such relations are needed when a shock propagates in a two-phase mixture, not when the interface separates two pure (or nearly pure) fluids. In the single phase limit, as the model tends to the Euler equations, correct shock dynamics is computed in the nearly pure phase. Difficulties arise when the two phases are in non negligible proportions, such as for example in solid alloys, composite materials, granular mixtures. In the weak shock limit such relations have been obtained Saurel et al. [2007b]. Their validity for strong shocks has been then checked against all available experiments in the literature in the same reference, showing good agreement. The corresponding system of jump relations reads,

\[
Y_k = Y^0_k, \quad \rho(u - \Sigma) = \rho^0(u^0 - \Sigma) = m, \quad p - p^0 + m^2(v - v^0) = 0, \quad e_k - e^0_k + \frac{p + p^0}{2}(v_k - v^0_k) = 0,
\]

(28)

where \(\Sigma\) is the shock speed and \(v = \frac{1}{\rho}\) the specific volume. Variables with superscript 0 denote the state upstream of the shock.

Riemann solver building with Eq. (28) has been done in Petitpas et al. [2007]. But imposing the shocked state is a given unsteady computation is challenging. Indeed, cell average of the volume fraction produce skid effects and the (strong) shock becomes a succession of weak shocks. A method based on artificial heat exchanges among the phases to partition correctly the shock energy among the phases was derived in Saurel et al. [2009]. Another method, simpler and more general was derived in Petitpas et al. [2009] and relies on extra transport equations relative to the Hugoniot pole:

\[
\frac{\partial p_0}{\partial t} + \mathbf{u} \cdot \nabla p_0 = 0, \quad \frac{\partial v^0_k}{\partial t} + \mathbf{u} \cdot \nabla v^0_k = 0.
\]

(29)

These pole coordinates are used in the energy jump relation \(e_k - e^0_k + \frac{p + p^0}{2}(v_k - v^0_k) = 0\) that are directly used in the pressure relaxation solver. Indeed, a pressure relaxation solver consists in the resolution of the following system:

\[
e_k(p, v_k) - e^0_k(p^0_k, v^0_k) + \tilde{p}(v_k - v^0_k) = 0, \quad k = 1, 2,
\]

with \(\alpha_1 + \alpha_2 = 1\), where \(\tilde{p} = p (\text{the relaxed pressure})\) at any current point and \(\tilde{p} = \frac{p + p^0}{2}\) inside the shock layer that need detection with the PNE flow model. The partition formula
are given in Petitpas et al. [2009]. This method has however an important limitation, as the considered shock must propagate in a uniform mixture. Imposing given shock conditions in these non-conservative flow model with general initial conditions is still an open research area. But it is not a limitation for the computation of flows with interfaces with (nearly) pure fluids.

### 3.3. Methods for models in both temperature and pressure equilibrium

These models are the ones used to model cavitating and boiling flows. As an extra equilibrium condition is added (temperature equilibrium) one of the partial differential equation vanishes and the best option is to remove the volume fraction equation that is non-conservative. The flow model now involves 4 partial differential equations (two masses, one mixture momentum and one mixture energy equation) and is fully conservative and hyperbolic. Excepting surface tension terms that need special care as discussed later, the numerical approximation of this flow model is straightforward. The HLLC Riemann solver is recommended and is used with the wave’s speeds of the Kapila model, that are easier to compute than that of the temperature-pressure equilibrium (TPE) model. As these wave speeds are greater than that of the TPE model, better stability and robustness is obtained in the computations. Details of the overall algorithm are given in Saurel et al. [2016]. We now address extra physics computations.

### 3.4. Approach for phase transition

For given mass and energy of a two-phase mixture, in both temperature and pressure equilibrium, equal phases Gibbs free energy,

\[
g_1(T, p) = g_2(T, p),
\]

where \(g_k\) denotes the free energy of species \(k\), provides enough information to determine the thermodynamic state and concentrations [Le Metayer et al. 2013], by solving the non-linear system

\[
\begin{align*}
v_{\text{mix}} &= Y_1 v_1(T, p) + (1 - Y_1) v_2(T, p), \\
e_{\text{mix}} &= Y_1 e_1(T, p) + (1 - Y_1) e_2(T, p).
\end{align*}
\]

Eq. (30) is equivalent to \(p = p_{\text{sat}}(T)\) or \(T = T_{\text{sat}}(p)\) which reduces the previous system to

\[
\begin{align*}
v_{\text{mix}} &= Y_1 v_{\text{sat}}(p) + (1 - Y_1) v_{2\text{sat}}(p), \\
e_{\text{mix}} &= Y_1 e_{\text{sat}}(p) + (1 - Y_1) e_{2\text{sat}}(p).
\end{align*}
\]

This system involves two unknowns, \(p\) and \(Y_1\) and it is simple to solve unless the state crosses the phase diagram boundaries into one of the single phases. Rather than solving this non-linear system a particularly simple and robust alternative method has been proposed in [Chiapolino et al. 2016]. It is based on a Minmod type procedure applied to the mass transfer source term of Eq. (20) expressed equivalently as,

\[
\frac{\partial \rho Y_1}{\partial t} + \nabla \cdot (\rho Y_1 \mathbf{u}) = \rho \nu (Y_1^* - Y_1)
\]

where \(Y_1^*\) denotes the mass fraction at thermodynamic equilibrium and \(\nu\) a relaxation parameter that tends to infinity. From the definition given in Eq. (32), the following
estimates of the mass fraction at equilibrium are determined,

\[ Y_{1m}^\epsilon = \frac{v_{\text{mix}}^\epsilon - v_{\text{sat}}^2}{v_{\text{sat}}^1 - v_{\text{sat}}^2}, \quad Y_{1e}^\epsilon = \frac{e_{\text{mix}}^\epsilon - e_{\text{sat}}^2}{e_{\text{sat}}^1 - e_{\text{sat}}^2}. \] (34)

The variations between the current local mass fraction are computed as \( \delta Y_{1m}^\epsilon = Y_{1m}^\epsilon - Y_1 \) and \( \delta Y_{1e}^\epsilon = Y_{1e}^\epsilon - Y_1 \). These two variations may have the same sign or opposite sign and their product, \( \chi = \delta Y_{1m}^\epsilon \delta Y_{1e}^\epsilon \), can be used to estimate the mass fraction at equilibrium, by

\[ Y_1^* = \begin{cases} Y_1, & \text{if } \chi < 0, \\ Y_1 + \text{sgn}(\delta Y_{1m}^\epsilon) \min(|\delta Y_{1m}^\epsilon|, |\delta Y_{1e}^\epsilon|), & \text{otherwise.} \end{cases} \] (35)

The mass fraction \( Y_1 \) is then set to the equilibrium estimate value \( Y_1^* \). This method is particularly simple to manage at single phase bounds, or when the state evolves from two-phase to single phase, crossing the saturation dome bounds. Extension to multicomponent gas mixtures is given in [Chiapolino et al. 2017a].

### 3.5. Controlling the thickness of diffuse interfaces

Diffuse interface methods based on the models presented formerly are simple and efficient in a wide range of complex flow situations, even at high pressure, temperature, and velocity conditions. However, their numerical implementation with shock/interface capturing numerical methods tends to produce solutions that exhibit excessive numerical diffusion. This can be seen clearly in low-speed transient conditions. Several approaches have been developed to alleviate this weakness. Here, we highlight some of the solutions that have been used successfully to prevent the artificial smearing of contact interfaces by capturing methods in resolved interface simulations. For simplicity, we refer to \( \alpha_k \) as \( \phi \) below, unless stated otherwise, and consider the behavior of the volume fraction governing equation surrounding an interface, that is usually detected by requiring that

\[ \phi(1 - \phi) > \epsilon, \]

where \( \epsilon \) is chosen typically in the range \( 10^{-2} \) to \( 10^{-4} \).

#### 3.5.1. Interface compression technique

The idea behind the compression technique is to modify the volume fraction equation (here for the Euler model) as follows

\[ \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \mathcal{U}_o \mathbf{n} \cdot \nabla \left[ \epsilon_h |\nabla \phi| - \phi(1 - \phi) \right], \] (36)

where \( \mathcal{U}_o \) is a mobility parameter, usually taken to be large with respect to the characteristic speeds in the flow, \( \epsilon_h \) is a lengthscale that defines the desired thickness of the interface, that should be chosen larger than the grid spacing, and \( \mathbf{n} = \nabla \phi / |\nabla \phi| \) denotes the local normal vector of the interface. The term in the right-hand side of Eq. (36) dominates when \( \mathcal{U}_o \) is large and drives the profiles of \( \phi \) to the equilibrium profile, defined by the vanishing of the term in square brackets in Eq. (36), given by

\[ \phi = \frac{1}{2} \left[ 1 + \tanh \left( \frac{n}{2\epsilon_h} \right) \right], \]

where \( n \) denotes a normal coordinate across the interface. This idea was first proposed by Olsson et al. [2007] in the context of incompressible flows, and extended by Gresho et al. [1984]
Figures 2 and 3 illustrate the effects of interface compression and sharpening on the simulation of shock-bubble interactions. Figure 2 shows the volume fraction comparison between simulations without (left) and with (right) interface compression, using the same resolution. The shock traveled from left to right. Improvements in the solution with compression are evident. Figure 3 presents a density comparison with and without interface sharpening, also using the same resolution and showing the shock traveling from left to right.

To compressible flow and thermodynamic consistency, the Kapila model was extended to the Kapila model by Tiwari et al. [2013]. Figure 2 demonstrates a shock in water, generated by a region of 40 MPa overpressure, interacting with an air cavity without and with interface compression [Shukla et al. 2010]. Improvements in the solution with interface compression are self-explanatory. The compression terms were discretized with a second-order centered scheme. Efficient techniques to solve the volume fraction equation with compression for large $U_o$ are discussed in Shukla [2014].

**3.5.2. Interface sharpening technique.** The second method is also an Eulerian sharpening algorithm referred to as the tangent of hyperbola for interface capturing (THINC), see Shyue and Xiao [2014]. This technique was first applied to the Allaire et al. [2002] model.
The key idea of this method is to replace the linear reconstruction of \( \phi(x) \) from the cell-averaged \( \bar{\phi}(x) \), used in second-order MUSCL-type methods, by a non-linear reconstruction of the form

\[
\phi(x) = \frac{1}{2} \left( 1 + \tanh \left[ \beta \left( \frac{x - x_{i-1/2}}{\Delta x} - \bar{x}_o \right) \right] \right),
\]

here exemplified for a one-dimensional arrangement in the cell \([x_{i-1/2}, x_{i+1/2}]\) with \( \bar{\phi}_i \) increasing in the positive \( x \) direction, where \( \bar{x}_o \) is the unknown location of the interface and \( \beta \approx 2 \) a user parameter. Imposing the conservation constraint

\[
\bar{\phi}_i = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \phi(x) dx,
\]

on the cell \( C_i \) with \( \Delta x = x_{i+1/2} - x_{i-1/2} \) and inverting for the unknown \( \bar{x}_o \), we have

\[
\bar{x}_o = \tanh^{-1} \left[ \alpha - \delta \exp(\beta(2\bar{\phi}_i - 1)) \right],
\]

where \( \alpha = (\tanh \beta)^{-1} \) and \( \delta = (\sinh \beta)^{-1} \). Once \( \bar{x}_o \) is known, \( \phi(x) \) can be evaluated at any \( x \) from Eq. (37), as required by the construction of numerical fluxes. This carries over transparently to high-order methods. An example of the method applied to a Mach 1.22 shock wave traveling over an R22 gas bubble.

### 3.5.3. TVD limiter technique

A third method recently developed to address excessive numerical diffusion in unstructured meshes is discussed in Chiapolino et al. [2017b]. This method can be extended to an arbitrary number of fluid components and it is based on the MUSCL reconstruction scheme applied to Eq. (13). First, the limiter function of all fields is set to zero and second, a first-order TVD limiter is used for \( \phi \). Figure 4 shows the classical representation of the limiter function as a function of the slope ratio \( r \), see LeVeque [2002] for reference discussion about limiters. The approach is unusual with MUSCL type schemes where gradient limiters always belong to the second-order TVD region. The limiter used for volume fraction computation resides in part outside the second-order region and consequently it is inappropriate for smooth flows, but it behaves well for discontinuous fields, such as the volume fraction at interfaces. Results from an example simulation is shown in Figure 5 for a Mach 1.5 shock interacting with Krypton-air bubble in an unstructured mesh.
3.6. Numerical anisotropy

The methods described in previous sections can be used in conjunction with structured or unstructured grids and for problems concerned with mixtures or resolved interfaces. In addition, one can use the formulations discussed earlier for simulations of coarse (engineering) or fine (research) level of detail or complexity. If one is interested in highly-accurate simulations, specially for resolved interfaces, it is desirable to employ advanced numerical methods. This pertains to low numerical dissipation but also to low phase errors and low geometrical anisotropy errors because the flows of interest here can quickly become geometrically complex. Preserving geometrical detail in these simulations is helped by minimizing numerical anisotropy (the imprint of the grid). This can be accomplished by the use of a triangle-based mesh. The interesting point to outline is the difference between computed results with Superbee (left) and the new “Overbee” limiter (right); the latter showing clear improvements. When time evolves, the solution with Superbee becomes more and more diffused, while that obtained with the Overbee limiter remains resolved.
Figure 7
Computation of a liquid oxygen fragmentation by a coaxial hydrogen gaseous flow in conditions of cryotechnic engines combustion restart. Computed mass fraction contours with and without phase change. Details are given in [Chiapolino et al. 2017a].

of approximately isotropic discretization methods, see the wave propagation method [Bale et al. 2002], or simply by utilizing high-order methods. For example, figure 6 shows a comparison of two spherical bubble collapse simulations with the same mesh and with a low- and high-order numerical method (second order HLLC and 5th-order WENO, respectively). Here, an initially spherical bubble residing in a Cartesian cubic mesh implodes due to higher pressure outside the bubble and the results shown correspond to the time when the bubble reached minimum size, see Tiwari et al. [2013] for details. Evidently, the high-order method preserves the sphericity of the bubble much better.

4. SOME RECENT RESULTS
To illustrate capabilities of diffuse interface methods several computational results are shown with various physics.

Interfaces with phase change The flow model of the section on boiling flows is considered in the absence of gravity and surface tension for the computation of an oxygen liquid jet atomisation with a coaxial hydrogen gas flow. Such situation is representative of fuel injection systems in cryotechnic combustion chambers of space launchers. Computed results shown in the Figure 8 compare the effects of phase change on the liquid oxygen dynamics.

The same flow model is considered in the presence of both gravity and surface tension effects to deal with DNS-like simulation of boiling flows. As the flow evolves in low Mach number conditions, simple time integration methods are adopted. In that.
Figure 8
Computed boiling flow with a liquid initially at saturation and containing three nucleation sites. Constant and uniform heat flux is imposed at the bottom wall. Vapour mass fraction contours are shown at times 0, 50, 100, 200, 300 and 400 ms. Similar results are obtained when the initial condition is free of nucleation sites. Details are given in Le Martelot et al. [2014].

Solid-fluid interfaces The Kapila model and its pressure non-equilibrium variant can be extended to hyperelastic materials following Favrie et al. [2009]. Extra equations are obviously needed to express the stress tensor present in solids. Plastic transition can be considered as well following Ndanou et al. [2015]. The Kapila model enables dynamic interfaces appearance in fluids, as a consequence of pressure relaxation effects. When this capability is combined with plastic transition it results in dynamic fragmentation and crack propagation. An example is shown in Figure 9 with the impact of a solid projectile at high speed on a solid plate.

Bubble clouds (Adams and Komoutsakos, Carlos)
Tiwari et al. [2015]
Shocks bubbles (Colonius)
5. FUTURE RESEARCH DIRECTIONS

Diffuse interface formulations have shown important progresses and a growing range of capabilities in the last two decades. Nevertheless, many fundamental research issues are still outstanding and further progresses is desirable. We mention here some of the important outstanding topics that deserve attention, in our opinion.

- While a lot of progress has been accomplished, a complete resolution of the ‘best’ treatment of non-conservative terms in the governing equations of diffused interface methods would be desirable. In particular, an understanding of which method(s) lead to converged solutions, not only in one dimensional problems but also in multiple dimensions. For example, it is hard to impose at the discrete level a given system of shock relations. This is a challenging problem that is compound by the potential nonlinearities present in the equations of state, which may complicate the stability of existing methods.
- A comparative analysis of which sharpening/compression method produces the best results, and what are the conditions of enhanced formation for each method.
works best in different circumstances.

- The development of robust solvers for flows at extreme high and low densities. For example, robust and realizable methods for the study of interactions of two-phase flow with strong shocks, high Mach numbers, shock/shock interactions, near vacuum conditions (cavitation), etc.

- The improvement of methods for low Mach number flows. This requires development of efficient preconditioning techniques for two-phase DNS-like flow simulations.

- The development of simple and well-posed (convex) equations of state to deal with phase change. Since diffuse interface models are hyperbolic, cubic equations of state have to be reconsidered, modified, and simplified to be inserted in the various relaxation solvers (for mechanical and thermodynamical equilibrium).

- Extension of the existing methods to more sophisticated fluids, such as non-Newtonian materials, elastic-plastic fluids with damage.

- Finally, there is a growing need to develop well-defined test problems where validation of the numerical methods can be performed. For example, it is not routine in two-phase flow simulation to carry out convergence studies of the solution as the grid is refined in two- and three-dimensional problems. This does not only happen because the simulations can be computationally challenging, but also because one needs well-posed problems that have unique solutions.

The outcome of this research is slowly, but steadily, producing research tools and methods that will inevitably lead to better understanding of compressible two-phase flow physics, from laminar to turbulent flows.

**DISCLOSURE STATEMENT**

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**Appendix: Equations of State**

A convenient equation of state used to model compressible fluids is the Noble-Abel stiffened gas (NASG) EOS, expressed as

\[ p_k = \left( \gamma_k - 1 \right) \rho_k \left( \frac{e_k - q_k}{1 - \rho_k b_k} \right) - \gamma_k p_{\infty,k}, \]  

where \( \gamma_k, p_{\infty,k} \) and \( b_k \) are characteristic of material \( k \) and \( q_k \) represents the reference energy of phase \( k \); details can be found in [Le Metayer and Saurel 2016]. This is a generalization of the well-known stiffened gas (SG) EOS to include covolume effects, i.e., short distance repulsive effects. The original SG EOS was extended for the unification through the
internal energy contribution and attractive effects through the term $-\gamma_k p_{\infty,k}$. All basic physical molecular effects are thus considered in the NASG formulation, resulting in an improved thermodynamic description of matter compared to SG. When two phases are present the corresponding mixture EOS is given by

$$p(\rho, e, \alpha_1) = \rho e - \left( \frac{\alpha_1 (1 - \rho_1 b_1) \gamma_1 p_{\infty,1}}{\gamma_1 - 1} + \frac{\alpha_2 (1 - \rho_2 b_2) \gamma_2 p_{\infty,2}}{\gamma_2 - 1} \right).$$

(41)

This mixture EOS is needed with the Kapila and the pressure non-equilibrium model.

**LITERATURE CITED**


