AIX-MARSEILLE UNIVERSITÉ

Laboratoire de Mécanique et d'Acoustique -UMR CNRS 7031-

THÈSE

pour obtenir le grade de DOCTEUR D'AIX-MARSEILLE UNIVERSITÉ

Discipline : Mécanique Énergétique École Doctorale 353 : Sciences pour l'Ingénieur présentée et soutenue publiquement

par

Alexandre CHIAPOLINO

le 18 Décembre 2018

QUELQUES CONTRIBUTIONS À LA MODÉLISATION ET SIMULATION NUMÉRIQUE DES ÉCOULEMENTS DIPHASIQUES COMPRESSIBLES

Some contributions to the theoretical modeling and numerical simulation of compressible two-phase flows

Directeur de thèse : Professeur Richard Saurel - LMA - Aix-Marseille Université

JURY

Rémi Abgrall,	Professeur des universités - Universität Zürich - Switzerland (Rapporteur)
Patrick Bontoux,	Directeur de Recherche CNRS - M2P2 - Aix-Marseille Université (Examinateur)
Bénédicte Cuenot,	Directrice de Recherche - CERFACS - Toulouse (Examinatrice)
Sébastien Ducruix,	Directeur de Recherche CNRS - EM2C Centrale Supélec - Université Paris-Saclay (Rapporteur)
Richard Saurel,	Professeur des universités - LMA - Aix-Marseille Université (Directeur)
Thomas Schmitt,	Chargé de Recherche CNRS - EM2C Centrale Supélec - Université Paris-Saclay (Examinateur)

 \grave{A} Serge Dusserre-Bresson

Acknowledgements

Je tiens à remercier le professeur Richard Saurel, non seulement pour son accueil dans son équipe, mais surtout pour m'avoir transmis sa passion pour la mécanique des fluides et la thermodynamique.

Richard a dirigé cette thèse pendant ces trois années. Il m'a laissé toute la liberté nécessaire à mon épanouissement personnel et scientifique, et a su rester disponible même lorsque d'autres obligations l'accaparaient. Pour tout ceci merci énormément.

J'exprime ma profonde reconnaissance envers les docteurs Jeaniffer Vides, François Fraysse, Damien Furfaro ainsi que les futurs docteurs Quentin Carmouze et Lucas David pour l'aide précieuse que j'ai pu trouver auprès d'eux durant cette aventure scientifique et humaine.

Je remercie Rémi Abgrall et Sébastien Ducruix, respectivement professeur et directeur de recherche, qui ont accepté de juger ce travail en tant que rapporteurs, ainsi que Bénédicte Cuenot, directrice de recherche, Patrick Bontoux, directeur de recherche, et Thomas Schmitt, chargé de recherche, qui ont accepté de participer au jury.

Merci également à Pierre Boivin, chargé de recherche, et au professeur Boniface Nkonga pour leur aide et leurs conseils avisés.

Enfin je souhaite remercier ma famille, ce travail est l'aboutissement d'un cursus universitaire que je n'aurai pas pu réaliser sans leur aide et leur soutien.

 $Ce\ travail\ de\ thèse\ a\ \acute{ete}\ financ\acute{e}\ par\ RS2N^1,\ par\ l'intermédiaire\ d'une\ bourse\ CIFRE.$

¹www.rs2n.eu

Contents

	Gen	neral introduction	1
Ι	Material interfaces		10
1	Sha	harpening diffuse interfaces with compressible fluids on unstructured meshes	
	1.1	Introduction	13
	1.2	Flow model	15
	1.3	Hyperbolic solver on unstructured meshes $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	21
	1.4	Gradient computation on unstructured meshes	24
	1.5	Development of a new limiter for Heaviside-type discontinuities	27
	1.6	Coupling with the diffuse interface formulation	41
	1.7	Validations	43
	1.8	Illustrations on unstructured meshes	47
	1.9	Conclusion	53
II	II Stiff phase transition phenomena 56		
2	\mathbf{A} si	mple and fast phase transition relaxation solver for compressible multicompo-	-
	nen	t two-phase flows	58
	2.1	Introduction	59
	2.2	Flow model	61
	2.3	Mixture equation of state	62
	2.4	Mixture speed of sound	64
	2.5	Phase transition model	65
	2.6	Thermochemical relaxation algorithm	68
	2.7	Extension to a multicomponent gas phase	72
	2.8	Extended thermodynamic closure	74

2.9	Phase transition model	3
2.10	Extended thermochemical relaxation algorithm	0
2.11	Algorithm's stability	4
2.12	Numerical results	5
2.13	Computational time, efficiency and simplicity	0
2.14	${\rm Multi-dimensional\ illustrations\ } \ldots $	1
2.15	Conclusion	6

III Equations of state

107

145

3	${\bf Extended\ Noble-Abel-Stiffened-Gas\ equation\ of\ state\ for\ sub-and-supercritical\ liquid-supercritical\ liquid-supercritical$		
	gas systems far from the critical point		
	3.1	Introduction	110
	3.2	Extended NASG EOS	112
	3.3	Saturation condition of the liquid-vapor couple $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	120
	3.4	Summary of the Extended NASG state functions	123
	3.5	Extended NASG parameters	124
	3.6	$Transition \ to \ supercritical \ fluids \ . \ . \ . \ . \ . \ . \ . \ . \ . \ $	128
	3.7	Two-phase flow illustrations	138
	3.8	Conclusion	144

IV Fluid dispersal at large scales

4	Mo	dels and methods for two-layer shallow water flows	147
	4.1	Introduction	148
	4.2	Hyperbolic two-layer shallow water model $\hdots \hdots \$	149
	4.3	Approximate Riemann solvers	155
	4.4	Results and validations	160
	4.5	Comparison of two-layer shallow water solutions versus two-dimensional two-fluid com-	
		putations	174
	4.6	Conclusion	181
	Gen	neral conclusion	182
Bi	Bibliography		184
Aj	Appendices 1		194

Appendix A Material interfaces		194
A.1	Sharpening contact discontinuities in single-phase flows	194
		100
Appen	dix B Stiff phase transition phenomena	196
B.1	Summary of the iterative algorithm computing phase transition between a liquid and a	
	multicomponent gas phase	196
Appendix C Equations of state 199		199
C.1	Convexity of the ENASG formulation	199
C.2	Maxwell's relations	201
C.3	Methodology to determine the various Extended NASG (ENASG) parameters	203
C.4	Connection temperature between the ENASG EOS and ideal gas formulation $\ . \ . \ .$	207
C.5	Towards the critical point	208
Appendix D Fluid dispersal at large scales 213		
D.1	Extended formulation with variable external pressure	213
A		91.0
Appen	Appendix ESummary21	
E.1	Résumé	216

General introduction

For several decades, two-phase flows have been a topic of rising interest within the scientific and industrial communities. This high degree of interest can be explained. The first reason is linked to the substantial development potential with regard to the high level of physics that two-phase flow models can take into account. Moreover in the current economic context, as industrial processes become more and more specific, the theoretical models developed in the past require nowadays important extensions and adaptations. Besides, the computing resources simultaneously booming, more massive and accurate numerical simulations can now be envisaged. Finally, two-phase flows are omnipresent in industry and in nature as well. In this context, the present thesis addresses compressible two-phase flow modeling in the frame of space, energy and safety areas.

The research work presented in this manuscript is highly linked to a continued need of scientific expertises destined to the above-mentioned industrial communities. Those possess indeed many applications involving a large range of highly transient physical phenomena, where the compressibility of the materials is of utmost importance. Within this framework, a fundamental and applied research has been developed with respect to the following research topics:

- Interface motion and related instabilities,
- Stiff evaporation and condensation phenomena,
- Equations of state for sub-and-supercritical liquid-gas systems,
- Dispersion of non-miscible fluids.

Those problematics are indeed present in many industrial situations. Knowledge of the involved physical phenomena is of paramount importance for the correct operating conditions of industrial systems and for safety purposes as well. In this context, the present thesis addresses the design of theoretical models and numerical methods to describe physical phenomena occurring in industrial systems more and more sophisticated.

The dynamics of interfaces, phase transition phenomena or the thermodynamics of liquid and gas phases as well as two-phase mixtures are part of the physics present within such multiphase flows. The present research work addresses these topics as well as gas dispersal computations involving large time and space scales.

Figure 1 illustrates a portion of such physics in an application reminiscent of multiphase flows evolving in cryotechnic rocket engines. Dimensioning combustion chambers and injection systems of cryotechnic engine of the space launching systems of Ariane 6 is of typical interest. In this Ph.D. thesis, this technical area is addressed through the ANR SUBSUPERJET project. This Ariane-6 launcher will be the first rocket engine able to be reignited multiple times while in space for commercial purposes, namely: dropping several satellites on distinct orbits. In such combustion chambers, intense phase change phenomena are expected as well as combustion of resulting gases. A temperature rise is naturally expected, resulting in supercritical flow conditions. However, the treatment of combustion reactions is out of the scope of the present manuscript.

This project involves three of the above-mentioned research thematics. Indeed, before the engine reaches supercritical conditions, the flow consists of a liquid oxygen jet surrounded by a high speed gaseous hydrogen flow. The entrance of the liquid jet into the combustion chamber obviously involves the dynamics of material interfaces that must be captured correctly by an appropriate numerical method. In addition, under such thermodynamic circumstances, those interfaces are expected to get evaporated and this phase transition is meant to play a significant role within the two-phase flow. Finally the thermodynamics of pure phases as well as mixtures, considered through appropriate equations of state, is of paramount importance and is also an important motivation for the present research work.

Sharpening diffuse interfaces

Part of this manuscript dwells in the extension of a theory partly initiated by the advisor of this thesis, Professor Richard Saurel. This theory addresses the treatment of interfaces between two fluids and two continuous media. Pioneering work in this direction was done with "Volume of Fluid" (VOF) methods (Hirt and Nichols (1981) [2]) in the frame of incompressible fluids. In this context, 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 subvolumes occupied by the phases and several mass balance equations. Later, extensions to compressible fluids were done in Saurel and Abgrall (1999) [3], [4] and Kapila et al. (2001) [5]. This approach often called "diffuse interface" is initially linked to the computation of mixture cells that hydrodynamic codes have to handle. Those mixture cells are inevitable because of the numerical dissipation, inherent to all numerical methods. In particular, they are responsible for many difficulties regarding the numerical resolution and can yield computational failures.

The main idea of the diffuse interface strategy is to consider numerical mixture cells as physical



Figure 1: Density $(kg.m^{-3}, top)$ and temperature (K, bottom) profiles of a liquid oxygen jet surrounded by vapor at high speed entering a combustion chamber of a cryotechnic rocket engine. Shear effects induce jet fragmentation. The filaments separating the main liquid core and the gas gradually vanish as a consequence of evaporation. Details are given in Chiapolino et al. (2017) [1]. In this situation, three research topics addressed in this Ph.D. thesis are illustrated. Material interfaces separating liquid oxygen and gas phase are present and subject to phase transition that modifies significantly the two-phase flow dynamics. In such circumstances, the thermodynamics of pure phases as well as the one of the two-phase mixture is essential. Since the two-phase flow is expected to result in a supercritical flow, an extension of the thermodynamics is consequently necessary. These research areas are addressed in Chapters 1, 2 and 3 while Chapter 4 deals with fluid dispersal situations involving much larger time and space scales.

multiphase mixtures, via an appropriate modeling method. The resulting hyperbolic system allows the resolution of each continuous medium as well as the interfacial zone via a unique system of partial deferential equations, solved in each numerical cell with the same numerical scheme (Saurel and Le Métayer (2001) [6]).

This approach yields some advantages. The most obvious relies on its coding simplicity as well as its robustness since the very same algorithm is used throughout the entire computational domain. Conservation is guaranteed for the mixture whereas conventional algorithms only guarantee mass conservation at best. Interface conditions are perfectly matched, even during the coupling of complex media in the presence of shock waves and mass transfer (evaporation, condensation, detonation, ...). Particularly, this approach is the only one able to describe the appearance of interfaces that would not be initially present as it is the case with cavitation or spallation phenomena.

In these references, a hyperbolic modeling approach where the phases are separate is developed. It is to say that each fluid possesses its own thermodynamics (thus its own equation of state) and its own system of equations. The satisfaction of the interface conditions is simultaneously ensured by relaxation processes and by the treatment of non-conservative terms present in the equations.

Over the last years, extra physics extensions have been addressed: chemical reactions [7], phase change [8], surface tension [9], solid-fluid [10], plastic transformation [11], to cite a few. Diffuse interface methods have shown their ability to address a wide range of difficult flow situations. However, progress is required at the level of numerical accuracy. Indeed, the main limitation of these diffuse interface methods is related to their excessive numerical diffusion. This unphysical dissipation is essential to the stability of those methods but is too often unreasonable, especially with long-time computations dealing with unstructured meshes. This last point is nonetheless crucial in view of the intended industrial problems. While diffuse interface methods allow to take into account physics increasingly richer, the excessive artificial diffusion is still present and may corrupt the computed results as their analyses are affected by this lingering liability.

This problematic is undertaken in Chapter 1 where a new, very simple but dramatically efficient, numerical method relying on diffuse interface models is proposed to control the artificial dissipation which remains essential in the frame of these methods. As it will be seen further, the simplicity and efficiency of diffuse interface models are kept but the quality of computed results is significantly improved at the price of slight but subtle code modifications.

This method can be placed in the framework of the "MUSCL" numerical method (Monotonic Upstream-centered Scheme for Conservation Laws) very used in production codes. In this framework, various efforts have been done in the direction of limitation or control of numerical smearing of contact discontinuities. For instance, Shyue and Xiao (2014) [12] examined a flux limiter combined with a hyperbolic tangent reconstruction. This technique was first applied to the Allaire et al. (2002) [13]

model. The key idea of this method is to replace the linear reconstruction of the volume fraction α from the cell-averaged $\bar{\alpha}_i$, used in second-order MUSCL-type methods, with a non-linear hyperbolic tangent reconstruction. This method provides excellent results on structured grids and its extension to unstructured meshes seems possible. It is an Eulerian-sharpening algorithm referred to as the tangent of hyperbola for interface capturing. However, this strategy seems inappropriate for flow computations involving more than two fluids. Additional efforts are consequently required in view of the intended industrial applications.

In this manuscript, an approach relying on the Total Variation Diminishing (TVD) limiter technique is considered. The TVD notion was first presented in the original work of Harten (1983) [14] who proposed this concept to characterize oscillation free schemes. In such context, the use of limiter functions is mandatory. Those are indeed essential to ensure that the numerical scheme maintains its TVD property and consequently remains stable. Later a graphical analysis was presented by Sweby (1984) [15], who defined the so-called first-order TVD area. In the same contribution Sweby completed the TVD theory by introducing the second-order TVD area that is actually delimited by the Superbee limiter function developed by Roe [16]. Most of the existing limiter functions lie inside the second-order TVD region, the first-order one (upper region) is inappropriate for continuous fields and shock waves.

However, only interfaces are of interest in Chapter 1. Those are Heaviside-type discontinuous fields and require thereby a specific attention. In this special context, the research work presented in the next chapter reconsiders the TVD region of interest. As it will be seen later, when dealing with Heaviside-type discontinuities only, the first-order TVD area (upper region) is this actual restriction of the Total Variation Diminishing theory.

This statement will be clarified in Chapter 1 where a new limiter named "Overbee" is created for the specific case of interfaces. Unlike conventional limiters, the "Overbee" function is a first-order TVD limiter and is the cornerstone of the sharpening method developed in the next chapter. In this context, the limiter function of all fields is set to zero in the interfacial zone with the exception of the volume fraction (Heaviside-type discontinuity) where the new "Overbee" limiter is used. This approach is unusual in the context of MUSCL-type schemes, where most of the existing gradient limiters belong to the second-order TVD region. As the new limiter goes beyond the second-order area, it is consequently inappropriate for smooth flows and shock waves but behaves very well for Heaviside-type discontinuous fields like the volume fraction at interfaces as seen in Chapter 1.

The resulting numerical method is able to deal with both structured and unstructured meshes, multiple interfaces and multiple fluids. Those last characteristics are essential in view of real industrial applications. This research work has been published in Chiapolino et al. (2017) [17].

Phase transition solvers

Under specific thermodynamic conditions, material interfaces may be subject to phase transition. Knowledge of phase change phenomena is essential for many applications and must be taken into account in computer codes in order to reproduce the desired effects.

Cryogenic flows in rocket engines are for instance characterized by their multiphase, unsteady and multidimensional aspects in addition to their reacting properties through phase change phenomena playing significant roles. In such configurations, the state of the fluid must be predicted, as well as the thermodynamic state in combustion chambers. In the present manuscript, this research topic is linked to the filling of those combustion chambers with a cryogenic fuel.

During the ignition stage (for which the engine has not yet reached supercritical conditions), the flow consists of a liquid oxygen (LOX) jet surrounded by a high-speed gaseous hydrogen (H₂) flow, injected in conditions above the saturation point of the inner oxygen core. The aim of this operation is to produce a combustion reaction (not addressed in this document) within the gas phase (H₂ and O_2). Gaseous oxygen is then needed but is initially absent in the chamber. Phase change from liquid oxygen to vapor is consequently required.

From a physics point of view, phase transition happens when one of the two phases (liquid or vapor) is said to be metastable. This denomination refers to a state involving a thermodynamical disequilibrium. This can happen,

- Either when a liquid is overheated. Such situations appear for example through heat exchanges with the gas, or through an expansion wave that lowers the saturation temperature of the liquid. In that case, the liquid evaporates and becomes saturated vapor.
- Or when a vapor species is subcooled. It is to say that the temperature becomes lower than the saturation temperature at the current pressure. In that case, the vapor condensates into a liquid at saturation. This situation can happen for instance through a shock wave, as the liquid's temperature barely varies whereas the saturation temperature increases. Condensation can also appear near walls if those are cooled.

When one of these conditions is satisfied, phase transition phenomena appear and are often of utmost importance for many industrial applications. In such circumstances, the equation of state must reproduce the behavior of each fluid (liquid and vapor), as well as the behavior of the two-phase mixture appearing in the so-called saturation dome. Furthermore, additional non-condensable gases are present in practical applications. Those do not react and do not have any reason *a priori* to be in thermodynamic equilibrium with the liquid-vapor couple but must be taken into account in the mixture equation of state as well. In this context, Chapter 2 focuses on the theoretical modeling and the numerical treatment of phase transition. In our approach, phase change at material interfaces is treated by an instantaneous relaxation process involving Gibbs free energies (Saurel et al. (2008) [18]). This consists in a non-linear algebraic system that is made from the equilibrium conditions (equality of the temperatures, pressures and free energies of the phases) and mixture mass and mixture energy definitions. Its resolution is non-trivial and may yield unstable computations, particularly when the final state gets out of the two-phase domain to join one of the pure phases. Besides, additional complexity is added to the system when non-condensable gases are present. This situation is however present in many practical applications. The most common way to compute such phase change situations is to directly solve the corresponding system via complex root-finding procedures, sometimes draining more CPU time than the flow computation itself. As such strategy may be detrimental to the computation, it motivates the introduction of a new relaxation method where the solution relaxes weakly (smoothly during time evolution) to the correct solution, on the basis of some estimates. This new method developed in Chapter 2 happens to be stable, accurate, fast and particularly simple to code. This work has been the subject of two publications in scientific journals, Chiapolino et al. (2017) [1], [19].

Construction of equations of state

Moreover, equations of state used to describe the thermodynamic behavior of the different phases have their own ranges of validity. In view of future industrial applications, extension of these ranges of validity is necessary. Several forms of equation of state (EOS) can be found in the literature (see Le Métayer (2003, 2013) [20], [21] for more details). Each form is more or less complex depending on the medium to represent and the transformations that may occur.

When envisioning the whole phase diagram presenting liquid, vapor and supercritical states, the most common thermodynamic option relies on cubic equations of state. Such type of thermodynamic modeling is particularly attractive as it involves all possible effects occurring in matter, namely: agitation, attraction and repulsion, with one unique formulation by foreseeing the transition from one state into another. Its particular interest for phase transition modeling relies on variable attractive effects responsible, at least qualitatively, for cohesion of liquids. Those effects vanish when the density becomes low. Cubic equations of state are thereby well-suited, at least in appearance, for the thermodynamic description of liquid, vapor and supercritical state as well. However, this type of thermodynamic modeling involves serious theoretical and numerical difficulties as listed in Chapter 3. Among these complexities, the loss of convexity within the two-phase region and consequently the loss of hyperbolicity of related flow models is a severe flaw of cubic equations of state.

The "philosophy" of diffuse interface methods relies on convex equations of state and hyperbolic systems. The convexity property is indeed essential both for theoretical and numerical points of view. The recent Noble-Abel-Stiffened-Gas (NASG) EOS (Le Métayer and Saurel (2016) [22]) is a wellposed formulation involving the three above-mentioned molecular forces of a fluid and is consequently appealing.

To address supercritical conditions, large temperature and pressure variation ranges are considered in Chapter 3. Nevertheless, the NASG EOS is only well-suited in a limited temperature range [22]. Wherefore, an extension of the NASG EOS is necessary in view of the intended industrial applications. A novel convex equation of state is consequently developed in Chapter 3 and presents an alternative to well-known cubic equations of state. The formulation is named ENASG with "E" standing for "Extended". With the ENASG description, attractive and repulsive effects depend on the temperature and the density respectively whereas the NASG equation of state considers these effects constant, restricting consequently its range of validity. This work has been published in Chiapolino and Saurel (2018) [23].

Large-scale dispersion

In another framework, Chapter 4 deals with fluid dispersal at both large time and space scales. Many situations may involve fluid dispersal in large urban or natural places after an important period of time. Consequently, this topic is of interest to the safety community as gas dispersal may yield severe consequences. Figure 2 illustrates circumstances of typical interest. In the present example, a cloud of chlorine is spread to the surrounding of the area of "La Défence" in Paris, France, due to the explosion of a TNT charge. At early times, the explosion stage is to be treated by an appropriate flow model such as the one presented in Hank et al. (2014) [24]. This Ph.D. thesis focuses on the dispersal of the resulting dense gases happening at much longer times. The evolution of dense gases is also of interest to the safety community as the gases spreading throughout large places may be dangerous chemical species.

This technical area motivates the design of a new two-layer shallow water type system. Indeed, in such context one of the difficulties is to address long-time computations involving large-scale numerical domains while providing accurate results at a reasonable cost in CPU time.

The two-layer shallow water strategy is consequently attractive as it allows to address 2D simulations to mimic 3D results. However, it also involves serious theoretical and numerical difficulties related to the conditional hyperbolicity of most mathematical systems and their non-conservative character.

This problematic is undertaken in Chapter 4 where a new strictly hyperbolic two-layer shallow water type model is developed. Pressure disequilibrium and fluid compressibility are responsible for its well-posedness. Its numerical resolution is treated as well through a HLL-type Riemann solver and provides an attractive alternative over conventional multi-fluid flow models to deal with fluid dispersal



Figure 2: Dispersion of a chlorine cloud spreading under gravity effects and weather conditions. In the present case, a mixture of air and chlorine was set to motion by the explosion of a TNT charge placed near the area of "La Défence" in Paris, France. The evolution of the resulting dense and toxic chlorine cloud is observed at t = 3.24 s after the detonation. Its spreading throughout the city at much larger periods of time is of interest to the safety community and motivates the work presented in Chapter 4. The present simulation is adapted with permission from Hank (2012) [25] (see also Hank et al. (2014) [24]).

computations involving large time and space scales. This work has also been valued by a scientific publication, Chiapolino and Saurel (2018) [26].

The overall contents of this manuscript may be of interest to "Computational Fluid Dynamics" (CFD) practitioners working on multiphase flows. At the cost of some repetitiveness, each chapter is almost self-contained and has plenty of cross-referencing, so that the reader may decide to start reading this manuscript in the middle or jump to the last chapter.

Part I

Material interfaces

Introduction

As their name suggests, diffuse interface methods rely on numerical diffusion. This artificial dissipation is essential to ensure robustness and stability of any flow computation where discontinuities are present. However, this numerical diffusion is often unreasonable, especially at long times and with unstructured-mesh computations.

Diffuse interface computations rely on discontinuity capturing (instead of "tracking" or "reconstruction") but progress is still needed to handle these interfaces with the minimum amount of points. In certain situations this may become pathologic, for instance if physical dissipation such as mass diffusion must be differentiated from numerical dissipation.

The following chapter attempts to provide an efficient method reducing the dissipation zone around interfaces while keeping simplicity and stability of diffuse interface methods. Phase transition is omitted and a multiphase flow formulation able to cope with interfaces of simple mechanical contact is considered.

Over the years several methods, more or less complex and efficient, have been developed to lower the numerical dissipation, inherent to all numerical methods. However, those are mainly devoted to Cartesian grids and to this day, there are no simple and efficient numerical methods able to deal with unstructured meshes and an arbitrary number of fluids. These characteristics are major features nonetheless, in view of real practical applications.

At the price of slight but subtle code modifications, a very simple, robust and efficient numerical method is developed in Chapter 1 and is able to deal with both structured and unstructured meshes, this property being very important. Besides, multiple interfaces and multiple fluids can be treated with the proposed method, this asset being significant as well. The method relies on a new flux limiter developed in the following chapter. This limiter is named "Overbee" and is a major asset for the numerical capture of interfaces.

For the sake of simplicity, the diffuse interface model of Saurel et al. (2009) [27] is used in the following chapter. As recalled further, Saurel et al.'s model is a two-phase flow formulation involving interfaces which simplifies the numerical resolution of the mechanical-equilibrium two-phase flow model of Kapila et al. (2001) [5]. However, the proposed method is not restricted to this specific formulation but can deal with any two-phase flow models involving material interfaces.

Chapter 1

Sharpening diffuse interfaces with compressible fluids on unstructured meshes

Abstract

Diffuse interface methods with compressible fluids, considered through hyperbolic multiphase flow models, have demonstrated their capability to solve a wide range of complex flow situations in severe conditions (both high and low speeds). These formulations can deal with the presence of shock waves, chemical and physical transformations, such as cavitation and detonation. Compared to existing approaches able to consider compressible materials and interfaces, these methods are conservative with respect to mixture mass, momentum, energy and are entropy preserving. Thanks to these properties they are very robust. However, in many situations, typically in low transient conditions, numerical diffusion at material interfaces is excessive. Several approaches have been developed to lower this weakness. In the present contribution, a specific flux limiter is proposed and inserted into conventional MUSCL-type schemes, in the frame of the diffuse interface formulation of Saurel et al. (2009) [27]. With this limiter, interfaces are captured with 3 ± 1 mesh points depending on the test problem, showing significant improvement in interface representation compared to conventional limiters, such as for example Superbee. The method works on both structured and unstructured meshes and its implementation in existing codes is simple. Computational examples showing method capabilities and accuracy are presented.

1.1 Introduction

The present contribution deals with the computation of compressible flows with material interfaces. As soon as the computational domain involves more than one fluid or material, a fundamental difficulty arises, as an extra type of discontinuity appears in addition to shocks and contact discontinuities, present in single-phase flows. An interface separates two materials possibly governed by the same set of balance equations (for example interfaces separating air and liquid water) but with different thermodynamics. As soon as the interface moves in a given cell, this latter becomes a mixture cell and the computation of the thermodynamic state becomes problematic. The fluids have significantly different densities and internal energies, these latter ones being different from the density and internal energy of the mixture in the computational cell as well. It is not possible to compute the cell thermodynamics and in particular the pressure without extra information. In this frame, several approaches have been developed along several decades.

The first class of methods attempts to avoid appearance of mixture cells by maintaining sharp interface profiles. Lagrangian [28] and "Arbitrary Lagrangian Eulerian" (ALE) methods [29] track interfaces but are limited by mesh distortions of arbitrary amplitude [30]. Front tracking [31] attempted to reduce these distortions by considering fixed meshes and moving interfaces, tracked by Lagrangian markers. This was done at the price of limitations, such as the management of several flow solvers, as well as interface distortions involving geometrical singularities, resulting in computational issues.

To progress in the direction of simplicity and generality, the Level Set Method [32] was adapted to compressible fluids and the Ghost Fluid Method [33] was used to compute approximate thermodynamic state in mixture cells and particularly pressure. To avoid 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 Ghost Fluid Method is used to transfer the boundary conditions at interfaces through specific extrapolations from one set of Euler equations to the other. Although apparently simple, this method still needs efforts to improve robustness in severe flow conditions, to maintain conservation and address extra physics.

The last family of methods devoted to mixture cells is termed "diffuse interface methods" (DIM). Two subclasses of DIM are present in the literature. The first one considers physically diffuse interfaces, having a visco-capillary structure [34]. Here the spatial resolution must be less than the interface width, *i.e.* a few nanometers. Also, the equation of state is aimed to describe phase transition between a liquid and its vapor through a cubic-type equation of state. To the authors' knowledge, this approach has never shown its capability to compute interfaces between immiscible fluids (water and air for example). Its seems restricted to small scale computations of phase transition.

The second subclass of DIM addresses mixture cells having computational origins instead of physi-

cal ones. Pioneering work in this direction was done with "Volume of Fluid" (VOF) methods [2] in the frame of incompressible fluids. 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 subvolumes occupied by the phases and several mass balance equations. Extensions of this approach to compressible fluids were done in [3] and [5].

Contrarily to shocks, captured with the help of some artificial viscosity, the computation of interfaces separating materials with different thermodynamics has no viscous regularization. As shown in [3], [5], [35], the computation of mixture thermodynamics can be achieved through relaxation effects in multiphase mixtures. In this frame, as pure materials, far from interfaces, are governed by hyperbolic systems (Euler equations or more sophisticated models), it is natural to address hyperbolic models of diffuse interfaces.

The present contribution is placed in this framework. The simplicity of the implementation of diffuse interface methods is a key point for the computation of complex flows, with distorted interfaces, shocks and interactions among them. Insertion of these methods into existing CFD compressible flow codes is in general easy.

In this frame, Abgrall (1996) [36] considered interfaces separating two ideal gases. Shyue (1998) [37] and Saurel and Abgrall (1999) [4] considered liquid-gas interfaces and added evolution equations for the Stiffened-Gas equation of state parameters to compute mixture cells' thermodynamics. These methods were generalized and rationalized with the help of multiphase flow modeling [3], [5], [13], [27], [38], [39], [40], to cite a few.

In 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. The interfaces are captured and not tracked or reconstructed. Such an approach is mandatory in most compressible flow computations as interface deformations are arbitrarily complex.

These methods are permanently improved, for example to reduce artificial smearing and sharpen interfaces [12], [41], [42] as well as to increase the order of approximation and global accuracy [43].

Extra physics extensions have been addressed as well: chemical reactions [7], phase change [8], surface tension [9], solid-fluid [10], plastic transformation [11], to cite a few.

The main limitation of these diffuse interface methods is related to their excessive numerical diffusion, typically four mesh points and even more. This is not problematic for fast transient flows as the interfaces are in general maintained sharp during sufficiently long time, but becomes problematic at least for slow transient flows. Several contributions have been done to maintain or restore sharp interfaces. Shyue (2006) [44] adapted the interface reconstruction method of Youngs (1982) [45] to a diffuse interface model of compressible fluids. Pantano and coworkers (2010, 2013) [41], [42] adapted the sharpening method of Olsson and Kreiss (2005) [46] to another diffuse interface model. Kokh

and Lagoutiere (2010) [47] promoted another method based on a downwind limiter. Shyue and Xiao (2014) [12] examined another limiter, combined with a hyperbolic tangent reconstruction. It is clear that this research area is very active and that various directions are under investigation.

The present contribution addresses interface sharpening on unstructured meshes. With the help of mild modifications of existing flux limiters in conventional MUSCL methods [48], interfaces are captured with 3 ± 1 mesh points depending on the test problem, improving significantly quality of the results.

The chapter is organized as follows. The considered flow model is recalled in Section 1.2. The hyperbolic flow solver on unstructured meshes is summarized in Section 1.3. In the frame of unstructured meshes and MUSCL methods (Monotonic Upstream-centered Scheme for Conservation Laws), gradient computations have importance, as detailed in Section 1.4. The two main ingredients constituting the present sharpening method are successively detailed in Sections 1.5 and 1.6,

- Development of a specific flux limiter.
- Coupling with a diffuse interface formulation.

The last sections 1.7 and 1.8 deal with validations and illustrations of the method capabilities.

1.2 Flow model

The almost sharp algorithm developed in the present chapter considers the diffuse interface model of Saurel et al. (2009) [27]. This model is a pressure non-equilibrium variant of Kapila et al.'s model (2001) [5] that facilitates consideration of non-conservative terms. The sharpening algorithm can also be applied to simplified versions of these models, such as for example, models given in [13] and [38] as well as variants [40]. Furthermore, the method also applies to more general models such as Baer and Nunziato's (1986) [49]. The model of reference [27] is recalled hereafter:

$$\begin{cases} \frac{\partial \alpha_k}{\partial t} + \mathbf{u}. \operatorname{grad}\left(\alpha_k\right) = \mu(p_k - p_I), \\ \frac{\partial \left(\alpha_k \rho_k e_k\right)}{\partial t} + \operatorname{div}\left(\alpha_k \rho_k e_k \mathbf{u}\right) + \left(\alpha_k p_k\right) \operatorname{div}\left(\mathbf{u}\right) = -p_I \mu(p_k - p_I), \\ \frac{\partial \left(\alpha_k \rho_k\right)}{\partial t} + \operatorname{div}\left(\alpha_k \rho_k \mathbf{u}\right) = 0, \\ \frac{\partial \left(\rho \mathbf{u}\right)}{\partial t} + \operatorname{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + p\underline{I}\right) = 0, \end{cases}$$
(1.2.1)

with k varying from 1 to the number of fluids considered. The notations are conventional in the two-phase flow literature. α_k , ρ_k , p_k , e_k denote respectively the volume fraction, density, pressure and internal energy of phase k. **u** represents the center of mass velocity. The mixture internal energy is defined as $e = \sum Y_k e_k$ where $Y_k = (\alpha_k \rho_k)/\rho$ denotes the mass fraction of phase k. The mixture

density and pressure are defined as $\rho = \sum \alpha_k \rho_k$ and $p = \sum \alpha_k p_k$. The interfacial pressure appearing in the right-hand side reads,

$$p_I = \frac{\sum \frac{p_k}{Z_k}}{\sum \frac{1}{Z_k}},\tag{1.2.2}$$

where $Z_k = \rho_k c_k$ denotes the acoustic impedance of fluid k. The entropy equations read,

$$\frac{\partial \left(\alpha_k \rho_k s_k\right)}{\partial t} + div(\alpha_k \rho_k s_k \mathbf{u}) = \frac{\mu (p_I - p_k)^2}{T_k}.$$
(1.2.3)

System (1.2.1) is hyperbolic with wave speeds u, u + c, u - c with the following definition for the square sound speed: $c^2 = \sum Y_k c_k^2$. It is convenient to write this system in compact form as,

$$\frac{\partial U}{\partial t} + div\{F(U)\} + B(U)\,div\,(\mathbf{u}) = \mu S(U),\tag{1.2.4}$$

with,

$$U = \begin{pmatrix} \alpha_k \\ \alpha_k \rho_k e_k \\ \alpha_k \rho_k \\ \rho \mathbf{u} \end{pmatrix} \quad F(U) = \begin{pmatrix} \alpha_k \mathbf{u} \\ \alpha_k \rho_k e_k \mathbf{u} \\ \alpha_k \rho_k \mathbf{u} \\ \rho \mathbf{u} \otimes \mathbf{u} + p\underline{I} \end{pmatrix} \quad B(U) = \begin{pmatrix} -\alpha_k \\ \alpha_k p_k \\ 0 \\ 0 \end{pmatrix} \quad S(U) = \begin{pmatrix} p_k - p_I \\ p_I(p_I - p_k) \\ 0 \\ 0 \end{pmatrix}.$$
(1.2.5)

This system is non-conservative and is subject to multiple weak solutions. The aim being to couple two systems of Euler equations with different thermodynamics across the diffuse interface, the flow model must tend to the appropriate Euler equations with corresponding jump conditions on both sides of the interface when the volume fractions tend to 0 and 1. Such aim is reached by adding Eq. (1.2.6):

$$\frac{\partial \left(\rho E\right)}{\partial t} + div \left(\mathbf{u} \left[\rho E + p\right]\right) = 0, \qquad (1.2.6)$$

with E the mixture total energy $(E = e + \frac{1}{2}\mathbf{u}^2)$. In this frame, the equation of state must correspond to the one of the appropriate phase (as guaranteed by Eq. (1.2.9)) in the same limit when the volume fractions tend to 0 and 1.

This "forcing" of appropriate Rankine-Hugoniot conditions is simple and accurate when dealing with pure (or nearly pure) fluids separated by interfaces. The situation becomes much more complex when one of the media is a mixture with phases in non-negligible proportions. The difficulty corresponds to the correct partition of the shock energy among the phases. Progresses in this direction were done in Saurel et al. (2007) [50], Petitpas et al. (2007) [51], Petitpas et al. (2009) [7], Schoch et al. (2013) [52], but this is out of the scope of the present chapter as the interfaces considered herein separate two pure (or nearly pure) fluids.

The formulation based on (1.2.4)-(1.2.6) with equation of state (EOS) (1.2.9) tends to the appropriate equations on both sides of the interface separating pure fluids, with appropriate shock relations. But the flow model must also enforce interface conditions of equal pressures and equal normal velocities. As it involves a single velocity, the second interface condition is immediately satisfied. To fulfill the condition of equal pressures, stiff pressure relaxation is done through the pressure relaxation parameter μ that tends to infinity. Such a method is now well-accepted (Saurel and Abgrall (1999) [3], Saurel et al. (2009) [27]) and its efficiency has been demonstrated on many examples. This method does not require resolution of stiff ordinary differential equations (ODEs), as will be summarized later.

At the end of the pressure relaxation step, the volume fractions at mechanical equilibrium are determined and the mixture EOS (1.2.9) is used to compute the pressure in agreement with the total energy evolution (1.2.6).

As the numerical integration of the non-conservative internal energy equations necessarily lacks of accuracy, there is no guarantee that the computed internal energies e_k are in agreement with the mixture pressure p and their respective equations of state $e_k = e_k(p, \rho_k)$. To enforce thermodynamic compatibility, the internal energies are reset with the computed pressure at mechanical equilibrium with the EOS (1.2.9) and their respective EOSs: $e_k(p, \rho_k)$. The global procedure is summarized in System (1.2.7) where the two stiff relaxations (pressure relaxation and internal energy reset) are present in the right-hand side,

$$\begin{cases} \frac{\partial U}{\partial t} + div\{F(U)\} + B(U) \, div \, (\mathbf{u}) &= \mu S(U) + \frac{1}{\epsilon} R(U, \rho E), \\ \frac{\partial \left(\rho E\right)}{\partial t} + div \left(\mathbf{u} \left[\rho E + p\right]\right) &= 0. \end{cases}$$
(1.2.7)

Internal energy reset is done through the relaxation vector $R(U, \rho E)$ defined as,

$$R(U, \rho E) = \begin{pmatrix} 0 \\ \alpha_k \rho_k (e_k(p, \rho_k) - e_k) \\ 0 \\ 0 \\ 0 \end{pmatrix},$$
(1.2.8)

where p is the mixture pressure computed with the mixture total energy,

$$p = p(U, \rho E) = \frac{\left(\rho E - \frac{1}{2}\rho \mathbf{u} \cdot \mathbf{u}\right) - \sum \left(\frac{\alpha_k(1-\rho_k b_k)\gamma_k p_{\infty,k}}{\gamma_k - 1}\right)}{\sum \left(\frac{\alpha_k(1-\rho_k b_k)}{\gamma_k - 1}\right)}.$$
(1.2.9)

The mixture EOS (1.2.9) can be derived explicitly or implicitly from any convex EOS $p_k(\rho_k, e_k)$ and definition of mixture internal energy $\rho e = \sum \alpha_k \rho_k e_k(p_k, \rho_k)$ under pressure equilibrium condition $p = p_k$. The mixture EOS (1.2.9) above is derived from the NASG EOS, used for each fluid,

$$p_k(\rho_k, e_k) = \frac{(\gamma_k - 1)\,\rho_k e_k}{1 - \rho_k b_k} - \gamma_k p_{\infty,k}.$$
(1.2.10)

NASG stands for Noble-Abel-Stiffened-Gas (Le Métayer and Saurel (2016) [22]). It is a generalization of the Stiffened-Gas (SG) EOS, to covolume effects to improve its range of validity and accuracy, at the price of mild modifications. Associated parameters are given for example in [22], [53].

The numerical approximation of System (1.2.7) is achieved with three distinct steps: hyperbolic evolution, relaxation of the phase pressures and reset of the phase internal energies. Those three steps are briefly recalled hereafter.

Hyperbolic evolution

At the beginning of this step, the following relation is satisfied at the current time denoted n,

$$\sum_{k} (\alpha_k \rho_k e_k)^n = (\rho E)^n - \frac{1}{2} \rho^n \|\mathbf{u}^n\|^2.$$
(1.2.11)

The associated dynamics is driven by the following set of non-conservative equations, describing the evolution of U as well as the evolution of ρE ,

$$\begin{cases} \frac{\partial U}{\partial t} + div\{F(U)\} + B(U) \, div \, (\mathbf{u}) = 0, \\ \frac{\partial \left(\rho E\right)}{\partial t} + div \left(\mathbf{u}[\rho E + p]\right) = 0. \end{cases}$$
(1.2.12)

This system is evolved during a time step Δt . In the following, the superscript ⁽¹⁾ will indicate the output variables coming from this hyperbolic step. When this latter is fully computed, the sum of the phase internal energies is in general different from its definition,

$$\sum_{k} (\alpha_k \rho_k e_k)^{(1)} \neq (\rho E)^{(1)} - \frac{1}{2} \rho^{(1)} \|\mathbf{u}^{(1)}\|^2.$$

This feature is particularly true for discontinuous solutions. This inconsistency vanishes with the following corrections.

Pressure relaxation

At this point, the vector $U^{(1)}$ and $(\rho E)^{(1)}$ are available and used as inputs of System (1.2.13). During the second step, the phase pressures are relaxed according to,

$$\begin{cases} \frac{\partial U}{\partial t} &= \mu S(U), \\ \frac{\partial (\rho E)}{\partial t} &= 0. \end{cases}$$
(1.2.13)

Rather than solving (1.2.13) that involves the pressure relaxation rate μ , the combination of the various ODEs results in the following non-linear algebraic system,

$$\begin{cases} e_k \left(p^{(2)}, \rho_k^{(2)} \right) - e_k^{(1)} - p^{(2)} \left(\frac{1}{\rho_k^{(2)}} - \frac{1}{\rho_k^{(1)}} \right) = 0, \\ \sum_k \left(\frac{(\alpha_k \rho_k)^{(1)}}{\rho_k^{(2)}} \right) = 1, \end{cases}$$
(1.2.14)

where $\rho_k^{(1)}$, $(\alpha_k \rho_k)^{(1)}$ and $e_k^{(1)}$ come from the previous hyperbolic step. The superscript ⁽²⁾ denotes here the relaxed pressure state. System (1.2.14) is solved with Newton's method [27]. When only two fluids are considered, an exact solution is available (given here for the Stiffened-Gas EOS),

$$p^{(2)} = \frac{1}{2} \Big[A_1 + A_2 - (p_{\infty,1} + p_{\infty,2}) \Big] + \sqrt{\frac{1}{4} \Big[A_2 - A_1 - (p_{\infty,2} - p_{\infty,1}) \Big]^2 + A_1 A_2},$$
(1.2.15)

with,

$$A_{1} = \frac{\frac{\alpha_{1}^{(1)}}{\gamma_{1}} \left(p_{1}^{(1)} + p_{\infty,1} \right)}{\frac{\alpha_{1}^{(1)}}{\gamma_{1}} + \frac{\alpha_{2}^{(1)}}{\gamma_{2}}} \quad \text{and} \quad A_{2} = \frac{\frac{\alpha_{2}^{(1)}}{\gamma_{2}} \left(p_{2}^{(1)} + p_{\infty,2} \right)}{\frac{\alpha_{1}^{(1)}}{\gamma_{1}} + \frac{\alpha_{2}^{(1)}}{\gamma_{2}}}.$$
 (1.2.16)

When $\rho_k^{(2)}$ are computed, new volume fractions are deduced as $\alpha_k^{(2)} = \frac{(\alpha_k \rho_k)^{(1)}}{\rho_k^{(2)}}$. However, the computed phase internal energies at relaxed pressure $e_k\left(p^{(2)}, \rho_k^{(2)}\right)$ are, once more, incompatible with the mixture total energy (in the presence of shocks) and the next and final step attempts to remedy to this.

Internal energy reset

At this point, the variables coming from the hyperbolic step (1) and the pressure relaxation one (2) are available. Another relaxation process is achieved, this time regarding the internal energies of the phases. The corresponding system is then,

$$\begin{cases} \frac{\partial U}{\partial t} &= \frac{1}{\epsilon} R(U, \rho E), \\ \frac{\partial (\rho E)}{\partial t} &= 0, \end{cases}$$
(1.2.17)

in the asymptotic limit where $\epsilon \to 0$. During this step, only the phase internal energies are reset as,

$$e_k^{(3)} = e_k \left(p^{(3)}, \rho_k^{(2)} \right).$$
 (1.2.18)

Here the superscript $^{(3)}$ denotes the pressure computed with the mixture EOS (1.2.9), based on the mixture total energy (invariant through steps 1-2-3) and the volume fractions after pressure relaxation

 $(\alpha_k^{(2)})$. As the internal energies $e_k^{(3)}$ are computed with the mixture pressure $p^{(3)}$ through EOS (1.2.9), those are now compatible with the conservation of the mixture internal energy,

$$\sum_{k} (\alpha_k \rho_k e_k)^{(3)} = (\rho E)^{(3)} - \frac{1}{2} \rho^{(3)} \|\mathbf{u}^{(3)}\|^2.$$

The time step update is now complete and reads,

$$U^{n+1} = U^{(3)}$$
 and $(\rho E)^{n+1} = (\rho E)^{(3)}$.

It is worthwhile to note that the variables $(\alpha_k \rho_k)^{n+1}$, $(\rho \mathbf{u})^{n+1}$ and $(\rho E)^{n+1}$ are already updated at the end of the first hyperbolic step. The pressure relaxation step provides the updates of the volume fractions α_k^{n+1} and the energy reset step restores thermodynamic compatibility between the EOS (1.2.9), the mixture energy definition (1.2.11) and the phase EOSs (1.2.18),

$$\begin{cases} (\alpha_k \rho_k)^{n+1} = (\alpha_k \rho_k)^{(3)} = (\alpha_k \rho_k)^{(2)} = (\alpha_k \rho_k)^{(1)}, \\ (\rho \mathbf{u})^{n+1} = (\rho \mathbf{u})^{(3)} = (\rho \mathbf{u})^{(2)} = (\rho \mathbf{u})^{(1)}, \\ (\rho E)^{n+1} = (\rho E)^{(3)} = (\rho E)^{(2)} = (\rho E)^{(1)}, \\ \alpha_k^{n+1} = \alpha_k^{(3)} = \alpha_k^{(2)}, \\ e_k^{n+1} = e_k^{(3)}. \end{cases}$$
(1.2.19)

The overall method can thus be summarized as follows. Considering the flow model (1.2.4)-(1.2.6), a quasi-conservative-variable vector U is defined, as well as a primitive-variable vector W,

$$U = \begin{pmatrix} \alpha_k \\ \alpha_k \rho_k e_k \\ \alpha_k \rho_k \\ \rho \mathbf{u} \\ \rho E \end{pmatrix}, \quad W = \begin{pmatrix} \alpha_k \\ \rho_k \\ p_k \\ \mathbf{u} \end{pmatrix}.$$
(1.2.20)

and the method summarizes as:

- Solve the Riemann problem of System (1.2.4)-(1.2.6) (without relaxation terms) at each cell boundary with favorite solver. The HLLC solver [54] is recommended as this system involves 3 waves only. Such solver preserves positivity of density, mass and volume fractions.
- Evolve all flow variables with a Godunov-type method (or higher order variants).
- Determine the relaxed pressure by solving (1.2.14).
- Compute the mixture pressure with the mixture equation of state, EOS (1.2.9).

- Reset the internal energies with the computed pressure from Eq. (1.2.9) and respective EOSs, $e_k = e_k(\rho_k, p)$. During this step, the internal energies are computed by the mixture pressure, determined itself by the mixture internal energy, computed from the mixture total energy equation which is conservative and unambiguously updated.

The interface sharpening algorithm developed in the present chapter acts only during the hyperbolic step. The pressure relaxation and reset steps being unchanged and detailed in [27], the reader is referred to that reference. The hyperbolic step is recalled hereafter and the new flux limiter, rendering interfaces sharp is presented afterwards.

1.3 Hyperbolic solver on unstructured meshes

To develop the interface-sharpening algorithm, numerical resolution of the non-conservative system (Eqs. (1.2.4)-(1.2.6)) has to be addressed. The Godunov-type method given in [27] is extended hereafter to unstructured meshes. Second-order type extension is done with a MUSCL-type method summarized hereafter. Denoting by $V_i(P_i)$ and $V_j(P_j)$ two elements with cell centers P_i and P_j delimited by the boundary S_{ij} (see Fig. 1.1), the space-time Taylor expansion at the point P_{ij} , barycenter of S_{ij} , from the point P_i of a primitive variable W reads,

$$W_L(P_{ij}) = W(P_i) + \vec{r}_{ij} \cdot \nabla W(P_i) + \triangle t \frac{\partial W(P_i)}{\partial t}, \quad \vec{r}_{ij} = \overrightarrow{P_i P_{ij}}.$$
(1.3.1)

Similar expansion at P_{ij} from P_j reads,

$$W_R(P_{ij}) = W(P_j) + \vec{r}_{ji} \cdot \nabla W(P_j) + \triangle t \frac{\partial W(P_j)}{\partial t}, \quad \vec{r}_{ji} = \overrightarrow{P_j P_{ij}}.$$
(1.3.2)



Figure 1.1: Schematic representation of an unstructured mesh made of triangles. \bullet centers of the cells, \blacktriangle centers of the faces. The Riemann problem is solved on each face of the triangles.

The reconstructed solutions at left $W_L(P_{ij})$, and at right $W_R(P_{ij})$, are used as initial conditions for the Riemann problems in order to obtain more accurate numerical fluxes. The MUSCL-type scheme takes into account both data reconstruction and time evolution with the following sequence of computations.

Spatial reconstruction at cell boundaries

The spatial reconstruction step uses the preceding formulas (1.3.1), (1.3.2) without the time derivative, this one being approximated in the next predictor step,

$$W_L^n(P_{ij}) = W^n(P_i) + \vec{r}_{ij} \cdot \nabla W^n(P_i), \quad \vec{r}_{ij} = \overrightarrow{P_i P_{ij}}.$$
(1.3.3)

Similar expansion at P_{ij} from P_j reads,

$$W_R^n(P_{ij}) = W^n(P_j) + \vec{r}_{ji} \cdot \nabla W^n(P_j), \quad \vec{r}_{ji} = \overrightarrow{P_j P_{ij}}.$$
(1.3.4)

Superscript ⁿ denotes the current time step. During this step the gradients $\nabla W^n(P_i)$ and $\nabla W^n(P_j)$ are computed with the method recalled in Section 1.4. The primitive variables W are preferred to quasi-conservative ones U as they preserve uniform velocity and pressure at interfaces. Extrapolation (1.3.3) and (1.3.4) yields a second-order-in-space discretization. At this time, reconstructed variables are available at left $W_L^n(P_{ij})$ and right $W_R^n(P_{ij})$ of the cell faces.

Half-time step evolution

The cell-center-variable-state vector U_i^n is evolved during a half-time step with the conventional Godunov method, requiring Riemann problem resolutions at cell faces,

$$U_i^{n+1/2} = U_i^n - \frac{\triangle t}{2V_i} \sum_{j=1}^{N faces} \left(S_{ij} F_{ij}^{*n} \right).$$
(1.3.5)

Superscript * denotes the solution of the Riemann problem. During this step, the primitive variables at left $W_L^n(P_{ij})$ and right $W_R^n(P_{ij})$ (Eqs. (1.3.3), (1.3.4)) of cell faces come from the previous spatialreconstruction-at-cell-boundary step and are used as initial data of the Riemann problems providing the fluxes F_{ij}^{*n} at the cell faces. The non-conservative volume fraction equations are evolved with the following scheme:

$$\alpha_{k,i}^{n+1/2} = \alpha_{k,i}^n - \frac{\Delta t}{2V_i} \sum_{j=1}^{N \, faces} S_{ij} \Big[(S_m \alpha_k)_{ij}^{*n} - \alpha_{k,i}^n \, S_{m \, ij}^{*n} \Big], \tag{1.3.6}$$

where S_m denotes the contact wave speed projected along the face normal vector, solution of the Riemann problem. Regarding the non-conservative internal energy equations, similar approximation of the corresponding equations is used by assuming the product $(\alpha_k p_k)$ constant during the time step,

$$(\alpha_k \rho_k e_k)_i^{n+1/2} = (\alpha_k \rho_k e_k)_i^n - \frac{\Delta t}{2V_i} \sum_{j=1}^{N \, faces} S_{ij} \Big[(\alpha_k \rho_k e_k S_m)_{ij}^{*n} + (\alpha_k p_k)_i^n S_{m\,ij}^{*n} \Big]. \tag{1.3.7}$$

The lack of accuracy in the internal energy computation resulting from the present scheme is not crucial. The internal energies are only used to estimate the pressure of the phases at the end of the hyperbolic step, before relaxation. The relaxation step gives a first correction to the internal energies, in agreement with the second law of thermodynamics. A second correction is made with the help of the mixture total energy and mixture EOS (1.2.9) [27]. Thereby, a single value of the pressure is available for the next step and for the various phases.

Full-time step evolution

The previous cell-center and quasi-conservative vector $U_i^{n+1/2}$ is converted into the primitive one $W_i^{n+1/2}$ as this latter is preferable for the extrapolation step:

$$W_L^{n+1/2}(P_{ij}) = W^{n+1/2}(P_i) + \vec{r}_{ij} \cdot \nabla W^n(P_i), \quad \vec{r}_{ij} = \overrightarrow{P_i P_{ij}}.$$
 (1.3.8)

Similar expansion at P_{ij} from P_j reads,

$$W_R^{n+1/2}(P_{ij}) = W^{n+1/2}(P_j) + \vec{r}_{ji} \cdot \nabla W^n(P_j), \quad \vec{r}_{ji} = \overrightarrow{P_j P_{ij}}.$$
 (1.3.9)

The gradients $\nabla W^n(P_i)$ and $\nabla W^n(P_j)$ come from the first spatial reconstruction step and add robustness to the method as no combination of gradients computed at time t^n and $t^{n+1/2}$ is made. From the extrapolated variables at left $W_L^{n+1/2}(P_{ij})$ and right $W_R^{n+1/2}(P_{ij})$, a second Riemann problem is solved yielding more accurate numerical fluxes. The solution vector is then evolved during the full-time step with the conventional Godunov method for the various quasi-conservative variables,

$$U_i^{n+1} = U_i^n - \frac{\triangle t}{V_i} \sum_{j=1}^{N \text{ faces}} \left(S_{ij} F_{ij}^{*n+1/2} \right), \qquad (1.3.10)$$

while spacial care is taken for the non-conservative variables,

$$\begin{cases} \alpha_{k,i}^{n+1} = \alpha_{k,i}^{n} - \frac{\Delta t}{V_{i}} \sum_{j=1}^{N faces} S_{ij} \Big[(S_{m}\alpha_{k})_{ij}^{*n+1/2} - \alpha_{k,i}^{n+1/2} S_{mij}^{*n+1/2} \Big], \\ (\alpha_{k}\rho_{k}e_{k})_{i}^{n+1} = (\alpha_{k}\rho_{k}e_{k})_{i}^{n} - \frac{\Delta t}{V_{i}} \sum_{j=1}^{N faces} S_{ij} \Big[(\alpha_{k}\rho_{k}e_{k}S_{m})_{ij}^{*n+1/2} + (\alpha_{k}p_{k})_{i}^{n+1/2} S_{mij}^{*n+1/2} \Big]. \end{cases}$$
(1.3.11)

Then, another pressure relaxation step is done followed by mixture EOS (1.2.9) pressure computation and internal energy reset.

This MUSCL-type scheme is thus summarized in three steps,

- Spatial reconstruction at cell boundaries.

- Half-time step evolution (prediction) followed by pressure relaxation.
- Full-time step evolution followed by another pressure relaxation step.

Figure 1.2 displays a schematic representation of the procedure. The MUSCL-type scheme presented previously requires to solve two Riemann problems per time step but only one gradient computation of the various flow variables. This point is addressed in the following section.



Figure 1.2: Schematic representation of the MUSCL-type numerical scheme. At time t^n , values at the faces $W_L^n(P_{ij})$ and $W_R^n(P_{ij})$ (Eqs. (1.3.3), (1.3.4)), reconstructed via the gradients $\nabla W^n(P_i)$, are used as initial data of a Riemann problem providing fluxes F_{ij}^{*n} . The solution evolves at time $t^{n+1/2}$ via the Godunov-type scheme (Eqs. (1.3.5), (1.3.6), (1.3.7)). At this intermediate time, the previous gradients are used to reconstruct the solution at the faces $W_L^{n+1/2}(P_{ij})$ and $W_R^{n+1/2}(P_{ij})$, (Eqs. (1.3.8), (1.3.9)). Those states are used as initial data of a second Riemann problem providing fluxes $F_{ij}^{*n+1/2}$. Finally, values at cell center U_i^n are updated to U_i^{n+1} with Godunov-type scheme using $F_{ij}^{*n+1/2}$, (Eqs. (1.3.10), (1.3.11)).

1.4 Gradient computation on unstructured meshes

A robust and accurate method for the computation of gradient variables is based on least squares approximation. This method is perhaps the simplest and the cheapest approach on unstructured grids. It is based on multiple Taylor expansions about P_i and a cloud of neighboring cells,

$$W_{j} = W_{i} + \overrightarrow{P_{i}P_{j}} \cdot \vec{e_{x}} \frac{\partial W_{i}}{\partial x} + \overrightarrow{P_{i}P_{j}} \cdot \vec{e_{y}} \frac{\partial W_{i}}{\partial y} + \overrightarrow{P_{i}P_{j}} \cdot \vec{e_{z}} \frac{\partial W_{i}}{\partial z} + O\left(\|\overrightarrow{P_{i}P_{j}}\|^{2}\right)$$

$$= W_{i} + \Delta x_{ij} \frac{\partial W_{i}}{\partial x} + \Delta y_{ij} \frac{\partial W_{i}}{\partial y} + \Delta z_{ij} \frac{\partial W_{i}}{\partial z} + O\left(\|\overrightarrow{P_{i}P_{j}}\|^{2}\right).$$

(1.4.1)

Using Eq. (1.4.1) with a set of neighbors results in the following system:

$$\begin{pmatrix} w_1 \triangle x_{i1} & \cdots & w_1 \triangle z_{iN} \\ \vdots & \ddots & \vdots \\ w_N \triangle x_{iN} & \cdots & w_N \triangle z_{iN} \end{pmatrix} \begin{pmatrix} \frac{\partial W_i}{\partial x} \\ \frac{\partial W_i}{\partial y} \\ \frac{\partial W_i}{\partial z} \end{pmatrix} = \begin{pmatrix} w_1 (W_1 - W_i) \\ \vdots \\ w_N (W_N - W_i) \end{pmatrix} \Leftrightarrow AX = B, \quad (1.4.2)$$

with,

$$w_j = \frac{1}{\triangle x_{ij}^2 + \triangle y_{ij}^2 + \triangle z_{ij}^2} \quad j = 1, \cdots, N$$

where N is the number of neighboring elements. The introduction of weights w_j allows to control numerical instabilities (division by small numbers) when the mesh is skewed. In three dimensions, a minimum of three neighboring elements is necessary to solve the system. When the number of available neighbors is greater than three, then the system is over-determined and solution of minimum residual ||AX - B|| is addressed. A classical way to solve this over-determined system is to multiply both sides by the transpose matrix. A square system (the so-called normal equations) is obtained: $AX = B, A^T AX = A^T B$, and the solutions reads, $X = (A^T A)^{-1} A^T B$.

The main issue regarding this methodology is linked with the condition number of the matrix A, cond(A). If it is big (ill-conditioned) then the system of normal equations $A^TAX = A^TB$ yields a condition number even bigger, $cond(A)^2$. A large condition number is highly undesirable as its numerical solution may be very difficult to achieve accurately. A second approach is to use a QR decomposition. Q is an orthogonal matrix $(Q^TQ = \underline{I})$ and R is an upper-triangle matrix:

$$AX = B$$
, $QRX = B$, $RX = Q^T B$, $X = R^{-1}Q^T B$.

In this framework, QR decomposition is performed using Gram-Schmidt algorithm. It is important to note that for non-moving meshes, the factors $(A^TA)^{-1}A^T$ or $R^{-1}Q^T$ are computed once for all at the beginning of the computation, so that the whole least squares method only yields one matrix-vector product per element.

The direct neighbors of the considered cell are used. Nevertheless, some configurations may require to extend the gradient computation to the indirect neighbors. This configuration is slightly more complex but is sometimes necessary. This situation is depicted in Fig. 1.3.

In the presence of discontinuities, the solution vector cannot be decomposed into Taylor series. In order to avoid oscillation appearances, the gradients are limited. In this framework, the Barth and Jespersen (1989) [55] approach is employed. To avoid reconstructed solution at the face exceeding minimum or maximum values at cell centers on each side of the face (TVD property consequence), the gradient is scaled by factor Θ . The primitive variables W are used during this step,



Figure 1.3: Schematic representation of the direct and indirect neighbors of the cell P_0 on an unstructured mesh made of triangles, for gradient computation. The cell of interest P_0 is represented as the shaded cell. On the left, only the direct neighbors are represented as the darker cells. On the right, the indirect neighbors are represented in addition as the darkest cells.

$$W = \begin{pmatrix} \alpha_k \\ \rho_k \\ p_k \\ \mathbf{u} \end{pmatrix}.$$

The reconstruction at the center of the face separating P_i and P_j "to the left" becomes,

$$W_{ij}^{lim} = W_i + \Theta_i \vec{r}_{ij} \cdot \nabla W_i,$$

with

$$\Theta_i = \min\left(\theta\left(\phi_{ij}\right)\right), \quad j \in neigh(i),$$

and

$$\phi_{ij} = \begin{cases} \frac{W^{max} - W_i}{2(W_{ij}^{n\,lim} - W_i)} & \text{if } \left(W_{ij}^{n\,lim} - W_i\right) > 0, \\ \frac{W^{min} - W_i}{2(W_{ij}^{n\,lim} - W_i)} & \text{if } \left(W_{ij}^{n\,lim} - W_i\right) < 0, \\ 1 & \text{if } \left(W_{ij}^{n\,lim} - W_i\right) = 0, \end{cases}$$
(1.4.3)

with $W_{ij}^{n\,lim} = W_i + \vec{r}_{ij}$. ∇W_i , the unlimited reconstruction solution and W^{max} , W^{min} respectively the maximum and minimum value between the current cell and all its direct neighbors.

 $\theta(\phi_{ij})$ is limiter dependent. For instance,

$$\theta(\phi_{ij}) = max \Big[0, min(\beta \phi_{ij}, 1), min(\phi_{ij}, \beta) \Big], \qquad (1.4.4)$$

gives the Minmod limiter [56] for $\beta = 1$ and the Superbee limiter [16] for $\beta = 2$. In the sharpening method that follows, a specific limiter is used for the volume fraction computation in the vicinity of interfaces only.

1.5 Development of a new limiter for Heaviside-type discontinuities

The present interface-sharpening algorithm consists in a specific flux limiter to insert into the former MUSCL-type scheme. Many gradient limiters are available in the literature in order to prevent local extrema and sharpen discontinuities. Among them the Minmod, van Leer and Superbee limiters are often used. The Ultrabee limiter is another one [16], very accurate for one-dimensional advection of discontinuous profiles. It handles discontinuities in one point only (see for example Leonard (1991) [57], Toro (1997) [58]).

However, when dealing with smooth functions, the Ultrabee limiter produces unacceptable results. It adds "negative numerical viscosity" (locally) and results in wrong "steepening" and "squaring" of the solution profiles.

Nevertheless, flows involving non-miscible fluids present volume fraction discontinuities at interfaces rendering the Ultrabee limiter an interesting candidate. The Ultrabee limiter has been intensively used in the sharpening method of Kokh and Lagoutiere (2010) [47]. However, this method seems restricted to Cartesian grids.

The present chapter aims at computing "sharp-but-still-diffuse" interfaces on unstructured meshes. To this end, a specific limiter is considered and inserted into the compressible two-phase flow model considered previously.

The sought-after function is aimed to deal with multi-dimensional computations, compressive enough to sharpen discontinuous profiles, but diffusive enough to ensure stability. As stated in Sidilkover and Roe (1995) [59], "artificial compression" may be used in multi-dimensional computations to improve the resolution of discontinuities. This feature is not to be used in smooth regions as some undesirable effects may appear. However it can lead to significant improvements in resolving discontinuous profiles.

The investigation of the "artificial compression or interface sharpening" prompted the work of this chapter. In the present manuscript, several modifications of the Superbee limiter are examined in order to:

– Sharpen discontinuities for simple transport equations.
- Maintain stability.
- Work on multi-D with unstructured meshes.

Flux limiters are well-understood in 1D (van Leer (1979) [48], Sweby (1984) [15]) but a clear theory is lacking for multi-dimensional computations. The present investigations are based on numerical experiments, in one and two dimensions, with and without coupling with the diffuse interface flow model. Various modifications of the Superbee limiter are considered as options A, B, C, D, E and F shown in Fig. 1.5. In this figure, the first-order TVD region is presented as the shaded region. The TVD property is briefly recalled hereafter, for more details or discussions, the reader is referred to [14], [15], [58], [60], [61], [62], [63] for example.

Ideally, a second-order accuracy is used while guaranteeing that no nonphysical oscillations arise. The notion of total variation (TV) is a measurement of oscillations in the solutions. The total variation of a solution Q is defined by,

$$TV(Q^n) = \sum_{i=-\infty}^{\infty} |Q_i^n - Q_{i-1}^n|,$$

and the method is called total variation diminishing (TVD) if, for any set of data Q^n , the values Q^{n+1} computed by the method satisfy,

$$TV(Q^{n+1}) \le TV(Q^n).$$
 (1.5.1)

The TVD notion was first presented in the original work of Harten (1983) [14] who proposed this concept to characterize oscillation free schemes. In the same contribution, Harten introduced a fundamental tool to obtain an algebraic proof that the resulting method is TVD.

Later, the Lax-Wendroff scheme (1960) [64] prompted the work of Sweby (1984) [15] who introduced the first and second-order TVD regions. Lax-Wendroff scheme is known to be non-TVD and [15] attempted to remedy to this drawback by introducing a function $\theta(\phi)$. ϕ is a ratio of gradient variables, as it will be detailed further.

To design a TVD method, the function $\theta(\phi)$ should satisfy the following relations,

$$0 \leq \frac{\theta\left(\phi\right)}{\phi} \leq 2 \text{ and } 0 \leq \theta\left(\phi\right) \leq 2.$$

These constraints are rewritten concisely as,

$$0 \le \theta(\phi) \le minmod(2, 2\phi). \tag{1.5.2}$$

This defines the first-order TVD region in a ϕ - θ plane. The curve $\theta(\phi)$ must lie in this region, shown

as the shaded region in Fig. 1.4.



Figure 1.4: Sweby TVD regions. The shaded region of the left figure represents the Sweby region of first-order TVD methods. The dashed line $\theta = 1$ (Lax-Wendroff (1960) [64]) and the dash-dotted line $\theta = \phi$ (Beam-Warming (1976) [65]) are displayed and led to the Sweby region of second-order TVD methods [15] represented as the shaded region of the right figure.

This graphical analysis of (1.5.2) was first presented by Sweby (1984) [15], who analyzed a wide class of flux-limiter methods. In the same reference, Sweby introduced the second-order TVD region depicted in Fig. 1.4 as well. According to [15], for any second-order accurate method, it is better to take θ as a convex combination of $\theta = 1$ (Lax-Wendroff (1960) [64]) and $\theta = \phi$ (Beam-Warming (1976) [65]). Other choices apparently give too much compression and smooth data such as a sine wave tends to turn into a square wave as time evolves. Imposing this additional restriction provides the second-order TVD region of Sweby depicted in Fig. 1.4.

However, as only Heaviside-type discontinuities are aimed to be sharpened in the present framework, those other choices are to be reconsidered as they may provide compression of discontinuities. In that sense, the second-order TVD region of Sweby may no longer be a restriction and the first-order TVD region (upper area) is to be reconsidered. As this latter goes beyond the second-order area, it may provide extra compression while remaining TVD. The first numerical experiments are depicted in Fig. 1.5.

In the following, one-dimensional advection of a Heaviside function ψ at prescribed velocity is computed as a reference test. Numerical solutions of this equation are examined in 1D first and



Figure 1.5: Modifications of the Superbee limiter (A, B, C, D, E and F) considered for the various numerical experiments. The dashed lines represent the various options and the full lines represent the conventional Superbee limiter. The first-order TVD region is shown as the shaded region.

multi-D secondly. The corresponding advection equation reads,

$$\frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} = 0. \tag{1.5.3}$$

Nevertheless, it is demonstrated (see Leveque (1992) [66], Toro (1997) [58] for details) that the actual equation solved by a Godunov-type scheme is,

$$\frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} = \zeta \frac{\partial^2 \psi}{\partial x^2} \quad \text{with} \quad \zeta = \frac{1}{2} \Delta x \, u \, (1 - |c|) \quad \text{and} \quad c = \frac{u \Delta t}{\Delta x}. \tag{1.5.4}$$

The viscous term $\zeta \frac{\partial^2 \psi}{\partial x^2}$ corresponds to the numerical viscosity of the scheme and vanishes when Δx tends to zero. It also vanishes when |c| = 1, which is only of the academic importance. It thus appears that the dependence on both cell size and CFL number has to be considered with the various experimental limiters. The results of the first test series are given in Fig. 1.6 with a CFL number of 0.8. As the present chapter is based on MUSCL schemes and unstructured meshes, gradient computations have to be specified. As mentioned earlier, least squares approximation is appropriate for unstructured meshes and its 1D analogue corresponds to the centered approximation,

$$\left(\frac{\partial\psi}{\partial x}\right)_{i} = \frac{1}{2\triangle x} \left(\psi_{i+1} - \psi_{i-1}\right), \qquad (1.5.5)$$

with i denoting the current cell.

All tests presented in Fig. 1.6 use this approximation for gradient computation and show much better results than the conventional Superbee limiter thanks to their first-order TVD behavior.

While test F tends to Superbee as it is quite close, all other variants present comparable results and capture the discontinuities with two mesh points.

In the following, it would be interesting to build a limiter which can be reduced to the upper boundary of the second-order TVD area, that corresponds to the Superbee limiter, and can be increased to the extreme boundary of the first-order TVD region as well, in order to provide a class of compressive flux limiters for Heaviside-type discontinuities.

To this end, option A is selected as it lies along both first and second-order TVD boundaries with an intermediate constant region. Figure 1.7 examines various variants of option A by experimenting various levels of the plateau region. Those tests are named G, H, I and J and are presented in Fig. 1.7. Figure 1.8 displays the results with CFL = 0.8.

Again, all tests show clear improvements compared to the conventional Superbee limiter. In the following, the first-order TVD boundary (test J of Fig. 1.7) keeps being analyzed by modifying the mesh size and the CFL number. Figure 1.9 provides the results obtained with limiter of test J for meshes of 100, 1000 and 10,000 cells with CFL = 0.8.

In addition, it is interesting to see the behavior of the present compressive limiter when the



Figure 1.6: Comparison of the various limiters A, B, C, D, E and F shown in Fig. 1.5 (full circle symbols •) to the Superbee limiter (diamond symbols \diamond) for the simple transport of a Heaviside function ψ at prescribed velocity. The advection speed is 100 m.s⁻¹. The dashed lines represent the initial condition and the full lines represent the exact solution. Here $\Delta x = 0.01$ m corresponding to 100 cells. The final time is $t \approx 4$ ms and CFL = 0.8.



Figure 1.7: Modifications of the Superbee limiter (G, H, I and J) considered for the various numerical experiments. The first-order TVD region of Sweby is presented in this figure as the shaded region. The dashed lines represent the various options and the full lines represent the Superbee limiter.



Figure 1.8: Comparison of the various limiters G, H, I and J shown in Fig. 1.7 (full circle symbols •) to the Superbee limiter (diamond symbols \diamond) for the simple transport of a Heaviside function ψ at prescribed velocity. The advection speed is 100 m.s⁻¹. The dashed lines represent the initial condition and the full lines represent the exact solution. Here $\Delta x = 0.01$ m corresponding to 100 cells. The final time is $t \approx 4$ ms and CFL = 0.8.

gradients are computed according to the upwind $(\psi_{i+1} - \psi_i)$ and downwind formulas $(\psi_i - \psi_{i-1})$. Their ratio,

$$\phi_i = \frac{\psi_i - \psi_{i-1}}{\psi_{i+1} - \psi_i},\tag{1.5.6}$$

is used as argument in the limiter as it is the conventional method for one dimensional computations (see Toro (1997) [58] for example).



Figure 1.9: Comparison of the limiter J shown in Fig. 1.7 (full circle • and square \blacksquare symbols) to the Superbee limiter (diamond \diamond and triangle \triangle symbols) for the simple transport of a Heaviside function ψ at prescribed velocity. The advection speed is 100 m.s⁻¹. The dashed lines represent the initial condition. The full lines represent the exact solution. The left column displays the results with gradients computed with the least squares method (Eq. (1.5.5)) and the right column with the upwind-downwind formulas (Eq. (1.5.6)). Final time: $t \approx 4$ ms. Meshes: 100 cells (top), 1000 cells (middle), 10,000 cells (bottom). CFL = 0.8.

When the upwind and downwind formulas (Eq. (1.5.6)) are used with the Superbee limiter, discontinuities are captured with four points (results of the right column of Fig. 1.9) while the first-order TVD method (option J of Fig. 1.7) requires two points only.

However, multi-slope computation as Eq. (1.5.6) is inappropriate for unstructured meshes. The least squares method (Eq. (1.5.5)) is convenient for unstructured meshes but the numerical diffusion is excessive as seen in Fig. 1.9. The present limiter captures the discontinuities with the same amount of cells whether the least squares method (Eq. (1.5.5)) or the upwind-downwind formulas (Eq. (1.5.6)) are used. This is a major feature as only two mesh points are required to capture the discontinuities for all mesh resolutions.

The next test (Fig. 1.10) uses a 100-cell mesh and a longer simulation time. The final time is about 10 times longer than the previous tests and CFL numbers of 0.8 and 0.1 are considered with gradients computed with the least squares method (Eq. (1.5.5)) and the upwind-downwind formulas (Eq. (1.5.6)). The boundary conditions are periodic.



Figure 1.10: Comparison of the limiter J shown in Fig. 1.7 (full circle • and square \blacksquare symbols) to the Superbee limiter (diamond \diamond and triangle \triangle symbols) for the simple transport of a Heaviside function ψ at prescribed velocity (100 m.s⁻¹). The dashed lines represent the initial condition. The full lines represent the exact solution. The graphs at top display the results with gradients computed with the least squares method (Eq. (1.5.5)) and the graphs at bottom with the upwind-downwind formulas (Eq. (1.5.6)). Final time: $t \approx 44$ ms. Mesh: 100 cells, CFL = 0.8 (left figures) and CFL = 0.1 (right figures). The boundary conditions are periodic.

The present limiter handles both high and low CFL numbers. Again the number of points required to capture the discontinuities remains the same for both gradient computation methods (least squares method and downwind formulas) whereas the Superbee limiter presents significantly different results. The Superbee limiter lies along the upper boundary of the second-order TVD region of Sweby. This region is able to deal with discontinuities as well as smooth solutions. However, when dealing with Heaviside-type discontinuities only, according to the numerical experiments, the upper boundary of the first-order TVD region seems to be the actual restriction and provides significant improvement over the second-order TVD region.

Similarly to Sweby who introduced a class of flux limiters which includes both extremes of the upper and lower boundaries of the second-order TVD region with the limiter,

$$\theta\left(\phi_{ij}\right) = max \Big[0, min(\beta\phi_{ij}, 1), min(\phi_{ij}, \beta)\Big], \quad 1 \le \beta \le 2, \tag{1.5.7}$$

we propose the following limiter that includes the upper boundaries of the first and second-order TVD regions,

$$\theta(\phi_{ij}) = max \Big[0, min \Big[2, 2\phi_{ij}, max \big[min(2\phi_{ij}, \beta), min\{(2-\beta)\phi_{ij} + 2(\beta-1), \phi_{ij}\} \big] \Big] \Big], \quad 1 \le \beta \le 2.$$
(1.5.8)

Both limiters (1.5.7) and (1.5.8) are depicted in Fig. 1.11. Many other compressive limiters can be considered according to the numerical experiments. The present limiter is proposed here as Eq. (1.5.8) is convenient. For $\beta = 1$, it reduces to the upper boundary of the second-order TVD region corresponding to the Superbee limiter. For $\beta = 2$, it increases to the upper boundary of the first-order TVD region. Because of this feature, the proposed limiter is named "Overbee". The parameter β corresponds to the height of the constant region of the present limiter and controls the amount of artificial compression while remaining TVD as the constraint $0 \le \theta(\phi) \le minmod(2, 2\phi)$ is satisfied.

In the specific case $\beta = 2$, this formulation simplifies to,

$$\theta\left(\phi_{ij}\right) = max \Big[0, min \big[2\phi_{ij}, 2\big]\Big]. \tag{1.5.9}$$

As shown latter, this limit is of particular interest.

Two-dimensional transport

Two-dimensional computations are now considered. In the following, the previously developed limiter (1.5.8) is used with $\beta = 2$. The limiter then lies along the boundary of the first-order TVD region. $\beta = 2$ will be used in all the following tests as it corresponds to the maximum value of interest and to the maximum amount of artificial compression while remaining TVD.

The various tests are schematically depicted in Fig. 1.12. In this section, 2D-Cartesian-structured meshes are used.



Figure 1.11: Graphical representation of the proposed limiter (1.5.8) on the left and Sweby's limiter (1.5.7) on the right. Both limiters use $\beta = 1.5$ for this example. The dark gray shaded region represents the region of first-order TVD methods (left figure). The light gray shaded region represents the region of second-order TVD methods (left and right figures).



Figure 1.12: Schematic representation of the initial conditions of simple transport tests on a twodimensional-Cartesian-structured grid. On the left, the rotation of Zalesak's disk is studied. In this configuration, the velocity is set to $u_x = y - 0.5$ and $u_y = 0.5 - x$ with x, y the coordinates of the cell centers. Non-reflecting boundary conditions are used. The mesh consists in 100×100 cells. On the right, the advection of a square profile along a diagonal is studied. The advection speed is 100 m.s^{-1} in both directions (x, y). Non-reflecting boundary conditions are used. The mesh consists in 200×200 cells.

The first test deals with the rotation of Zalesak's disk. Inside the disk, function ψ is set to 1 and 0 outside. With 2D Cartesian grids made of squares, the least squares method (Eq. 1.4.2) reads,

$$\nabla \psi_{ij} = \begin{pmatrix} \frac{\partial \psi}{\partial x} \\ \frac{\partial \psi}{\partial y} \end{pmatrix}_{ij} = \begin{pmatrix} \frac{1}{2\Delta x} \left(\psi_{i+1,j} - \psi_{i-1,j} \right) \\ \frac{1}{2\Delta y} \left(\psi_{i,j+1} - \psi_{i,j-1} \right) \end{pmatrix}.$$
 (1.5.10)

Figure 1.13 compares the results obtained with the Superbee limiter and the previously developed function with a CFL number of 0.5. The discontinuity is clearly sharpened with the new limiter whereas the least squares method with Superbee limiter produces much more diffusion. Figure 1.13 shows the computed profile of function ψ along x at given y = 0.65 m. About 4 cells are needed to capture the discontinuity with the new limiter whereas Superbee needs about 9 cells.

The next test examines the advection of a square profile along a diagonal. As previously, inside the square, function ψ is set to 1 and 0 outside. For this test, as a consequence of transport along diagonal direction, the influence of the indirect neighbors is studied in addition to the direct ones. As the mesh is made of squares, the stencil used in the computation of gradients is depicted in Fig. 1.14.

Gradient computation with the least squares method reduces to,

$$\nabla\psi_{ij} = \begin{pmatrix} \frac{\partial\psi}{\partial x} \\ \frac{\partial\psi}{\partial y} \end{pmatrix}_{ij} = \begin{pmatrix} \frac{1}{6\Delta x} \left(\psi_{i+1,j} + \psi_{i+1,j-1} + \psi_{i+1,j+1} - \psi_{i-1,j} - \psi_{i-1,j+1} - \psi_{i-1,j-1}\right) \\ \frac{1}{6\Delta y} \left(\psi_{i,j+1} + \psi_{i+1,j+1} + \psi_{i-1,j+1} - \psi_{i,j-1} - \psi_{i+1,j-1} - \psi_{i-1,j-1}\right) \end{pmatrix}.$$
(1.5.11)

The results are given in Fig. 1.15 with CFL = 0.5. Again the least squares method with the conventional Superbee limiter provides a much more diffused discontinuity than the developed new limiter.

Diagonal transport induces distortions when only the direct neighbors are used in the gradient computation via Eq. (1.5.10). The present limiter does its part nonetheless. This drawback is linked to the mesh geometry and the advection direction. It can hardly be seen when the conventional Superbee limiter is used as the square is quite diffused. Nevertheless, this drawback is fixed when the indirect neighbor cells are used in addition via Eq. (1.5.11). The square keeps its shape and remains sharp. For this example, as the mesh structure and the test case itself are simple, the addition of the indirect neighbors has negligible extra CPU cost.

We now have in hands a simple MUSCL-type method to transport accurately Heaviside-type discontinuities with limited diffusion, independent of time and *CFL*.



Figure 1.13: Comparison of the Superbee limiter (left) and the new limiter (right) with $\beta = 2$. Rotation of Zalesak's disk with the situation depicted in Fig. 1.12. Eight values of isocontours of ψ are displayed within the range [0.1-0.9] in both top figures. The results are given at $t \approx 6.3$ s (one full rotation). The figures at bottom show the ψ profile versus x at a given y = 0.65 m. The solid lines represent the initial conditions. The full diamond and circle symbols represent respectively the results provided by Superbee (left) and "Overbee" (right). Cartesian mesh: 100×100 , CFL = 0.5.

		i, j+1			i - 1, j + 1	i, j+1	i+1, j+1	
	i-1,j	i, j	i+1, j		i-1,j	i, j	i+1, j	
j ↑		i,j-1			i-1, j-1	i, j-1	i+1, j-1	

Figure 1.14: Schematic representation of the direct and indirect neighbors of the cell (i, j) on a Cartesian structured mesh, for gradient computation. The cell of interest (i, j) is represented as the shaded cell. On the left, only the direct neighbors are represented as the darker cells. On the right, the indirect neighbors are represented in addition as the darkest cells.

1.6 Coupling with the diffuse interface formulation

The aim of this section is to use the previously developed limiter to sharpen interfaces in the diffuse interface formulation (1.2.4)-(1.2.6). However, because it goes beyond the second-order region of TVD methods (Fig. 1.4) this limiter fails with continuous and shock waves. Therefore, interfaces have to be detected, and the "Overbee" limiter has to be used at interfaces only.

At interfaces, pressure and velocity must be invariant while volume fractions must be as sharp as possible. Near interfaces, the pressure and velocity gradients are very weak but the density gradient is not. To avoid oscillations resulting from bad limiter combinations, all flow variables are computed with zero gradient at interfaces, except volume fractions. It is therefore important to detect interfaces and use a specific procedure in corresponding cells.

To this end, an interface indicator is developed. The interfaces are detected with the help of the volume fractions as follows,

$$\alpha_k^n \alpha_j^n > \epsilon, \quad \text{and} \quad j \neq k.$$
 (1.6.1)

It consists in using the products of phase volume fractions that correspond to Gaussian functions centered at interfaces. According to the numerical experiments, using $\epsilon \simeq 10^{-2}$ seems to be a fair choice. Another efficient filter can be considered as well,

$$|\alpha_k^n(i) - \alpha_k^n(l)| > \epsilon, \quad \text{with} \quad l = 1, \cdots, N \tag{1.6.2}$$

where N is the number of neighboring elements and i denotes the present cell. Equation (1.6.2) allows to deal with variables presenting bounds different from 0 and 1 unlike filter (1.6.1). In the rest of the chapter, filter (1.6.1) is used only.



Figure 1.15: Comparison of the Superbee limiter (left column) and the new limiter (right column) with $\beta = 2$. Advection of a square along the diagonal with the situation depicted in Fig. 1.12. The results at top are computed with gradients based on direct neighbors. At bottom, the intermediate neighbors are used in addition. Eight values of isocontours of ψ are displayed within the range [0.1-0.9] in all figures. The results are given at $t \approx 7$ ms. Cartesian mesh: 200×200 , CFL = 0.5. Direct and intermediate neighbors are mandatory to keep the correct shape, at least for this example.

1.7 Validations

The "Overbee" limiter is now used in two-phase flow computations. The capabilities of the present method are first highlighted on one-dimensional tests. The Stiffened-Gas (SG) EOS (1.2.9) is used in this chapter with the parameters given in Table 1.1. Note that with the SG EOS, the co-volume parameter b_k is not used and is set to 0.

3

Table 1.1: Stiffened-Gas coefficients of the tested fluids.

Advection problem

First let us consider a pure advection problem. A column of liquid water is advected at velocity 100 m.s⁻¹. The initial density of liquid water is set to 1000 kg.m⁻³. The second fluid is air with initial density set to 1 kg.m⁻³. The atmospheric conditions are considered (p = 0.1 MPa). Nearly pure fluid conditions are initially used as $\alpha_{air} = 10^{-6}$ in the liquid phase and $\alpha_{air} = 1 - 10^{-6}$ in the gas phase. The results are given in Fig. 1.16 at time $t \approx 5$ ms. The Superbee flux limiter (Eq. (1.5.7) with $\beta = 2$) is used in the flow solver except regarding the volume fractions computed alternatively with the "Overbee" limiter (Eq. (1.5.8) with $\beta = 2$).

This test is the analogue of the previous advection of a Heaviside function ψ . Figure 1.16 shows that the mixture pressure and velocity are free of spurious oscillations. The volume fractions and the mixture density are clearly sharpened compared to the least squares method with the conventional Superbee limiter.

It appears that volume fraction profiles are slightly more diffused compared to the previous advection tests. The CFL being now based on sound speed, much more time steps are required to reach the final simulation time, resulting in extra diffusion.

In the following, the method is tested on situations involving both continuous and discontinuous waves in addition to interfaces.

Liquid-gas shock tube test

A two-phase shock tube test is now considered. It consists in a one-meter long tube containing two chambers separated by an interface at the location x = 0.75 m. Each chamber contains nearly pure fluid. The liquid is water with initial density $\rho_{water} = 1000 \text{ kg.m}^{-3}$ and the initial density of the gas phase is $\rho_{gas} = 10 \text{ kg.m}^{-3}$.



Figure 1.16: Comparison of the present interface-sharpening method versus the conventional method (without sharpening) with Superbee limiter. Advection of a liquid water column with coupling of flow model (1.2.4)-(1.2.6) and volume fraction sharpening. The advection speed is 100 m.s⁻¹. The dashed lines represent the initial conditions: p = 0.1 MPa, $\rho_{water} = 1000$ kg.m⁻³, $\rho_{air} = 1$ kg.m⁻³, u = 100 m.s⁻¹. The diamond symbols \diamond represent the solution with the Superbee limiter used for all flow variables. The full circle symbols \bullet represent the solution when interface sharpening is used in addition (Eq. (1.5.8), $\beta = 2$). The full lines represent the exact solution. Final time: $t \approx 5$ ms. Mesh: 100 cells. CFL = 0.8.

The left chamber contains a very small amount of gas, $\alpha_{gas} = 10^{-6}$ and the initial pressure is set to 1 GPa. The right chamber contains the same fluids but the volume fractions are reversed. The initial pressure is set to 0.1 MPa. In both chambers, the fluids are initially at rest. The results are shown in Fig. 1.17 at time $t \approx 240 \ \mu$ s with a 200-cell mesh. A close-up view of the interface capture is displayed in Fig. 1.18. The Sweby flux limiter (Eq. (1.5.7)) is used in the hydrodynamic solver with $\beta = 1.35$, except with respect to the volume fractions, when sharpening is active. When the interface is detected, Eq. (1.5.8) is used with $\beta = 2$.



Figure 1.17: Liquid-gas shock tube computation with and without interface sharpening. The dashed lines represent the initial conditions: $p^{left} = 1$ GPa, $p^{right} = 0.1$ MPa, $\rho_{water} = 1000$ kg.m⁻³, $\rho_{gas} = 10$ kg.m⁻³, $u^{left} = u^{right} = 0$ m.s⁻¹, $\alpha_1^{left} = 1 - 10^{-6}$, $\alpha_1^{right} = 10^{-6}$. The diamond symbols \diamond represent the solution with Sweby's limiter (Eq. (1.5.7), $\beta = 1.35$). The full circle symbols \bullet represent the exact solution. Final time: $t \approx 240 \ \mu$ s. Mesh: 200 cells. CFL = 0.5.

The mixture density and volume fraction graphs show that the interface is sharpened with the new limiter. In addition, Fig. 1.18 shows that the pressure and velocity are unchanged in the interface region.



Figure 1.18: Liquid-gas shock tube computation with and without interface sharpening. Close-up view on the interface region. The dashed lines represent the initial conditions: $p^{left} = 1$ GPa, $p^{right} = 0.1$ MPa, $\rho_{water} = 1000$ kg.m⁻³, $\rho_{gas} = 10$ kg.m⁻³, $u^{left} = u^{right} = 0$ m.s⁻¹, $\alpha_1^{left} = 1 - 10^{-6}$, $\alpha_1^{right} = 10^{-6}$. The diamond symbols \diamond represent the solution with Sweby's limiter (Eq. (1.5.7), $\beta = 1.35$). The full circle symbols \bullet represent the solution when interface sharpening is used in addition (Eq. (1.5.8), $\beta = 2$). The full lines represent the exact solution. Final time: $t \approx 240 \ \mu$ s. Mesh: 200 cells. CFL = 0.5.

1.8 Illustrations on unstructured meshes

In the following, the capabilities of the present limiter are highlighted with two-phase flow computations on unstructured meshes.

Advection

This test consists in advecting a liquid water column, initially shaped as Zalesak's disc, into surrounding air. The numerical domain is a square of 1 m by 1 m. The initial conditions are schematically represented in Fig. 1.19. A mesh made of about 50,000 triangles is used. The initial density of liquid water and air are set to 1000 kg.m⁻³ and 1 kg.m⁻³ respectively. The atmospheric conditions are considered (p = 0.1 MPa). Nearly pure fluid conditions are initially used as $\alpha_{min} = 10^{-6}$ and $\alpha_{max} = 1 - 10^{-6}$. The advection speed is 100 m.s⁻¹ in both directions (x, y). Figure 1.20 displays the results obtained with the Superbee limiter (Eq. (1.5.7), $\beta = 2$) and the new function (Eq. (1.5.8), $\beta = 2$). The isocontours of volume fractions are presented, showing enhancements of the present method. For this test, as a consequence of transport along diagonal direction, the influence of the indirect neighbors is studied in addition to the direct ones. When only the direct neighbors are considered, Zalesak's disc tends to become asymmetric. This drawback is lowered when the indirect neighbors are used in addition. For this test, including the indirect neighbors required additional computational cost of about 8% with a commercial computer using 8 cores and MPI architecture. Figure 1.21 shows the cells activated by filter (1.6.1), where the new limiter is active. About 4 cells are detected with (1.6.1) and the interface is always sharper than this zone with the new limiter.



Figure 1.19: Schematic representation of the various two-dimensional tests. The figure on the left represents an advection test of a liquid water column shaped as Zalesak's disc. Non-reflecting boundary conditions are used for this test. The figure in the middle represents a shock tube test where the interface is accelerated by a shock wave moving towards a krypton bubble. The krypton bubble is initially located at x = 0.26 m and y = 0.04 m. Wall boundaries are considered except for the right one considered as non-reflecting. The figure on the right represents an underwater explosion test. The boundaries are non-reflecting.



Figure 1.20: Comparison of the present interface-sharpening method (right figures) versus the Superbee limiter (left figures). Two dimensional advection test of Zalesak-disc shaped liquid water column. The results at top are computed with gradients based on direct neighbors. At bottom, the intermediate neighbors are used in addition. Eight values of the volume fraction isocontours are displayed within the range [0.1-0.9] in all figures. The initial conditions are p = 0.1 MPa, $\rho_{water} = 1000$ kg.m³, $\rho_{air} = 1$ kg.m³, $u_x = u_y = 100$ m.s⁻¹. Final time: $t \approx 7$ ms. Mesh $\approx 50,000$ triangles. CFL = 0.8.



Figure 1.21: Two dimensional advection test of Zalesak-disc shaped liquid water column of Fig. 1.20 (computation with indirect neighbors in addition to the direct ones). The figure on the left represents the cells computed by the interface indicator (Eq. (1.6.1)) (not to be confused with the interface cells required to capture the interface). On the right, cells of water are shown. $t \approx 0.7$ ms. Mesh $\approx 50,000$ triangles. CFL = 0.8.

Air-krypton-shock-interaction

This test addresses both interfaces and shocks. As pressure and density gradients are not collinear, vorticity appears through Richtmyer-Meshkov instabilities [67], [68]. In this section a bubble filled with krypton is considered. The surrounding gas is air. The SG parameters are given in Table 1.1. The geometry is schematically represented in Fig. 1.19 and the initial conditions are given in Table 1.2. Those conditions consist in a low pressure chamber filled with air at atmospheric pressure. The second chamber is filled with shocked air, resulting in the propagation of a left-facing shock at Mach number $M \approx 1.5$. The Mach number is defined as $M = \sigma/c_0$ with σ the speed of the incident shock wave and c_0 the speed of sound in the surrounding air at atmospheric conditions. The bubble of krypton at atmospheric conditions is initially set in the low pressure chamber. Again, nearly pure fluid conditions are initially used as $\alpha_{min} = 10^{-6}$ and $\alpha_{max} = 1 - 10^{-6}$.

Location	Density $(kg.m^{-3})$	Pressure (Pa)	$u_x (\mathrm{m.s}^{-1})$	$u_y \; ({\rm m.s^{-1}})$
Air (post-shock)	2.35	252,840	-230.3	0
Air (pre-shock)	1.29	101, 325	0	0
Krypton	3.506	101, 325	0	0

Table 1.2: Initial conditions of the interface-shock interaction test.

Figure 1.22 presents the corresponding computed results at various times. A mesh of about 60,000 triangles (computing only half of the domain for symmetry reasons) is used. The Superbee limiter

(Eq. (1.5.7), $\beta = 2$) is used in the hydrodynamic solver with both computations (conventional and sharpening). In this flow configuration, the bubble is filled with krypton which is heavier than the surrounding air ($\rho_{krypton} = 3.506 \text{ kg.m}^{-3}$ and $\rho_{air} = 1.29 \text{ kg.m}^{-3}$). The gas properties (densities and acoustic impedances $Z = \rho c$) are strongly different. In addition to these differences, combination of pressure and density gradients induces vorticity as shown in Fig. 1.22. However, at first instants, these effects are dominated by compression ones. During that stage, the transmitted shock wave through krypton is slower than the incident one through air. At further instants, vorticity effects develop and become dominant. As shown in Fig. 1.22, filaments are created initially at top and bottom of the bubble in the flow direction. Then a vortex ring issued from their rolling-up gets formed and grows with time. For more details on the physics of this interaction, see Layes and Le Métayer (2007) [69] for instance.

The benefit of the present method is clearly seen in Fig. 1.22. The mixture zone is much reduced at the interface when the volume fraction computation is done with the "Overbee" limiter (Eq. (1.5.8), $\beta = 2$). The numerical gain is especially visible at the rolling regions of the krypton bubble. As time goes on, the numerical dissipation gets more intense with the conventional method, while the interface and the rolls are clearly distinguishable with the new method. Figure 1.23 presents the cells detected by the interface indicator (Eq. (1.6.1)). Again, about 4 cells are detected with Eq. (1.6.1) and the interface is always sharper than this zone with the new limiter. The additional neighbors provide no significant differences for this test and require additional CPU cost of about 8% (distributed memory parallel implementation using 8 cores).

Underwater explosion

The computational test that follows corresponds to a high pressure gas bubble settled underwater, close to the water-air surface. Such a situation occurs when an underwater explosion bubble reaches the surface. Relevant literature on the subject may be found in Holt (1977) [70], Grove and Menikoff (1990) [71]. The detonation is treated as a constant volume explosion resulting in high pressure gas products at high density. Liquid water surrounding the charge is considered initially at atmospheric conditions. The air above is at rest and at atmospheric conditions as well. The initial situation is shown in Fig. 1.19 and the initial data are summarized in Table 1.3. Three different fluids are considered with thermodynamic data given in Table 1.1. Near pure fluid conditions are initially used as $\alpha_{min} = 10^{-6}$ and $\alpha_{max} = 1 - 2.10^{-6}$.

Due to the high pressure differential between detonation products and surrounding water, a strong shock is emitted into the water while an expansion wave propagates into the gas. The liquid-gas interface is set to intense motion and the bubble deforms. Another wave diffraction occurs at the liquidair interface, resulting in the motion of the two liquid-gas interfaces. The bubble grows intensively



Figure 1.22: Comparison of the present interface-sharpening method (Eq. (1.5.8), $\beta = 2$) versus Superbee limiter (Eq. (1.5.7), $\beta = 2$). The test consists in a krypton-bubble/air configuration where a left-facing shock wave moving at M = 1.5 interacts with the interface. Eight values of the volume fraction isocontours are displayed within the range [0.1-0.9] in all figures. The left column corresponds to the results with the Superbee limiter and the right column with the present compressive limiter. The results are shown at times: $t \approx 0.013$ ms, $t \approx 0.155$ ms and $t \approx 0.297$ ms. The reference time $t_0 = 0$ corresponds to the moment when the shock wave interacts with the interface. Mesh $\approx 60,000$ triangles (computing only half of the domain for symmetry reasons), CFL = 0.5. Only the direct neighbors are used for this test.



Figure 1.23: Krypton bubble shock interaction test of Fig. 1.22. The figure on the left represents the cells computed by the interface indicator (Eq. (1.6.1)) (not to be confused with the interface cells required to capture the interface). On the right, the krypton bubble cells are displayed. The results are given at time: $t \approx 0.155$ ms. The reference time $t_0 = 0$ corresponds to the moment when the shock wave interacts with the interface. Mesh $\approx 60,000$ triangles (computing only half of the domain for symmetry reasons), CFL = 0.5. Only the direct neighbors are used for this test.

Material	Density $(kg.m^{-3})$	Pressure (Pa)
Air Detonation products	$1.225 \\ 1250 \\ 1200$	$101,325$ 10^9
Water	1000	101, 325

Table 1.3: Initial conditions of the underwater explosion test.

resulting in a thin liquid layer appearance between the air and the detonation products. This layer is stretched during time evolution and finally breaks into several fragments.

Phase transition has not been considered in these computations, nor surface tension and viscosity. Fragment size selection is thus numerical. However, the method is able to fragment a liquid film subjected to tension. Indeed, if the single phase Euler equations were solved, the pressure would be negative due to liquid tension and discrepancy with the interface condition where air is present (at positive pressure) would appear. With the present diffuse interface formulation (Eqs. (1.2.4)-(1.2.6)), thanks to the small amount of air present in the liquid, sub-scale bubbles grow during pressure relaxation, maintaining pressure positivity and resulting in the dynamic appearance of new interfaces, which result in the formation of fragments. Such break-up is done automatically as a result of stretching [27]. Such simplified modeling of cavitation is in principle representative enough in explosion situations such as the present case.

Figure 1.24 shows the isocontours of the liquid water volume fraction. The mesh consists in approximately 75,000 triangles (computing only half of the domain for symmetry reasons). The

Minmod limiter (Eq. (1.5.7) with $\beta = 1$) is used in the hydrodynamic solver for both methods (conventional and sharpening). When an interface is located via filter (1.6.1), either the Superbee or the "Overbee" function is used for volume fraction computation. The improvement with the present method is clearly visible. At the end of the simulation, the break-up of the liquid water layer is barely seen with the conventional Superbee limiter whereas the fragmentation process is clearly observable with the new limiter. Figure 1.25 presents the cells detected by filter (1.6.1). Again, about 4 cells are detected with (1.6.1) and the interface is always sharper than this zone with the new limiter. The additional neighbors provide no significant differences for this test and require additional CPU cost of about 8% (distributed memory parallel implementation using 8 cores).

1.9 Conclusion

A simple interface sharpening method bas been built, especially devoted to the computation of compressible two-phase flows. The method has been presented in the context of Saurel et al. (2009) [27] diffuse interface model but can be implemented in the models of Allaire et al. (2002) [13], Massoni et al. (2002) [38], Pelanti and Shyue (2014) [40] and many others. The method relies on a specific limiter for the volume fraction computation in MUSCL-type schemes. This limiter is TVD and deals with Heaviside-type discontinuities only as it is compressive but diffusive enough to behave satisfactorily in multi-D computations. Insertion of this limiter into diffuse interface formulations requires detection of interfaces. A simple indicator function is used for this aim. The developed algorithm thus uses two main ingredients,

- localization of interfaces via an interface indicator,
- volume fraction gradient limitations with the "Overbee" limiter (a first-order TVD limiter).

Computational examples have shown capabilities of the present method. It is able to capture interfaces in two mesh points, improving significantly quality of the results, at the price of slight modifications. The present work has been developed in the context of two-phase flows with inmiscible fluids. A reduced version is given in Appendix A.1 for the computation of contact discontinuities with the Euler equations, in the single phase limit.

Acknowledgements

This work has been done in cooperation with Prof. Boniface Nkonga. The authors would like to acknowledge Dr. Jeaniffer Vides and Dr. François Fraysse for participating in valuable discussions. Part of this work has been carried out in the framework of the ANR-14-CE22-011 (SUBSUPERJET) Project.



Figure 1.24: Comparison of the present compressive limiter (figures on the right, Eq. (1.5.8), $\beta = 2$) versus the Superbee limiter (figures on the left, Eq. (1.5.7), $\beta = 2$). Underwater explosion test. Eight values of the volume fraction isocontours are displayed within the range [0.1-0.9] in all figures. The results are shown at times: $t \approx 1.8$ ms, $t \approx 22$ ms and $t \approx 29$ ms. Mesh $\approx 75,000$ triangles (computing only half of the domain for symmetry reasons), CFL = 0.1. Only the direct neighbors are used for this test.



Figure 1.25: Underwater explosion test of Fig. 1.24. The figure on the left represents the cells computed by the interface indicator (Eq. (1.6.1)) (not to be confused with the interface cells required to capture the interfaces). On the right, the liquid water cells are displayed. The results are given at time: $t \approx 1.2$ ms. Mesh $\approx 75,000$ triangles (computing only half of the domain for symmetry reasons), CFL = 0.1. Only the direct neighbors are used for this test.

Part II

Stiff phase transition phenomena

Introduction

The present part of this manuscript focuses on the treatment of phase transition in compressible multiphase flows through a fast thermochemical relaxation solver and the building of an appropriate mixture equation of state. When a system reaches thermodynamic equilibrium, the mechanical, thermal and molecular exchanges between liquid and vapor phases are in balance. Thermodynamic equilibrium thus corresponds to the combination of the mechanical, thermal and chemical equilibria.

Mechanical and thermal equilibrium solvers have been successfully developed in Le Métayer et al. (2013) [72] and are consequently out of the scope of this research work. Chemical equilibrium has also been addressed in [72] through a stiff relaxation solver. However, this latter happens to be computationally expensive and may be unstable as a result of non-linearities. Also transition to single phase bounds of pure liquid and pure vapor is problematic.

While reaching chemical equilibrium, mass transfer takes place between the liquid and its vapor. In order to isolate the specific difficulties related to the chemical equilibrium, from both theoretical and numerical points of view, a mixture two-phase model involving implicitly both thermal and mechanical equilibria is considered in the following chapter. It is indeed important to consider the simplest model involving the pertinent physics. Such reduction is equivalent to considering the two-phase flow model of Saurel et al. (2009) [27] presented in Chapter 1 with stiff temperature relaxation in addition to the pressure one. Besides, as mentioned in Chapter 2, a large range of applications can be considered with such reduced model (see Saurel et al. (2016) [8] for more details).

In this work, as in Le Métayer et al. (2013) [72], mass transfer is treated by an instantaneous thermochemical relaxation process regarding Gibbs free energies (Saurel et al. (2008) [18]). It consists in a non-linear algebraic system that is made from the equilibrium conditions (equality of the temperatures, pressures and free energies of the phases) and mixture mass and mixture energy definitions. Its numerical resolution is non-trivial and may yield unstable computations, the culprit being the non-trivial relation linking pressure (p) and temperature (T) at saturation. Besides, additional complexity is added to the system when non-condensable gases are present. In such context, p and Tare not directly linked to the saturation curve but are related through the partial pressure of the vapor component in the multicomponent gas phase bringing extra difficulties. This situation is however present in many practical applications.

The most common way to compute such phase change situations is to directly solve the corresponding system via complex root-finding procedures as done in Le Métayer et al. (2013) [72]. Nevertheless, such strategy is computationally expensive and may be detrimental to the computation. Consequently, it motivates the introduction of a new relaxation method where the solution relaxes weakly to the correct solution, on the basis of some estimates. As a result, there is no non-linear system to solve and the transition from two-phase mixture to single phase flows is straightforward.

Chapter 2

A simple and fast phase transition relaxation solver for compressible multicomponent two-phase flows

Abstract

Determining liquid-vapor phase equilibrium is often required in multiphase flow computations. Existing equilibrium solvers are either accurate but computationally expensive, or cheap but inaccurate. The present chapter aims at building a fast and accurate specific phase equilibrium solver, specifically devoted to unsteady multiphase flow computations. The main idea constituting the present phase transition solver is first presented in the context of two-phase flows involving only a liquid and its corresponding vapor phase. In a second time, the solver's range of application is extended by considering a multicomponent gas phase instead of pure vapor, a necessary improvement in most practical applications. The solver proves easy to implement compared to common iterative procedures, and allows systematic CPU savings over 50%, at no cost in terms of accuracy. It is validated against solutions based on an accurate but expensive iterative solver. Its capability to deal with cavitating, evaporating and condensing two-phase flows is highlighted on severe test problems both 1D and 2D.

2.1 Introduction

Most multiphase flow computations face phase transition modeling and one of the difficulties is to adopt the correct mass transfer model, appropriate to a given situation. Some approaches deal with mixtures out of thermal and velocity equilibria. When it is possible to determine the specific interfacial area separating the liquid and gas phases, determination of the mass transfer rate may be done on the basis of Nusselt and Sherwood correlations. Such a method was derived for spray evaporation by Ambramzon and Sirignano (1989) [73] and atmospheric flows by Jacobson (2005) [74]. Generalization to flashing and condensing sprays was done in Furfaro and Saurel (2016) [75].

However, determination of the specific interfacial area in two-phase mixtures is possible only for droplets and bubbly flows. When the topology is arbitrary, only limit case computations are possible, assuming the absence of mass transfer if the interfacial area is supposed to be very small, or assuming infinitely fast mass transfer (local thermodynamic equilibrium) if the interfacial area is supposed to be very large. When such an assumption is made, an appropriate equilibrium solver is needed.

The present chapter deals with the building of such an equilibrium solver when non-equilibrium hyperbolic models, such as Baer and Nunziato's (1986) [49] are considered. However, the present method is not restricted to such a model, but is also valid for its reduced versions such as the 5-equation model of Kapila et al. (2001) [5] and its extension for cavitating flows, Saurel et al. (2008) [18], Le Martelot et al. (2013) [76]. The Homogeneous Relaxation Model (HRM) and Homogeneous Equilibrium Model (HEM) (Downar-Zapolski et al. (1996) [77], Barret et al. (2002) [78]) being also reduced versions of these models with respectively 4 and 3 equations, the present phase transition solver similarly applies to them.

The theoretical link between these models was derived on the basis of asymptotic analysis in Saurel et al. (2008) [18], and more systematically by Lund (2012) [79]. Basically the present phase transition solver may be used each time both liquid and gas compressibility are considered, as all formerly cited models consider this effect, and this effect is responsible for their hyperbolic nature.

The 5-4-3-equation models are able to consider mixtures of fluids evolving respectively in mechanical, mechanical and thermal, and thermodynamic equilibrium. As they involve a single velocity (velocity disequilibrium is indeed absent), they are restricted mainly to specific applications such as:

- Cavitating flows, as it appears impossible in practice to address specific interfacial area determination and consequently model velocity slip. Computational examples of such flows are given for instance in Singhal et al. (2002) [80], Petitpas et al. (2009) [81], Le Martelot et al. (2013) [76] and Saurel et al. (2016) [8].
- Flashing and condensing flows, as they are high-speed flows and subject to stiff thermodynamic relaxation.

Interfacial flows, as the same equations deal with the direct numerical simulation of boiling flows at sub-bubble scale (Le Martelot et al. (2014) [82], Saurel et al. (2016) [8]).

Therefore the equilibrium solver addressed in the present work is a key point of the 7-5-4-3-equation hyperbolic two phase flow models as it computes local thermodynamic equilibrium, this feature being important in many situations. In the frame of flows where only the liquid and vapor phases coexist, the building of such an equilibrium solver has been addressed in Orbey et al. (1998) [83], Allaire et al. (2007) [84], Faccanoni et al. (2012) [85] and Le Métayer et al. (2013) [72] on the basis of a highly non-linear algebraic model based on the saturation conditions, mixture mass and mixture energy definitions. This system may cause difficulties as a result of non-linearities and single phase bounds of pure liquid and pure vapor, where it becomes ill-posed.

In the present chapter a novel approach is promoted where the solution relaxes weakly (smoothly during time evolution) to the correct solution, on the basis of some estimates. After providing the background and context of the model in Sections 2.2, 2.3, 2.4 and 2.5, the main idea constituting the present solver is detailed in Section 2.6:

 "Limitation" of the relaxation term, following a Minmod-type procedure, reminiscent of slope limiters in high-order hyperbolic solvers (van Leer et al. (1979) [48]).

This treatment leads to a faster procedure than the usual iterative process: reported computational times can be halved with the new algorithm. In addition, the algorithm described hereafter presents a very simple implementation, which is also a significant improvement over iterative procedures.

In the first place, we will focus on two-phase flow configurations where only a liquid and its corresponding vapor coexist within the medium. Indeed, it is worth focusing on this specific case as a first step, as this latter presents enough complexities as it is. When only liquid and vapor phases are present within the two-phase flow, the thermodynamic equilibrium directly translates into $p^* = p_{sat}(T^*)$ with p^* and T^* being respectively the equilibrium pressure and equilibrium temperature. p_{sat} denotes the saturation pressure.

In a second time (Section 2.7), a multicomponent gas phase is considered instead of a pure vapor phase. A necessary extension in view of the intended industrial applications. In such context, p^* and T^* are not directly linked to the saturation curve but are related through the partial pressure of the vapor component in the multicomponent gas phase.

The thermodynamic closure of the two-phase flow model is necessary reconsidered in Sections 2.7, 2.8 and 2.9. The thermochemical relaxation solver is consequently reconsidered as well in Sections 2.10 and 2.11. The last sections, 2.12, 2.13 and 2.14, are dedicated to displaying and validating the algorithm capabilities, through a series of 1D and 2D test cases involving cavitating, evaporating and condensing flows.

2.2 Flow model

The phase transition relaxation solver may be used with models mentioned previously (with 7, 5, 4 and 3 partial differential equations) but its presentation is simplified in the context of the 4-equation model (often called HRM) as the solver directly connects the 4 and 3-equation models. When dealing with more sophisticated formulations, for instance the 7-equation model, extra ingredients have to be presented, such as velocity and pressure relaxation solvers (see for example [86]). Here, there is a single step that makes the connection from the 4-equation model (modeling mixtures out of thermodynamic equilibrium) and the 3-equation model (mixtures in full equilibrium). Therefore, for the sake of simplicity the 4-equation model (HRM) is considered in the present chapter as the starting point. The corresponding hyperbolic flow model reads,

$$\begin{cases} \frac{\partial \rho}{\partial t} + div(\rho \mathbf{u}) = 0, \\ \frac{\partial(\rho \mathbf{u})}{\partial t} + div(\rho \mathbf{u} \otimes \mathbf{u} + p\underline{I}) = 0, \\ \frac{\partial(\rho E)}{\partial t} + div([\rho E + p]\mathbf{u}) = 0, \\ \frac{\partial(\rho Y_l)}{\partial t} + div(\rho Y_l \mathbf{u}) = 0, \end{cases}$$
(2.2.1)

alternatively, the last equation can be written as,

$$\frac{\partial(\rho_l \alpha_l)}{\partial t} + div(\rho_l \alpha_l \mathbf{u}) = 0,$$

where $Y_{l,g}$, $\alpha_{l,g}$, $\rho_{l,g}$ denote respectively the mass fraction, the volume fraction and the material density of the liquid ($_l$ subscript) and gas ($_g$ subscript) phases. ρ represents the mixture density, **u** represents the mixture centre of mass velocity, p denotes the mixture pressure and E the mixture total energy ($E = e + u^2/2$). The mixture internal energy is defined as $e = Y_l e_l + Y_g e_g$. System (2.2.1) is currently restricted to two fluids. Besides, mass transfer has been omitted as it is addressed later.

System (2.2.1) is clearly reminiscent of the reactive (or multicomponent) Euler equations widely used in chemically reacting flows. However, the thermodynamic closure differs significantly from the one used in gas mixtures since each phase is assumed to occupy its own volume. Indeed the mixture equation of state (EOS) is a consequence of the following algebraic system:

$$\begin{cases} T_{l} = T_{g} = T, \\ e = Y_{l}e_{l}(p,T) + Y_{g}e_{g}(p,T), \\ p_{l} = p_{g} = p, \\ v = Y_{l}v_{l}(p,T) + Y_{g}v_{g}(p,T), \end{cases}$$
(2.2.2)

where v_l , v_g and v are respectively the specific volumes of the liquid, gas, and mixture. T denotes the mixture temperature.

In this system, the two phases are in mechanical and thermal equilibria and each fluid is assumed to occupy its own volume. This is significantly different from ideal gas mixtures modeled through Dalton's law. Indeed, Dalton's law supposes that each fluid occupies the entire available volume and supposes that the mixture pressure is the sum of the partial pressures:

$$p = \sum_{k} p_{partial,k}.$$

For ideal gases, it is fairly conceivable that each molecule is free to move through the entire volume. For a liquid-gas mixture, the liquid cannot occupy the entire space. Its density would no longer make sense and neither would the notion of its liquid state.

System (2.2.1) is closed by the consequent mixture equation of state (EOS) that arises from Eqs. (2.2.2).

2.3 Mixture equation of state

In this frame, both liquid and gas require their own equation of state (EOS), with parameters carefully chosen to fit the phase diagram. The building of such EOS has been addressed in Le Métayer et al. (2004) [53], on the basis of the Stiffened-Gas (SG) EOS, an improved formulation (NASG) being available as well [22]. The main formulas for the SG EOS read for a given phase k = l, g,

$$\begin{pmatrix}
p_{k}(\rho_{k}, e_{k}) = \rho_{k}(\gamma_{k} - 1)(e_{k} - q_{k}) - \gamma_{k}p_{\infty,k}, \\
T_{k}(p_{k}, \rho_{k}) = \frac{p_{k} + p_{\infty,k}}{\rho_{k}(\gamma_{k} - 1)C_{v,k}}, \\
g_{k}(p_{k}, T_{k}) = (\gamma_{k}C_{v,k} - q_{k}')T_{k} - C_{v,k}T_{k}\ln\left(\frac{T_{k}^{\gamma_{k}}}{(p_{k} + p_{\infty,k})^{\gamma_{k} - 1}}\right) + q_{k}, \\
c_{k}(p_{k}, \rho_{k}) = \sqrt{\gamma_{k}\frac{p_{k} + p_{\infty,k}}{\rho_{k}}},
\end{cases}$$
(2.3.1)

where the following parameters are needed for each phase: γ_k , $p_{\infty,k}$, $C_{v,k}$, q_k , and q'_k . From Eqs. (2.3.1), two other relations are found,

$$\begin{cases} v_k(p_k, T_k) = \frac{(\gamma_k - 1)C_{v,k}T_k}{p_k + p_{\infty,k}}, \\ e_k(p_k, T_k) = \frac{p_k + \gamma_k p_{\infty,k}}{p_k + p_{\infty,k}}C_{v,k}T_k + q_k. \end{cases}$$
(2.3.2)

As shown in [53] there is no difficulty to obtain these parameters once the saturation curves $(p_{sat}(T), v_{g,sat}(T), v_{l,sat}(T), h_{g,sat}(T), h_{l,sat}(T))$ are known. Saturation pressure and temperature

obeying formulation (2.3.1) are linked through the saturation curve,

$$\ln(p_{sat} + p_{\infty,g}) = A + \frac{B}{T_{sat}} + C\ln(T_{sat}) + D\ln(p_{sat} + p_{\infty,l}), \qquad (2.3.3)$$

with

$$A = \frac{C_{p,l} - C_{p,g} + q'_g - q'_l}{C_{p,g} - C_{v,g}}, \quad B = \frac{q_l - q_g}{C_{p,g} - C_{v,g}}, \quad C = \frac{C_{p,g} - C_{p,l}}{C_{p,g} - C_{v,g}}, \quad D = \frac{C_{p,l} - C_{v,l}}{C_{p,g} - C_{v,g}}, \quad (2.3.4)$$

which comes from the equality of the Gibbs free energies g_l and g_g of the Stiffened-Gas EOS (2.3.1) (see [53] for details).

For liquid water and steam, the fluid parameters optimized in the [300 - 500] K temperature range are given in Table 2.1.

Coefficients	Liquid phase	Vapor phase
$C_p ~({\rm J/kg/K})$	4267	1487
$C_v ~({ m J/kg/K})$	1816	1040
γ	2.35	1.43
P_{∞} (Pa)	10^{9}	0
$q~({ m J/kg})$	$-1167 imes 10^3$	2030×10^3
$q'~({\rm J/kg/K})$	0	-23×10^3

Table 2.1: Stiffened-Gas coefficients for water determined in the temperature range [300 - 500] K.

These parameters are used in the computational examples (Figs. 2.5, 2.6 and 2.8) of the present chapter. With the mixture thermodynamic closure (2.2.2), it is straightforward to derive the following analytical relations for the mixture temperature, energy and pressure, that correspond to the mixture EOS:

$$\begin{cases} T = T(p, v, Y_l), \\ e = e(p, T, Y_l), \\ p = p(v, e, Y_l). \end{cases}$$
(2.3.5)

The thermodynamic closure presented in [53] or its improved formulation [22] is very convenient, as the above relations (2.3.5) are fully explicit for the mixture [8, 82]. Combining Eqs. (2.2.2) and (2.3.5), the mixture temperature reads,

$$T(p, v, Y_l) = v \left(\frac{(\gamma_l - 1)Y_l C_{v,l}}{p + p_{\infty,l}} + \frac{(\gamma_g - 1)Y_g C_{v,g}}{p + p_{\infty,g}} \right)^{-1},$$
(2.3.6)
the mixture internal energy reads,

$$e(p,T,Y_l) = Y_l \left(C_{v,l} T \frac{p + \gamma_l p_{\infty,l}}{p + p_{\infty,l}} + q_l \right) + Y_g \left(C_{v,g} T \frac{p + \gamma_g p_{\infty,g}}{p + p_{\infty,g}} + q_g \right),$$
(2.3.7)

and the pressure reads,

$$p(v, e, Y_l) = \frac{1}{2} \left(A_l + A_g - (p_{\infty,l} + p_{\infty,g}) \right) + \sqrt{\frac{1}{4} \left(A_g - A_l - (p_{\infty,g} - p_{\infty,l}) \right)^2 + A_l A_g},$$
(2.3.8)

with

$$A_{k} = \frac{Y_{k}(\gamma_{k}-1)C_{v,k}}{Y_{l}C_{v,l}+Y_{g}C_{v,g}} \left(\frac{e - (Y_{l}q_{l}+Y_{g}q_{g})}{v} - p_{\infty,k}\right),$$
(2.3.9)

where the subscript $_k$ denotes liquid (l) and gas (g) phases (see Le Martelot et al. (2014) [82] for details).

Albeit the apparent simplicity of the thermodynamic closure chosen, the phase transition model presented here may be extended to other thermodynamic closures given each phase EOS is convex. Such extension is immediate with the NASG EOS [22] and will be addressed in Section 2.8 in the context of two-phase flows involving a multicomponent gas phase.

2.4 Mixture speed of sound

The "reactive" Euler equations govern the propagation of three waves throughout space (Fig. 2.1). The middle wave (traveling along u) is a contact discontinuity, while the left and right waves (traveling along $u \pm c$, c being the speed of sound) are non-linear acoustic waves and can be either shocks or rarefactions.



Figure 2.1: Schematic representation in a (x, t) diagram of the three waves present in the flow model (2.2.1).

With the thermodynamic closure (2.2.2), System (2.2.1) is hyperbolic with wave speeds u, u + c

and u - c. The sound speed for this system is given in Le Martelot et al. (2014) [82],

$$c^{2} = \frac{1}{2} \Biggl\{ \left[e - (Y_{l}q_{l} + Y_{g}q_{g}) \right] (a_{1} + a_{2}) + \frac{\frac{1}{2} \left(\frac{\partial R_{1}}{\partial \rho} \right)_{e} R_{1} + \left(\frac{\partial R_{2}}{\partial \rho} \right)_{e}}{\sqrt{\frac{1}{4}R_{1}R_{1} + R_{2}}} + \frac{p}{\rho^{2}} \left(\rho \left(a_{1} + a_{2} \right) + \frac{\frac{1}{2} \left(\frac{\partial R_{1}}{\partial e} \right)_{\rho} R_{1} + \left(\frac{\partial R_{2}}{\partial e} \right)_{\rho}}{\sqrt{\frac{1}{4}R_{1}R_{1} + R_{2}}} \right) \Biggr\},$$
(2.4.1)

where

$$\begin{aligned} a_1 &= \frac{Y_l (\gamma_l - 1) C_{v,l}}{Y_l C_{v,l} + Y_g C_{v,g}}, \\ a_2 &= \frac{Y_g (\gamma_g - 1) C_{v,g}}{Y_l C_{v,l} + Y_g C_{v,g}}, \end{aligned}$$
(2.4.2)
$$R_1 &= a_2 \rho \left[e - (Y_l q_l + Y_g q_g) \right] - a_2 p_{\infty,g} - a_1 \rho \left[e - (Y_l q_l + Y_g q_g) \right] + a_1 p_{\infty,l} - p_{\infty,g} + p_{\infty,l}, \\ R_2 &= a_1 a_2 \{ \rho \left[e - (Y_l q_l + Y_g q_g) \right] - p_{\infty,l} \} \{ \rho \left[e - (Y_l q_l + Y_g q_g) \right] - p_{\infty,g} \} . \end{aligned}$$

This sound speed can then be compared with a simpler approximation of the sound speed given by Wood (1930) [87]:

$$\frac{1}{\rho c^2} = \frac{\alpha_l}{\rho_l c_l^2} + \frac{\alpha_g}{\rho_g c_g^2}.$$
(2.4.3)

As shown in Fig. 2.2, Wood's expression (2.4.3) for the sound speed is always slightly greater than the sound speed given by Eq. (2.4.1). It is thus more convenient (and simpler) for computational purposes related to the hyperbolic solver.

2.5 Phase transition model

When phase transition is addressed in System (2.2.1), the equations for the mixture mass, momentum and energy are unaffected, and only the mass fraction equation is modified through Gibbs free energy relaxation terms. The analysis of the entropy production associated with System (2.2.1) is addressed in Saurel et al. (2008) [18] and leads to the following admissible formulation of the mass transfer terms,

$$\frac{\partial \left(\rho Y_l\right)}{\partial t} + div(\rho \mathbf{u} Y_l) = \rho \nu (g_g - g_l), \qquad (2.5.1)$$

where $g_k = h_k - Ts_k$ denotes the phase k Gibbs free energy with h_k and s_k being respectively the specific enthalpy and specific entropy. $\nu(A_I, p, T)$ represents a relaxation parameter that controls the rate at which thermodynamic equilibrium is reached. It is a function of the interfacial area A_I ,



Figure 2.2: The speed of sound of System (2.2.1) given by Eq. (2.4.1) is compared with Wood's sound speed, Eq. (2.4.3). Full view and close up. The thick lines represent Wood's sound speed. The dashed lines represent the augmented Euler's sound speed. The two-phase mixture is made of liquid water and air at atmospheric conditions.

pressure and temperature. Its determination is possible only when the interfacial area A_I is available, as with droplets and bubbly flows. In this framework, when a fluid is metastable, ν is considered very big, so that relaxation to thermodynamic equilibrium is immediate.

The consideration of mass transfer in Eq. (2.5.1) combined with the equations of mass, momentum and energy of System (2.2.1) does imply,

$$\frac{\partial \left(\rho s\right)}{\partial t} + div(\rho s \mathbf{u}) = \frac{\rho \nu (g_g - g_l)^2}{T},$$

where the mixture entropy is defined as $s = Y_l s_l + Y_g s_g$. Obviously this formulation does respect the second law of thermodynamics,

$$\frac{\partial\left(\rho s\right)}{\partial t}+div(\rho s\mathbf{u})\geqslant0.$$

Using a fractional step method, phase transition is decoupled of transport and wave propagation. At each time step of the flow solver, the following equation has to be resolved for the mass fraction Y_l ,

$$\frac{\partial \left(\rho Y_l\right)}{\partial t} = \rho \frac{\left(Y_l^* - Y_l\right)}{\tau},\tag{2.5.2}$$

where Y_l^* is the liquid mass fraction at thermodynamic equilibrium. This equation trivially solves to a solution exponentially tending to Y_l^* , with a characteristic time τ . In this work, τ is assumed to be smaller than the other characteristic times of the flow model: stiff relaxation is considered. As a consequence, solving Eq. (2.5.1) at every time step reduces to setting $Y_l = Y_l^*$ after each hyperbolic step.

With the infinitely fast mass transfer relaxation strategy, it is interesting to represent the effective thermodynamic path that the fluid undergoes during the phase change process. Figure 2.3 represents this effective thermodynamic path.



Figure 2.3: The isentrope of the liquid and the one of the gas are connected with a kinetic path corresponding to a mass transfer between the two states (liquid and vapor). The metastable states are immediately transformed into a mixture at equilibrium. The effective thermodynamic path is represented. The slope of the isentrope is purposely exaggerated in order to insist on the fact that this slope is weak but non-zero.

At the two-phase zone boundaries, the connection between the liquid's isentrope (or the vapor's) and the one of the two-phase mixture is made continuously through the thermodynamic path represented in Fig. 2.3. It is also worth mentioning that the use of the thermochemical relaxation solver allows to omit the integration of stiff source terms.

Although the specific volume $v = 1/\rho$ and energy e do not vary in the mixture during thermodynamic relaxation, the pressure and temperature do, also reaching their equilibrium values (p^*, T^*) on the saturation curve, since $g_l = g_g$ is equivalent to the saturation condition: Eq. (2.3.3). The phase transition model thus reduces to computing the equilibrium state (p^*, T^*, v, e, Y_l^*) , at every time step, from the state described by (p, T, v, e, Y_l) , as represented schematically in Fig. 2.4.



Figure 2.4: Representation of a control volume in the flow model during the phase transition step in the context of a flow involving only a liquid and its own vapor.

With the thermodynamic closure (2.2.2) presented above, the equilibrium state satisfies,

$$\begin{cases} p^*(v, e, Y_l^*) = p_{sat} \left(T^*(v, e, Y_{l_i}^*) \right), \\ v = Y_l^* v_l(p^*, T^*) + (1 - Y_l^*) v_g(p^*, T^*), \\ e = Y_l^* e_l(p^*, T^*) + (1 - Y_l^*) e_g(p^*, T^*), \end{cases}$$
(2.5.3)

unless there is a solution in which the mixture is a pure phase (resp. $Y_l^* = 0$ or $Y_l^* = 1$), with a temperature respectively above or below the saturation temperature. The above non-linear system can be solved following an iterative algorithm such as Le Métayer et al.'s (2013) [72] but the aim of the present work is to offer a simpler and faster alternative.

2.6 Thermochemical relaxation algorithm

Let us recall that with an iterative approach, the goal of the thermochemical relaxation is to compute accurately Y_l^* , the liquid mass fraction at equilibrium (or alternatively Y_g^*), while with the present method, the aim is to reach the same solution but gradually (typically 2 or 3 time steps).

The first step is to check with pure fluid existence. For numerical reasons, pure fluid conditions are considered via $\epsilon \to 0$, typically on the order of 10^{-8} . To do this, $Y_l^* = \epsilon$ and $Y_l^* = 1 - \epsilon$ are successively assumed. Under these assumptions, the pressures are computed by use of the equation of state for the mixture (2.3.5),

$$p = p(v, e, Y_l),$$

since v and e are invariant through phase transition. The associated temperatures are then computed through Eq. (2.3.6),

$$T = T(v, p, Y_l).$$

The corresponding temperatures are compared to the saturation one at the current pressure $(T_{sat}(p))$,

$$\begin{cases} \text{if } (Y_l = \epsilon \quad \text{and} \quad T > T_{sat}) \quad \text{then} \quad Y_l^* = \epsilon \quad (\text{overheated vapor}), \\ \text{if } (Y_l = 1 - \epsilon \quad \text{and} \quad T < T_{sat}) \quad \text{then} \quad Y_l^* = 1 - \epsilon \quad (\text{subcooled liquid}). \end{cases}$$
(2.6.1)

If one of the two inequalities is fulfilled the equilibrium liquid mass fraction Y_l^* is fully determined and no further computation is required. If none of the above statements is true, then necessarily,

$$\epsilon < Y_l^* < 1 - \epsilon, \quad p^* \text{ is unknown},$$
(2.6.2)

and System (2.5.3) has to be resolved. The difficulty resides in the non-trivial relationship between

the saturation pressure and saturation temperature arising from Eq. (2.3.3):

$$T_{sat}(p) = -\frac{B}{C.W\left(-\frac{Be^{A/C}p^{-1/C}(p+p_{\infty,l})^{D/C}}{C}\right)},$$
(2.6.3)

where W is the Lambert function¹, which cannot be expressed analytically, calling for an iterative method such as Newton's.

The idea of the algorithm is to start from a rough estimate of the equilibrium pressure $p^* = p$, and the associated equilibrium temperature $T^* = T_{sat}(p)$ and reach gradually the solution. Since the pressure and temperature are related at saturation, the liquid internal energy $e_l(p,T)$ and specific volume $v_l(p,T)$ become two functions depending on p only, and two values for Y_l^* as functions of the initial pressure p are obtained from System (2.5.3), by either using the mixture mass definition,

$$Y_l^m(p) = \frac{v - v_g(p)}{v_l(p) - v_g(p)},$$
(2.6.4)

or the mixture internal energy definition,

$$Y_l^e(p) = \frac{e - e_g(p)}{e_l(p) - e_g(p)}.$$
(2.6.5)

Indeed, these two formulas are only equal if p is exactly the equilibrium pressure p^* , which is not the case *a priori* since the process is not isobaric.

Based on these two guesses, a strategy inspired by flux limiters used in high-order schemes [48] is adopted. Let us introduce the ratio of the liquid mass fraction variations induced by the mass $(Y^m - Y)$ and internal energy $(Y^e - Y)$ guesses for the equilibrium mass fraction,

$$r = \frac{Y_l^m(p) - Y_l}{Y_l^e(p) - Y_l}.$$

An estimate of the equilibrium mass fraction is then obtained as,

$$\begin{cases} \text{if } \mathbf{r} < 0, & Y_l^* = Y_l \\ \text{if } 0 < \mathbf{r} < 1, & Y_l^* = Y_l^{mass} \\ \text{if } \mathbf{r} > 1, & Y_l^* = Y_l^{energy} \end{cases}$$

Alternatively, it also expresses as,

$$r = (Y_l^m(p) - Y_l) (Y_l^e(p) - Y_l), \qquad (2.6.6)$$

¹The Lambert W function is defined as $z = W(ze^z)$.

$$\begin{cases} \text{if } r < 0, \qquad Y_l^* = Y_l \\ \text{otherwise} \quad Y_l^* = Y_l + sgn \Big[Y_l^m(p) - Y_l \Big] \times Min \Big[|Y_l^m(p) - Y_l|, |Y_l^e(p) - Y_l| \Big]. \end{cases}$$
(2.6.7)

In the first case, the evolutions indicated by the two equilibrium guesses are discordant: one tends to evaporate whereas the other tends to condensate. The four quantities $(Y_l, Y_l^*, Y_l^m, Y_l^e)$ are then likely to be very close to one another, and no mass transfer is to be considered. In the other case, among (Y_l^m, Y_l^e) , the closest to the initial value Y_l is to be chosen. In that sense, the algorithm ensures equality of Eqs. (2.6.4) and (2.6.5) in the weak sense, rather than in the strong sense. When Y_l^* is determined, the entire Y_l field is reset for the next time step resolution.

Negative mass fractions are impossible to obtain with this algorithm. This can be seen from Fig. 2.5: slopes of Y_g^e and Y_g^m are of different sign. Since the crossing of the two lines occurs at a positive mass fraction (which is the *exact* solution), only one of Y_g^e and Y_g^m can be negative at a time. Following the algorithm, there are then two possibilities: if the initial Y_g (from the hyperbolic step) is between Y_g^e and Y_g^m , then nothing happens thanks to the Minmod-like limitation. If Y_g is not between Y_g^e and Y_g^m , then it is necessarily above the maximum of the two (since $Y_g > 0$), and the algorithm will automatically pick the closest estimation (which is then positive).

The reason for this algorithm efficiency is illustrated in Fig. 2.5, which presents the evolution of Y_l^m and Y_l^e as functions of the initial guess for the pressure, for a mixture initially away from thermodynamic equilibrium. It is seen that following the above algorithm, which in the depicted case returns $Y_l^* = Y_l^e$, gives a result within half a percent of the exact value, even though the initial state is quite far from equilibrium: 30 K below the saturation temperature at the initial pressure of 1 atm.



Figure 2.5: Evolution of Y_l^m and Y_l^e with p (thick dashed and dash-dotted lines resp.) corresponding to Eqs. (2.6.4) and (2.6.5). The exact values of Y_l^* and p^* are found at the crossing of the two lines (\blacklozenge). Initial state (\bullet): p = 1 atm, $Y_l = 0.2$, $T = T_{sat} - 30$ K= 343 K. The triangles represent the value of Y_l^m (\blacktriangle) and Y_l^e (\blacktriangledown) evaluated by the algorithm. Relative error between the exact solution Y_l^* and that obtained with the algorithm is indicated.

Accuracy of the relaxation algorithm is illustrated in Fig. 2.6. A shock tube containing liquid water and its own vapor is considered. In the present example, the tube is 1 meter long and the initial discontinuity is located at 0.5 meter. Boundary conditions are considered as non-reflecting. The computation that follows is addressed with the first-order Godunov method and the HLLC Riemann solver (see Toro (1997) [58], Saurel et al. (2016) [8], for details). Doing so, computed results are free of extra ingredients such as gradient limiters. As liquid and vapor coexist in the present context, the initial conditions correspond to both saturated liquid and vapor. Given initial pressures and mass fractions, the initial temperatures are computed with Eq. (2.3.3), initial mixture energy and specific volumes are deduced from the definitions given by Eqs. (2.2.2). Figure 2.6 presents the results obtained with the present relaxation solver and a classic root-finding procedure method such as Newton's.



Figure 2.6: Comparison of the present relaxation algorithm (thick lines) versus the iterative Newton's method (symbols). Shock tube test with a two-phase mixture involving a vanishing liquid phase. The dotted lines represent the solution without phase transition. The dashed lines represent the initial conditions: $p_l = 2 \cdot 10^5$ Pa, $p_r = 10^5$ Pa, $u_l = u_r = 0$ m.s⁻¹, $Y_l^{liq} = Y_r^{liq} = 0.01$. Final time: $t \approx 0.5$ ms. Mesh: 100 cells. For the sake of clarity, only 50 symbols out of 100 are plotted for the iterative Newton's method.

Excellent agreement is obtained between the present relaxation solver and the iterative method. Clearly the shock compression yields total evaporation while the rarefaction results in condensation. Appearance of pure vapor is computed without oscillations by the two methods. Note that the specific management of pure phases is handled by Eq. (2.6.1) for both algorithms ("Minmod-type" and iterative).

In view of the intended industrial applications, the thermodynamic closure of the two-phase flow must necessarily be extended to account for a multicomponent gas phase. The present thermochemical relaxation solver must consequently be adapted. The main idea constituting the present solver remains nonetheless unchanged (Minmod-like limitation). The basics of the previous thermochemical algorithm are indeed essential for the design of a simple, robust and fast solver able to deal with a liquid in equilibrium with a multicomponent gas phase. This problematic is addressed in the next sections.

2.7 Extension to a multicomponent gas phase

The work introduced in Section 2.6 [1] presents the basis required to build a simple and efficient thermochemical solver able to deal with a liquid and its vapor.

When only liquid and the corresponding vapor are present (previous sections), p and T are linked by the saturation curve $p = p_{sat}(T)$, simplifying somewhat the system to solve. In the present section, we aim at extending the model to liquid in equilibrium with a multicomponent gas phase. In this case, p and T are not directly on the saturation curve, but are related through the partial pressure of the vapor component in the multicomponent gas phase. This allows the well-known existence of water vapor in air at atmospheric conditions, albeit a temperature below the boiling point.

The range of flow solvers to which the present model applies is identical to its previous version: it is designed in association with non-equilibrium hyperbolic flow models, such as Baer and Nunziato's (1986) [49] and its reduced versions. This includes the 5-equation model of Kapila et al. (2001) [5] and its extension for cavitating flows [8, 18, 76], as well as formulations for thermal equilibrium two-phase mixtures such as the Homogeneous Relaxation Model (HRM) and Homogeneous Equilibrium Model (HEM) [77, 78].

The phase transition relaxation solver may be used with models mentioned previously (with 7, 5, 4 and 3 partial differential equations) but its presentation is simplified in the context of the 4-equation model (often called HRM). When dealing with more sophisticated formulations, as for example the 7-equation model, extra ingredients have to be presented, such as velocity, pressure and temperature relaxation solvers, as done for example in [72, 86]. Here, there is a single step that makes the connection from the 4-equation model (modeling mixtures out of thermodynamic equilibrium) and the 3-equation model (mixtures in full equilibrium).

Considering multicomponent effects within the gas phase needs additional mass balance equations,

$$\frac{\partial(\rho_g \alpha_g y_k)}{\partial t} + div(\rho_g \alpha_g y_k \mathbf{u}) = 0, \qquad (2.7.1)$$

where y_k denotes the k-th gas component mass fraction within the gas phase. In the thermodynamic closure considered in this study, and detailed in the next section, the gas phase is assumed to obey the ideal gas equation of state.

As the molar volume is independent of the gas constituent, it is equivalent to considering the constituents as ideally mixed within the gas phase (each occupying the whole gas phase volume), or assuming that each component within the gas phase occupies its own separate volume. The equivalence between these two approaches is clarified in the next section. Under the latter assumption, all mass balance equations can be written as:

$$\frac{\partial(\rho Y_k)}{\partial t} + div(\rho Y_k \mathbf{u}) = 0,$$

where the subscript $_k$ refers to the various physical and chemical components. In the following, let us introduce the following convention:

-k = 1 for the liquid,

- -k=2 for the gas component corresponding to vapor of species 1,
- $-k = 3, \ldots, N$ for the remaining gas components, considered non-condensable in this work.

This notation for the species conservation equation is more convenient, as Y_k is now the mass fraction for the k-th species in the entire mixture (containing both liquid and gas), so that the conservation equation for each species within the gas phase is of the same form as the liquid mass conservation equation.

The extended two-phase flow model consequently reads,

$$\begin{cases} \frac{\partial \rho}{\partial t} + div(\rho \mathbf{u}) = 0, \\ \frac{\partial(\rho \mathbf{u})}{\partial t} + div(\rho \mathbf{u} \otimes \mathbf{u} + p\underline{I}) = 0, \\ \frac{\partial(\rho E)}{\partial t} + div([\rho E + p]\mathbf{u}) = 0, \\ \frac{\partial(\rho Y_k)}{\partial t} + div(\rho Y_k \mathbf{u}) = 0, \end{cases}$$
(2.7.2)

with

$$E = e + \frac{1}{2}\mathbf{u}^2, \quad e = \sum_{k=1}^{N} Y_k e_k.$$

Mass transfer has been omitted in System (2.7.2) as it is addressed later. System (2.7.2) is clearly reminiscent of the reactive (or multicomponent) Euler equations widely used in chemically reacting flows. However, like in previous sections, the thermodynamic closure differs significantly from the one used in gas mixtures as examined hereafter.

2.8 Extended thermodynamic closure

This section presents the equations of state (EOS) used for each pure component as well as the mixture equation of state. Preliminarily, let us demonstrate the equivalence between the ideal gas mixture model that follows Dalton's law, and a gas phase where each constituent is assumed to occupy its own volume, in the specific context of temperature and pressure equilibria.

To this aim, the question of the gaseous mixture model is to be asked. Should we consider that the pressure within the gaseous mixture obeys Dalton's law, or should we consider, like in the liquid-vapor mixture case (see Section 2.2), that all pressures are equal (liquid, vapor, non-condensable gases)?

Basically, it boils down to an ideal gaseous mixture, or a mixture where all gaseous species are assumed to evolve in their own separate volume. This essential question is schematically depicted in Fig. 2.7. In order to clarify this statement, let us come back to the mixture rules for some ideal gases following the two possible options: ideal mixture or separate species. Note also that for the sake of clarity, we will use the mass fractions y_k in the next analyses. Indeed, those are the mass fractions of the chemical species of the gaseous mixture. Though, to remain consistent with the convention introduced previously, the index counting will start at 2 as it corresponds to the first gas component (vapor). We will come back to the mass fractions Y_k of the entire mixture (containing both liquid and gas phases) when building the equation of state of the two-phase mixture.



Figure 2.7: Representation of a control volume in the flow model according to Dalton's law (left figure) and the separate phase approach (right figure). This illustration represents a liquid, its own vapor and the atmospheric air as a non-condensable gas. The two approaches are different as Dalton's law considers an ideal mixture of gases whereas the other option considers all the gas constituents as separate.

The gas phase is ideally mixed: Dalton's law

The gas phase is analyzed under the assumption of a gaseous mixture respecting Dalton's law. The index 2 is the index of the vapor which is the first constituent of the gas phase. The ideal gas EOS is considered. With this approach, the associated mixture rules are:

$$\begin{cases} T = T_k & : \text{ mixture in temperature equilibrium,} \\ V = V_k & : \text{ each chemical species occupies the entire volume,} \\ p = \sum_{k=2}^{N} p_{partial, k} & : \text{ the mixture pressure is the sum of partial pressures} \\ e = \sum_{k=2}^{N} y_k e_k & : \text{ mixture internal energy definition.} \end{cases}$$

In this context, the ideal gas law for a given species reads,

$$p_{partial, k}V_k = n_k \hat{R}T_k$$
 and becomes $p_{partial, k}V = n_k \hat{R}T$.

Consequently the gas mixture pressure expresses,

$$pV = \left(\sum_{k=2}^{N} p_{partial,\,k}\right) V = \left(\sum_{k=2}^{N} n_k\right) \hat{R}T,\tag{2.8.1}$$

where \hat{R} denotes the universal gas constant in molar units and n_k is the number of moles of species k. The ideal gas Joule's relation, Mayer's relation and the ratio of the specific heats are now used,

$$\begin{cases} e_k = C_{v,k} T_k + q_k = \frac{\hat{C}_{v,k}}{W_k} T_k + q_k, \\ \hat{R} = \hat{C}_{p,k} - \hat{C}_{v,k}, \\ \gamma_k = \frac{\hat{C}_{p,k}}{\hat{C}_{v,k}} = \frac{C_{p,k}}{C_{v,k}}, \quad \hat{C}_{v,k} = \frac{\hat{R}}{\gamma_k - 1}, \end{cases}$$
(2.8.2)

and lead to the following relation expressing the internal energy of a gaseous constituent,

$$e_k = \frac{\hat{R}T}{W_k \left(\gamma_k - 1\right)} + q_k.$$

In this relation, W_k denotes the molar mass and γ_k the polytropic coefficient of chemical species k. $C_{p,k}$ and $C_{v,k}$ are the heat capacities at constant pressure and volume respectively and q_k is the reference energy of fluid k. Note that the superscript defines the molar values. In relation (2.8.1), the temperature is deduced from the caloric equation of state for the gas mixture. Indeed, the definition of the mixture internal energy yields,

$$e = \hat{R}T\left(\sum_{k=2}^{N} \frac{y_k/W_k}{\gamma_k - 1}\right) + \sum_{k=2}^{N} y_k q_k.$$
 (2.8.3)

The combination of Eqs. (2.8.1), (2.8.2) and (2.8.3) leads to the gaseous mixture pressure relation,

$$p = \left(\sum_{k=2}^{N} \frac{n_k}{V}\right) \left(\frac{e - \sum_{k=2}^{N} y_k q_k}{\sum_{k=2}^{N} \frac{y_k/W_k}{\gamma_k - 1}}\right) = \left(\sum_{k=2}^{N} \frac{n_k}{V}\right) \left(\frac{e - \sum_{k=2}^{N} y_k q_k}{\sum_{k=2}^{N} \frac{y_k \hat{C}_{v,k}}{W_k \hat{R}}}\right).$$
 (2.8.4)

Let us now manipulate Eq. (2.8.4). Making use of the next decomposition,

$$\begin{cases} \frac{n}{V} = \frac{nW}{VW} = \frac{\rho}{W},\\ \sum_{k=2}^{N} \frac{n_k}{V} = \frac{n}{V} = \frac{\rho}{W}, \end{cases}$$
(2.8.5)

and by using the mass definition and the ideal gas EOS, the following relations arise,

$$\begin{cases} \rho_k = \frac{m_k}{V}, \\ y_k = \frac{m_k}{m} = \frac{m_k}{V} \frac{V}{m} = \frac{\rho_k}{\rho}, \\ p_{partial, k} = \rho_k \frac{\hat{R}}{W_k} T = \rho \frac{y_k}{W_k} \hat{R} T, \end{cases}$$

where m_k and m denote respectively the mass of species k and the mass of the gaseous mixture. According to the ideal gas EOS, the gas mixture pressure reads,

$$p = \rho \frac{\hat{R}}{W} T. \tag{2.8.6}$$

Using Dalton's law properties, the gas mixture pressure also expresses as,

$$\begin{cases} p = \sum_{k=2}^{N} p_{partial, k}, \\ p = \rho \left(\sum_{k=2}^{N} \frac{y_k}{W_k} \right) \hat{R}T. \end{cases}$$
(2.8.7)

Identifying Eqs. (2.8.6) and (2.8.7), it appears that,

$$\frac{1}{W} = \sum_{k=2}^{N} \frac{y_k}{W_k}.$$
(2.8.8)

Then, from Eq. (2.8.5),

$$\sum_{k=2}^{N} \frac{n_k}{V} = \frac{\rho}{W} = \rho \sum_{k=2}^{N} \frac{y_k}{W_k}.$$
(2.8.9)

Using Eqs. (2.8.4) and (2.8.9), the gas mixture pressure for a gaseous mixture respecting Dalton's law finally reads,

$$p = \frac{\rho\left(\sum_{k=2}^{N} \frac{y_k}{W_k}\right) \left(e - \sum_{k=2}^{N} y_k q_k\right)}{\sum_{k=2}^{N} \frac{y_k/W_k}{\gamma_k - 1}} = \frac{\hat{R}\rho\left(\sum_{k=2}^{N} \frac{y_k}{W_k}\right) \left(e - \sum_{k=2}^{N} y_k q_k\right)}{\sum_{k=2}^{N} \frac{y_k \hat{C}_{v,k}}{W_k}}.$$
 (2.8.10)

A mixture polytropic coefficient can be defined as well. Mayer's relation for ideal gases stats:

$$\hat{C}_p - \hat{C}_v = \hat{R}.$$

The polytropic coefficient is the ratio of the specific heats: $\gamma = \frac{\hat{C}_p}{\hat{C}_v} = \frac{C_p}{C_v}$. Mayer's relation can then be written as:

$$\gamma = 1 + \frac{\hat{R}}{\hat{C}_v} = 1 + \frac{R}{C_v}.$$

Applying this relation to the gas mixture, the mixture polytropic coefficient is found. Using Eq. (2.8.8), relation (2.8.10) expresses as:

$$p = \rho \frac{\hat{R}}{W} \frac{e - \bar{q}}{C_{vm}} = \rho R \frac{e - \bar{q}}{C_{vm}},$$

with $R = \frac{\hat{R}}{W}$, $\bar{q} = \sum_{k=2}^{N} y_k q_k$ and $C_{vm} = \sum_{k=2}^{N} \frac{y_k \hat{C}_{v,k}}{W_k}$. It is then straightforward to find,

$$\begin{split} \gamma &= 1 + \frac{R}{C_{vm}} &= 1 + \frac{\hat{R}/W}{C_{vm}}, \\ \gamma &= 1 + \frac{\hat{R}\sum_{k=2}^{N} \frac{y_{k}}{W_{k}}}{\sum_{k=2}^{N} \frac{y_{k}\hat{C}_{v,k}}{W_{k}}} &= \frac{\left(\sum_{k=2}^{N} \frac{y_{k}\hat{C}_{v,k}}{W_{k}}\right) + \hat{R}\sum_{k=2}^{N} \frac{y_{k}}{W_{k}}}{\sum_{k=2}^{N} \frac{y_{k}\hat{C}_{v,k}}{W_{k}}} = \frac{\left(\sum_{k=2}^{N} \frac{y_{k}\hat{C}_{v,k}}{W_{k}}\right) + \hat{R}/W}{\sum_{k=2}^{N} \frac{y_{k}\hat{C}_{v,k}}{W_{k}}} \\ \gamma &= \frac{C_{vm} + R}{C_{vm}} &= \frac{C_{pm}}{C_{vm}}. \end{split}$$

This well-known result does validate this approach. The opposite mixture model is now to be considered.

Each gas constituent occupies its own volume in pressure and temperature equilibria

We now consider another configuration with separate chemical species. Corresponding mixture rules are,

$$T = T_k$$
 : mixture in temperature equilibrium,
 $v = \sum_{k=2}^{N} y_k v_k$: the total specific volume is the sum of fluid specific subvolumes,
 $p = p_k$: pressure equilibrium among the chemical species,
 $e = \sum_{k=2}^{N} y_k e_k$: mixture internal energy definition.

The ideal gas law for a given species now reads,

$$p_k V_k = n_k \hat{R} T_k$$
 and becomes $p_k V_k = n_k \hat{R} T$.

In mass units, it expresses as,

$$p_k = \frac{n_k W_k}{V_k} \frac{\hat{R}}{W_k} T = \rho_k \frac{\hat{R}}{W_k} T.$$

Consequently, the specific volume of a given chemical species as a function of pressure and temperature reads,

$$v_k = \frac{\hat{R}}{W_k} \frac{T}{p_k}.$$

This result is inserted into the specific volume definition,

$$v = \sum_{k=2}^{N} y_k v_k,$$

yielding,

$$v = \frac{T}{p} \sum_{k=2}^{N} \left(\frac{y_k \hat{R}}{W_k} \right),$$

and

$$p = \rho \hat{R}T \sum_{k=2}^{N} \left(\frac{y_k}{W_k}\right).$$
(2.8.11)

In this last equation, both pressure and temperature equalities have been used. Using the ideal gas EOS and the definition of the mixture internal energy (which is unchanged), the mixture temperature expresses,

$$\begin{cases} e_k = C_{v,k}T_k + q_k = \frac{\hat{C}_{v,k}}{W_k}T_k + q_k, \\ e = \sum_{k=2}^N (y_k C_{v,k}T) + \sum_{k=2}^N (y_k q_k), \\ T = \frac{e - \sum_{k=2}^N (y_k q_k)}{\sum_{k=2}^N (y_k C_{v,k})}. \end{cases}$$
(2.8.12)

Equation (2.8.12) is manipulated with the help of Mayer's relation (2.8.2), resulting in the same relation as in the preceding analysis (Dalton's law, Eq. (2.8.3)),

$$e = \hat{R}T\left(\sum_{k=2}^{N} \frac{y_k/W_k}{\gamma_k - 1}\right) + \sum_{k=2}^{N} y_k q_k.$$
 (2.8.13)

Eliminating the temperature by combining Eqs. (2.8.11) and (2.8.13), the mixture pressure for ideal gases under the assumption of a separate-phase mixture is obtained,

$$p = \frac{\rho\left(\sum_{k=2}^{N} \frac{y_k}{W_k}\right) \left(e - \sum_{k=2}^{N} y_k q_k\right)}{\sum_{k=2}^{N} \frac{y_k/W_k}{\gamma_k - 1}} = \frac{\hat{R}\rho\left(\sum_{k=2}^{N} \frac{y_k}{W_k}\right) \left(e - \sum_{k=2}^{N} y_k q_k\right)}{\sum_{k=2}^{N} \frac{y_k \hat{C}_{v,k}}{W_k}}.$$
(2.8.14)

It then appears that Eqs. (2.8.10) and (2.8.14) are exactly the same. Consequently, when several ideal gases are present, the two mixture models (Dalton's law and separate phases) assuming thermal and mechanical equilibria are strictly equivalent. This is an essential observation for the determination of the mixture equation of state of the present 4-equation model. The previous remark no longer makes sense for mixtures of fluids governed by a NASG-type equation of state [22] as Dalton's law is not valid anymore. A liquid for instance cannot occupy the whole multiphase volume (except of course if it is a one-phase configuration).

The separate-phase strategy of Section 2.2 can then be repeated without any ambiguity for the building of the mixture equation of state in the context of a mixture made of a liquid, its vapor and any non-condensable gases evolving in both mechanical and thermal equilibria. Note that the vapor and the non-condensable gases must be considered as ideal gases for the previous analysis to be valid.

EOS for pure constituent

In this frame, it is assumed that each gaseous constituent (k = 2, ..., N) obeys the ideal gas equation of state. The EOS coefficients for the vapor (species k = 2) must be carefully computed, in accordance with the liquid (k = 1) EOS, as to fit the phase diagram. The building of such an EOS has been addressed in Le Métayer et al. (2004) [53], on the basis of the Stiffened-Gas (SG) EOS. In later developments, the same authors proposed the "Noble-Abel-Stiffened-Gas" (NASG) EOS [22], which improves considerably the liquid specific volume accuracy by taking into account the repulsive molecular effects in addition to those already present in the SG EOS (agitation and attraction). The main formulas for the NASG EOS read for a given constituent k = 1, ... N (liquid, vapor, gas),

$$\begin{cases} p_{k}(v_{k}, e_{k}) = (\gamma_{k} - 1)\frac{(e_{k} - q_{k})}{v_{k} - b_{k}} - \gamma_{k}p_{\infty,k}, \\ T_{k}(p_{k}, v_{k}) = \frac{(v_{k} - b_{k})(p_{k} + p_{\infty,k})}{(\gamma_{k} - 1)C_{v,k}}, \\ g_{k}(p_{k}, T_{k}) = (\gamma_{k}C_{v,k} - q_{k}')T_{k} - C_{v,k}T_{k}\ln\left(\frac{T_{k}^{\gamma_{k}}}{(p_{k} + p_{\infty,k})^{\gamma_{k} - 1}}\right) + b_{k}p_{k} + q_{k}, \\ c_{k}(p_{k}, v_{k}) = \sqrt{\frac{\gamma_{k}v_{k}^{2}(p_{k} + p_{\infty,k})}{v_{k} - b_{k}}}, \end{cases}$$
(2.8.15)

where the following parameters are needed for each phase: γ_k , $p_{\infty,k}$, $C_{v,k}$, q_k , q'_k and b_k . These parameters are constant coefficients characteristic of the thermodynamic properties of the fluid. Among

them the coefficient b_k represents the covolume of the fluid. g_k denotes the phase Gibbs free energy of fluid k, $g_k = h_k - Ts_k$ with h_k and s_k respectively the specific enthalpy and entropy. c_k denotes the speed of sound of fluid k.

The following results can be adapted to the SG EOS framework by setting $b_k = 0$. For all gaseous constituents (k = 2, ..., N), $b_k = 0$ and $p_{\infty,k} = 0$, and the above system reduces to the ideal gas EOS. Note that, for the k-th gaseous constituent, the pressure p_k is based on the subvolume containing the constituent. It is therefore equal to the pressure of the whole gas phase, and not to the partial pressure of the constituent in the gas phase. In the following, it is explicitly stated when a partial pressure is introduced.

The same strategy as in [22] and [53] is repeated in order to find a formulation connecting the saturation pressure and temperature, by equating the liquid and the vapor chemical potentials $g_1 = g_2$, leading to the following equation:

$$\ln(p_{sat} + p_{\infty,2}) = A + \frac{B + E \, p_{sat}}{T_{sat}} + C \ln(T_{sat}) + D \ln(p_{sat} + p_{\infty,1}), \qquad (2.8.16)$$

where,

$$A = \frac{C_{p,1} - C_{p,2} + q'_2 - q'_1}{C_{p,2} - C_{v,2}}, \qquad B = \frac{q_1 - q_2}{C_{p,2} - C_{v,2}},$$

$$C = \frac{C_{p,2} - C_{p,1}}{C_{p,2} - C_{v,2}}, \qquad D = \frac{C_{p,1} - C_{v,1}}{C_{p,2} - C_{v,2}}, \qquad E = \frac{b_1 - b_2}{C_{p,2} - C_{v,2}}.$$
(2.8.17)

For liquid water and steam, the NASG fluid parameters, determined in the [300 - 500] K temperature range are given in Table 2.2. In the same table, the coefficients for air² are given (in the frame of the ideal gas assumption).

Coefficients	Liquid water	Water vapor	air
$C_p (\mathrm{J/kg/K})$	4285	1401	1007
$C_v ~({ m J/kg/K})$	3610	955	719
γ	1.19	1.47	1.4
P_{∞} (Pa)	7028×10^5	0	0
$q~({ m J/kg})$	-1177788	2077616	0
$q'~({ m J/kg/K})$	0	14317	0
$b~({ m m}^3/{ m kg})$	$6.61 imes 10^{-4}$	0	0
W (g/mol)	18	18	29

Table 2.2: Noble-Abel-Stiffened-Gas (NASG) coefficients for water and air determined in the temperature range [300 - 500] K.

These parameters are used in the following computational examples. A comparison between the NASG

 $^{^{2}}$ Note that we only consider mass transfer between liquid and vapor, so the reference energies of the other gas components have no importance. If other mass transfers are to be considered (between gas species), reference energies have to be set appropriately.



EOS and experimental data is displayed in Fig. 2.8, showing good agreement.

Figure 2.8: Comparison between experimental and theoretical saturation curves for liquid l water and steam v with coefficients determined in the temperature range [300 - 500] K. The symbols represent the experimental data. The thick lines represent the NASG theoretical saturation curves and the dash-dotted lines represent the SG theoretical saturation curves. p_{sat} denotes the saturation pressure, L_v the latent heat, h the specific enthalpy and v the specific volume. The SG coefficients are given in Table 2.1 and the NASG coefficients are given in Table 2.2.

Mixture equation of state

Each constituent is assumed to follow the NASG EOS (reduced to the ideal gas EOS for gaseous constituents). However the mixture equation of state, based on mechanical and thermal equilibria has yet to be built. Under the assumption of mechanical and thermal equilibria, an inherent assumption

of the 4-equation model, we have:

$$\begin{cases} T = T_k \quad \forall k, \\ p = p_k \quad \forall k, \\ v = \sum_{k=1}^N Y_k v_k, \\ e = \sum_{k=1}^N Y_k e_k. \end{cases}$$
(2.8.18)

As shown at the beginning of this section, considering (2.8.18) for the mixture of gases is equivalent to Dalton's law. Therefore the computed mixture pressure for the gas mixture is in agreement with both Dalton's law in the gas mixture and with the liquid-gas interface condition of equal pressures. Consequently, System (2.8.18) summarizes correctly the separate-phase mixture model between the liquid and the gas mixture on one hand and the ideal gas mixture on the other hand.

From the expressions given in Eqs. (2.8.15) for pure constituents, the specific volumes and internal energies read,

$$\begin{cases} v_k(p_k, T_k) = \frac{(\gamma_k - 1)C_{v,k}T_k}{p_k + p_{\infty,k}} + b_k, \\ e_k(p_k, T_k) = \frac{p_k + \gamma_k p_{\infty,k}}{p_k + p_{\infty,k}} C_{v,k}T_k + q_k, \end{cases}$$
(2.8.19)

which can be rewritten to give two expressions for the temperature (since $T_k = T, \forall k$),

$$T = \frac{v - \sum_{k=1}^{N} Y_k b_k}{\sum_{k=1}^{N} \frac{Y_k (\gamma_k - 1)C_{v,k}}{p + p_{\infty,k}}},$$
(2.8.20)

$$T = \frac{e - \sum_{k=1}^{N} Y_k q_k}{\sum_{k=1}^{N} Y_k C_{v,k} \left(\frac{p + \gamma_k p_{\infty,k}}{p + p_{\infty,k}}\right)}.$$
 (2.8.21)

Equating these two expressions, and taking into account that $p_{\infty,k} = 0$ and $b_k = 0, \forall k > 1$, a quadratic expression for the mixture pressure is obtained as,

$$p = \frac{b + \sqrt{b^2 + 4ac}}{2a},\tag{2.8.22}$$

with

$$\begin{cases} a = \bar{C}_{v}, \\ b = \left(\frac{e - \bar{q}}{v - \bar{b}}\right) \left(\bar{C}_{p} - \bar{C}_{v}\right) - p_{\infty,1}\bar{C}_{v} - p_{\infty,1}Y_{1}\left(C_{p,1} - C_{v,1}\right), \\ c = \left(\frac{e - \bar{q}}{v - \bar{b}}\right) p_{\infty,1}\left[\bar{C}_{p} - \bar{C}_{v} - Y_{1}\left(C_{p,1} - C_{v,1}\right)\right], \end{cases}$$
(2.8.23)

where mixture quantities are introduced,

$$\bar{C}_v = \sum_{k=1}^N Y_k C_{v,k}, \quad \bar{C}_p = \sum_{k=1}^N Y_k C_{p,k}, \quad \bar{q} = \sum_{k=1}^N Y_k q_k, \quad \bar{b} = \sum_{k=1}^N Y_k b_k.$$
(2.8.24)

Although not trivial, Eq. (2.8.22) ensures the strict positivity of the mixture pressure p: if $Y_1 \neq 1$, both a and c are strictly positive leading to p > (b + |b|)/a. The mixture pressure is then strictly positive. When $Y_1 = 1$, a > 0 and c = 0, and the strict positivity of the pressure is less trivial to demonstrate. However, combining Eqs. (2.8.19) and (2.8.23) in this limit leads to b > 0, and consequently p > 0, where p follows the NASG EOS for the pure liquid phase. Let us add that when $Y_1 = 0$ (absence of liquid), the pressure equation (2.8.22) reduces to

$$p = \left(\frac{e - \bar{q}}{v}\right) \frac{(\bar{C}_p - \bar{C}_v)}{\bar{C}_v}$$

which after substituting $e = \sum_{k=2}^{N} Y_k e_k$, and noticing that $(\bar{C}_p - \bar{C}_v) = \sum_{k=2}^{N} Y_k \hat{R} / W_k$ for ideal gases, leads to,

$$p = \sum_{k=2}^{N} Y_k \rho \hat{R} T / W_k;$$

or, in other words, the classical Dalton's Law for the gas mixture. This provides an additional verification as to the possibility of considering each gas constituent to be in its own volume, as already discussed. Albeit the apparent simplicity of the thermodynamic closure chosen, the phase transition model presented here may be extended to other thermodynamic closures provided each phase EOS is convex.

2.9 Phase transition model

When phase transition is addressed between the liquid and its vapor, only the conservation equations of the first two constituents are modified as,

$$\begin{cases} \frac{\partial(\rho Y_1)}{\partial t} + div(\rho Y_1 \mathbf{u}) &= \rho\nu(g_2 - g_1),\\ \frac{\partial(\rho Y_2)}{\partial t} + div(\rho Y_2 \mathbf{u}) &= -\rho\nu(g_2 - g_1), \end{cases}$$
(2.9.1)

where g_k denotes the phase k Gibbs free energy $g_k = h_k - Ts_k$ with h_k and s_k respectively the specific enthalpy and entropy and $\nu(A_I, p, T)$ represents a relaxation parameter that controls the rate at which thermodynamic equilibrium is reached. It is a function of the specific interfacial area A_I , pressure and temperature. Its determination is possible only when the interfacial area A_I is available, as with droplets and bubbly flows (see Furfaro and Saurel (2016) for example [75]) and sometimes for stratified flows. A natural way to determine this exchange area would be to use a very fine mesh to capture interfaces at all spatial scales. However this strategy would require tremendous computing resources and can hardly be envisaged when considering large-scale problems. Nevertheless a realistic method in specific limit situations is to consider instantaneous thermodynamical relaxation between phases by the use of additional source terms [72]. In the present work, ν is considered very large, so that relaxation to thermodynamic equilibrium is immediate.

During the phase transition process, the mixture specific volume $v = 1/\rho$ and energy e do not vary. The mass fractions for all gas species other than the vapor $(Y_{k\geq 3})$ also remain constant. However, pressure and temperature do vary, reaching their equilibrium values (p^*, T^*) . The phase transition model thus reduces to computing the equilibrium state (p^*, T^*, Y_k^*) , at every time step, from the state described by (p, T, v, e, Y_k) .

Since pressure and temperature are functions of (v, e, Y_k) , and v and e are constant during the phase transition, the primary goal of the procedure is to compute accurately Y_1^* , since Y_2^* is linked through mass conservation,

$$Y_2^* = 1 - Y_1^* - \sum_{k \ge 3} Y_k.$$

In our approach, phase transition is decoupled of transport and wave propagation using a fractional step method, essentially reducing the model to setting $Y_1 = Y_1^*$ and $Y_2 = Y_2^*$ after each hyperbolic step (resolution of System (2.7.2) without mass transfer).

Link between the mass fractions Y_k of the two-phase flow and the mass fractions y_k of the gaseous phase

The separate-phase strategy is used since the presence of liquid naturally imposes this approach when envisioning the whole two-phase flow mixture. However, it has been demonstrated previously that within the gas phase, Dalton's law is actually equivalent to the separate-phase approach in the specific context of ideal gases evolving in both mechanical and thermal equilibria.

The equality of Gibbs free energies $g_1 = g_2$ implies that the partial pressure of the vapor component is equal to the saturation pressure at the current temperature,

$$p_{partial,2} = p_{sat}(T). \tag{2.9.2}$$

Let us first examine the thermodynamic description of the gaseous mixture. According to Dalton's mixture rules, the partial pressure of the vapor species is linked to the volume occupied by the gaseous mixture, to the number of moles and to the temperature as,

$$p_{partial,2}V_g = n_2 RT_g$$

with V_g the volume of the gaseous phase. The pressure of the gaseous mixture is obtained as the sum of the partial pressures, that implies,

$$pV_g = \hat{R}T\sum_{k=2}^N n_k$$

We now define the molar fraction of the vapor species as,

$$x_v = \frac{n_2}{\sum_{k=2}^N n_k}$$

With this definition, the following equation is obtained,

$$x_v = \frac{p_{partial,2}}{p} = \frac{p_{sat}(T)}{p}.$$
 (2.9.3)

This molar fraction is now to be converted into mass fraction,

$$x_v = \frac{\frac{y_2}{W_2}}{\sum_{k=2}^{N} \frac{y_k}{W_k}},$$
(2.9.4)

where y_k represent the mass fractions of the chemical species within the gas phase and are not to be confused with the mass fractions of the whole two-phase flow Y_k . Hence,

$$\sum_{k=2}^{N} y_k = y_2 + \sum_{k=3}^{N} y_k = 1,$$
(2.9.5)

and

$$\begin{cases} v_g = \left(1 - \sum_{k=3}^N y_k\right) v_2(p,T) + \sum_{k=3}^N y_k v_k(p,T), \\ e_g = \left(1 - \sum_{k=3}^N y_k\right) e_2(p,T) + \sum_{k=3}^N y_k e_k(p,T), \end{cases}$$
(2.9.6)

with the subscript $_g$ denoting the combined group of gaseous components. Those last equations are important because it has been previously demonstrated that they lead to Dalton's law for the gaseous mixture. Using Eqs. (2.9.3) and (2.9.4), another equation linking the saturation pressure and the current one is obtained as,

$$p_{sat}(T) = \frac{\frac{y_2}{W_2}}{\sum_{k=2}^N \frac{y_k}{W_k}} p.$$

The pressure p is the one obtained by the 4-equation model (before Gibbs free energy relaxation) and the mass fractions are those transported by the very same model. Indeed, as it will be seen further, there exist simple relations that convert the mass fractions of the two-phase flow Y_k into those of the gaseous mixture y_k .

From Eq. (2.9.3), the saturation relation is used to find the temperature in the gaseous mixture, which is also the temperature of the two-phase flow, at the end of the Gibbs free energy relaxation process:

$$T = T_{sat}(p_{sat}) = T_{sat}(x_v p).$$

$$(2.9.7)$$

Naturally, this temperature is different from the one of the 4-equation system (before Gibbs free energy relaxation). With this temperature (that will be the one of the fluids after the relaxation process converges to the equilibrium state), the following definitions are considered,

$$\begin{cases} v = Y_1 v_1(p, T) + (1 - Y_1) v_g(p, T), \\ e = Y_1 e_1(p, T) + (1 - Y_1) e_g(p, T). \end{cases}$$

Note that the separate-phase approach is now used within the whole two-phase flow. Indeed, since a condensed phase (liquid) is present in the considered flow, only this approach is valid when dealing with a mixture containing a liquid and some gases. Thereby Y_k are used and define the mas fractions of the components present in the two-phase flow.

We now inject Eqs. (2.9.6) into these identities and find,

$$\begin{cases} v = Y_1 v_1(p,T) + (1-Y_1) \left(1 - \sum_{k=3}^N y_k \right) v_2(p,T) + (1-Y_1) \sum_{k=3}^N y_k v_k(p,T), \\ e = Y_1 e_1(p,T) + (1-Y_1) \left(1 - \sum_{k=3}^N y_k \right) e_2(p,T) + (1-Y_1) \sum_{k=3}^N y_k e_k(p,T). \end{cases}$$

Analyzing these last equations, it appears that,

$$Y_k = (1 - Y_1) y_k \quad \text{with} \quad k \ge 3,$$

and then,

$$y_k = \frac{Y_k}{(1 - Y_1)}$$
 with $k \ge 3.$ (2.9.8)

Hence,

$$\begin{cases} v = Y_1 v_1(p, T) + \left(1 - Y_1 - \sum_{k=3}^N Y_k\right) v_2(p, T) + \sum_{k=3}^N Y_k v_k(p, T), \\ e = Y_1 e_1(p, T) + \left(1 - Y_1 - \sum_{k=3}^N Y_k\right) e_2(p, T) + \sum_{k=3}^N Y_k e_k(p, T). \end{cases}$$

We then obtain the following definitions,

$$\begin{cases} Y_1^m = \frac{v - \left(1 - \sum_{k=3}^N Y_k\right) v_2(p, T) - \sum_{k=3}^N Y_k v_k}{v_1(p, T) - v_2(p, T)}, \\ Y_1^e = \frac{e - \left(1 - \sum_{k=3}^N Y_k\right) e_2(p, T) - \sum_{k=3}^N Y_k e_k}{e_1(p, T) - e_2(p, T)}. \end{cases}$$

That is to say,

$$\left\{ \begin{array}{l} Y_1^m = \frac{v - v_g(p,T)}{v_1(p,T) - v_2(p,T)}, \\ Y_1^e = \frac{e - e_g(p,T)}{e_1(p,T) - e_2(p,T)}. \end{array} \right.$$

It is important to note that in these relations,

$$\begin{cases} v_g = \left(1 - \sum_{k=3}^N Y_k\right) v_2(p,T) + \sum_{k=3}^N Y_k v_k(p,T), \\ e_g = \left(1 - \sum_{k=3}^N Y_k\right) e_2(p,T) + \sum_{k=3}^N Y_k e_k(p,T). \end{cases}$$

Also, it is worth mentioning that if $Y_{3\to N} = 0$, then Eqs. (2.6.4) and (2.6.5) of Section 2.6 in the context of a liquid evolving with its own vapor only are recovered.

All these relations are now expressed in terms of mass fractions of the two-phase mixture. Let us then convert relation (2.9.4) with those previously-mentioned mass fractions. Using Eq. (2.9.5), the relation,

$$x_v = \frac{\frac{y_2}{W_2}}{\sum_{k=2}^N \frac{y_k}{W_k}},$$

becomes,

$$x_v = \frac{\frac{1 - \sum_{k=3}^{N} y_k}{W_2}}{\frac{1 - \sum_{k=3}^{N} y_k}{W_2} + \sum_{k=3}^{N} \frac{y_k}{W_k}}.$$

Thanks to relation (2.9.8), this last equation becomes,

$$x_{v} = \frac{\frac{1 - \sum_{k=3}^{N} \frac{Y_{k}}{(1 - Y_{1})}}{W_{2}}}{\frac{1 - \sum_{k=3}^{N} \frac{Y_{k}}{(1 - Y_{1})}}{W_{2}} + \sum_{k=3}^{N} \frac{\frac{Y_{k}}{(1 - Y_{1})}}{W_{k}}},$$

that is to say,

$$x_v = \frac{\frac{1 - Y_1 - \sum_{k=3}^{N} Y_k}{W_2}}{\frac{1 - Y_1 - \sum_{k=3}^{N} Y_k}{W_2} + \sum_{k=3}^{N} \frac{Y_k}{W_k}}.$$

Finally, by use of the saturation constraint,

$$Y_2 = 1 - Y_1 - \sum_{k=3}^{N} Y_k;$$

the sought-after relation is found,

$$x_v = \frac{Y_2/W_2}{Y_2/W_2 + \sum_{k=3}^N Y_k/W_k} = \frac{Y_2/W_2}{\sum_{k=2}^N Y_k/W_k}.$$
(2.9.9)

This equation will simplify dramatically the building of the thermochemical relaxation algorithm as this notation is much more convenient. The mass fractions Y_k , before relaxation, are known from the hyperbolic step.

Expression of the thermochemical equilibrium

When only liquid and vapor are present $(Y_{k\geq 3} = 0)$, as in Section 2.6 [1], the thermochemical equilibrium directly translates into $p^* = p_{sat}(T^*)$, independently of Y_1^* . Here an extra complexity is added, as the vapor *partial* pressure in the gas phase is equal to the saturation pressure at the current temperature.

The relation between p^* and T^* then depends on the composition of the multicomponent gas $Y_{k\geq 2}$. Within ideal gas mixtures, the vapor partial pressure is directly proportional to the vapor molar fraction:

$$p_{partial} = \frac{Y_2/W_2}{\sum_{k \ge 2} Y_k/W_k} p,$$
(2.9.10)

so that the expression satisfied at thermochemical equilibrium is

$$p_{sat}(T^*) = p_{partial} = \frac{Y_2^*/W_2}{\sum_{k \ge 2} Y_k^*/W_k} p^*.$$
(2.9.11)

This relation is indeed essential as it allows equilibrium of liquid and multicomponent gas in conditions below saturation (for instance, existence of water vapor at ambient temperature and pressure).

Solution of a simplified problem

Instead of solving thermochemical equilibrium at constant $v^* = v$, $e^* = e$ and $Y_{k\geq 3}^* = Y_{k\geq 3}$, and computing (p^*, T^*, Y_1^*) , let us assume $p^* = p$, $T^* = T$ and $Y_{k\geq 3}^* = Y_{k\geq 3}$ are constant, and v and eare varying. The thermochemical equilibrium problem is straightforward to solve analytically in these conditions:

Case 1 $T > T_{sat}(p)$: the mixture is necessarily purely gaseous. We then have $Y_1^* = 0$.

Case 2 $T < T_{sat}(p)$: the mixture can be purely gaseous when the vapor quantity does not exceed its saturation limit, to be established hereafter. If this value is reached, then liquid is present.

The attainable limit for the vapor mass fraction before condensation in the multicomponent gas is obtained by solving $p_{partial} = p_{sat}(T)$. Using Eq. (2.9.10), one gets,

$$Y_2^{sat} = \frac{p_{sat}(T)W_2}{p - p_{sat}(T)} \sum_{k \ge 3} Y_k / W_k.$$
 (2.9.12)

Below the saturation temperature, we then have,

$$Y_2^* = \min\left(Y_2^{sat}, 1 - \sum_{k \ge 3} Y_k\right).$$
 (2.9.13)

The equilibrium mass fraction Y_2^* cannot exceed the available room $(1 - \sum_{k\geq 3} Y_k)$, nor can it exceed the saturation limit, after which liquid is present. Y_1^* is then deduced from mass conservation. Figure 2.9 shows the solution for Y_1^* and Y_2^* of this simple problem, for a mixture of liquid water, water vapor and air (N = 3), at atmospheric pressure, and a mixture temperature of 350 K. On the right-hand side of the plot, there is so much air content that water vapor is diluted enough (below the saturation limit), and no liquid is present. On the left part, Y_2^* varies linearly with Y_3 , as a consequence of the saturation relation $p_{partial} = p_{sat}(T)$. The figure also indicates the variation of the mixture specific volume, which increases up to the saturation limit (since the liquid fraction diminishes), and then decreases, because air is heavier than water vapor.



Figure 2.9: Equilibrium mass fractions obtained from water liquid/vapor, as a function of the air mass fraction. Conditions: atmospheric pressure, T=350 K. Dashed line: Y_1^* , dash-dotted: Y_2^* . The thick line represents the specific volume obtained for the mixture in these conditions.

This simplified problem is convenient for two reasons: it illustrates well the problem to be solved, and also provides a simple way to compute initial conditions in a simulation.

When the problem is to be solved at constant (v, e), instead of (p, T), an analytic approach is no

longer possible, and the problem has to be solved numerically. In the following section, we present an alternative to a tedious iterative process.

2.10 Extended thermochemical relaxation algorithm

The idea of our method is to gradually reach the exact solution (typically in 1 to 3 time steps of the flow solver), by providing a fair approximation for Y_1^* , while iterative approaches, such as the one promoted in Le Métayer et al. (2013) [72], directly computes the exact solution. In that direction, we will follow a similar strategy as in our previous work (Section 2.6) [1], extended to the fact that the relation between pressure and saturation pressure is modified compared to Eq. (2.9.11), and now depends on the result (since the partial pressure is a function of Y_2). First, let us bound the equilibrium mass fractions Y_1^* and Y_2^* ,

$$\begin{cases} Y_{min} = \epsilon, \\ Y_{max} = 1 - Y_{min} - \sum_{k=3}^{N} Y_k, \end{cases}$$
(2.10.1)

with $\epsilon \to 0$ for numerical purposes, typically on the order of 10^{-8} . As in our previous work (Section 2.6) [1], we first assume $Y_1^* = Y_{min}$, to check if the system has a solution without liquid. Under this assumption, pressure and temperature are computed by use of the mixture equation of state (2.8.20) and (2.8.22),

$$\begin{cases} p = -p(v, e, Y), \\ T = -T(v, e, Y), \end{cases}$$

since the mixture variables v and e are invariant through phase transition. Additionally, we compute the corresponding partial pressure for vapor Eq. (2.9.10), and compare it to the saturation pressure Eq. (2.8.16). If the partial pressure is below the saturation pressure, no liquid is present and the solution is $Y_1^* = Y_{min}$ and $Y_2^* = Y_{max}$. Note that, unlike in Section 2.6 [1], there is no need to check the existence of the pure liquid phase: no matter how small ϵ is chosen, there will always be a (very small) solution for Y_2^* satisfying that its partial pressure is equal to the saturation pressure. Section 2.11 (about the algorithm's stability) provides additional comments and clarify this last feature. If $Y_1^* \neq Y_{min}$, the following system has to be solved:

$$\begin{cases} p_{partial} = x_v^* \cdot p^* = p_{sat}(T^*), \\ v = Y_1^* v_1(p^*, T^*) + Y_2^* v_2(p^*, T^*) + \sum_{k=3}^N Y_k v_k(p^*, T^*), \\ e = Y_1^* e_1(p^*, T^*) + Y_2^* e_2(p^*, T^*) + \sum_{k=3}^N Y_k e_k(p^*, T^*), \end{cases}$$
(2.10.2)

leaving us with three equations for three unknowns (p^*, T^*, Y_1^*) . The vapor molar fraction x_v^* is defined as,

$$x_v^* = \frac{Y_2^*/W_2}{Y_2^*/W_2 + \sum_{k=3}^N Y_k/W_k}.$$
(2.10.3)

We will now evaluate three approximate expressions for Y_1^* . Rewriting the specific volume definition from System (2.10.2) leads to the following approximate expression,

$$Y_1^m(p,T) = \frac{v - v_g(p,T)}{v_1(p,T) - v_2(p,T)}, \quad \text{with} \quad v_g(p,T) = \left(1 - \sum_{k=3}^N Y_k\right) v_2(p,T) + \sum_{k=3}^N Y_k v_k(p,T).$$
(2.10.4)

Any mass fraction computed from this formula after the hyperbolic step will satisfy the mass conservation $\forall (p, T)$. Similarly, we can rewrite the specific mixture energy definition from System (2.10.2),

$$Y_1^e(p,T) = \frac{e - e_g(p,T)}{e_1(p,T) - e_2(p,T)}, \quad \text{with} \quad e_g(p,T) = \left(1 - \sum_{k=3}^N Y_k\right) e_2(p,T) + \sum_{k=3}^N Y_k e_k(p,T).$$
(2.10.5)

Equations for $Y_2^m(p,T)$ and $Y_2^e(p,T)$ (expressed for the vapor phase instead of the liquid phase) can be obtained as,

$$Y_2 = 1 - Y_1 - \sum_{k=3}^{N} Y_k.$$

In Section 2.6 [1], these two functions of (p,T) could be reduced to functions of p in finding the equilibrium as $p = p_{sat}(T)$ for a liquid-vapor mixture. As shown in Eq. (2.9.11), the new relation $p_{partial} = p_{sat}(T^*)$ includes an additional dependence on Y_2^* (or, equivalently, on Y_1^*), leading to Eq. (2.9.11), reminded here:

$$Y_2^{sat}(p,T) = \frac{p_{sat}(T)W_2}{p - p_{sat}(T)} \sum_{k \ge 3} Y_k / W_k.$$
(2.10.6)

The exact solution to the problem relies on determining pressure and temperature satisfying all three equations of System (2.10.2), or, equivalently:

$$Y_2^m(p^*, T^*) = Y_2^e(p^*, T^*) = Y_2^{sat}(p^*, T^*).$$

This is illustrated in Fig. 2.10, for a set of conditions initially out of equilibrium (30 K below saturation).



Figure 2.10: Illustration of the algorithm for the multicomponent phase transition solver. From light gray to dark gray: $Y^m(p^*, T^*), Y^e(p^*, T^*), Y^{sat}(p^*, T^*)$. The exact solution to the problem is found at the intersection of the three surfaces. The value from hyperbolic step corresponds to the initial conditions of the algorithm: $Y_2 = 2.Y_2^*$ (far from equilibrium) at p = 1 atm, $T = T_{sat}(p) - 30$ K = 343 K, and $Y_3 = 0.1$. Here, computations lead to $Y_2^* = 0.1$, $Y^m = 0.11$, $Y^e = 0.09$, $Y^{sat} = 0.03$, so that the algorithm retains Y^m , within 10% of the exact solution.

In this graph,

- the light gray surface represents the mass conservation condition: $Y_2^m(p,T)$,
- the medium gray surface represents the energy conservation condition: $Y_2^e(p,T)$,
- the dark gray surface, represents the thermochemical equilibrium condition: $Y_2^{sat}(p,T)$.

The algorithm consists in computing three approximations for Y_2^* :

- $Y^m = Y_2^m(p,T)$ is evaluated for the initial values of (p, x_v) (from the hyperbolic step), and $T = T_{sat}(x_v \cdot p),$
- $Y^e = Y_2^e(p,T)$ is evaluated for the initial values of (p, x_v) (from the hyperbolic step), and $T = T_{sat}(x_v \cdot p),$
- $Y^{sat} = Y_2^{sat}(p, T)$ is evaluated at the initial (p, T).

As in Section 2.6 [1], the idea of this method is then to pick the value with the smallest variation, under the condition that all three associated mass transfers are of the same sign. This idea is reminiscent of the well-known Minmod slope limiter widely used in high-order CFD solvers for limitation of gradients. In other words, we introduce:

$$\begin{cases} r_1 = (Y^m - Y_2) (Y^e - Y_2), \\ r_2 = (Y^m - Y_2) (Y^{sat} - Y_2), \end{cases}$$
(2.10.7)

where Y_2 is the initial mass fraction (from the hyperbolic step), and Y^m, Y^e, Y^{sat} are three estimates for the equilibrium Y_2^* ,

- If $r_1 < 0$, or $r_2 < 0$, no mass transfer happens: $Y_2^* = Y_2$.
- Else, the minimum mass transfer is used. For instance, if Y^m is the closest value to Y_2 (out of Y^m, Y^e, Y^{sat}), then $Y_2^* = Y^m$.

Under the latter condition, it can be implemented as:

$$Y_2^* = Y_2 + sgn\left[Y^m - Y_2\right] \times Min\left[|Y^m - Y_2|, |Y^e - Y_2|, |Y^{sat} - Y_2|\right].$$
(2.10.8)

Summary of the procedure:

1) Search for a solution without liquid

- The limit case $Y_l^* \to \epsilon$ is considered with computation of the pressure and temperature according to the mixture equations of state (2.8.20) and (2.8.22). Additionally the corresponding saturation pressure and partial pressure for vapor are computed according to Eqs. (2.8.16) and (2.9.10).
- If the partial pressure is below the saturation pressure, no liquid is to be considered and the solution is $Y_1^* = Y_{min}$ and $Y_2 = Y_{max}$ according to Eq. (2.10.1).

2) If liquid is present, thermodynamic equilibrium is to be computed

- Computation of the liquid mass fraction at equilibrium Y_1^* is done according to the Minmod-like procedure Eqs. (2.10.7), (2.10.8) using Eqs. Y^m (2.10.4), Y^e (2.10.5), Y^{sat} (2.10.6), and the EOS (2.8.19).

2.11 Algorithm's stability

In the present work's context, we can find a value for the vapor mass fraction $Y_2 = Y_{vap}$, no matter the conditions given, as traces of non-condensable gas are present $Y_3 = Y_{air}$. For instance, at 300 K and 1 atm for a mixture of liquid water, vapor water and air, assuming $Y_3 = \epsilon$ (which can be as small as numerically allowed) will lead to a very small but non-zero Y_2 . With these considerations, the transition from "pure" liquid into two-phase mixture is continuous.

Additionally, let us note that presence of air in water is physical (dissolved), and can be estimated through Henry's law. For instance, in ambient conditions, the air mass fraction dissolved is of the order of $Y_3 = 10^{-5}$, leading to a value of Y_2 of the same order, satisfying System (2.10.2). Indeed, such low values do not have significant effect on mean density and energy, which remain close to the pure phase values.

In practical computations presented in the following, unless stated otherwise, a small value is set for Y_3 in the "pure" liquid, and Y_2 is computed accordingly, following Eq. (2.9.13) for the initial prescribed pressure and temperature.

Another key property responsible for the algorithm's stability is that $\forall (p,T)$ (a priori away from the equilibrium point), the exact solution for Y_2^* always lies between the minimum and maximum values of $Y_2^m(p,T)$, $Y_2^e(p,T)$, $Y_2^{sat}(p,T)$. This is clearly visible in Fig. 2.10. Although we have not proved this result because of the non-linear dependence of $p_{sat}(T)$ (as in our previous contribution, Section 2.6 [1]), we have not found a case in which this does not apply. As a consequence:

- If $Y_2 > Y_2^*$ initially, mass transfer will be activated only if Y^m, Y^e and Y^{sat} are all smaller than Y_2 . Given the above property, one of them at least is superior to Y_2^* . The algorithm then cannot "overestimate" the mass transfer.

- The same thing can be said when $Y_2 < Y_2^*$ initially.
- Last but not least, since $0 < Y_2 < 1 \sum_{k \ge 3} Y_k$ (given the hyperbolic step is properly implemented) and the exact solution also satisfies $0 < Y_2^* < 1 \sum_{k \ge 3} Y_k$, the approximate solution from the algorithm can never go out of bounds.

2.12 Numerical results

In the current context, non-condensable gases are present. The proposed relaxation solver is to be compared to an iterative algorithm such as the one promoted in Le Métayer et al. (2013) [72]. Unlike this last algorithm, the notion of vapor molar fraction and partial pressures in the gas phase must be taken into account, bringing additional difficulties. The corresponding iterative solver is consequently recalled and modified in Appendix B.1.

To illustrate robustness and accuracy of the relaxation algorithm, a shock tube containing liquid water, its own vapor and some non-condensable air is considered, with variable initial conditions. Shock tube tests appear as excellent benchmarks as the flow contains shock waves, contact discontinuities and rarefaction fans that create some arduous conditions. In this section, the tube is 1 meter long and the initial discontinuity is located at 0.5 meter. Boundary conditions are non-reflecting ones. The computations that follow are addressed with the MUSCL method using van Leer's slope limiter and the HLLC Riemann solver (see Toro (1997) [58], Saurel et al. (2016) [8] for details). This section compares the results obtained with the present relaxation solver and the classic root-finding method given in Appendix B.1. Unless stated otherwise, the one-dimensional simulations are carried out on meshes with 100 cells.

Shock tube test with a mixture far from the phase bounds

A two-phase mixture with initial mass fractions set to $Y_1 = 0.1$ (liquid), $Y_2 = 0.2$ (vapor) and $Y_3 = 0.7$ (air) is considered throughout the entire tube with an initial pressure ratio of 2, resulting in the presence of initial density and temperature discontinuities. In order to find an initial thermodynamic equilibrium, the temperatures in both chambers are deduced as,

$$T = T_{sat} (x_v p) \quad \text{with} \quad x_v = \frac{Y_2/W_2}{Y_2/W_2 + \sum_{k=3}^N Y_k/W_k}.$$
 (2.12.1)

The mixture density is then computed as,

$$\rho = \frac{1}{v} \quad \text{with} \quad v = \sum_{k=1}^{N} Y_k v_k(p, T),$$
(2.12.2)

where $v_k(p,T)$ is given by Eq. (2.8.19). The results are shown at time $t \approx 1$ ms in Fig. 2.11.



Figure 2.11: Comparison of the present relaxation algorithm (thick lines) versus the iterative solver (symbols). Shock tube test with a two-phase mixture made of liquid water, vapor water and air. The dotted lines represent the solution without phase transition. The dashed lines represent the initial conditions: $p_l = 2 \cdot 10^5$ Pa, $p_r = 10^5$ Pa, $u_l = u_r = 0$ m.s⁻¹, $Y_1^{left} = Y_1^{right} = 0.1$, $Y_2^{left} = Y_2^{right} = 0.2$ and $Y_3^{left} = Y_3^{right} = 0.7$. Final time: $t \approx 1$ ms. Mesh: 100 cells. For the sake of clarity, only 50 symbols out of 100 are plotted for the iterative method.

Excellent agreement is obtained between the present relaxation solver and the iterative method. The shock compression yields evaporation and the expansion wave results in condensation in this example.

Shock tube test with a mixture with air in major proportions

Mass fractions of the previous test were given as inputs and the temperatures were deduced in order to respect initial thermodynamic equilibrium. Let us now consider a different point of view. As it is easier to measure or impose temperature in a given flow, it is now used as initial input. Pressures, velocities and the mass fraction of the non-condensable gas (air) remain inputs as well. Proportions of liquid and vapor are then deduced according to Eq. (2.9.13).

The following test considers a shock tube with an initial pressure ratio of 2 and initial temperature of T = 293 K throughout the tube. The air mass fraction is initially set to $Y_3 = 0.98$ in the whole tube. The liquid and vapor mass fractions are then deduced as $Y_1 \simeq 1.073 \cdot 10^{-2}$ and $Y_2 \simeq 9.263 \cdot 10^{-3}$ in the left chamber and $Y_1 \simeq 1.186 \cdot 10^{-3}$ and $Y_2 \simeq 1.881 \cdot 10^{-2}$ in the right chamber. The results are shown at time $t \approx 1$ ms in Fig. 2.12.

Excellent agreement is obtained between the two solvers. The shock compression results in total evaporation of the liquid water and the rarefaction results in condensation. Disappearance of liquid water is computed without oscillations by the two methods. Note that the specific management of pure phases is handled by Eq. (2.10.1) for both algorithms ("Minmod-type" and iterative).

Shock tube test with a mixture mainly made of liquid water

Mass fractions from the previous test case are reversed by considering $Y_3 = 10^{-5}$ and T = 293K initially throughout the tube, corresponding to a subcooled liquid. The following test considers a shock tube with an initial pressure ratio of 2. The liquid and vapor mass fractions are then deduced as $Y_1 \simeq 0.9999899$ and $Y_2 \simeq 9.426 \cdot 10^{-8}$ in the left chamber and $Y_1 \simeq 0.99989$ and $Y_2 \simeq 1.919 \cdot 10^{-7}$ in the right chamber. The results are shown at time $t \approx 1.5$ ms in Fig. 2.13.

Excellent agreement is again obtained between the two solvers. The liquid phase having the highest internal heat capacity, the resulting flow is quasi-isothermal despite the slight evaporation and condensation processes appearing through the shock and rarefaction.

Double expansion test with a two-phase mixture mainly made of liquid water

The following test mimics cavitation in an initial subcooled liquid. The initial pressure, temperature and air mass fractions are respectively 1 bar, T = 293 K and $Y_3 = 10^{-5}$ throughout the entire tube. The liquid and vapor mass fractions are then deduced as $Y_1 \simeq 0.99989$ and $Y_2 \simeq 1.919 \cdot 10^{-7}$ in



Figure 2.12: Comparison of the present relaxation algorithm (thick lines) versus the iterative solver (symbols). Shock tube test with a two-phase mixture with air in major proportions. The dotted lines represent the solution without phase transition. The dashed lines represent the initial conditions: $p_l = 2 \cdot 10^5$ Pa, $p_r = 10^5$ Pa, $u_l = u_r = 0$ m.s⁻¹, $Y_1^{left} \simeq 1.073 \cdot 10^{-2}$, $Y_1^{right} \simeq 1.186 \cdot 10^{-3}$, $Y_2^{left} \simeq 9.263 \cdot 10^{-3}$, $Y_2^{right} \simeq 1.881 \cdot 10^{-2}$ and $Y_3^{left} = Y_3^{right} = 0.98$. Final time: $t \approx 1$ ms. Mesh: 100 cells. For the sake of clarity, only 50 symbols out of 100 are plotted for the iterative method. Full liquid evaporation is correctly computed by both methods.



Figure 2.13: Comparison of the present relaxation algorithm (thick lines) versus the iterative solver (symbols). Shock tube test with a two-phase mixture mainly made of liquid water. The dotted lines represent the solution without phase transition. The dashed lines represent the initial conditions: $p_l = 2 \cdot 10^5 \text{ Pa}, p_r = 10^5 \text{ Pa}, u_l = u_r = 0 \text{ m.s}^{-1}, Y_1^{left} \simeq 0.9999899, Y_1^{right} \simeq 0.999899, Y_2^{left} \simeq 9.45 \cdot 10^{-8}, Y_2^{right} \simeq 1.919 \cdot 10^{-7} \text{ and } Y_3^{left} = Y_3^{right} = 10^{-5}$. Final time: $t \approx 1.5 \text{ ms}$. Mesh: 100 cells. For the sake of clarity, only 50 symbols out of 100 are plotted for the iterative method.
the left and right chambers. The initial velocity is set to -1 m.s^{-1} at left and $+1 \text{ m.s}^{-1}$ at right. The results are shown at time $t \approx 3.5$ ms in Fig. 2.14.



Figure 2.14: Comparison of the present relaxation algorithm (thick lines) versus the iterative solver (symbols). Double expansion test with a mixture mainly made of liquid water. The dotted lines represent the solution without phase transition. The dashed lines represent the initial conditions: $p_l = p_r = 10^5$ Pa, $u_l = -1$ m.s⁻¹, $u_r = +1$ m.s⁻¹, $Y_1^{left} = Y_1^{right} \simeq 0.99989$, $Y_2^{right} = Y_2^{right} \simeq 1.919 \cdot 10^{-7}$ and $Y_l^{air} = Y_r^{air} = 10^{-5}$. Final time: $t \approx 3.5$ ms. Mesh: 100 cells. For the sake of clarity, only 50 symbols out of 100 are plotted for the iterative method.

Excellent agreement is again obtained between the two solvers. Appearance of vapor in the liquid is computed without oscillations by the two methods.

2.13 Computational time, efficiency and simplicity

All computational examples considered in this multicomponent-gas-phase context led to the same observation: the present relaxation solver is much faster than the iterative algorithm given in Appendix B.1. The CPU saving is at least 50% in all reported cases. The main argument for this time gain is related to its simplicity: the relaxation solver is direct whereas the iterative method requires solving a non-linear-algebraic system that may cause difficulties as a result of non-linearities. Besides, the root-finding method requires the calculation of the saturation pressure via Eq. (2.8.16) at each iterative

step, which itself requires an iterative method.

In practical applications, fine discretization is usually used on zones of interest. However, as the method is not iterative, and converges after some time steps, it is interesting to address its robustness and accuracy in situation with both coarse space and time resolutions. To this end, Fig. 2.15 repeats the test case already presented in Fig. 2.12, with a 10-cell mesh and first-order Godunov numerical scheme. These results are very reasonable, illustrating the robustness of the method and its correct behavior even on coarse meshes.

Results for the same test case are also given in Fig. 2.15 for a higher-order solver (MUSCL scheme with the Superbee limiter), on a 1000-cell mesh. Again, excellent agreement is found between the present relaxation solver and the iterative method. Robustness of the present method thus seems quite independent of mesh resolution and order of accuracy of the numerical scheme.



Figure 2.15: Comparison of the present relaxation algorithm (thick lines) versus the iterative solver (symbols). Shock tube test with a two-phase mixture mainly made of air, computed on coarse (left figure) and fine (right figure) meshes to assess method robustness. The dashed lines represent the initial conditions: $p_l = 2 \cdot 10^5$ Pa, $p_r = 10^5$ Pa, $u_l = u_r = 0$ m.s⁻¹, $Y_1^{left} \simeq 1.073 \cdot 10^{-2}$, $Y_1^{right} \simeq 1.186 \cdot 10^{-3}$, $Y_2^{left} \simeq 9.263 \cdot 10^{-3}$, $Y_2^{right} \simeq 1.881 \cdot 10^{-2}$ and $Y_3^{left} = Y_3^{right} = 0.98$. Final time: $t \approx 0.5$ ms. The figure on the left represents the solution with a 10-cell mesh and first-order Godunov numerical scheme. The figure on the right represents the solution with a 1000-cell mesh and MUSCL scheme with Superbee limiter. For the sake of clarity, only 50 symbols out of 1000 are plotted for the iterative method in the figure on the right. The relaxation method and iterative one tend to the same solution even with the coarse mesh.

2.14 Multi-dimensional illustrations

Evaporating liquid jet

In this section, the capabilities of the flow model are illustrated on an evaporating liquid jet configuration in conditions typical of cryotechnic rocket engines during the ignition phase (for which the engine has not yet reached supercritical conditions). The flow consists of a coaxial liquid oxygen jet surrounded by a high-speed hydrogen flow, injected in conditions above the saturation point of the inner oxygen core, which then evaporates whilst being destabilized. Such a case is very challenging, because there is initially no vapor oxygen, and the phase transfer model developed is the only possible term for vapor production. The Stiffened-Gas EOS is used, the parameters for oxygen and hydrogen are given in Table 2.3.

Coefficients	Liquid phase (O_2)	Vapor phase (O_2)	Hydrogen (H_2)
$C_p ~({\rm J/kg/K})$	1702	780	14256
$C_v ~({ m J/kg/K})$	695	531	10183
γ	2.45	1.47	1.4
P_{∞} (bar)	1062	0	0
$q~({ m J/kg})$	-258000	6900	-1.2×10^6
$q'~({\rm J/kg/K})$	0	-9280	0

Table 2.3: Stiffened-Gas coefficients for the simulation of the evaporating liquid jet.

The 2D computations are carried out on a simplified geometry given in Fig. 2.16.



2.5

2.5

Figure 2.16: Geometrical data for half the computational domain of the evaporating liquid jet.

G

Η

0

100

40

40

The inlet boundary conditions correspond to two subsonic inflows:

-2

-20

С

D

- central flow made of nearly pure liquid oxygen, at 100 K and 30 m.s⁻¹, pressure 3 MPa along segment AB of Fig. 2.16,
- peripheral flow made of nearly pure gaseous hydrogen, at 150 K and 200 m.s⁻¹, with the pressure of 3 MPa along segment DE of Fig. 2.16,

and one subsonic outlet, along segments GH and HI, where non-reflecting subsonic boundary condition is imposed at 3 MPa. The remaining walls are treated as symmetric boundary conditions. The mesh consists of about 360,000 triangles, with a spatial discretization varying from 0.1 mm in the jet to 0.6 mm in the far field.

The small scale destabilization of the liquid jet requires to extend the numerical solver presented in Saurel et al. (2016) [8] to second order. This was achieved following the MUSCL scheme with the Superbee limiter, as detailed for example in Toro (1997) [58].

Two computations have been carried out on the same mesh, with the aim of studying the effect of the thermochemical relaxation on jet destabilization. The contours of mass fraction of liquid oxygen as obtained with and without evaporation effects are compared in Figs. 2.17.a and 2.17.b, showing serious changes due to phase transition.





d) with phase change: Y_2

Figure 2.17: Fragmentation of a liquid O_2 jet by a coaxial high-speed H_2 current. The results from Figs. b), c) and d) are from the same computation, whereas Fig. a) is taken at the same time, from a computation without phase transition. All results present mass fraction contours, on the same color map. Figs. a) and b) compare the liquid mass fraction of oxygen without and with phase transfer. Fig. d) shows the contour of vapor oxygen resulting from the liquid jet evaporation. Fig. c) represents the sum $Y_1 + Y_2$ (Fig. b+d), showing a total mass fraction of oxygen, to be compared to the case without mass transfer (Fig. a).

As expected, the filaments separating the main liquid core and the gas gradually vanish as a consequence of evaporation, resulting in much steeper contours of liquid mass fraction in the vicinity of the jet, and very few pockets of liquid with significant life time. Figure 2.17.d shows the contour of

vapor oxygen (which indeed remains at zero in the case without phase transfer). Figure 2.17.c plots the total oxygen mass fraction contour $(Y_1 + Y_2)$. It can also be compared to Fig. 2.17.a.

Although the results in terms of total mass fraction for oxygen qualitatively seem close whether or not the mass transfer is activated, it is clear that the vapor mass fraction is of utmost importance for future works, which shall include the gaseous combustion between vapor oxygen and hydrogen.

Capillary effects are not included in these simulations, as the intense velocity gradients make them negligible in the present jet destabilization conditions. However, capillary effects may be of importance when the filaments start separating from the jet and will be included in future works, following the approach presented in Le Martelot et al. (2014) [82].

Explosive liquid water dispersal into air

The present relaxation solver has been presented in the context of the 4-equation formulation. This model considers mechanical and thermal equilibria but thermochemical disequilibrium. However the relaxation solver is not restricted to such a model and can be extended to non-equilibrium hyperbolic flow models, such as Baer and Nunziato's (1986) [49] and its reduced versions. This last model is a 7-equation formulation assuming mechanical, thermal and chemical disequilibria. Thereby, finding local thermodynamic equilibrium requires extra ingredients such as velocity, pressure and temperature relaxation solvers such as the ones given in [72, 86]. We propose here to repeat the explosive liquid water dispersal test presented in Furfaro and Saurel (2015) [88] with the 4 and 7-equation models. The test consists in a cylindrical gas-liquid explosion schematically represented in Fig. 2.18. The results are given in Fig. 2.19.



Figure 2.18: Schematic representation of the cylindrical gas-liquid explosive system. A cylindrical explosive charge is surrounded by a liquid water layer. The internal cylinder is 160 mm long with a 52 mm radius and is initially filled with nearly pure dense gas (1500 kg/m³) at high pressure (7000 MPa). The external cylinder is 160 mm long with a 96 mm radius and is initially filled with nearly pure liquid water (1000 kg/m³) at atmospheric pressure (0.1 MPa). Atmospheric conditions with nearly pure gas (1 kg/m³) at 0.1 MPa are considered around both cylinders.



Figure 2.19: Vapor mass fraction created during a 2D cylindrical gas-liquid explosive dispersal. The figure compares the results obtained with the 4-equation model (mechanical and thermal equilibria, top) and with the 7-equation model (total disequilibrium, bottom) after relaxation of the velocities, pressures, temperatures following the relaxation solvers presented in [72] and phase transition consideration through the relaxation method presented in this chapter. The results computed by both models are in close agreement.

No noticeable changes are visible in Fig. 2.19 illustrating the capabilities of the relaxation solver to model phase change in both 7-equation and 4-equation models. An evaporation front is clearly visible with both models.

2.15 Conclusion

A simple relaxation solver has been built, able to deal with phase transition between a liquid phase and a multicomponent gas phase. Computational examples have shown that the method converges to the same solution as methods based on iterative (and exact) equilibrium solvers. The Minmod-type treatment of the source term is the main ingredient of the thermochemical relaxation algorithm.

Several features are in favor of the present solver compared to iterative ones:

- CPU savings over 50%,
- high simplicity of implementation and verification,
- increased robustness with high-order methods.

This is reached without any noticeable loss of accuracy.

This research can be continued in many directions. Among them, consideration of supercritical fluids in the same theoretical frame appears important. This task is undertaken in Chapter 3. Another perspective deals with the consideration of combustion effects within the gas phase.

Acknowledgements

This work has been done in cooperation with Dr. Pierre Boivin. Dr. Damien Furfaro and Dr. François Fraysse are gratefully acknowledged for carrying out the simulations presented in Fig. 2.19.

Part of this work has been carried out in the framework of the Labex MEC (ANR-10-LABX-0092) and of the A*MIDEX project (ANR-11-IDEX-0001-02), funded by the «Investissements d'Avenir» French Government program managed by the French National Research Agency (ANR). We also acknowledge funding from ANR through project SUBSUPERJET, ANR-14-CE22-0014.

Part III

Equations of state

Introduction

The three states of a fluid (liquid, vapor, supercritical) present radically different thermodynamic behaviors. For instance, the speed of sound of a liquid is generally higher than the sound speed of a gas. The standard density is also representative of a fluid, as well as its compressibility and its heat capacity. The most common thermodynamic description relies on cubic equations of state (EOS), the basic prototype being the van der Waals (VdW) EOS. Indeed, the VdW EOS involves all possible effects occurring in matter, *i.e.* agitation, attraction and repulsion within a unique formulation. This thermodynamic modeling is consequently attractive as it is able to describe (at least qualitatively) liquid, vapor and supercritical states as well as two-phase mixtures. Unfortunately, the use of this EOS, as all cubic ones, implies a loss of hyperbolicity (through the convexity of the EOS) within the two-phase mixture region. An isentropic curve is represented in Fig. 2.20 and displays this behavior.



Figure 2.20: Thermodynamic path according to the van der Waals representation in the (p, v) plan alongside an isentropic curve. The square speed of sound $c^2 = -v^2 (\frac{\partial P}{\partial v})_s$ is well-defined in the pure liquid zone where the slope of the isentrope is negative as well as in the pure gas zone, but it is not defined in the two-phase zone.

Cubic EOSs present an inadmissible behavior regarding acoustic wave propagation during phase change. In the present manuscript, convex EOSs are addressed and used in hyperbolic two-phase flow models, phase transition being considered through the stiff thermochemical relaxation solver of Chapter 2. The recent Noble-Abel-Stiffened-Gas (NASG) equation of state (Le Métayer and Saurel (2016) [22]) is a well-posed formulation that involves the various molecular effects present in matter while remaining simple. Nevertheless, the NASG EOS is only well-suited in a limited temperature range [22]. In Chapter 3, large temperature and pressure variation ranges are considered to address supercritical conditions. Consequently, the range of validity of the convex NASG EOS is to be extended in view of future industrial applications. This topic is addressed in the next chapter where the ENASG equation of state is developed ("E" stands for "Extended"). Its particular interest relies on variable attractive and repulsive effects that consequently extend the range of validity of the NASG description where they are considered constant.

Chapter 3

Extended Noble-Abel-Stiffened-Gas equation of state for sub-and-supercritical liquid-gas systems far from the critical point

Abstract

The Noble-Abel-Stiffened-Gas (NASG) equation of state (Le Métayer and Saurel (2016) [22]) is extended to variable attractive and repulsive effects to improve the liquid phase accuracy when large temperature and pressure variation ranges are considered. The transition from pure phase to supercritical state is of interest as well. The gas phase is considered through the ideal gas assumption with variable specific heat rendering the formulation valid for high temperatures. The liquid equationof-state constants are determined through the saturation curves making the formulation suitable for two-phase mixtures at thermodynamic equilibrium. The overall formulation is compared to experimental characteristic curves of the phase diagram showing good agreement for various fluids (water, oxygen). Compared to existing cubic equations of state the present one is convex, a key feature for computations with hyperbolic flow models.

3.1 Introduction

Modeling liquid-gas systems with or without phase transition is an old research topic in the physics community but still challenging at both theoretical and computational levels. The most common thermodynamical approach relies on cubic equations of state (EOS), the van der Waals one being the basic prototype. Indeed, this EOS involves all relevant molecular effects present in matter, *i.e.*, thermal agitation, short distance repulsive forces and long range attractive ones. It is thus able to deal, at least qualitatively, with pure liquid, pure gas and two-phase mixture. This EOS, as all cubic ones, is aimed to close flow models based on balance equations of mass, momentum and energy for the mixture. The Euler equations are one of the relevant possible options, as well as more sophisticated ones aimed to model capillary effects, such as the Cahn and Hilliard (1958) [34] model for example. In this context, the thermodynamical state is determined from two internal variables only, the density and the internal energy of the mixture, or alternatively the density and the temperature, depending on the formulation of the equations. This approach consequently seems simple, but involves serious difficulties and limitations:

- The first and certainly the most obvious and limiting is related to its inability to deal with liquid and non-condensable gas separated by well-defined interfaces, such as for example interfacial flows of liquid water and air. The thermodynamics of these two media being considered as discontinuous, specific theoretical and numerical treatments have been addressed. In this context, Arbitrary Lagrangian Eulerian (Hirt et al. (1974) [29]), Interface Reconstruction (Youngs (1984) [89]), Front Tracking (Glimm et al. (1998) [31]), Level-Set (Fedkiw et al. (1999) [33]), anti-diffusion (Kokh and Lagoutiere (2010) [90]) methods are possible options. Another approach relies on continuous models with extra internal variables, such as volume and mass fractions and extended equation of state. Examples of such models are the Kapila et al. (2001) [5] one and its extension with phase transition (Saurel et al. (2008) [18]), to cite a few. With these formulations the same equations are solved everywhere routinely, in pure liquid, pure gas and interface which becomes a diffuse zone. These models are indeed often named "diffuse interface methods" (Saurel and Pantano (2018) [91]). In this approach, hyperbolic models with relaxation are considered and each phase evolves in its own volume, with its own thermodynamics. In particular there is no need to address cubic formulations. When phase transition is addressed, it occurs through mass transfer terms that can be considered finite rate (Saurel et al. (2008) [18], Furfaro and Saurel (2016) [75]) or assumed stiff when the physical knowledge of the phase change kinetics is insufficiently documented (Le Métayer et al. (2013) [72], Chiapolino et al. (2017) [1], [19], Chapter 2) or unnecessary.
- The second limitation is related to the lack on convexity of cubic EOSs, having dramatic con-

sequences on sound propagation during phase transition. The square sound speed becomes negative in the spinodal decomposition zone, such behavior being unphysical.

- The third limitation is related to the description of phase transition with such EOSs. Cubic equations
 of state consider phase transition as a thermodynamic process and not a kinetic one. It is unclear
 at this level whether cubic EOSs are limited to the description of global two-phase mixtures with
 many interfaces and not local ones, at the scale of a single interface.
- The fourth, but possibly not the last, is related to the numerical treatment of boundary conditions (BC) in practical compressible flow computations. Subsonic inflow and outflow BCs rely on stagnation enthalpy and entropy invariance coupled to Riemann invariants that can be defined and computed correctly only if the equation of state is well-posed. The second issue related to EOS convexity consequently reemerges at this level. Moreover, the practical expression of Riemann invariants may be inextricable with these EOSs.

This list of arguments gives motivations to the present work where an extended version of the Noble-Abel-Stiffened-Gas (NASG, Le Métayer and Saurel (2016) [22]) EOS is examined to:

- Represent the thermodynamics of pure liquid, pure vapor and supercritical fluid. Combination of the pure liquid and pure vapor EOSs must be able to represent as accurately as possible the two-phase region.
- Each phase EOS must be convex in its respective domain.
- The EOS must be as simple as possible, while remaining accurate, to simplify practical computations and building of mixture EOS in hyperbolic multiphase flow models.

Hyperbolic multiphase flow models have demonstrated their ability to solve a wide range of complex flow situations in severe conditions. Material interface problems [17] (Chapter 1), chemical reactions [7], phase change [8] (Chapter 2), surface tension [9], solid-fluid [10], plastic transformation [11], dense and dilute flows [92], shallow water flows [26] (Chapter 4) can be cited for instance. In these flow models, compressibility of each phase is responsible for the hyperbolic character of the equations and an appropriate and convex EOS is required for each fluid.

The NASG EOS combines relevant physics and simplicity. Its predictions are in a good agreement with experimental data but in restricted temperature range, [300 - 500] K for example with liquid water at saturation. This limitation is linked to constant attractive and repulsive effects. Indeed, this assumption no longer holds when larger pressure and temperature ranges are addressed.

The present contribution aims at extending the liquid NASG EOS to variable attractive and repulsive effects to improve its range of validity, a necessary improvement in view of future engineering applications. The thermodynamics of the liquid and vapor phases must be combined correctly to reproduce the phase diagram and relevant properties, such as the latent heat of phase change and saturation pressure for example. Building of appropriate EOSs in this direction was done by Le Métayer et al. (2004) [53] and Le Métayer and Saurel (2016) [22] with extended "Stiffened-Gas" (SG) formulations. In the present contribution, the proposed EOS is also meant to describe transitions from pure fluids to supercritical state.

Such transition is indeed essential in some industrial applications such as flows evolving in combustion chambers of cryotechnic rocket engines as well as combustion systems of modern automotive engines for the sake of reduced pollutant emissions and fuel consumption.

The determination of the corresponding EOS parameters is of interest as well. For gases, the new formulation reduces to the ideal gas description. Variable heat capacities can easily be considered with such formulation making the equation of state able to deal with supercritical fluids at high temperatures.

This chapter is organized as follows. The determination of the novel liquid EOS is described in Section 3.2. Among the different relations, the Gibbs free energies of the liquid-vapor couple provide the saturation conditions. Those latter ones are developed in Section 3.3 and the overall formulation is summarized in Section 3.4. Experimental and theoretical curves are compared in Section 3.5, considering water and oxygen at saturation. The abilities of the proposed EOS are illustrated in Section 3.6 with transitions from sub to supercritical state. Practical applications are illustrated in Section 3.7.

3.2 Extended NASG EOS

The following Extended NASG EOS (ENASG) is considered as a postulate,

$$p(e,v) = \frac{(\gamma - 1)(e - q)}{v - b(v)} - \gamma p_{\infty}(e,v), \qquad (3.2.1)$$

with
$$p_{\infty}(e, v) = p_{\infty}(T) = p_{\infty,1}T + p_{\infty,0}$$
 and $b(v) = b_1v + b_0$, (3.2.2)

where p, T, v, e and q represent respectively, the pressure, temperature, specific volume, specific internal energy and reference energy of a corresponding single phase fluid. q and γ are parameters considered as constant coefficients and are meant to be characteristics of the thermodynamic properties of the fluid. Note that in this formulation, we are yet to define γ as the heat capacity ratio ($\gamma = C_p/C_v$) of the fluid. However, γ is still considered as $\gamma > 1$. Further calculations will show that this condition remains essential for the sake of convexity and thermodynamic consistency of the ENASG EOS (see Section 3.3). b(v) represents the covolume, modeling short range repulsive effects. The term $\gamma p_{\infty}(T)$ represents attractive ones, present in condensed matter only.

In the NASG formulation, the parameters b and p_{∞} are considered constant, yielding simplicity while ensuring presence of the main molecular forces present in a fluid. Besides, as the formulation is close to the ideal gas expression, it facilitates the resolution of the Riemann problem (Plohr (1988) [93], Menikoff and Plohr (1989) [94], Cocchi and Saurel (1997) [95]). The Riemann problem is indeed the cornerstone of numerical methods used to solve hydrodynamic problem, see Toro (1997) [58] for example.

The simplicity of the corresponding formulas is beneficial to the theoretical analysis and computational efficiency. This section aims at extending the liquid NASG EOS to deal with large pressure and temperature variations while remaining simple and convex.

In this work, simple linear dependencies on the specific volume and temperature have been added to the NASG EOS regarding respectively the covolume b(v) and attractive pressure $p_{\infty}(T)$. The formulation is meant to be convex and thermodynamically consistent. These two points are addressed hereafter. Inverting Eq. (3.2.1), the internal energy reads,

$$e(v,T) = \left(\frac{p(v,T) + \gamma p_{\infty}(T)}{\gamma - 1}\right) \left[v - b(v)\right] + q.$$

$$(3.2.3)$$

From postulate (3.2.1) or its alternative (3.2.3) form, the aim is now to derive the thermal EOS p = p(v, T) and the caloric one e = e(v, T).

Thermal and caloric EOSs

Thermal and caloric EOSs must fulfill the compatibility condition,

$$\frac{\partial}{\partial v} \left[\left(\frac{\partial f}{\partial T} \right)_v \right]_T = \frac{\partial}{\partial T} \left[\left(\frac{\partial f}{\partial v} \right)_T \right]_v, \tag{3.2.4}$$

that is precisely the first Maxwell's relation, where f represents the Helmholtz free energy defined by,

$$f = e - Ts,$$

where s denotes the specific entropy. With the help of the thermodynamic definition of pressure and entropy, $p = -\left(\frac{\partial f}{\partial v}\right)_T$ and $s = -\left(\frac{\partial f}{\partial T}\right)_v$, identity (3.2.4) transforms to a more convenient expression linking the thermal EOS p(v,T) and the caloric one e(v,T),

$$\left(\frac{\partial e}{\partial v}\right)_T = T \left(\frac{\partial p}{\partial T}\right)_v - p. \tag{3.2.5}$$

From postulate (3.2.3), the following partial derivatives arise,

$$\left(\frac{\partial e}{\partial T}\right)_{v} = \left(\frac{v - b(v)}{\gamma - 1}\right) \left[\left(\frac{\partial p}{\partial T}\right)_{v} + \gamma p_{\infty,1}\right],\tag{3.2.6}$$

$$\left(\frac{\partial e}{\partial v}\right)_T = \left(\frac{v - b(v)}{\gamma - 1}\right) \left(\frac{\partial p}{\partial v}\right)_T + \left(\frac{1 - b_1}{\gamma - 1}\right) \left[p + \gamma p_{\infty}(T)\right].$$
(3.2.7)

As the thermal capacity at constant volume is defined as,

$$C_v = \left(\frac{\partial e}{\partial T}\right)_v,\tag{3.2.8}$$

combining Eqs. (3.2.6) and (3.2.8) results in,

$$\left(\frac{\partial p}{\partial T}\right)_v = \frac{(\gamma - 1)C_v}{v - b(v)} - \gamma p_{\infty,1}.$$
(3.2.9)

The preceding relation (3.2.9) is now integrated over the temperature T leading to,

$$p(v,T) = \frac{(\gamma - 1)C_v T}{v - b(v)} - \gamma p_{\infty,1}T + K(v), \qquad (3.2.10)$$

where K(v) is a function depending on the specific volume v. Expression (3.2.10) is differentiated over v and at constant temperature T yielding,

$$\left(\frac{\partial p}{\partial v}\right)_T = -\frac{(1-b_1)(\gamma-1)C_vT}{\left[v-b(v)\right]^2} + \frac{dK(v)}{dv}.$$
(3.2.11)

Afterwards, relation (3.2.7) is inserted into Maxwell's relation (3.2.5) resulting in,

$$\left(\frac{\partial p}{\partial v}\right)_T = \frac{(\gamma - 1)T}{v - b(v)} \left(\frac{\partial p}{\partial T}\right)_v - \frac{\gamma \left[p + p_\infty(T)\right]}{v - b(v)} + \frac{b_1 \left[p + p_\infty(T)\right]}{v - b(v)}.$$
(3.2.12)

Expressions (3.2.9) and (3.2.10) are now introduced into relation (3.2.12) leading to,

$$\left(\frac{\partial p}{\partial v}\right)_T = -\frac{(\gamma - 1)C_v T(1 - b_1)}{\left[v - b(v)\right]^2} - \frac{K(v)(\gamma - b_1) + \gamma p_\infty(T)(1 - b_1)}{v - b(v)} + \frac{p_{\infty,1}\gamma T(1 - b_1)}{v - b(v)}.$$
 (3.2.13)

The equality between Eqs. (3.2.11) and (3.2.13) yields a first-order ordinary differential equation,

$$\frac{dK(v)}{dv} + \frac{K(v)(\gamma - b_1) + \gamma p_{\infty,0}(1 - b_1)}{v - b(v)} = 0.$$
(3.2.14)

The solution of Eq. (3.2.14) is given by,

$$K(v) = \frac{cst}{(\gamma - b_1) \left[v - b(v) \right]^{\frac{\gamma - b_1}{1 - b_1}}} - \frac{\gamma p_{\infty,0}(1 - b_1)}{\gamma - b_1}.$$
(3.2.15)

Inserting Eq. (3.2.15) into (3.2.10), the thermal equation of state reads,

$$p(v,T) = \frac{(\gamma - 1)C_v T}{v - b(v)} - p'_{\infty}(T) - \frac{d}{\left[v - b(v)\right]^{\frac{\gamma - b_1}{1 - b_1}}},$$
(3.2.16)

where $d = -cst/(\gamma - b_1)$ is a constant to be determined and the "attractive" pressure $p'_{\infty}(T)$ is defined as,

$$p'_{\infty}(T) = \gamma p_{\infty,1}T + \frac{\gamma p_{\infty,0}(1-b_1)}{\gamma - b_1}.$$
(3.2.17)

In the present approach, as in Le Métayer et al. (2004) [53] and Le Métayer and Saurel (2016) [22], each fluid, liquid and gas, is governed by the same EOS, here Eq. (3.2.16) but with different parameters unlike cubic EOSs. The term $p'_{\infty}(T)$ is important for the liquid state whereas the second attractive term $d/[v - b(v)]^{\frac{\gamma-b_1}{1-b_1}}$, reminiscent of cubic EOSs, is important for dense gases. However, this coefficient yields conditional convexity (see Appendix C.5). The same observation holds for cubic EOSs. As this section aims to build an unambiguously convex EOS, the parameter d is set to zero. Note that d = 0 is a particular solution of Eq. (3.2.14). The corresponding ENASG EOSs then read,

$$p(v,T) = \frac{(\gamma - 1)C_v T}{v - b(v)} - p'_{\infty}(T), \qquad (3.2.18)$$

$$e(v,T) = C_v T + \frac{\gamma p_{\infty,0} [v - b(v)]}{\gamma - b_1} + q.$$
(3.2.19)

With the help of the caloric EOS (3.2.19), the temperature expresses as,

$$T(e,v) = \frac{e-q}{C_v} - \frac{\gamma p_{\infty,0} [v-b(v)]}{C_v (\gamma - b_1)},$$
(3.2.20)

and yields,

$$p(e,v) = \frac{(\gamma - 1)(e - q)}{v - b(v)} - \gamma p_{\infty} \left(T(e,v) \right).$$
(3.2.21)

Note that Eqs. (3.2.18), (3.2.19), (3.2.20) and (3.2.21) reduce to the NASG expressions if $p_{\infty,1} = 0$ and $b_1 = 0$. Also, inserting Eq. (3.2.18) into Eq. (3.2.21), the internal energy expresses,

$$e(p,T) = \left(\frac{p + \gamma p_{\infty}(T)}{p + p'_{\infty}(T)}\right) C_v T + q.$$
(3.2.22)

The expressions of the thermal and caloric EOSs being now available, the other thermodynamic variables may be obtained from the knowledge of the two independent variables p and T. This task is addressed hereafter.

Expression of the entropy

Expression of the specific entropy is mandatory to express the Gibbs free energy, a key function to address phase transition. The entropy formulation must fulfill the compatibility relation,

$$\frac{\partial}{\partial p} \left[\left(\frac{\partial g}{\partial T} \right)_p \right]_T = \frac{\partial}{\partial T} \left[\left(\frac{\partial g}{\partial p} \right)_T \right]_p, \qquad (3.2.23)$$

that is precisely the second Maxwell's relation, where g represents the Gibbs free energy defined by,

$$g = h - Ts,$$

where *h* represents the specific enthalpy. As the thermodynamic definition of entropy and specific volume implies $s = -\left(\frac{\partial g}{\partial T}\right)_p$ and $v = \left(\frac{\partial g}{\partial p}\right)_T$, identity (3.2.23) transforms to a more convenient expression,

$$\left(\frac{\partial s}{\partial p}\right)_T = -\left(\frac{\partial v}{\partial T}\right)_p.$$
(3.2.24)

With the help of Eq. (3.2.18), the partial derivative expresses,

$$\left(\frac{\partial v}{\partial T}\right)_p = -\left(\frac{1}{1-b_1}\right) \left(\frac{-(\gamma-1)C_v}{p+p'_{\infty}(T)} + \frac{\gamma p_{\infty,1}(\gamma-1)C_vT}{\left[p+p'_{\infty}(T)\right]^2}\right).$$
(3.2.25)

Also, by use of Maxwell's rule (3.2.24), the next equations arise,

$$\left(\frac{\partial s}{\partial p}\right)_T = \left(\frac{1}{1-b_1}\right) \left(\frac{-(\gamma-1)C_v}{p+p'_{\infty}(T)} + \frac{\gamma p_{\infty,1}(\gamma-1)C_vT}{\left[p+p'_{\infty}(T)\right]^2}\right),\tag{3.2.26}$$

$$s(p,T) = \left(\frac{1}{1-b_1}\right) \left(-(\gamma-1)C_v \ln\left[p + p'_{\infty}(T)\right] - \frac{\gamma p_{\infty,1}(\gamma-1)C_v T}{p + p'_{\infty}(T)}\right) + K(T).$$
(3.2.27)

Equation (3.2.18) is now inserted into Eq. (3.2.27) and yields,

$$s(v,T) = \left(\frac{1}{1-b_1}\right) \left(-(\gamma-1)C_v \ln\left[\frac{(\gamma-1)C_v T}{v-b(v)}\right] - \gamma p_{\infty,1}[v-b(v)]\right) + K(T).$$
(3.2.28)

This last equation admits the partial derivative,

$$\left(\frac{\partial s}{\partial T}\right)_v = -\frac{(\gamma - 1)C_v}{T(1 - b_1)} + \frac{dK(T)}{dT}.$$
(3.2.29)

The definition of the thermal capacity at constant volume may be used under the following form,

$$\left(\frac{\partial s}{\partial T}\right)_v = \frac{C_v}{T}.\tag{3.2.30}$$

Consequently, the next equation arises,

$$dK(T) = C_v \frac{dT}{T} + \frac{(\gamma - 1)C_v}{(1 - b_1)} \frac{dT}{T},$$

and is directly integrated yielding a temperature-dependent function K(T),

$$K(T) = C_v \ln(T) + \frac{(\gamma - 1)C_v}{(1 - b_1)} \ln(T) + q', \qquad (3.2.31)$$

where q' is defined as a constant (reference entropy). Equation (3.2.31) is now embedded in Eq. (3.2.28). After some algebraic manipulations, the resulting equation reads,

$$s(v,T) = C_v \ln(T) - \frac{\gamma p_{\infty,1} \left[v - b(v) \right]}{1 - b_1} + \frac{(\gamma - 1)C_v}{(1 - b_1)} \ln \left[v - b(v) \right] - \frac{(\gamma - 1)C_v}{(1 - b_1)} \ln \left[(\gamma - 1)C_v \right] + q'.$$

As the last term of this equation is constant, it is convenient to define,

$$q'' = -\frac{(\gamma - 1)C_v}{(1 - b_1)} \ln\left[(\gamma - 1)C_v\right] + q'.$$
(3.2.32)

The entropy equation consequently reads,

$$s(v,T) = C_v \ln(T) + \frac{(\gamma - 1)C_v}{(1 - b_1)} \ln\left[v - b(v)\right] - \frac{\gamma p_{\infty,1}[v - b(v)]}{1 - b_1} + q''.$$
(3.2.33)

Obviously, definition (3.2.30) is satisfied. Equation (3.2.18) is now inserted into (3.2.33), yielding,

$$s(p,T) = C_v \ln(T) + \frac{(\gamma - 1)C_v}{(1 - b_1)} \ln\left(\frac{(\gamma - 1)C_vT}{p + p'_{\infty}(T)}\right) - \frac{\gamma p_{\infty,1}(\gamma - 1)C_vT}{\left[1 - b_1\right]\left[p + p'_{\infty}(T)\right]} + q''.$$
(3.2.34)

The relation s(p,T) being now available, it is worth analyzing the expression of the heat capacity at constant pressure. Equation (3.2.34) admits as partial derivative,

$$\left(\frac{\partial s}{\partial T}\right)_{p} = \frac{C_{v}}{T} + \frac{(\gamma - 1)C_{v}}{(1 - b_{1})T} - \left(\frac{\gamma p_{\infty,1}(\gamma - 1)C_{v}}{\left[1 - b_{1}\right]\left[p + p_{\infty}'(T)\right]}\right) \left(1 + \frac{p + p_{\infty}'(T) - \gamma p_{\infty,1}T}{p + p_{\infty}'(T)}\right).$$
 (3.2.35)

As the heat capacity is defined as,

$$\left(\frac{\partial s}{\partial T}\right)_p = \frac{C_p}{T},\tag{3.2.36}$$

the ENASG thermal capacity at constant pressure consequently reads,

$$C_p(T) = C_v + \frac{(\gamma - 1)C_v}{(1 - b_1)} - \left(\frac{\gamma p_{\infty,1}(\gamma - 1)C_v T}{\left[1 - b_1\right]\left[p + p'_{\infty}(T)\right]}\right) \left(1 + \frac{p + p'_{\infty}(T) - \gamma p_{\infty,1}T}{p + p'_{\infty}(T)}\right).$$
(3.2.37)

It then appears that $C_p \neq \gamma C_v$. However, if $p_{\infty,1} = 0$ and $b_1 = 0$, then the preceding relation reduces to,

$$C_p = C_v + (\gamma - 1)C_v = \gamma C_v,$$

and the NASG thermal capacity at constant pressure is recovered. Note also that this feature is valid for the Stiffened-Gas (SG) ($b_0 = 0$) and ideal gas ($b_0 = 0$ and $p_{\infty,0} = 0$) equations of state as well.

Equation (3.2.34) can be manipulated to obtain an entropy relation closer to the NASG one. Indeed, after some algebraic manipulations, Eq. (3.2.34) can be written as,

$$s(p,T) = C_v \left[\ln(T) + \ln\left(\frac{T}{p + p'_{\infty}(T)}\right)^{\frac{\gamma - 1}{1 - b_1}} \right] - \frac{\gamma p_{\infty,1}(\gamma - 1)C_v T}{\left[1 - b_1\right] \left[p + p'_{\infty}(T)\right]} + \frac{(\gamma - 1)C_v}{1 - b_1} \ln\left[(\gamma - 1)C_v\right] + q''.$$

Using Eq. (3.2.32), the last term of this equation reduces to,

$$\frac{(\gamma - 1)C_v}{1 - b_1} \ln\left[(\gamma - 1)C_v\right] + q'' = q'.$$

Equation (3.2.34) consequently transforms to,

$$s(p,T) = C_v \ln\left(\frac{T^{\frac{\gamma-b_1}{1-b_1}}}{\left[p + p'_{\infty}(T)\right]^{\frac{\gamma-1}{1-b_1}}}\right) - \frac{\gamma p_{\infty,1}(\gamma-1)C_v T}{\left[1 - b_1\right]\left[p + p'_{\infty}(T)\right]} + q'.$$
(3.2.38)

Under form (3.2.38), it is straightforward to see that the relation does reduce to the NASG equation if $p_{\infty,1} = 0$ and $b_1 = 0$.

At this point, the caloric, thermal and entropy equations of state are determined. The next step is to check positivity of the sound speed as it is a key feature in fluid dynamics.

Speed of sound

The sound speed is defined as,

$$c^{2} = -v^{2} \left(\frac{\partial p}{\partial v}\right)_{s}.$$
(3.2.39)

The pressure is expressed as a function of the specific volume and the specific entropy by combining relations (3.2.18) and (3.2.38),

$$p(v,s) = \frac{\exp\left(\frac{s-q''}{C_v}\right)\exp\left(\frac{\gamma p_{\infty,1}\left[v-b(v)\right]}{C_v(1-b_1)}\right)\left[(\gamma-1)C_v - \gamma p_{\infty,1}\left[v-b(v)\right]\right]}{\left[v-b(v)\right]^{\frac{\gamma-b_1}{1-b_1}}} - \frac{\gamma p_{\infty,0}(1-b_1)}{\gamma-b_1}, \quad (3.2.40)$$

with

$$q'' = -\frac{(\gamma - 1)C_v}{(1 - b_1)} \ln\left[(\gamma - 1)C_v\right] + q'.$$
(3.2.41)

The ENASG speed of sound consequently expresses after some algebraic manipulations as,

$$c^{2}(p,v) = -v^{2}\gamma p_{\infty,1}\left(p + \frac{\gamma p_{\infty,0}(1-b_{1})}{\gamma-b_{1}}\right)\left(\frac{\gamma-1}{(\gamma-1)C_{v}-\gamma p_{\infty,1}[v-b(v)]} + \frac{1}{C_{v}}\right) + \left(\frac{p + \frac{\gamma p_{\infty,0}(1-b_{1})}{\gamma-b_{1}}}{(\gamma-1)C_{v}-\gamma p_{\infty,1}[v-b(v)]}\right)\left(\frac{v^{2}(\gamma-b_{1})(\gamma-1)C_{v}}{v-b(v)}\right).$$
(3.2.42)

It is worth mentioning that Eq. (3.2.42) reduces to,

$$c^{2}(p,v) = \frac{v^{2}(p+p_{\infty,0})\gamma}{v-b_{0}},$$
(3.2.43)

if $p_{\infty,1} = 0$ and $b_1 = 0$, that corresponds to the NASG speed of sound. It also appears that $c^2 > 0$ unambiguously if $p_{\infty,1} \le 0$, $p_{\infty,0} \ge 0$ and $b_1 < 1$. Obviously v - b(v) must be positive as well.

For a liquid state, the attractive effects summarized by the terms $p_{\infty}(T)$ and $p'_{\infty}(T)$ are expected to decrease when the temperature rises. The conditions $p_{\infty,1} \leq 0$ and $p_{\infty,0} \geq 0$ are consequently in agreement with the physics to represent, at least qualitatively. The same observation holds for the repulsive effects summarized by the covolume b(v). When the density decreases, those short distance effects are expected to vanish as the liquid tends to become a dense gas. Condition $b_1 < 1$ is then not restrictive for liquids. Also, it is worth noticing from Eq. (3.2.42), that

$$p_{\infty,1} \neq \left(\frac{\gamma - 1}{v - b(v)}\right) \frac{C_v}{\gamma},$$

must be satisfied for the ENASG sound speed function to be defined. However, as the right-hand side of this relation is necessarily positive, considering $p_{\infty,1} \leq 0$ satisfies unambiguously this condition.

The two linear dependencies $p_{\infty}(T)$ and b(v) are thus in agreement with the description of a liquid state. As it will be seen further, those simple functions result in predictions in very good agreement with experimental data.

This set of liquid EOS relationships results in a convex formulation, this feature being essential both for theoretical and numerical considerations. Indeed, sufficient conditions to ensure convexity are summarized by,

$$p_{\infty,1} \le 0, \quad p_{\infty,0} \ge 0 \quad \text{and} \quad b_1 < 1,$$
(3.2.44)

related calculations being given in Appendix C.1.

For the gas phase, the attractive effects are expected to increase with the temperature but this evolution is not in agreement with the convexity condition (3.2.44). Gas attractive effects are thus removed by setting $p_{\infty,0} = 0$ and $p_{\infty,1} = 0$, reducing the formulation to the Noble-Abel (NA) EOS with a variable covolume b(v).

However, covolume effects alone are not enough to describe dense gases near the critical point. Attractive effects are needed in addition (see Appendix C.5) but yield conditional convexity. As it will be seen further, the ideal gas EOS is well-suited for fluids evolving away from the critical point, either at low temperatures where thermal capacities can be considered constant or at much higher ones where heat capacities are meant to evolve with the temperature.

Thereby, for the sake of simplicity, covolume effects are removed as well reducing the formulation to the ideal gas description. Consequently, the saturated vapor phase lacks of accuracy near the critical point since attractive effects are absent but the overall formulation remains convex, a key feature for computational fluid dynamics.

For ENASG formulation completion, the expression of the saturation condition of the liquid-vapor couple must be determined. This task is addressed in the next section.

3.3 Saturation condition of the liquid-vapor couple

Thermodynamic equilibrium is considered when the fluids are in pressure, temperature and Gibbs free energies $(g_l = g_v)$ equilibria. The saturation condition results from these equilibria. As,

$$g(p,T) = h(p,T) - Ts(p,T),$$
(3.3.1)

the enthalpies of pure constituents must be determined first. The enthalpy is defined as,

$$h(p,T) = e(p,T) + pv(p,T).$$
 (3.3.2)

Combining Eqs. (3.2.18) and (3.2.21), the enthalpy of the ENASG EOS reads,

$$h(p,T) = \left(\frac{C_v T}{p + p'_{\infty}(T)}\right) \left(\frac{\gamma \left[p + p_{\infty}(T)\right] - pb_1 - \gamma b_1 p_{\infty}(T)}{1 - b_1}\right) + \frac{pb_0}{1 - b_1} + q.$$
(3.3.3)

Note that the partial derivative of Eq. (3.3.3) gives after some algebraic manipulations,

$$\left(\frac{\partial h}{\partial T}\right)_{p} = C_{v} + \frac{(\gamma - 1)C_{v}}{(1 - b_{1})} - \left(\frac{\gamma p_{\infty,1}(\gamma - 1)C_{v}T}{\left[1 - b_{1}\right]\left[p + p_{\infty}'(T)\right]}\right) \left(1 + \frac{p + p_{\infty}'(T) - \gamma p_{\infty,1}T}{p + p_{\infty}'(T)}\right).$$
 (3.3.4)

Equation (3.2.37) is then recovered and the definition of the thermal capacity at constant pressure is satisfied, providing extra verification,

$$C_p = T\left(\frac{\partial s}{\partial T}\right)_p = \left(\frac{\partial h}{\partial T}\right)_p.$$
(3.3.5)

Note that if $p_{\infty,1} \leq 0$, $b_1 < 1$ and $\gamma > 1$, then the thermodynamic condition $C_p > C_v$ is ensured. These conditions are the same that preserve convexity of the formulation. Note also that $\gamma \neq C_p/C_v$, so it cannot be defined as the heat capacity ratio. However, the condition $\gamma > 1$ remains for the sake of thermodynamic consistency of the ENASG EOS.

Thanks to Eqs. (3.2.38), (3.3.1) and (3.3.3), the Gibbs free energy of a pure constituent expresses as,

$$g(p,T) = \left[\left(\frac{C_v}{1-b_1} \right) \left(\frac{\gamma \left[p + p_{\infty}(T) \right] - pb_1 - \gamma b_1 p_{\infty}(T)}{p + p'_{\infty}(T)} \right) - q' \right] T - C_v T \ln \left(\frac{T^{\frac{\gamma - b_1}{1-b_1}}}{\left[p + p'_{\infty}(T) \right]^{\frac{\gamma - 1}{1-b_1}}} \right) + \frac{pb_0}{1-b_1} + q + \frac{\gamma p_{\infty,1}(\gamma - 1)C_v T^2}{\left[1 - b_1 \right] \left[p + p'_{\infty}(T) \right]}.$$
(3.3.6)

Solution of the equation,

$$g_l(p,T) = g_v(p,T),$$
 (3.3.7)

provides the saturation pressure as a function of temperature $p_{sat}(T)$. Subscripts l and v denote respectively the liquid and vapor states.

The equality of Gibbs free energies of both phases corresponds to phase equilibrium and leads to

the following expression linking pressure and temperature,

$$\ln\left[p + p'_{\infty,v}(T)\right] = \frac{C_{v,l}(1 - b_{1,v})}{(1 - b_{1,l})(\gamma_v - 1)C_{v,v}} \left(\frac{\gamma_l\left[p + p_{\infty,l}(T)\right] - pb_{1,l} - \gamma_l b_{1,l} p_{\infty,l}(T)}{p + p'_{\infty,l}(T)}\right) \\ - \left(\frac{1}{\gamma_v - 1}\right) \left(\frac{\gamma_v\left[p + p_{\infty,v}(T)\right] - pb_{1,v} - \gamma_v b_{1,v} p_{\infty,v}(T)}{p + p'_{\infty,v}(T)}\right) + \frac{(q'_v - q'_l)(1 - b_{1,v})}{(\gamma_v - 1)C_{v,v}} \\ \frac{B + Ep}{T} + C\ln(T) + D\ln\left[p + p'_{\infty,l}(T)\right] - T\left(\frac{\gamma_v p_{\infty,1,v}}{p + p'_{\infty,v}(T)} - \frac{\gamma_l p_{\infty,l,l}D}{p + p'_{\infty,l}(T)}\right),$$
(3.3.8)

with

$$B = \frac{(q_l - q_v)(1 - b_{1,v})}{(\gamma_v - 1)C_{v,v}}, \qquad C = \left(\frac{(\gamma_v - b_{1,v})C_{v,v}}{1 - b_{1,v}} - \frac{(\gamma_l - b_{1,l})C_{v,l}}{1 - b_{1,l}}\right) \left(\frac{1 - b_{1,v}}{(\gamma_v - 1)C_{v,v}}\right), \qquad D = \frac{(\gamma_l - 1)C_{v,l}(1 - b_{1,v})}{(\gamma_v - 1)C_{v,v}(1 - b_{1,l})}, \qquad E = \left(\frac{b_{0,l}}{1 - b_{1,l}} - \frac{b_{0,v}}{1 - b_{1,v}}\right) \left(\frac{1 - b_{1,v}}{(\gamma_v - 1)C_{v,v}}\right).$$
(3.3.9)

Relation (3.3.8) provides a unique value of the pressure for a given temperature and implicitly represents the theoretical saturated pressure as a function depending on the temperature. Numerical resolution is needed to compare the predictions with experiments, as will be examined later. When $p_{\infty,1,k}$ and $b_{1,k}$ are set to zero, the preceding relation reduces to,

$$\ln\left[p + p_{\infty,0,v}\right] = A + \frac{B + Ep}{T} + C\ln(T) + D\ln\left[p + p_{\infty,0,l}\right],$$
(3.3.10)

with

$$A = \frac{\gamma_{l}C_{v,l} - \gamma_{v}C_{v,v} + q'_{v} - q'_{l}}{\gamma_{v}C_{v,v} - C_{v,v}}, \qquad B = \frac{q_{l} - q_{v}}{\gamma_{v}C_{v,v} - C_{v,v}}, C = \frac{\gamma_{v}C_{v,v} - \gamma_{l}C_{v,l}}{\gamma_{v}C_{v,v} - C_{v,v}}, \qquad D = \frac{\gamma_{l}C_{v,l} - C_{v,l}}{\gamma_{v}C_{v,v} - C_{v,v}}, \qquad E = \frac{b_{0,l} - b_{0,v}}{\gamma_{v}C_{v,v} - C_{v,v}}.$$
(3.3.11)

The NASG relation is then recovered. The whole ENASG formulation is summarized in the next section and is compared with experimental data in the following ones.

3.4 Summary of the Extended NASG state functions

The different liquid ENASG functions of common use are,

$$\begin{split} \left(\begin{array}{l} p(e,v) &= \frac{(\gamma-1)(e-q)}{v-b(v)} - \gamma p_{\infty}\left(T(e,v)\right), \\ v(p,T) &= \frac{(\gamma-1)C_vT}{(1-b_1)(p+p'_{\infty}(T))} + \frac{b_0}{(1-b_1)}, \\ e(p,T) &= \left(\frac{p+\gamma p_{\infty}(T)}{p+p'_{\infty}(T)}\right) C_vT + q, \\ h(p,T) &= \left(\frac{C_vT}{p+p'_{\infty}(T)}\right) \left(\frac{\gamma[p+p_{\infty}(T)] - pb_1 - \gamma b_1 p_{\infty}(T)}{1-b_1}\right) + \frac{pb_0}{1-b_1} + q, \\ s(p,T) &= C_v \ln\left(\frac{T^{\frac{\gamma-b_1}{1-b_1}}}{\left[p+p'_{\infty}(T)\right]^{\frac{\gamma-1}{1-b_1}}}\right) - \frac{\gamma p_{\infty,1}(\gamma-1)C_vT}{\left[1-b_1\right]\left[p+p'_{\infty}(T)\right]} + q', \\ g(p,T) &= \left[\left(\frac{C_v}{1-b_1}\right) \left(\frac{\gamma[p+p_{\infty}(T)] - pb_1 - \gamma b_1 p_{\infty}(T)}{p+p'_{\infty}(T)}\right) - q'\right]T - C_vT \ln\left(\frac{T^{\frac{\gamma-b_1}{1-b_1}}}{\left[p+p'_{\infty}(T)\right]^{\frac{\gamma-1}{1-b_1}}}\right) \\ &+ \frac{pb_0}{1-b_1} + q + \frac{\gamma p_{\infty,1}(\gamma-1)C_vT^2}{\left[1-b_1\right]\left[p+p'_{\infty}(T)\right]}, \\ c^2(p,v) &= -v^2\gamma p_{\infty,1}\left(p + \frac{\gamma p_{\infty,0}(1-b_1)}{\gamma-b_1}\right) \left(\frac{\gamma^2(\gamma-b_1)(\gamma-1)C_v}{v-\gamma p_{\infty,1}\left[v-b(v)\right]} + \frac{1}{C_v}\right) \\ &+ \left(\frac{p + \frac{\gamma p_{\infty,0}(1-b_1)}{\gamma-b_1}\left[v-b(v)\right]}\right) \left(\frac{v^2(\gamma-b_1)(\gamma-1)C_v}{v-b(v)}\right), \end{split}$$
(3.4.1)

with

$$T(e,v) = \frac{e-q}{C_v} - \frac{\gamma p_{\infty,0} \left[v - b(v) \right]}{C_v (\gamma - b_1)},$$

$$p_{\infty}(e,v) = p_{\infty}(T) = p_{\infty,1}T + p_{\infty,0}, \quad p'_{\infty}(T) = \gamma p_{\infty,1}T + \frac{\gamma p_{\infty,0}(1-b_1)}{\gamma - b_1} \quad \text{and} \quad b(v) = b_1v + b_0.$$

Those different functions are in agreement with the fundamental relations of Maxwell analyzed in Appendix C.2 and are thermodynamically consistent and convex under conditions $p_{\infty,1} \leq 0$, $p_{\infty,0} \geq 0$ and $b_1 < 1$. The whole formulation reduces to the NASG EOS if $p_{\infty,1} = 0$ and $b_1 = 0$. In addition, the ideal gas description is recovered if $p_{\infty,0} = 0$, $b_0 = 0$ and is used for the sake of convexity and simplicity of the gas-phase formulation. The corresponding formulas thus read,

$$\begin{cases} p(e,v) = \frac{(\gamma-1)(e-q)}{v}, \\ v(p,T) = \frac{(\gamma-1)C_vT}{p}, \\ e(T) = C_vT + q, \\ h(T) = \gamma C_vT + q, \\ s(p,T) = C_v \ln\left(\frac{T^{\gamma}}{p^{\gamma-1}}\right) + q', \\ g(p,T) = \left(\gamma C_v - q'\right)T - C_vT \ln\left(\frac{T^{\gamma}}{p^{\gamma-1}}\right) + q, \\ c^2(p,v) = \gamma pv. \end{cases}$$
(3.4.2)

In these formulations (ENASG and ideal gas), heat capacities are considered constant. This assumption is fair for the liquid phase. It is also valid for the gas phase evolving at low temperatures. However, this assumption fails at high temperatures motivating consideration of variable heat capacities as introduced in Section 3.6. This situation is typical of supercritical fluids at high temperatures.

3.5 Extended NASG parameters

The method used in this work to determine the different EOS parameters is summarized in Appendix C.3. The liquid parameters are computed with experimental saturation data as in Le Métayer and Saurel (2016) [22], but unlike this last reference the gas parameters are chosen regardless of the saturation conditions. The present method is directly applied to water and oxygen liquid-gas couples as countless engineering applications involve those two fluids. Safety studies of thermohydraulic systems of power plants and flows in cryotechnic rocket engines can be cited for instance. This latter example involves specific situations where transitions from pure fluid into two-phase mixture are present as well as transition to supercritical state. In the same context, combustion systems of modern automotive engines also involve transitions from pure phase to both two-phase mixture and supercritical fluid. Tables 3.1 and 3.2 provide the associated parameters of the ENASG EOS (3.4.1), (3.4.2).

Figures 3.1 and 3.2 compare the present theoretical predictions to experimental data at saturation for water and oxygen.

The ENASG EOS (3.4.1) presents good agreement with liquid experimental data at saturation. The saturated pressure resulting from the equality of the liquid and vapor Gibbs free energies is rather good as well. Away from the critical point, the vapor phase, described by the ideal gas expressions (3.4.2), is also in good agreement with experimental data. However, the saturated vapor phase necessarily lacks of accuracy near the critical point as the attractive effects have been removed in order to keep an unambiguously convex formulation.



Figure 3.1: Comparison between experimental and theoretical saturation curves for liquid l and vapor v water. Symbols represent experimental data. The thick lines represent the theoretical saturation curves obtained with the Extended NASG EOS (ENASG) reducing to the ideal gas description for the vapor phase, Eqs. (3.4.1) and (3.4.2). The thin lines represent results obtained with the original NASG EOS also reducing to the ideal gas formulation for the vapor phase. p_{sat} denotes the saturation pressure, L_v the latent heat, h the specific enthalpy and ρ the density.



Figure 3.2: Comparison between experimental and theoretical saturation curves for liquid l and vapor v oxygen. Symbols represent experimental data. The thick lines represent the theoretical saturation curves obtained with the Extended NASG EOS (ENASG) reducing to the ideal gas description for the vapor phase, Eqs. (3.4.1) and (3.4.2). The thin lines represent results obtained with the original NASG EOS also reducing to the ideal gas formulation for the vapor phase. p_{sat} denotes the saturation pressure, L_v the latent heat, h the specific enthalpy and ρ the density.

Coefficients	ENASG_{Liq}	$ENASG_{gas}$	NASG_{Liq}	$NASG_{gas}$
γ	1.0147	1.3079	1.1807	1.5377
$C_v ~({ m J/kg/K})$	4014	1500	3630	856
b_1	-0.6050	0	0	0
$b_0 \ (\mathrm{m}^3/\mathrm{kg})$	1.5196×10^{-3}	0	6.8428×10^{-4}	0
$p_{\infty,1} (\mathrm{Pa/K})$	-471025	0	0	0
$p_{\infty,0}$ (Pa)	307078403	0	664961465	0
$q (\mathrm{J/kg})$	-1112426	1947630	-1178154	2176064
$q'~({\rm J/kg/K})$	-22049	1136	-10742	4863

Table 3.1: Extended NASG (ENASG) coefficients for water. The NASG parameters are also given and determined with the method given in Le Métayer and Saurel (2016) [22] except for the liquid reference entropy q' that is computed with the NASG reduction of Eq. (C.3.10) (see Appendix C.3). The NASG water parameters are determined with N = 201 experimental saturation points in the temperature range $T_{exp} \in [300 - 500]$ K.

Coefficients	ENASG_{Liq}	$ENASG_{gas}$	NASG_{Liq}	$NASG_{gas}$
γ	1.0281	1.3985	1.6610	1.4730
$C_v ~({ m J/kg/K})$	1535	652	1016	548
b_1	-0.6721	0	0	0
$b_0 \ (\mathrm{m}^3/\mathrm{kg})$	1.3131×10^{-3}	0	5.7003×10^{-4}	0
$p_{\infty,1} (\mathrm{Pa/K})$	-324997	0	0	0
$p_{\infty,0}$ (Pa)	50890107	0	196815802	0
$q~({ m J/kg})$	-278134	-1589	-285545	6528
$q'~({\rm J/kg/K})$	-3691	4237	8171	4650

Table 3.2: Extended NASG (ENASG) coefficients for oxygen. The NASG parameters are also given and determined with the method given in Le Métayer and Saurel (2016) [22] except for the liquid reference entropy q' that is computed with the NASG reduction of Eq. (C.3.10) (see Appendix C.3). The NASG oxygen parameters are determined with N = 41 experimental saturation points in the temperature range $T_{exp} \in [60 - 100]$ K.

The results of the original NASG EOS (Le Métayer and Saurel (2016) [22]) are plotted as well in Figs. 3.1 and 3.2 for comparison. The corresponding parameters are given in Tables 3.1 and 3.2. As the attractive pressure is constant in such formulation, liquid density necessarily lacks of accuracy away from its reference temperature range. However, as the ideal gas parameters have been determined thanks the saturation curve in [22] (unlike the present work, see Appendix C.3), the vapor enthalpy and latent heat are in slightly better agreement than the present ENASG EOS (3.4.1), (3.4.2).

The present chapter aims at building an overall EOS able to deal with pure liquid, pure vapor and supercritical phases, while being as accurate as possible at saturation. When thermodynamic conditions remain close to the saturation ones and away from the critical point, the original NASG EOS with its associated parameters (Le Métayer and Saurel (2016) [22]) is preferred as the formulation is simpler than the ENASG one and yields excellent results as seen in Figs. 3.1 and 3.2.

However, as the original method [22] uses the saturation curves both for liquid and vapor phases

when determining the corresponding parameters, the NASG EOS lacks of accuracy away from the saturation conditions. This will be illustrated in the following section. As it will be seen later, the overall ENASG EOS presents good agreement with experimental data away from the saturation conditions while being rather satisfying at saturation (except for the vapor phase near the critical point as discussed earlier).

In the next section, the theoretical behavior of the ENASG EOS is analyzed with thermodynamic conditions corresponding to the transition from single phase to supercritical state.

3.6 Transition to supercritical fluids

This section deals with fluids transitioning from a pure phase to supercritical state as schematically illustrated in Fig. 3.3.



Figure 3.3: The saturation curve is composed of the boiling and the dew curves separating the twophase mixture zone and the pure phase zones. Beyond the critical isotherm, there is no transition between the liquid and the gaseous state. The fluid is neither liquid nor gas, it is said to be supercritical. Phase transition can happen either through the saturation dome corresponding to liquid-vapor phase change, or through the critical isotherm corresponding to a pure-phase-to-supercritical-state transition.

At high temperatures, the assumption of constant heat capacities no longer holds for the supercritical phase. The ideal gas description can still be fairly assumed in the supercritical state but variable heat capacities are required when reaching a certain temperature. Consequently, the following definition of heat capacity (at constant volume or pressure) is considered:

$$\begin{cases} C_v = C_{v,0} & \text{if } T \leq T_0, \\ C_v = C_v(T) & \text{otherwise,} \end{cases}$$
(3.6.1)

where $C_{v,0}$ denotes the constant heat capacity given in Tables 3.1 and 3.2. T_0 is the temperature at

which the assumption of constant heat capacities starts to fail. In this work, at such temperature the fluid is necessarily supercritical. These temperatures are reported in Table 3.3 for water and oxygen.

For ideal gases, Mayer's relation $C_p(T) - C_v(T) = R$ holds and the ratio of heat capacities reads $\gamma(T) = \frac{C_p(T)}{C_v(T)}$. In these relations, $R = \hat{R}/W$ where \hat{R} denotes the universal gas constant and W the molar mass. In the present work, $C_p(T)$ is estimated via the NASA polynomial expression [96],

$$C_p(T) = R \Big[a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \Big], \qquad (3.6.2)$$

with corresponding parameters reported in Table 3.3.

Fluid	T_0 (K)	a_1	$a_2 \; ({\rm K}^{-1})$	$a_3 \; ({\rm K}^{-2})$	$a_4 \; ({\rm K}^{-3})$	$a_5 ({\rm K}^{-4})$
$\begin{array}{c} \mathrm{H}_{2}\mathrm{O}\\ \mathrm{O}_{2} \end{array}$	$\begin{array}{c} 1000\\ 400 \end{array}$	$3.31570 \\ 3.78246$	$\begin{array}{c} 2.10648 \times 10^{-3} \\ -2.99673 \times 10^{-3} \end{array}$	$\begin{array}{c} -3.76340\times 10^{-7} \\ 9.84730\times 10^{-6} \end{array}$	$\begin{array}{c} 3.47520 \times 10^{-11} \\ -9.68129 \times 10^{-9} \end{array}$	$-1.70335 \times 10^{-15} \\ 3.24373 \times 10^{-12}$

Table 3.3: Parameters of the NASA polynomial expression [96] for the heat capacity at constant pressure, Eq. (3.6.2).

Proceeding similar derivations as in Section 3.2, the ideal gas formulation yields,

$$\begin{cases} p(v,T) = \frac{RT}{v}, \\ e(T) = \int C_v(T)dT + q, \\ h(T) = \int C_p(T)dT + q, \\ s(p,T) = \int C_p(T)\frac{dT}{T} - R\ln(p) + q', \\ c^2(T) = \gamma(T)RT = \frac{C_p(T)}{C_v(T)}RT, \\ C_p(T) - C_v(T) = R. \end{cases}$$
(3.6.3)

As explained in Appendix C.3, the γ parameter of the gas phase is determined thanks to Mayer's relation as to ensure $[\gamma(T) - 1]C_v(T) = R$. Note that the ideal gas reduction of the NASG EOS (Le Métayer and Saurel (2016) [22]), with its associated original method to determine the different coefficients, does not ensure the preceding Mayer's relation as the gas parameters are determined with the saturation curves.

Liquid-to-supercritical-state transition

The liquid phase is described with the ENASG EOS as its particular interest resides in variable repulsive and attractive effects. In the transcritical zone, attractive and repulsive molecular forces are the dominant effects of the fluid. Thereby, the ENASG EOS is also used to describe liquids transitioning to their supercritical state. The transition is then continuous. At much higher temperatures, thermal agitation becomes the dominant effect. The ideal gas description is then to be used in this context. However, as two different EOSs are used through different parameters, the continuity between the ENASG EOS and its ideal gas reduction is not trivial.

Indeed, the two EOSs must be connected in order to make a continuous formulation. For a given pressure, there exists a connection temperature where the two EOSs are equal. Nevertheless, those connection temperatures are *a priori* dependent on the variable of interest.

Equations (3.4.1) and (3.4.2) provide expressions of the different variables for the ENASG and ideal gas EOSs. Equality of both expressions provides the connection temperature that is the positive solution of a quadratic equation,

$$aT^2 + bT + c = 0. ag{3.6.4}$$

Note that the admissible range of the sought-after temperature is known as this latter is necessarily higher than the critical one (T_c) and must ensure $p + p_{\infty,l}(T) > 0$ and $p + p'_{\infty,l}(T) > 0$. Note also that Eq. (3.6.4) is available only if the heat capacities are constant. An iterative method is required otherwise, but this situation (high temperatures, $T \ge T_0$) is not to be encountered in this work as the fluid is necessarily supercritical and the ENASG EOS is not to be used (see Section 3.7). The different parameters of the quadratic equation (3.6.4) are provided in Appendix C.4.

In the following, two isobars are considered for both fluids (water and oxygen). The first one is rather close (230 bar for water and 60 bar for oxygen) to the critical pressure (220 bar for water and 50 bar for oxygen) and the second is much higher (500 bar for water and 200 bar for oxygen). Figures 3.4, 3.5, 3.6 and 3.7 show results corresponding to the transition from pure liquid to the supercritical state as schematically represented in Fig. 3.3.

As seen in Figs. 3.4, 3.5, 3.6 and 3.7, the liquid ENASG EOS (3.4.1) presents excellent agreement with experimental data. Passed the critical temperature T_c , the ENASG EOS is also used until connection with the ideal gas EOS and yields good agreement as well.

At the temperature of connection, the ideal gas EOS is considered with constant heat capacities until the temperature T_0 is reached. From this temperature, variable thermal capacities are used. Consequently, the ideal gas formulation is rather well-suited in the supercritical state. At such high temperatures, thermal agitation is indeed expected to be the dominant effect determining the properties of the fluid. The fundamental assumption of the ideal gas description (molecules free to evolve regardless of the others) then reappears in such thermodynamic conditions. The results computed with the ideal gas expression in the supercritical state are in excellent agreement with experimental data with the exception of the specific volume of supercritical water that presents a lesser agreement.

The results of the overall ENASG formulation are in good agreement with experimental data at



Figure 3.4: Comparison between experimental and theoretical isobar for water. The symbols represent the experimental isobar p = 230 bar. Beyond the critical temperature $T_c = 646$ K, the liquid transforms to supercritical state. The thick solid lines represent the Extended NASG (ENASG) EOS, reducing to the ideal gas description for the supercritical phase, Eqs. (3.4.1), (3.4.2) and (3.6.3). The thin solid lines represent the original NASG EOS also reducing to the ideal gas formulation for the supercritical phase. The dashed lines represent the van der Waals (VdW) theoretical predictions and the dash-dotted lines represent the Soave-Redlich-Kwong (SRK) ones. The critical temperature is indicated with the dotted lines. From this temperature, the liquid ENASG EOS is extended and joins the ideal gas EOS (except for the sound speed). The temperature $T_0 = 1000$ K at which variable heat capacities are considered is indicated in dotted lines as well.



Figure 3.5: Comparison between experimental and theoretical isobar for water. The symbols represent the experimental isobar p = 500 bar. Beyond the critical temperature $T_c = 646$ K, the liquid transforms to supercritical state. The thick solid lines represent the Extended NASG (ENASG) EOS, reducing to the ideal gas description for the supercritical phase, Eqs. (3.4.1), (3.4.2) and (3.6.3). The thin solid lines represent the original NASG EOS also reducing to the ideal gas formulation for the supercritical phase. The dashed lines represent the van der Waals (VdW) theoretical predictions and the dash-dotted lines represent the Soave-Redlich-Kwong (SRK) ones. The critical temperature is indicated with the dotted lines. From this temperature, the liquid ENASG EOS is extended and joins the ideal gas EOS (except for the sound speed). The temperature $T_0 = 1000$ K at which variable heat capacities are considered is indicated in dotted lines as well.



Figure 3.6: Comparison between experimental and theoretical isobar for oxygen. The symbols represent the experimental isobar p = 60 bar. Beyond the critical temperature $T_c = 154$ K, the liquid transforms to supercritical state. The thick solid lines represent the Extended NASG (ENASG) EOS, reducing to the ideal gas description for the supercritical phase, Eqs. (3.4.1), (3.4.2) and (3.6.3). The thin solid lines represent the original NASG EOS also reducing to the ideal gas formulation for the supercritical phase. The dashed lines represent the van der Waals (VdW) theoretical predictions and the dash-dotted lines represent the Soave-Redlich-Kwong (SRK) ones. The critical temperature is indicated with the dotted lines. From this temperature, the liquid ENASG EOS is extended and joins the ideal gas EOS (except for the sound speed). The temperature $T_0 = 400$ K at which variable heat capacities are considered is indicated in dotted lines as well.



Figure 3.7: Comparison between experimental and theoretical isobar for oxygen. The symbols represent the experimental isobar p = 200 bar. Beyond the critical temperature $T_c = 154$ K, the liquid transforms to supercritical state. The thick solid lines represent the Extended NASG (ENASG) EOS, reducing to the ideal gas description for the supercritical phase Eqs. (3.4.1), (3.4.2) and (3.6.3). The thin solid lines represent the original NASG EOS also reducing to the ideal gas formulation for the supercritical phase. The dashed lines represent the van der Waals (VdW) theoretical predictions and the dash-dotted lines represent the Soave-Redlich-Kwong (SRK) ones. The critical temperature is indicated with the dotted lines. From this temperature, the liquid ENASG EOS is extended and joins the ideal gas EOS (except for the sound speed). The temperature $T_0 = 400$ K at which variable heat capacities are considered is indicated in dotted lines as well.

both pressures close to the critical one and much higher. They also show the good behavior of the ENASG EOS when dealing with conditions away from the saturation ones.

As seen in Figs. 3.4, 3.5, 3.6 and 3.7, the extension of the liquid ENASG EOS results in good agreement with experimental data and provides a continuous formulation in the transcritical zone.

The only discontinuous thermodynamic variable is the speed of sound. This is clearly seen in Fig. 3.7 for example. Regarding the sound speed, the liquid ENASG EOS is not extended beyond the critical temperature as the formulation may not connect to the ideal gas expression. The discontinuous speed of sound at the critical temperature appears to be in practice similar to situations involving large sound-speed variations such as the transition from a pure fluid into a two-phase mixture at equilibrium, which does not cause practical difficulties. Obviously, this flaw is not encountered with cubic EOSs.

The ENASG EOS is also compared to cubic ones in the preceding figures. The van der Waals (VdW) [97] and Soave-Redlich-Kwong (SRK) [98] are used in this work. Detailed reviews of cubic equations of state can be found in Wei and Sadus (2000) [99] for instance.

As shown in Figs. 3.4 and 3.5, the cubic EOSs present poor accuracy regarding liquid water. However, the supercritical phase is well-described and the transition from liquid to supercritical state is naturally continuous since a unique formulation is used for both phases.

When oxygen is considered (Figs. 3.6 and 3.7), the VdW EOS shows very good results regarding the supercritical phase but is unable to represent properly the liquid state. Nevertheless, the SRK EOS presents excellent agreement with experimental data both for liquid and supercritical phases.

Vapor-to-supercritical-state transition

Much lower pressures (30 bar for water and 10 bar for oxygen) are considered in Figs. 3.8 and 3.9. Consequently, the three states of the corresponding fluids are involved (liquid, vapor, supercritical) and the vapor phase transforms to supercritical fluid beyond the critical temperature (Fig. 3.3).

As seen in Fig. 3.8, the ENASG EOS is able to represent correctly the liquid water unlike the VdW and SRK ones. The vapor and supercritical phases are rather well-described with all EOSs (ideal gas, VdW, SRK) and with continuous formulations (except for the sound speed with the ideal gas EOS).

The ENASG EOS is also well-suited for oxygen as seen in Fig. 3.9. The VdW EOS is again unable to represent properly the liquid state but the SRK one presents excellent results.

Concluding remarks

The results of the present section illustrate the good behavior of the ENASG EOS (3.4.1) and its reduction to the ideal gas expression (3.4.2), (3.6.3) in situations away from the saturation thermodynamic conditions. Figures 3.4, 3.5, 3.6 and 3.7 show that the proposed EOS is able to deal


Figure 3.8: Comparison between experimental and theoretical isobar for water. The symbols represent the experimental isobar p = 30 bar. Beyond the critical temperature $T_c = 646$ K, the vapor transforms to supercritical state. The thick solid lines represent the Extended NASG (ENASG) EOS, reducing to the ideal gas description for vapor and supercritical phases, Eqs. (3.4.1), (3.4.2) and (3.6.3). The thin solid lines represent the original NASG EOS also reducing to the ideal gas formulation. The dashdotted lines represent the van der Waals (VdW) theoretical predictions and the dashed lines represent the Soave-Redlich-Kwong (SRK) ones. The critical temperature is indicated with the dotted lines. The temperature $T_0 = 1000$ K at which variable heat capacities are considered is indicated in dotted lines as well.



Figure 3.9: Comparison between experimental and theoretical isobar for oxygen. The symbols represent the experimental isobar p = 10 bar. Beyond the critical temperature $T_c = 154$ K, the vapor transforms to supercritical state. The thick solid lines represent the Extended NASG (ENASG) EOS, reducing to the ideal gas description for vapor and supercritical phases, Eqs. (3.4.1), (3.4.2) and (3.6.3). The thin solid lines represent the original NASG EOS also reducing to the ideal gas formulation. The dash-dotted lines represent the van der Waals (VdW) theoretical predictions and the dashed lines represent the Soave-Redlich-Kwong (SRK) ones. The critical temperature is indicated with the dotted lines. The temperature $T_0 = 400$ K at which variable heat capacities are considered is indicated in dotted lines as well.

with pure liquids and supercritical states in pressure conditions both close and much higher than the critical pressure. Figures 3.8 and 3.9 illustrate the good behavior of the overall formulation with much lower pressures as well. The liquid expression seems able to represent the whole liquid phase diagram including the saturation conditions and the transcritical zone with a unique set of parameters. The corresponding vapor and supercritical phases are described accurately as well with the ideal gas expressions, except near the critical point as attractive terms have been removed in order to remain unambiguously convex, as discussed earlier.

The results of the original NASG EOS (Le Métayer and Saurel (2016) [22]), with associated parameters given in Tables 3.1 and 3.2, are also plotted in Figs. 3.4, 3.5, 3.6, 3.7, 3.8 and 3.9 for comparison. As already discussed, the supercritical phase is inaccurate as the different parameters have been determined with the help of experimental saturation data.

Nevertheless, for flows evolving away from saturation and at pressures much lower than the critical one, the NASG EOS is preferred to the ENASG one for the sake of simplicity. However, its reduction to the ideal gas formulation should use parameters determined away from the saturation curves since the ones determined at the thermodynamic equilibrium [22] induce inaccuracy as seen in Figs. 3.4, 3.5, 3.6, 3.7, 3.8 and 3.9. The results at saturation may be slightly degraded but the overall formulation is expected to deal with multiple thermodynamic conditions.

3.7 Two-phase flow illustrations

In the following, two-phase flows subject to phase changes are of interest. When evaporation or condensation phenomena appear, instantaneous phase transition is considered through the stiff thermochemical relaxation solver of Chiapolino et al. (2017) [1], [19] (Chapter 2, Section 2.10). Note that in the present chapter, the specific management of pure phases is not handled by Eq. (2.10.1) but by the Minmod-type method (see Chapter 2, Section 2.10). For the sake of simplicity, the Homogeneous Relaxation Model (HRM) [77] is considered and is reminiscent of the reactive (or multicomponent) Euler equations widely used in chemically reacting flows. The corresponding system reads,

$$\frac{\partial \rho}{\partial t} + div(\rho \mathbf{u}) = 0,$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + div(\rho \mathbf{u} \otimes \mathbf{u} + p\underline{I}) = 0,$$

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

$$\frac{\partial(\rho Y_1)}{\partial t} + div(\rho Y_1\mathbf{u}) = \rho\nu(g_2 - g_1),$$

$$\frac{\partial(\rho Y_2)}{\partial t} + div(\rho Y_2\mathbf{u}) = -\rho\nu(g_2 - g_1),$$

$$\frac{\partial(\rho Y_k)}{\partial t} + div(\rho Y_k\mathbf{u}) = 0,$$
(3.7.1)

with

$$E = e + \frac{1}{2}\mathbf{u}^2, \quad e = \sum_{k=1}^N Y_k e_k.$$

System (3.7.1) considers implicitly mechanical and thermal equilibria. The thermodynamic equilibrium is reached through the instantaneous relaxation ($\nu \to \infty$) of Gibbs free energies $g_1 = g_2$ where the indexes 1 and 2 denote respectively the liquid and vapor phases (see [1], [19], Chapter 2, Section 2.7). The other constituents of the flow ($N = 3 \to N$) are considered as non-condensable gases. **u** represents the mixture centre of mass velocity and E the mixture total energy.

System (3.7.1) is closed by a mixture equation of state made from mechanical and thermal equilibria. In the first place, let us considered gaseous flows transitioning to a supercritical state. When the critical temperature is reached, liquid is no longer present and the ENASG EOS is not to be used. Following the strategy of Chiapolino et al. (2017) [1], [19] (Chapter 2, Section 2.8), two expressions of the mixture temperature can be found according to the definitions of the mixture mass and mixture energy,

$$T = T_k \quad \forall k, \quad p = p_k \quad \forall k, \quad v = \sum Y_k v_k, \quad e = \sum Y_k e_k, \tag{3.7.2}$$

with Y_k denoting the mass fraction of the chemical species k.

In practical computations, gaseous mixture can be considered if $Y_1 < \epsilon$ with $\epsilon \simeq 10^{-8}$. In that case, $k = 2 \rightarrow N$ and the combination of Eqs. (3.7.2) and (3.4.1) leads to,

$$T_{v} = \frac{pv}{\sum_{k=2}^{N} Y_{k}(\gamma_{k} - 1)C_{v,k}} \quad \text{and} \quad T_{e} = \frac{e - \sum_{k=2}^{N} Y_{k}q_{k}}{\sum_{k=2}^{N} Y_{k}C_{v,k}}.$$
(3.7.3)

Equality of T_v and T_e provides the mixture gas pressure,

$$p(e,v) = \frac{\left(e - \sum_{k=2}^{N} Y_k q_k\right) \sum_{k=2}^{N} Y_k (\gamma_k - 1) C_{v,k}}{v \sum_{k=2}^{N} Y_k C_{v,k}}.$$
(3.7.4)

Figure 3.10 shows such a situation where water vapor transforms into supercritical state through compression effects of a shock wave. A shock tube is indeed considered with liquid water, vapor water and air. In the high pressure chamber, air is initially in major proportions, $Y_3 \rightarrow 1$ with thermodynamic conditions p = 30 bar and T = 800 K. In the second chamber, water vapor is in major proportion $Y_2 \rightarrow 1$ with p = 1 bar and T = 600 K. The mixture is initially at thermodynamic equilibrium according to the conditions detailed in [19] (Chapter 2, Section 2.9, Eq. (2.9.13)). The ideal gas reduction of the ENASG EOS is used with parameters for water given in Table 3.1 while the only coefficients needed for air are: $C_{v,3} = 719$ J/kg/K and $\gamma_3 = 1.4$. Liquid is present but in negligible proportions so mixture equation of state (3.7.4) is used in practice. As seen in Fig. 3.10, the transition from "pure" vapor to supercritical state is naturally continuous when the temperature becomes higher than the critical one $T_c = 646$ K.



Figure 3.10: Shock tube test illustrating the transition from "pure" water vapor to supercritical state. The critical temperature is indicated with the dotted line. The thick lines represent the solution obtained with the mixture ENASG EOS reducing to Eq. (3.7.4) in the present example as liquid mass fraction is non-zero but in negligible proportions. The dashed lines represent the initial conditions. In the left chamber, air is initially in major proportions with $Y_3^{left} = 1 - 2 \cdot 10^{-7}$, p = 30 bar and T = 800 K. Liquid and vapor mass fractions are deduced as $Y_1^{left} \simeq 10^{-8}$ and $Y_2^{left} \simeq 1.9 \cdot 10^{-7}$. In the right chamber, water vapor is in major proportions with $Y_3^{right} = 10^{-7}$, p = 1 bar and T = 600 K. Liquid and vapor mass fractions are deduced as $Y_1^{right} \simeq 10^{-8}$ and $Y_2^{right} \simeq 0.99999989$. The test was carried out with Godunov time integration method and HLLC Riemann solver extended to second order: MUSCL scheme with Minmod flux limiter. The solution is given at $t \approx 0.3$ ms on a 1000-cell mesh using CFL = 0.8.

Let us now consider a situation where liquid is in major proportions. In that case, the combination of the mixture definitions (3.7.2) and the ENASG relations (3.4.1) leads to two quadratic expressions for the mixture temperature (note that only one liquid is considered in this work),

$$aT^2 + bT + c = 0, (3.7.5)$$

with the corresponding coefficients,

$$\begin{cases} a_v = \frac{\gamma_1 p_{\infty,1,1}}{p} \sum_{k=2}^N Y_k(\gamma_k - 1) C_{v,k}, \\ b_v = Y_1 \frac{(\gamma_1 - 1) C_{v,1}}{1 - b_{1,1}} + \left(1 + \frac{\gamma_1 p_{\infty,0,1}(1 - b_{1,1})}{(\gamma_1 - b_{1,1})p}\right) \left(\sum_{k=2}^N Y_k(\gamma_k - 1) C_{v,k}\right) + \left(\frac{Y_1 b_{0,1}}{1 - b_{1,1}} - v\right) \gamma_1 p_{\infty,1,1}, \\ c_v = \left(\frac{Y_1 b_{0,1}}{1 - b_{1,1}} - v\right) \left(p + \frac{\gamma_1 p_{\infty,0,1}(1 - b_{1,1})}{\gamma_1 - b_{1,1}}\right), \end{cases}$$

$$(3.7.6)$$

$$\begin{cases} a_e = Y_1 \gamma_1 p_{\infty,1,1} C_{v,1} + \gamma_1 p_{\infty,1,1} \sum_{k=2}^N Y_k C_{v,k}, \\ b_e = Y_1 \left(p + \gamma_1 p_{\infty,0,1} \right) C_{v,1} + \left(p + \frac{\gamma_1 p_{\infty,0,1} (1 - b_{1,1})}{\gamma_1 - b_{1,1}} \right) \left(\sum_{k=2}^N Y_k C_{v,k} \right) + (\bar{q} - e) \gamma_1 p_{\infty,1,1}, \quad (3.7.7) \\ c_e = (\bar{q} - e) \left(p + \frac{\gamma_1 p_{\infty,0,1} (1 - b_{1,1})}{\gamma_1 - b_{1,1}} \right), \end{cases}$$

where the mixture quantity is introduced:

$$\bar{q} = \sum_{k=1}^{N} Y_k q_k.$$
 (3.7.8)

Equality of the two positive solutions provides the mixture pressure p(e, v). An iterative method is required nonetheless. However, Eq. (3.7.4) is to be used where $Y_1 \leq \epsilon \rightarrow 0$ corresponds to a gaseous mixture.

The transition from supercritical state to "pure" liquid is now considered through a double expansion test. In Fig. 3.11, vapor water and air are present in negligible proportions and supercritical water undergoes expansion waves. Those induce pressure drop from 350 bar to about 226 bar. The final pressure then remains slightly above the critical one, $p_c = 220$ bar. They also induce temperature drop from 655 K to about 641 K. The final temperature is consequently inferior to the critical one $T_c = 646$ K resulting in transition from supercritical to liquid phase that is computed continuously.

A configuration where liquid-gas interfaces are present is now considered. Phase change is illustrated on the evaporating liquid jet configuration detailed in Chiapolino et al. (2017) [19] (Chapter 2, Section 2.14, Fig. 2.16). In this last reference, the mixture EOS is made from the NASG EOS for each fluid (reduced to SG in this test) and is reconsidered in the following in the frame of the ENASG EOS.

The conditions are typical of cryotechnic rocket engines during the ignition phase (for which the engine has not yet reached supercritical conditions). The flow consists of a coaxial liquid oxygen jet



Figure 3.11: Double expansion test illustrating the transition from supercritical state to "pure" liquid water. The critical pressure and temperature are indicated with the dotted lines. The thick lines represent the solution obtained with the mixture ENASG EOS. The dashed lines represent the initial conditions. Liquid water is initially in major proportions with $Y_1 = 1 - 2 \cdot 10^{-6}$, $Y_2 = Y_3 = 10^{-6}$, p = 350 bar, T = 655 K and $u = \pm 45$ m/s. The test was carried out with Godunov time integration method and HLLC Riemann solver extended to second order: MUSCL scheme with Minmod flux limiter. The solution is given at $t \approx 0.3$ ms on a 1000-cell mesh using CFL = 0.8.

surrounded by a high-speed hydrogen flow (non-condensable gas), injected in conditions above the saturation point of the inner oxygen core, which then evaporates whilst being destabilized. Such a case is very challenging, because there is initially no vapor oxygen, and mass transfer is the only possible term for vapor production. The ENASG EOS is used with parameters for oxygen given in Table 3.2 while the only coefficients needed for hydrogen are: $C_{v,3} = 10183 \text{ J/kg/K}, \gamma_3 = 1.4$ and $q_3 = -1.2 \cdot 10^6 \text{ J/kg}$. Mass transfer is treated with the thermochemical relaxation solver detailed in [19] (Chapter 2, Section 2.10). Figure 3.12 shows the density contours and the vapor mass fraction created.



Figure 3.12: Density and vapor mass fraction profiles of a liquid oxygen jet surrounded by hydrogen at high speed entering a combustion chamber of a cryotechnic rocket engine. Shear effects induce jet fragmentation. The filaments separating the main liquid core and the gas gradually vanish as a consequence of evaporation. The computation was done with the MUSCL scheme with Superbee limiter and CFL = 0.7. The solution is given at $t \approx 4.1$ ms. The mesh is unstructured and made of about 360,000 triangles.

As expected, the filaments separating the main liquid core and the gas gradually vanish as a consequence of evaporation and the created vapor mass fraction is of utmost importance for future works, which shall include the gaseous combustion between vapor oxygen and hydrogen. In that case, only the ideal gas reduction of the ENASG EOS is to be used with variable heat capacities.

3.8 Conclusion

The Noble-Abel-Stiffened-Gas (NASG) equation of state has been extended to variable attractive and repulsive effects to deal with liquids when large temperature and pressure ranges are considered. The liquid phase is well-described at thermodynamic conditions both near and away from the saturation ones with a convex formulation. The overall ENASG EOS reduces to the ideal gas description both for vapor and supercritical phases for the sake of convexity.

The transition from pure fluid to supercritical state is of interest as well, including at high pressures where the liquid directly transforms to supercritical fluid. The ENASG EOS proposes a solution in the direction of such transition while remaining convex, an essential property in computational fluid dynamics.

Two different liquid-gas couples have been addressed, water and oxygen, presenting respectively triatomic and diatomic molecular fluids. The overall formulation presents good agreement with experimental data. However, the saturated vapor phase necessarily lacks of accuracy near the critical point as attractive effects are absent.

Those latter ones seem nonetheless responsible for conditional convexity, a feature reminiscent of cubic equations of state.

The Extended NASG (ENASG) equation of state recovers the NASG one when the new introduced coefficients are set to zero. Its formulation remains quite simple, convex and is beneficial to the introduction of phase transition solvers such as the ones promoted in Chiapolino et al. (2017) [1], [19] (Chapter 2).

Acknowledgements

Part of this work has been carried out in the framework of the Labex MEC (ANR-10-LABX-0092) and of the A*MIDEX project (ANR-11-IDEX-0001-02), funded by the "Investissements d'Avenir" French Government program managed by the French National Research Agency (ANR). We also acknowledge funding from ANR through project SUBSUPERJET, ANR-14-CE22-0014.

Part IV

Fluid dispersal at large scales

Introduction

Gas dispersal at large time and space scales may appear in many urban places, industrial plants and natural environments. This topic is consequently of interest to the safety community as the gas dispersion may yield severe consequences.

In this manuscript, the situations of typical interest involve multiple dense gases. In this context, one of the difficulties is to address long-time simulations involving large-scale numerical domains while providing accurate results at a reasonable cost in CPU time.

The two-layer shallow water strategy is consequently an interesting candidate as it allows to address 2D simulations to mimic 3D results. The computational gain in CPU time is thereby expected to be tremendous compared to conventional multi-fluid approaches.

However, two-layer shallow water models present serious difficulties as well. Those are related to the conditional hyperbolicity of most models and to the presence of non-conservative terms in the corresponding theoretical formulations.

The research work presented in Chapter 4 addresses these problematics and provides solutions. A new two-layer shallow water system is introduced in the following chapter and its numerical resolution is treated as well through a HLL-type Riemann solver. The new system is strictly hyperbolic as a consequence of pressure disequilibrium and compressible character of the fluids.

Chapter 4

Models and methods for two-layer shallow water flows

Abstract

Two-layer shallow water models present at least two fundamental difficulties that are addressed in the present contribution. The first one is related to the lack of hyperbolicity of most existing models. By considering weak compressibility of the phases, a strictly hyperbolic formulation with pressure relaxation is obtained. It is shown to tend to the conventional two-layer model in the stiff pressure relaxation limit. The second issue is related to the non-conservative terms in the momentum equations. Analyzing the Riemann problem structure, local constants appear precisely at locations where the non-conservative products need definition. Thanks to these local constants, a locally conservative formulation of the equations is obtained, simplifying the Riemann problem resolution through a HLLtype Riemann solver. The method is compared to literature data, showing accurate and oscillation free solutions. Additional numerical experiments show robustness and accuracy of the method.

4.1 Introduction

Two-layer (and multi-layer) shallow water models are particularly useful in some limit cases of multi-fluid and variable density flows separated by nearly horizontal interfaces. These models govern the dynamics of incompressible fluids spreading under gravity effects. It can be for example:

- Flows of the same liquid but at different temperatures, resulting in density differences, such situation being typical of oceanic flows;
- Flows of two liquids of different densities;
- Flows of two gases evolving at low Mach number.

The two-layer approach is particularly interesting compared to multidimensional approaches, that consider vertical motion, as it enables much faster computations. It is also helpful when the height of one of the phases is arbitrarily small, as there is no need to spatially resolve it. Thereby, no numerical diffusion of the nearly horizontal interface is present and no interface tracking is needed. However, there are obviously some limitations with this approach:

- The vertical velocity component is neglected;
- The velocity is assumed uniform in cross sections of each layer.

Such type of modeling also involves serious difficulties. Indeed, most models are not hyperbolic, this issue having serious consequences both for propagation phenomenon, which becomes ill-posed, and for the design of numerical methods. A second serious difficulty appears as non-conservative terms are present in the momentum equations. The present chapter addresses these two difficulties and provides solutions.

In the frame of averaged (or homogenized) equations in fluid mechanics, the issue related to the lack of hyperbolicity appears in different type of models, such as those of non-equilibrium two-phase flows. Only a few models seem well-posed with this respect, (Marble (1963) [100], Baer and Nunziato (1986) [49], Saurel et al. (2017) [92]). There are mainly two types of remedy to cure this issue:

- Consider compressibility of the phases and deal with pressure relaxation [86]. This approach involves sound propagation in the phases and is particularly efficient in many situations. It has been adopted in the last two above-mentioned references.
- Consider turbulent effects in the phases, as they result in the appearance of a "turbulent sound speed" (Forestier et al. (1997) [101], Saurel et al. (2003) [102], Lhuillier et al. (2013) [103]). In the frame of shallow water flows, these effects have been studied in Richard and Gavrilyuk (2012) [104] and Gavrilyuk et al. (2016) [105].

In the present work, the first method is adopted and the fluids are considered weakly compressible. The resulting model is strictly hyperbolic and in the limit of stiff pressure relaxation, the conventional (non-hyperbolic) two-layer model is recovered. This approach is reminiscent of the model of Abgrall and Karni (2009) [106], except that extra pressure terms are present in the momentum equations of the new formulation. It also gives another interpretation of the relaxation approach, now based on compressibility and pressure effects.

The second issue is addressed as well and is related to the presence of non-conservative terms in the momentum equations. By examining the Riemann problem structure, it appears that local constants are present, at locations where the derivative of the Heaviside function emerges. Consequently the non-conservative products become well-defined. Also, local conservation laws are obtained and used in the frame of HLL-type Riemann solver.

The accuracy of the new solver is checked against results of Abgrall and Karni (2009) [106] as well as results obtained with a flow solver based on the VFRoe method of Gallouet and Masella (1996) [107] as it is able to deal, to some extent, with both conservative and non-conservative systems. The new method, based on HLL-type solver, shows results of high accuracy and is oscillation free.

This chapter is organized as follows. The two-layer hyperbolic model is presented in Section 4.2 and its stiff mechanical relaxation limit is examined. Both approximate VFRoe solver and non-conservative HLL solver are considered in Section 4.3. A Godunov-type scheme is derived in the same section. Results and validations are addressed in Sections 4.4 and 4.5. Conclusions are given in Section 4.6.

4.2 Hyperbolic two-layer shallow water model

The conventional two-layer shallow water model (Ovsyannikov (1979) [108]) reads,

$$\begin{cases} \frac{\partial(h_1\rho_1)}{\partial t} + \frac{\partial(h_1\rho_1u_1)}{\partial x} = 0, \\ \frac{\partial(h_1\rho_1u_1)}{\partial t} + \frac{\partial(h_1\rho_1u_1^2 + \frac{1}{2}\rho_1gh_1^2 + g\rho_2h_1h_2)}{\partial x} = \rho_2gh_2\frac{\partial h_1}{\partial x}, \\ \frac{\partial(h_2\rho_2)}{\partial t} + \frac{\partial(h_2\rho_2u_2)}{\partial x} = 0, \\ \frac{\partial(h_2\rho_2u_2)}{\partial t} + \frac{\partial(h_2\rho_2u_2^2 + \frac{1}{2}\rho_2gh_2^2)}{\partial x} = -\rho_2gh_2\frac{\partial h_1}{\partial x}. \end{cases}$$
(4.2.1)

 h_1 and h_2 denote the heights of the two layers, ρ_1 and ρ_2 represent the densities of the fluids, considered constant at this level, u_1 and u_2 denote the fluid velocities, averaged in each layer and g represents the gravity constant. Topography effects have been omitted for the sake of simplicity as well as friction with the bottom and between layers.

System (4.2.1) has been examined in Abgrall and Karni (2009) [106], Kurganov and Petrova (2009)

[109] and Monjarret (2015) [110] and appeared hyperbolic for small velocity drift only,

$$(u_1 - u_2)^2 < (h_1 + h_2)g\left(1 - \frac{\rho_2}{\rho_1}\right).$$
(4.2.2)

Moreover the wave speeds can hardly be computed, rendering the system intricate to solve numerically. A method is given in Kurganov and Petrova (2009) [109] to overcome this difficulty. In the present approach, pressure non-equilibrium effects result in an unconditionally hyperbolic formulation:

$$\frac{\partial h_1}{\partial t} + u_1 \frac{\partial h_1}{\partial x} = \frac{\mu(p_1 - p_0)}{\rho_1 c_1^2},$$

$$\frac{\partial (h_1 \rho_1)}{\partial t} + \frac{\partial (h_1 \rho_1 u_1)}{\partial x} = 0,$$

$$\frac{\partial (h_1 \rho_1 u_1)}{\partial t} + \frac{\partial (h_1 \rho_1 u_1^2 + h_1 p_1(\rho_1) + \frac{1}{2}\rho_1 g h_1^2 + g \rho_2 h_1 h_2)}{\partial x} = \rho_2 g h_2 \frac{\partial h_1}{\partial x} + p_0 \frac{\partial h_1}{\partial x},$$

$$\frac{\partial h_2}{\partial t} + u_2 \frac{\partial h_2}{\partial x} = \frac{\mu(p_2 - p_0)}{\rho_2 c_2^2},$$

$$\frac{\partial (h_2 \rho_2)}{\partial t} + \frac{\partial (h_2 \rho_2 u_2)}{\partial x} = 0,$$

$$\frac{\partial (h_2 \rho_2 u_2)}{\partial t} + \frac{\partial (h_2 \rho_2 u_2^2 + h_2 p_2(\rho_2) + \frac{1}{2}\rho_2 g h_2^2)}{\partial x} = -\rho_2 g h_2 \frac{\partial h_1}{\partial x} + p_0 \frac{\partial h_2}{\partial x}.$$
(4.2.3)

Two equations have been added and express the transport of the heights of the fluid layers that are assumed to vary as a function of pressure differentials $(p_k - p_0)$. p_k denotes the thermodynamic pressure of fluid k, given by barotropic (and convex) equations of state $p_k(\rho_k)$. Example of such equation of state (EOS) is,

$$p_k(\rho_k) = p_k^{(0)} + c_k^2 \left(\rho_k - \rho_k^{(0)} \right), \qquad (4.2.4)$$

with k = 1, 2. Other options, such as Tait EOS for instance are possible. We will see that the choice of the EOS is not important, only the related sound speed c_k has importance. p_0 denotes the (constant) atmospheric pressure and $p_k^{(0)} = p_0$.

The assumption of constant atmospheric pressure is quite realistic when dealing with flows of gases having different densities. When dealing with liquids and large hydrostatic effects, the model can be reformulated with extra pressure terms as a function of heights of the fluid layers, and does not cause extra fundamental issues than those already addressed in the present contribution. Such extension is given in Appendix D.1, but for the sake of simplicity of the presentation, this extended model is not considered in the rest of the chapter.

The pressure relaxation parameter μ is related to the fluid sound speeds and heights of layers. It controls the rate at which pressure equilibrium is reached. Following Saurel et al. (2017) [92], the first equation of System (4.2.3) can be written as,

$$\frac{d_1h_1}{dt} = \frac{h_1}{\tau} \frac{p_1 - p_0}{\rho_1 c_1^2}$$

where $\frac{d_1}{dt} = \frac{\partial}{\partial t} + u_1 \frac{\partial}{\partial x}$ and τ is the pressure relaxation time,

$$\tau = \frac{h_1}{c_1},$$
(4.2.5)

corresponding to the following pressure relaxation parameter estimate:

$$\mu \simeq \frac{h_1}{\tau} \simeq c_1. \tag{4.2.6}$$

In most situations, this relaxation time is of the order of $\frac{1}{100}$ second, meaning that the relaxation parameter μ is large: $\mu \simeq \text{Max}(\tau_1^{-1}, \tau_2^{-1})$ or alternatively $\mu \simeq \text{Min}(c_1, c_2)$. In practical computations, the relaxation time τ will be assumed of the same order as the computational time step and stiff pressure relaxation will be done at the end of each time step. Therefore, there is no need of precise knowledge of the pressure relaxation parameter μ .

This system is reminiscent of Baer and Nunziato's (1986) [49] model widely used in two-phase flow modeling. It is also reminiscent of Abgrall and Karni's (2009) [106] relaxation model, except that pressure terms have been added to the momentum equations $(h_1p_1(\rho_1) \text{ and } h_2p_2(\rho_2))$. To maintain mechanical equilibrium, extra non-conservative terms have been added in the right-hand side $(p_0 \frac{\partial h_k}{\partial x})$. These terms are not in contradiction with the total momentum conservation that reads:

$$\frac{\partial (h_1 \rho_1 u_1 + h_2 \rho_2 u_2)}{\partial t} + \frac{\partial \left[h_1 \rho_1 u_1^2 + h_1 p_1(\rho_1) + \frac{1}{2} \rho_1 g h_1^2 + g \rho_2 h_1 h_2 + h_2 \rho_2 u_2^2 + h_2 p_2(\rho_2) + \frac{1}{2} \rho_2 g h_2^2 - p_0 (h_1 + h_2)\right]}{\partial x} = 0.$$

Let us now examine some relevant properties to check validity of this formulation.

Hyperbolicity

System (4.2.3) is expressed in primitive-variable formulation (in the absence of source terms) as,

$$\frac{\partial W}{\partial t} + A(W)\frac{\partial W}{\partial x} = 0, \qquad (4.2.7)$$

with

$$W = \begin{pmatrix} h_1 \\ \rho_1 \\ u_1 \\ h_2 \\ \rho_2 \\ u_2 \end{pmatrix}, \quad A(W) = \begin{pmatrix} u_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & u_1 & \rho_1 & 0 & 0 & 0 \\ \frac{p_1 - p_0}{h_1 \rho_1} + g & \frac{c_1^2 + \frac{1}{2}gh_1}{\rho_1} & u_1 & g\frac{\rho_2}{\rho_1} & \frac{gh_2}{\rho_1} & 0 \\ 0 & 0 & 0 & u_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & u_2 & \rho_2 \\ g & 0 & 0 & \frac{p_2 - p_0}{h_2 \rho_2} + g & \frac{c_2^2 + \frac{1}{2}gh_2}{\rho_2} & u_2 \end{pmatrix}.$$
(4.2.8)

The wave speeds are solutions of det $(A(W) - \lambda \underline{I}) = 0$ resulting in,

$$(u_1 - \lambda)(u_2 - \lambda)\left[(u_2 - \lambda)^2 - \left(c_2^2 + \frac{1}{2}gh_2\right)\right]\left[(u_1 - \lambda)^2 - \left(c_1^2 + \frac{1}{2}gh_1\right)\right] = 0.$$
(4.2.9)

Six real and distinct eigenvalues appear as:

$$\begin{cases} \lambda_1 = u_1, \quad \lambda_2 = u_1 + \sqrt{c_1^2 + \frac{1}{2}gh_1}, \quad \lambda_3 = u_1 - \sqrt{c_1^2 + \frac{1}{2}gh_1}, \\ \lambda_4 = u_2, \quad \lambda_5 = u_2 + \sqrt{c_2^2 + \frac{1}{2}gh_2}, \quad \lambda_6 = u_2 - \sqrt{c_2^2 + \frac{1}{2}gh_2}. \end{cases}$$
(4.2.10)

Those eigenvalues correspond to the wave speeds emerging at a given initial discontinuity, as schematized in Fig. 4.1.



Figure 4.1: Schematic representation in the (x, t) diagram of the six waves (4.2.10) present in the flow model (4.2.3) and emerging at a given initial discontinuity.

System (4.2.3) is consequently strictly hyperbolic. This model is however relevant with respect to the physics expressed in (4.2.1) if it tends to the same equations when pressure relaxation is stiff. This limit is examined hereafter.

Stiff pressure relaxation limit

The mass and height equations of a given phase are analyzed:

$$\begin{cases} \frac{\partial h_k}{\partial t} + u_k \frac{\partial h_k}{\partial x} = \frac{\mu(p_k - p_0)}{\rho_k c_k^2},\\ \frac{\partial (h_k \rho_k)}{\partial t} + \frac{\partial (h_k \rho_k u_k)}{\partial x} = 0, \end{cases}$$

with k = 1, 2. Their combination results in,

$$\frac{d_k \rho_k}{dt} + \rho_k \frac{\partial u_k}{\partial x} = -\frac{\rho_k}{h_k} \frac{\mu \left(p_k - p_0\right)}{\rho_k c_k^2}$$

Inserting the phase k equation of state $p_k(\rho_k)$, the following pressure evolution equation is obtained,

$$\frac{d_k p_k}{dt} + \rho_k c_k^2 \frac{\partial u_k}{\partial x} = -\frac{\mu \left(p_k - p_0\right)}{h_k}$$

As the atmospheric pressure p_0 is constant, the last equation can be expressed as,

$$\frac{d_k(p_k - p_0)}{dt} + \rho_k c_k^2 \frac{\partial u_k}{\partial x} = -\frac{\mu \left(p_k - p_0\right)}{h_k}.$$

The phase pressure is expressed around the equilibrium state with the following expansion,

$$p_k = \left(p_k^{(0)} + \epsilon p_k^{(1)} + \ldots\right),\,$$

where

- ϵ is of the order of the inverse of pressure relaxation parameter ($\epsilon \simeq \mu^{-1} \simeq \tau$), tending to zero in most situations ($\epsilon \to 0^+$) as discussed earlier (see also Kapila et al. (2001) [5] for estimates in the context of granular flows),
- $-p_k^{(0)}$ and $p_k^{(1)}$ represent respectively the leading and first-order pressure terms of the Taylor expansion.

Inserting these definitions in the pressure evolution equation,

$$\frac{d_k\left(\left[p_k^{(0)} + \epsilon p_k^{(1)} + \dots\right] - p_0\right)}{dt} + \rho_k c_k^2 \frac{\partial u_k}{\partial x} = -\frac{\left[p_k^{(0)} + \epsilon p_k^{(1)} + \dots\right] - p_0}{h_k \epsilon},$$

the following results are obtained:

- At leading order (ϵ^{-1}) : $p_k^{(0)} = p_0$;
- At first order $p_k^{(1)} = -\rho_k c_k^2 h_k \frac{\partial u_k}{\partial x}$.

Inserting this last result in the height equations,

$$\frac{\partial h_k}{\partial t} + u_k \frac{\partial h_k}{\partial x} = \frac{\mu \left(p_k - p_0 \right)}{\rho_k c_k^2} \simeq \frac{p_k^{(1)}}{\rho_k c_k^2} \simeq -h_k \frac{\partial u_k}{\partial x}$$

they become,

$$\frac{\partial h_k}{\partial t} + \frac{\partial \left(h_k u_k\right)}{\partial x} \simeq 0.$$

The mass equations are unchanged while modifications in the momentum equations appear as a consequence of the equilibrium condition $(p_k = p_0)$. They finally result at leading order in,

$$\begin{cases} \frac{\partial \left(h_1\rho_1 u_1\right)}{\partial t} + \frac{\partial \left(h_1\rho_1 u_1^2 + \frac{1}{2}\rho_1 g h_1^2 + g \rho_2 h_1 h_2\right)}{\partial x} = \rho_2 g h_2 \frac{\partial h_1}{\partial x},\\ \frac{\partial \left(h_2\rho_2 u_2\right)}{\partial t} + \frac{\partial \left(h_2\rho_2 u_2^2 + \frac{1}{2}\rho_2 g h_2^2\right)}{\partial x} = -\rho_2 g h_2 \frac{\partial h_1}{\partial x}.\end{cases}$$

System (4.2.1) is recovered, complemented by two conservation equations for the heights, that are in agreement with the two mass equations as soon as the densities are constants.

It thus appears that System (4.2.3) tends to System (4.2.1) when pressure relaxation is stiff. As System (4.2.3) is hyperbolic, it is a good candidate to approximate (4.2.1) numerically with a two-step procedure:

- Solve the hyperbolic system (4.2.3) without source terms;
- Relax the pressures onto the atmospheric one and reset the heights.

This is similar to the method of Saurel and Abgrall (1999) [3] to compute flows with interfaces separating fluids. Before entering in the details of the hyperbolic solver, let us present the pressure relaxation process, that is particularly simple in the present context.

Stiff pressure relaxation solver

Let us consider for example EOS (4.2.4). Consequently, the densities as functions of pressures are given by:

$$\rho_k = \rho_k^{(0)} + \frac{p_k - p_k^{(0)}}{c_k^2}.$$
(4.2.11)

As the pressures relax to the atmospheric one $(p_k = p_k^{(0)} = p_0)$, the densities at relaxed pressure are just,

$$\rho_k^* = \rho_k^{(0)}, \tag{4.2.12}$$

where the superscript * denotes the relaxed pressure state. As the masses of each layer are computed by associated mass balance equations and are constant during the relaxation process,

$$m_k = h_k \rho_k = h_k^* \rho_k^*, \tag{4.2.13}$$

the heights at relaxed states are reset as,

$$h_k^* = \frac{h_k \rho_k}{\rho_k^{(0)}}.$$
(4.2.14)

The stiff pressure relaxation solver just consists in the reset of the heights of the fluids $h_k \to h_k^*$ and is independent of the equations of state. At this level, the relaxation method of Abgrall and Karni (2009) [106] is recovered. We now address the design of hyperbolic solvers.

4.3 Approximate Riemann solvers

Two different approximate methods are considered to solve the Riemann problem of System (4.2.3), the VFRoe method (Gallouet and Masella (1996) [107]) and a new HLL-type Riemann solver (Harten et al. (1983) [111]). As System (4.2.3) contains non-conservative terms, an approach dealing with both conservative and non-conservative systems is examined first.

VFRoe solver

The VFRoe method considers the equations in non-conservative formulation,

$$\frac{\partial W}{\partial t} + A(\overline{W})\frac{\partial W}{\partial x} = 0, \qquad (4.3.1)$$

with

$$W = (h_1, \ \rho_1, \ u_1, \ h_2, \ \rho_2, \ u_2)^T$$
 and $\overline{W} = \frac{W_L + W_R}{2}$,

where W_L and W_R are respectively the left and right-state vectors at a given cell boundary.

The VFRoe method considers the exact Riemann problem solution of (4.3.1). Note that (4.3.1) is a local linearization of the non-linear flow model (4.2.3) around state \overline{W} . The VFRoe solution is thus the exact solution of an approximate problem.

The exact solution of (4.3.1) may be found in many textbooks related to hyperbolic systems (LeVeque (2002) [60], Toro (2013) [112]) and can be summarized as follows,

$$W^* = W_L + \sum_{\overline{\lambda_i} < 0} \overline{a_i} \overline{R_i} = W_R - \sum_{\overline{\lambda_i} > 0} \overline{a_i} \overline{R_i}, \qquad (4.3.2)$$

where the wave strengths $\overline{a_i}$ are the coefficients resulting from the decomposition of the eigenvectors,

$$W_R - W_L = \sum_{\overline{\lambda_i}} \overline{a_i} \overline{R_i}.$$
(4.3.3)

For the sake of space, the right eigenvectors R_i and the wave strengths $\overline{a_i}$ are not detailed, associated formulas being considerably large. The main weakness of this method is related to the average \overline{W} which can be far from the solution of the non-linear problem, resulting in positivity issues especially when large amplitude waves are present.

With the help of the Riemann problem solution (4.3.2), the various equations of System (4.2.3) are updated with a Godunov-type method (stable under the conventional CFL condition) as,

$$h_{k,i}^{n+1} = h_{k,i}^n - \frac{\Delta t}{\Delta x} \left((h_k u_k)_{i+\frac{1}{2}}^* - (h_k u_k)_{i-\frac{1}{2}}^* \right) + \frac{\Delta t}{\Delta x} h_{k,i}^n \left(u_{k,i+\frac{1}{2}}^* - u_{k,i-\frac{1}{2}}^* \right), \tag{4.3.4}$$

$$(h_k \rho_k)_i^{n+1} = (h_k \rho_k)_i^n - \frac{\Delta t}{\Delta x} \left((h_k \rho_k u_k)_{i+\frac{1}{2}}^* - (h_k \rho_k u_k)_{i-\frac{1}{2}}^* \right), \tag{4.3.5}$$

$$(h_{1}\rho_{1}u_{1})_{i}^{n+1} = (h_{1}\rho_{1}u_{1})_{i}^{n} - \frac{\Delta t}{\Delta x} \left\{ \left(h_{1}\rho_{1}u_{1}^{2} + h_{1}(p_{1} - p_{0}) + \frac{1}{2}\rho_{1}h_{1}^{2} \right)_{i+\frac{1}{2}}^{*} - \left(h_{1}\rho_{1}u_{1}^{2} + h_{1}(p_{1} - p_{0}) + \frac{1}{2}\rho_{1}h_{1}^{2} \right)_{i-\frac{1}{2}}^{*} \right\} + \frac{\Delta t}{\Delta x} h_{1,i}^{n} \left\{ (-\rho_{2}gh_{2})_{i+\frac{1}{2}}^{*} - (-\rho_{2}gh_{2})_{i-\frac{1}{2}}^{*} \right\},$$

$$(4.3.6)$$

$$(h_{2}\rho_{2}u_{2})_{i}^{n+1} = (h_{2}\rho_{2}u_{2})_{i}^{n} - \frac{\Delta t}{\Delta x} \left\{ \left(h_{2}\rho_{2}u_{2}^{2} + h_{2}(p_{2} - p_{0}) + \frac{1}{2}\rho_{2}h_{2}^{2} + \rho_{2}gh_{1}h_{2} \right)_{i+\frac{1}{2}}^{*} - \left(h_{2}\rho_{2}u_{2}^{2} + h_{2}(p_{2} - p_{0}) + \frac{1}{2}\rho_{2}h_{2}^{2} + \rho_{2}gh_{1}h_{2} \right)_{i-\frac{1}{2}}^{*} \right\}$$

$$+ \frac{\Delta t}{\Delta x}h_{1,i}^{n} \left\{ \left((\rho_{2}gh_{2})_{i+\frac{1}{2}}^{*} - (\rho_{2}gh_{2})_{i-\frac{1}{2}}^{*} \right) \right\},$$

$$(4.3.7)$$

where n + 1 and n denote two consecutive time steps and superscript * denotes the VFRoe Riemann problem solution given by Eq. (4.3.2). Indexes i and $i \pm \frac{1}{2}$ denote respectively the center of the current numerical cell and its corresponding boundaries.

HLL-type Riemann solver

Let us consider a simplified solver, based on Rankine-Hugoniot conditions, such as the HLL solver. In this frame, the two extreme waves S_L and S_R are approximated following Davis (1988) [113] as,

$$\begin{cases} S_{L,k} = \min\left(u_{L,k} - \sqrt{c_{L,k}^2 + \frac{1}{2}gh_{L,k}} , u_{R,k} - \sqrt{c_{R,k}^2 + \frac{1}{2}gh_{R,k}}\right), \\ S_{R,k} = \max\left(u_{L,k} + \sqrt{c_{L,k}^2 + \frac{1}{2}gh_{L,k}} , u_{R,k} + \sqrt{c_{R,k}^2 + \frac{1}{2}gh_{R,k}}\right), \end{cases}$$
(4.3.8)

with k = 1, 2. The indexes L and R denote respectively the left and right states at a given cell boundary. The two extreme waves are considered as,

$$S_L = \min(S_{L,1}, S_{L,2}), \quad S_R = \max(S_{R,1}, S_{R,2}).$$
 (4.3.9)

The two contact waves u_1 and u_2 are considered as well for the transport of the heights h_1 and h_2 , as depicted in Fig. 4.2.



Figure 4.2: Schematic representation in the (x, t) diagram of the two extreme waves and the two contact waves considered for the transport of the two heights.

Regarding the transport equations, the exact Riemann problem solution is straightforward:

$$\begin{cases} h_1^* \left(\frac{x}{t} < u_1^*\right) = h_{1,L}, & h_1^* \left(\frac{x}{t} > u_1^*\right) = h_{1,R}, \\ h_2^* \left(\frac{x}{t} < u_2^*\right) = h_{2,L}, & h_2^* \left(\frac{x}{t} > u_2^*\right) = h_{2,R}. \end{cases}$$
(4.3.10)

These solutions indicate that the non-conservative terms have contributions between the two extreme waves S_R and S_L , at points where h_1 and h_2 are discontinuous. More precisely, only the discontinuity in h_1 needs attention, as the non-conservative terms involving the atmospheric pressure (considered constant) transform to fluxes,

$$p_0 \frac{\partial h_k}{\partial x} = \frac{\partial (p_0 h_k)}{\partial x}.$$

It thus remains to analyze only the non-conservative term,

$$\rho_2 g h_2 \frac{\partial h_1}{\partial x}$$

The solution states for $(\rho_2 h_2)$ are given by,

$$(\rho_2 h_2)_L^* = (\rho_2 h_2)_L \frac{u_{2,L} - S_L}{u_2^* - S_L}$$
 and $(\rho_2 h_2)_R^* = (\rho_2 h_2)_R \frac{u_{2,R} - S_R}{u_2^* - S_R}$.

A schematic representation is given in Fig. 4.3.



Figure 4.3: Schematic representation in the (x, t) diagram of the two levels $(\rho_2 h_2)_{L,R}^*$ in the Riemann problem solution.

These formulas need u_2^* for their practical use that is unknown at this level. However, according to the sign of the velocity difference $u_1^* - u_2^*$, only two instances may occur:

- If $u_1^* > u_2^*$, the $\rho_2 g h_2 \frac{\partial h_1}{\partial x}$ term becomes locally $g(\rho_2 h_2)_R^* \frac{\partial h_1}{\partial x}$. As $(\rho_2 h_2)_R^*$ is constant at the point where $\frac{\partial h_1}{\partial x}$ is discontinuous, the non-conservative term becomes locally;

$$\rho_2 g h_2 \frac{\partial h_1}{\partial x} = \frac{\partial \left[g \left(\rho_2 h_2 \right)_R^* h_1 \right]}{\partial x}$$

– If $u_1^* < u_2^*$, the same reasoning yields,

$$\rho_2 g h_2 \frac{\partial h_1}{\partial x} = \frac{\partial \left[g \left(\rho_2 h_2 \right)_L^* h_1 \right]}{\partial x}.$$

It thus appears that the momentum equations are locally conservative. However, their explicit determination and use require knowledge of both u_1^* and u_2^* that are themselves solutions of the integration of the momentum equations.

To simplify the algorithm, a single solution state is considered for the apparent densities $(\rho_k h_k)^*$

instead of the two $(\rho_k h_k)_L^*$ and $(\rho_k h_k)_R^*$ in the same spirit as in the HLL solver for the Euler equations:

$$(h_k \rho_k)^* = \frac{(h_k \rho_k)_R (u_{k,R} - S_R) - (h_k \rho_k)_L (u_{k,L} - S_L)}{S_L - S_R}.$$
(4.3.11)

Thanks to this approximation, the momentum equations become locally,

$$\left(\frac{\frac{\partial(h_1\rho_1u_1)}{\partial t}}{\frac{\partial(h_2\rho_2u_2)}{\partial t}} + \frac{\frac{\partial(h_1\rho_1u_1^2 + h_1[p_1(\rho_1) - p_0] + \frac{1}{2}\rho_1gh_1^2 + g\rho_2h_1h_2 - g(h_2\rho_2)^*h_1)}{\frac{\partial x}{\partial x}} = 0, \quad (4.3.12)$$

Denoting the momentum fluxes by,

$$\begin{cases} F_{1,mom} = h_1 \rho_1 u_1^2 + h_1 [p_1(\rho_1) - p_0] + \frac{1}{2} \rho_1 g h_1^2 + g \rho_2 h_1 h_2 - g(h_2 \rho_2)^* h_1, \\ F_{2,mom} = h_2 \rho_2 u_2^2 + h_2 [p_2(\rho_2) - p_0] + \frac{1}{2} \rho_2 g h_2^2 + g(h_2 \rho_2)^* h_1, \end{cases}$$

$$(4.3.13)$$

the momentum numerical fluxes are then given by,

$$F_{k,mom}^* = \frac{F_{k,mom,R}S_L - F_{k,mom,L}S_R + S_LS_R(U_{k,mom,L} - U_{k,mom,R})}{S_L - S_R},$$
(4.3.14)

with $U_{k,mom} = h_k \rho_k u_k$. The mass numerical fluxes are computed by the HLL approximation as well and read,

$$F_{k,mass}^* = \frac{(h_k \rho_k)_R S_L(u_{k,R} - S_R) - (h_k \rho_k)_L S_R(u_{k,L} - S_L)}{S_L - S_R}.$$
(4.3.15)

System (4.2.1) being non-conservative, the conservative variable-state vector and in particular the fluid velocities are also needed for the computations. With the help of Eqs. (4.3.12) and (4.3.13), the momentum variables are computed with the HLL approximation as,

$$(h_k \rho_k u_k)^* = \frac{F_{k,mom,R} - F_{k,mom,L} - S_R U_{k,mom,R} + S_L U_{k,mom,L}}{S_L - S_R}.$$
(4.3.16)

Using Eqs. (4.3.11) and (4.3.16), the speeds of the fluids are given by,

$$u_k^* = \frac{(h_k \rho_k u_k)^*}{(h_k \rho_k)^*}.$$
(4.3.17)

The associated Godunov-type method now reads,

$$\begin{pmatrix}
h_{k,i}^{n+1} = h_{k,i}^{n} - \frac{\Delta t}{\Delta x} \left((hu)_{k,i+\frac{1}{2}}^{*} - (hu)_{k,i-\frac{1}{2}}^{*} \right) + \frac{\Delta t}{\Delta x} h_{k,i}^{n} \left(u_{k,i+\frac{1}{2}}^{*} - u_{k,i-\frac{1}{2}}^{*} \right), \\
(h_{k}\rho_{k})_{i}^{n+1} = (h_{k}\rho_{k})_{i}^{n} - \frac{\Delta t}{\Delta x} \left(F_{k,mass,i+\frac{1}{2}}^{*} - F_{k,mass,i-\frac{1}{2}}^{*} \right), \\
(h_{1}\rho_{1}u_{1})_{i}^{n+1} = (h_{1}\rho_{1}u_{1})_{i}^{n} - \frac{\Delta t}{\Delta x} \left(F_{1,mom,i+\frac{1}{2}}^{*} - F_{1,mom,i-\frac{1}{2}}^{*} \right) + \frac{\Delta t}{\Delta x} h_{1,i}^{n} \left(-g \left[(h_{2}\rho_{2})_{i+\frac{1}{2}}^{*} - (h_{2}\rho_{2})_{i-\frac{1}{2}}^{*} \right] \right), \\
(h_{2}\rho_{2}u_{2})_{i}^{n+1} = (h_{2}\rho_{2}u_{2})_{i}^{n} - \frac{\Delta t}{\Delta x} \left(F_{2,mom,i+\frac{1}{2}}^{*} - F_{2,mom,i-\frac{1}{2}}^{*} \right) + \frac{\Delta t}{\Delta x} h_{1,i}^{n} \left(g \left[(h_{2}\rho_{2})_{i+\frac{1}{2}}^{*} - (h_{2}\rho_{2})_{i-\frac{1}{2}}^{*} \right] \right). \\
(4.3.18)$$

Efficiency of both VFRoe and HLL solvers are now investigated on various test problems of the literature.

4.4 **Results and validations**

It is important to address in priority the effects of the fluid EOS with the present relaxation approach. Indeed the model is hyperbolic as a consequence of compressibility terms in the momentum equations. Extra tests, where VFRoe and HLL solvers are compared, are addressed subsequently.

Effects of the artificial sound speed

The EOS (4.2.4) involves sound speed c_k that has influence on computed results, as shown hereafter in Figs. 4.4, 4.5 and 4.6. The examined configuration consists in a limit case where the initial height of the first fluid (lower layer) is as low as numerically admissible, so that only the upper layer (second fluid) evolves significantly. With this specific configuration, the solution of the two-layer shallow water system (4.2.3) is meant to be compared to the exact solution of the one-layer Saint-Venant equations.

A dam-break problem is used to this end. The following test is proposed in LeVeque's textbook (2002) [60] to illustrate behavior of the solution of the Saint-Venant equations. It consists in a dam, separating two levels of fluids, that bursts at time t = 0. All variables of the current test problem are in dimensionless units as done in [60]. This test is the shallow water equivalent of the shock-tube problem of gas dynamics and appears to be an excellent benchmark as the flow deals with shock and expansion waves that create arduous conditions. The constant gravity is normalized and reads g = 1. The numerical domain has a length set to 10 with a height discontinuity initially located in the middle. On the left of this discontinuity, the fluid is initially at h = 3 and h = 1 on the right. The fluid is initially at rest on either side of the discontinuity.

To mimic the Saint-Venant system with the two-layer model (4.2.3), the height of the first fluid is initially set to $h_1 = \epsilon = 10^{-6}$ throughout the whole numerical domain. Its density is set to $\rho_1 = 1.2$ and its velocity is set to $u_1 = 0$. The second fluid, placed above the first one, has initial heights $h_2 = 3$ at left and $h_2 = 1$ at right. Its density is set to $\rho_2 = 1$ and its velocity is set to $u_2 = 0$.

Figure 4.4 shows the results with constant sound speed set to $c_k = 100$. The same sound speed has been taken for both fluids for the sake of simplicity in this illustration. Also, two mesh resolutions are used in Fig. 4.4, a coarse one made of 100 cells (A) and a fine one made of 10,000 cells (B).



Figure 4.4: Comparison of the computed solutions with the present HLL-type Riemann solver (thick lines) versus the exact solution of the one-layer Saint-Venant equations (thin lines and symbols). Results on the left (A) use a 100-cell mesh while results on the right (B) use a 10,000-cell mesh. The two plots use constant sound speed set to $c_k = 100$ for both fluids. The dashed lines represent the initial conditions. For the sake of clarity, 50 symbols are plotted for the exact solution, shown at time $t \approx 2$. First-order Godunov-type numerical scheme is used with CFL = 0.9. Computed results are shown at the same time in full lines. Results at left (A) show a curved line where the shock and expansion waves have already exited the domain. Same computation is rerun with 10,000 cells (B) restoring the two waves inside the domain. All variables are in dimensionless units.

It appears that the speed of sound influences computed results. The wave speeds of the two-layer model (4.2.3) involve the effective sound speeds given by $\sqrt{c_k^2 + \frac{1}{2}gh_k}$ while the single-layer wave speed is \sqrt{gh} . When c_k is significantly greater than $\sqrt{\frac{1}{2}gh_k}$ (of the order of unity in the present example), excessive numerical diffusion is present, as shown in Plot A of Fig. 4.4 where $c_k = 100$ for both fluids. Indeed, at the current time, the left and right-facing waves are considerably dissipated and even exit the domain. However, this feature is purely numerical and the system does converge to the exact solution, as shown in Plot B of Fig. 4.4 that uses a fine grid made of 10,000 cells.

It thus appears that large sound speeds are admissible but result in excessive numerical diffusion. The effects of fluid compressibility and sound speed are then investigated by varying c_k from levels less than the admissible single phase bound $(c_k < \sqrt{\frac{1}{2}gh_k})$ to larger values. Corresponding results are shown in Fig. 4.5.

Numerical experiments of Fig. 4.5 indicate that the method becomes unstable when $c_k < \sqrt{\frac{1}{2}gh_k}$. Indeed, Plot C of Fig. 4.5 uses $c_k = 0.1 \times \sqrt{\frac{1}{2}gh_k}$ and presents spurious oscillations. These numerical



Figure 4.5: Influence of the artificial speed of sound. The computed solutions of the present HLL-type Riemann solver for the two-layer system are displayed in thick lines. The exact solution of the one-layer Saint-Venant equations is shown in thin lines and symbols. System (4.2.3) is solved with various sound speeds $c_k = \theta_k \sqrt{\frac{1}{2}gh_k}$. Plots C, D, E and F use respectively $\theta_k = 0.1$, $\theta_k = 2$, $\theta_k = 10$ and $\theta_k = 50$. The dashed lines represent the initial conditions: $h_1^{left} = h_1^{right} = 10^{-6}$, $u_1^{left} = u_1^{right} = 0$, $\rho_1 = 1.2$, $h_2^{left} = 3$, $h_2^{right} = 1$, $u_2^{left} = u_2^{right} = 0$, $\rho_2 = 1$. Final time: $t \approx 2$. All results use a 100-cell mesh. First-order Godunov-type numerical scheme is used with CFL = 0.9. For the sake of clarity, 50 symbols are plotted for the exact solution. An optimum appears for $\theta_k = 2$. All variables are in dimensionless units.

experiments suggest existence of a subcharacteristic condition:

$$c_k > \sqrt{\frac{1}{2}gh_k}.\tag{4.4.1}$$

In the upcoming computations, the following sound speed is used:

$$c_k = \theta_k \sqrt{\frac{1}{2}gh_k}, \quad \text{with} \quad \theta_k > 1, \quad k = 1, 2.$$
 (4.4.2)

 θ_k is a numerical parameter that controls the numerical diffusion as illustrated in Fig. 4.5.

In order to unambiguously fulfill the above-mentioned subcharacteristic condition (4.4.1), θ_k must be greater than unit. $\theta_k \in [2, 5]$ seems to be a fair choice as it is low enough to control numerical diffusion and high enough to ensure stability. Indeed, as seen in Plot D of Fig. 4.5, $\theta_k = 2$ provides accurate results whereas $\theta_k = 10$ (Plot E) and $\theta_k = 50$ (Plot F) show excessive numerical dissipation.

Figure 4.6 repeats the same test with $\theta_k = 2$ and a 1000-cell grid. The Godunov method (4.3.18) including non-conservative terms is extended to second order with the MUSCL-type method detailed for example in Toro (2013) [112] (see also Chiapolino et al. (2017) [17] (Chapter 1, Section 1.3) when non-conservative terms are present).

The results show excellent agreement with the exact solution. Besides, they also reveal that:

- Incompressible behavior is recovered as the densities ρ_k are constant;
- The two-layer shallow water model (4.2.3) tends to the single-layer Saint-Venant equations in the limit $h_1 \rightarrow \epsilon$;
- Second-order extension of the Godunov-type scheme (4.3.18) and associated non-conservative terms does not cause specific difficulties.

These various computations have been done with the HLL solver while the VFRoe one failed immediately, as it was unable to preserve positivity of the height h_1 . It is also important to note that the method does not require any fluid EOS, nor relaxation parameter, as Eq. (4.2.14) determines efficiently the heights at relaxed states. The only "thermodynamic" information is the sound speed, and more precisely θ_k in Eq. (4.4.2). The method is robust and accurate with $2 \le \theta_k \le 5$.

Effects of the fluid densities

The preceding dam-break problem showed that the two-layer shallow water model (4.2.3) is able to recover the single-layer Saint-Venant system in the limit $h_1 \rightarrow 0$. When the density ratio $r = \frac{\rho_2}{\rho_1}$ is small, the effects of the surrounding fluid (upper layer) are expected to become insignificant and the one-layer Saint-Venant solution is meant to be recovered as well.



Figure 4.6: Comparison of the computed solution with the present HLL-type Riemann solver (symbols) versus the exact solution of the one-layer Saint-Venant equations (thick lines). The numerical system uses an artificial sound speed reading $c_k = \theta_k \sqrt{\frac{1}{2}gh_k}$ with $\theta_k = 2$. The dashed lines represent the initial conditions: $h_1^{left} = h_1^{right} = 10^{-6}$, $u_1^{left} = u_1^{right} = 0$, $\rho_1 = 1.2$, $h_2^{left} = 3$, $h_2^{right} = 1$, $u_2^{left} = u_2^{right} = 0$, $\rho_2 = 1$. Final time: $t \approx 2$. Second-order MUSCL-type numerical scheme using van Leer's limiter (see [15], [62]) is considered with CFL = 0.5 and 1000 cells. For the sake of clarity, only 50 symbols out of 1000 are plotted for the HLL-type computation. All variables are in dimensionless units.

The forthcoming tests analyze the effects of the fluid densities on a configuration presenting initially a Heaviside function regarding the height of the first fluid (lower layer) located in the middle of the numerical domain. The first layer is initially at height h_1 above the flat ground and the top of the plateau is located at height h'_1 . The second fluid surrounds the lower layer and is set initially at constant height h_2 . The initial configuration is schematically depicted in Fig. 4.7 with data summarized in Table 4.1.



Figure 4.7: Schematic representation of the test problem analyzing the effects of the fluid densities. A fluid layer with a Heaviside profile is set to motion under gravity effects and interacts with the lighter fluid initially above with a Heaviside profile as well.

Test	$h_1 (m)$	h_1' (m)	h_2 (m)	$\rho_1 \; (\mathrm{kg.m^{-3}})$	$\rho_2 \; (\mathrm{kg.m^{-3}})$
G	4	10	20	1000	1
Η	10^{-6}	10	20	1000	1
Ι	4	10	20	1000	990
J	10^{-6}	10	20	1000	990
Κ	4	10	100	1000	990
\mathbf{L}	10^{-6}	10	100	1000	990

Table 4.1: Initial conditions of the test problem analyzing the effects of the fluid densities.

In all following tests, the gravity constant is set to $g = 10 \text{ m.s}^{-2}$ and the top of the Heaviside plateau is at $h'_1 = 10 \text{ m}$. The results are shown at time t = 1 s and computed on a 1000-cell mesh with second-order MUSCL-type scheme and CFL = 0.5. Figure 4.8 examines two different density ratios. Plots G and H consider $\rho_1 = 1000 \text{ kg.m}^{-3}$ and $\rho_2 = 1 \text{ kg.m}^{-3}$, this situation being typical of water-air configurations while Plots I, J, K and L consider $\rho_1 = 1000 \text{ kg.m}^{-3}$ and $\rho_2 = 990 \text{ kg.m}^{-3}$, a situation reminiscent of water-oil flows.

Besides, two different values of h_1 are used. The left column of Fig. 4.8 considers initially $h_1 = 4$ m while the right column uses $h_1 = 10^{-6}$ m. We will see that this initial data influences significantly computed results. All plots of Fig. 4.8 use $h_2 = 20$ m with the exception of Plots K and L that use a much larger height for the upper layer, $h_2 = 100$ m. This data also influences the results.

Small density ratio: $r = \frac{\rho_2}{\rho_1} \ll 1$

When the density ratio is small, such as the situation of Fig. 4.8 G and H considering a water-airtype configuration, the solutions of the two-layer system (4.2.3) are in excellent agreement with the exact solutions of the Saint-Venant model. For these two tests, $h'_1 = 10$ m, $h_2 = 20$ m and $h_1 = 4$ m for Plot G and $h_1 = 10^{-6}$ m for Plot H.

In Plot G of Fig. 4.8, the Heaviside profile of the lower layer gives rise to four waves moving in each direction. The extreme waves steepen through compression waves into two shocks, while the back waves spread out as rarefaction waves.

However, the solution in Plot H of Fig. 4.8 is significantly different as the initial height of the lower layer is as low as numerically acceptable (outside the Heaviside profile). Thereby the solution evolves continuously throughout the entire numerical domain as there is not enough fluid, regarding the lower layer (h_1) , to observe a compression process: expansion waves only are present.

Comparable densities: $r = \frac{\rho_2}{\rho_1} \rightarrow 1$

Plots I and J of Fig. 4.8 repeat the same test $(h'_1 = 10 \text{ m}, h_2 = 20 \text{ m}, h_1 = 4 \text{ m} (\text{Plot I})$ and $h_1 = 10^{-6} \text{ m} (\text{Plot J})$ but with a water-oil-type configuration. As expected, the solutions are different from the one-fluid solutions, as the two fluids are dense and interact each other, this interaction being taken into account by the two-fluid model only. The two-layer solutions are shown with full lines and the single-layer Saint-Venant solutions are shown with symbols, just to compare the limit solutions.

The interaction of the two fluids influences significantly the computed results as an interesting wave structure appears in Plot I of Fig. 4.8. Right and left-facing shock waves propagate faster than those of the single-layer system. These shocks induce height increase of the fluid layer. They are followed by expansion waves that decrease these heights. Contact waves follow these expansion waves, followed by extra expansion waves that decrease the initial height h'_1 .

The solution is quite different when $h_1 = 10^{-6}$ m initially (Plot J) where only two expansion waves are observable. The interaction of the two fluids influences the flow, as the first fluid moves more difficultly into the second one as a result of comparable densities.

Large upper layer

Plots K and L of Fig. 4.8 keep on analyzing the present density ratio (water-oil) but with a different height for the second fluid that is now set to $h_2 = 100$ m. Doing so, the domain is mainly filled with the upper layer and Plots K and L show that the first fluid moves into the second one difficultly. The



Figure 4.8: Influence of the density ratio between the two fluids. Two different density ratios are used: $r = \frac{\rho_2}{\rho_1} \ll 1$ and $r = \frac{\rho_2}{\rho_1} \rightarrow 1$. The computed solutions of the present HLL-type Riemann solver for the two-layer system are displayed in thick lines. The exact solutions of the one-layer Saint-Venant equations are shown in thin lines and symbols for comparison. System (4.2.3) uses an artificial sound speed reading $c_k = \theta_k \sqrt{\frac{1}{2}gh_k}$ with $\theta_k = 2$. The dashed lines represent the initial conditions. Final time: $t \approx 1$ s. All results use a 1000-cell mesh. Second-order MUSCL-type numerical scheme is used with Sweby's limiter ($\beta = 1.1$, see Chapter 1, Section 1.5, Eq. (1.5.7), see also [15]) and CFL = 0.5. For the sake of clarity, 50 symbols are plotted for the exact solutions of the single-layer model. On the column at left, the initial height is $h_1 = 4$ m and on the column at right $h_1 = 10^{-6}$ m. When the density ratio is small: $r = \frac{\rho_2}{\rho_1} \ll 1$, as in configurations G and H, the two-layer and single-layer models are in excellent agreement. Large differences appear when the density ratio increases as shown in configurations I, J, K and L.

difference of initial height for the first fluid $h_1 = 4$ m (Plot K) and $h_1 = 10^{-6}$ m (Plot L) is minor compared to the effect of the large layer of second fluid ($h_2 = 100$ m). As the entire domain is mainly filled with heavy fluids, the flow is slowly set to motion under gravity effects.

Concluding remarks

Those last results reveal that the two-fluid model (4.2.3) is able to recover the one-layer Saint-Venant system when the effects of the surrounding fluid are negligible, as expected. This behavior appears when the density ratio between the lightest fluid and the heaviest one is small: $r = \frac{\rho_2}{\rho_1} \ll 1$.

They also reveal the importance of the two-layer model when the density ratio is arbitrary. Indeed, the two-layer system is able to deal with interactions between fluids unlike the conventional one-fluid Saint-Venant model. Note that the previous tests have been computed with the HLL-type Riemann solver presented in Section 4.3, the VFRoe method being unable to keep positivity of the heights. Note also that drag effects are absent in these computations.

Comparison of VFRoe and HLL

The two solvers considered in the present chapter are tested on a flow configuration examined in Abgrall and Karni (2009) [106] and Kurganov and Petrova (2009) [109]. The following tests set gravity constant to $g = 10 \text{ m.s}^{-2}$ and density ratio to $r = \frac{\rho_2}{\rho_1} = 0.98$. Hereby, $\rho_1 = 1200 \text{ kg.m}^{-3}$ and $\rho_2 = 1176 \text{ kg.m}^{-3}$ are used. Initially, different heights are present from either side of the initial discontinuity and result in the creation of a flow under gravity effects. The numerical domain is 1 m long and the initial discontinuity is located at x = 0.5 m. On the left of this discontinuity, $h_1 = 0.5$ m and $h_2 = 0.5$ m. On the right, $h_1 = 0.45$ m and $h_2 = 0.55$ m. The initial conditions are schematically depicted in Fig. 4.9. The first-order Godunov-type scheme is used with CFL = 0.7 in the following tests. Doing so, the comparison between solvers is free of extra ingredients, such as gradient limiters.



Figure 4.9: Schematic representation of the test problem comparing the computed solutions with the present HLL-type Riemann solver and those computed with the VFRoe method. The initial conditions are $h_1^{left} = 0.5$ m, $h_1^{right} = 0.45$ m, $h_2^{left} = 0.5$ m, $h_2^{right} = 0.55$ m, $\rho_1 = 1200$ kg.m⁻³, $\rho_2 = 1176$ kg.m⁻³. The initial velocities are: $u_1^{left} = u_1^{right} = u_2^{left} = u_2^{right} = 0$ m.s⁻¹ in Figs. 4.10 and 4.11 and $u_1^{left} = u_1^{right} = u_2^{left} = 2.5$ m.s⁻¹ in Figs. 4.12 and 4.13.

Figure 4.10 displays the results obtained with the HLL-type solver and the VFRoe method on a



100-cell mesh. The initial velocity is set to $u_1 = u_2 = 0 \text{ m.s}^{-1}$ throughout the entire domain. The results are shown at time $t \approx 0.12$ s.

Figure 4.10: Comparison of the computed solution with the present HLL-type Riemann solver (thick lines) versus the computed solution with the VFRoe method (thin lines and symbols). The dashed lines represent the initial conditions: $h_1^{left} = 0.5 \text{ m}$, $h_1^{right} = 0.45 \text{ m}$, $h_2^{left} = 0.5 \text{ m}$, $h_2^{right} = 0.55 \text{ m}$, $u_1^{left} = u_1^{right} = u_2^{left} = u_2^{right} = 0 \text{ m.s}^{-1}$, $\rho_1 = 1200 \text{ kg.m}^{-3}$, $\rho_2 = 1176 \text{ kg.m}^{-3}$. For the first fluid, the numerical parameter reads $\theta_1 = 3.5$, for the second fluid, $\theta_2 = 3$. These parameters are minimum values for successful computations with VFRoe. Final time: $t \approx 0.12$ s. First-order Godunov-type numerical scheme is used with CFL = 0.7 and 100 cells. For the sake of clarity, only 50 symbols out of 100 are plotted for the VFRoe method.

The hyperbolic model (4.2.3) considers compressible fluids during the wave propagation stage. However, the pressure relaxation step restores incompressibility as shown in Fig. 4.10 where the densities ρ_1 and ρ_2 remain constant. The numerical solutions consist in 4 waves emerging from the initial discontinuity. Both methods predict the same solution qualitatively, but the VFRoe solver produces spurious oscillations while the HLL one is monotonic.

As initially $u_1^{left} = u_1^{right} = u_2^{left} = u_2^{right} = 0 \text{ m.s}^{-1}$, the velocity $\overline{u} = 0 \text{ m.s}^{-1}$ and the full state vector \overline{W} in the VFRoe solver induces singularities in the decomposition of the eigenvectors. To lower

this effect, different sound speeds (through θ_1 and θ_2) have been considered in the various fluids. In the absence of such correction, the VFRoe solver fails immediately. Consequently, $\theta_1 \neq \theta_2$ is used as well with the HLL-type solver for proper comparison.

Figure 4.11 addresses the same test problem on a 10,000-cell mesh, showing convergence to the same solution of both VFRoe and HLL. With refined mesh, the interfacial waves are clearly connected to a constant plateau spanning as time evolves. Besides the four-wave structure is clearly observable in the velocity plots.



Figure 4.11: Comparison of the computed solution with the present HLL-type Riemann solver (thick lines) versus the computed solution with the VFRoe method (thin lines and symbols). The dashed lines represent the initial conditions: $h_1^{left} = 0.5 \text{ m}$, $h_1^{right} = 0.45 \text{ m}$, $h_2^{left} = 0.5 \text{ m}$, $h_2^{right} = 0.55 \text{ m}$, $u_1^{left} = u_1^{right} = u_2^{left} = u_2^{right} = 0 \text{ m.s}^{-1}$, $\rho_1 = 1200 \text{ kg.m}^{-3}$, $\rho_2 = 1176 \text{ kg.m}^{-3}$. For the first fluid, the numerical parameter reads $\theta_1 = 3.5$, for the second fluid, $\theta_2 = 3$. Final time: $t \approx 0.12$ s. First-order Godunov-type numerical scheme is used with CFL = 0.7 and 10,000 cells. For the sake of clarity, only 50 symbols out of 10,000 are plotted for the VFRoe method. Both methods converge to the same solution.

The next test repeats the previous one with non-zero initial velocities. Those are set to $u_1 = u_2 = 2.5 \text{ m.s}^{-1}$ throughout the entire domain. This test was examined in Abgrall and Karni (2009) [106] and computed with both 400 and 10,000-cell meshes. The same grids are used here to compare the present model and HLL solver with the results given in [106]. Figure 4.12 shows the results at time $t \approx 0.07$ s with 400-cell mesh.



Figure 4.12: Comparison of the computed solution with the present HLL-type Riemann solver (thick lines) versus the computed solution with the VFRoe algorithm (thin lines and symbols). The dashed lines represent the initial conditions: $h_1^{left} = 0.5 \text{ m}$, $h_1^{right} = 0.45 \text{ m}$, $h_2^{left} = 0.5 \text{ m}$, $h_2^{right} = 0.55 \text{ m}$, $u_1^{left} = u_1^{right} = u_2^{left} = u_2^{right} = 2.5 \text{ ms}^{-1}$, $\rho_1 = 1200 \text{ kg.m}^{-3}$, $\rho_2 = 1176 \text{ kg.m}^{-3}$. For the first fluid, the numerical parameter reads $\theta_1 = 3.5$, for the second fluid, $\theta_2 = 3$. Final time: $t \approx 0.07 \text{ s}$. First-order Godunov-type numerical scheme is used with CFL = 0.7 and 400 cells. For the sake of clarity, only 50 symbols out of 400 are plotted for the VFRoe method.
As a consequence of non-zero initial velocities and fine mesh resolution, computational conditions are easier for the VFRoe-type solver that does not oscillate. The expected behavior is recovered. The heights and velocity profiles are transported to the right and the effects of gravity seen in Figs. 4.10 and 4.11 are still present. As expected the densities remain constant as a consequence of pressure relaxation. Figure 4.13 shows the results of the same test with 10,000-cell mesh.



Figure 4.13: Comparison of the computed solution with the present HLL-type Riemann solver (thick lines) versus the computed solution with the VFRoe algorithm (thin lines and symbols). The dashed lines represent the initial conditions: $h_1^{left} = 0.5 \text{ m}$, $h_1^{right} = 0.45 \text{ m}$, $h_2^{left} = 0.5 \text{ m}$, $h_2^{right} = 0.55 \text{ m}$, $u_1^{left} = u_1^{right} = u_2^{left} = u_2^{right} = 2.5 \text{ m.s}^{-1}$, $\rho_1 = 1200 \text{ kg.m}^{-3}$, $\rho_2 = 1176 \text{ kg.m}^{-3}$. For the first fluid, the numerical parameter reads $\theta_1 = 3.5$, for the second fluid, $\theta_2 = 3$. Final time: $t \approx 0.07 \text{ s}$. First-order Godunov-type numerical scheme is used with CFL = 0.7 and 10,000 cells. For the sake of clarity, only 100 symbols out of 10,000 are plotted for the VFRoe method.

The HLL-type solver and the VFRoe-type method are in excellent agreement and are in excellent agreement with the results given in Abgrall and Karni (2009) [106] as well.

It is interesting to examine the rate of convergence of the present method (HLL-type solver) and give comparison to existing methods. In Abgrall and Karni (2009) [106], only first-order computations were carried out while in Kurganov and Petrova (2009) [109], higher-order computational results are provided. Comparisons are consequently done with the results of figures 2.2, 2.3 and 2.4 of this last reference. The results are given in Fig. 4.14.

Figure 4.14 shows results comparable to those of Kurganov and Petrova (2009) [109] with all mesh



Figure 4.14: Rate of convergence of the present HLL-type solver. The second-order Godunov-type method is used with Minmod limiter ($\beta = 1$, see Chapter 1, Section 1.5, Eq. (1.5.7), see also [15]) and with four mesh resolutions. The thin solid lines represent results obtained with 100 cells (left column) and 400 cells (right column). The dash-dotted lines represent results obtained with 200 cells (left column) and 800 cells (right column). The thick solid lines represent the results obtained with 10,000 cells and considered as "reference" solution. The thick dashed lines represent the initial conditions: $h_1^{left} = 0.5 \text{ m}, h_1^{right} = 0.45 \text{ m}, h_2^{left} = 0.5 \text{ m}, h_2^{right} = 0.55 \text{ m}, u_1^{left} = u_1^{right} = u_2^{left} = u_2^{right} = 2.5 \text{ m.s}^{-1}, \rho_1 = 1200 \text{ kg.m}^{-3}, \rho_2 = 1176 \text{ kg.m}^{-3}$. For the two fluids, the numerical parameters read $\theta_1 = \theta_2 = 3$. Final time: $t \approx 0.07$ s. The CFL number is 0.7. A close-up view of the spanning plateau is provided at top with the h_1 profile. The overall height $h_1 + h_2 + B(x)$ is given in the middle. B(x) represents topography of the ground and is considered constant in the present work, B(x) = 0 m. For proper comparison with the results of Kurganov and Petrova (2009) [109] who considered B(x) = -1 m, unit is subtracted from $h_1 + h_2$. Finally the velocity profile u_1 is displayed at bottom.

sizes. The second-order MUSCL-type scheme provides velocity profiles accurate enough with both 400-cell and 800-cell meshes as observed in [109]. However, the velocity spike with the 800-cell mesh seems slightly greater than the reference solution and the close-up view on the height profiles reveals that only the 800-cell mesh cancels out sufficiently numerical dissipation and allows to observe properly the constant plateau. The same conclusions are obtained in Kurganov and Petrova (2009) [109].

Also, a slight oscillation is observed with the coarse mesh made of 100 cells. The same observation holds in [109]. However, the left and right-facing shocks, seen on the velocity profiles, differ from those observed in [109] where initial data seem to be not exactly the same as those of Abgrall and Karni (2009) [106]. The present results are nonetheless in agreement with the ones of Abgrall and Karni (2009) [106]. The overall height is consequently different from the results of Kurganov and Petrova (2009) [109]. Nevertheless, velocity profiles indicate that the present method seems to have a similar rate of convergence as the one of [109].

Note that for this test problem, $\theta_1 = \theta_2 = 2$ induces spurious oscillations, similar to those observed in Fig. 4.5, Plot C. Consequently, $\theta_1 = \theta_2 = 3$ is used for both fluids.

4.5 Comparison of two-layer shallow water solutions versus twodimensional two-fluid computations

The averaged (or homogenized) solution computed by the present one-dimensional two-layer shallow water system (4.2.3) is now compared to the solution of a multidimensional model involving material interfaces. As mentioned in the introduction, the two-layer approach is expected to provide comparable results with considerable computational savings.

In the following, the solution computed with the compressible two-phase flow model of Saurel et al. (2009) [27] is used as a reference solution. This model is a pressure disequilibrium system which tends, in its asymptotic limit of stiff pressure relaxation, to the model of Kapila et al. (2001) [5], able to compute fluid interfaces as diffuse numerical zones. Interface sharpening can be achieved with the method of Chiapolino et al. (2017) [17] (Chapter 1).

To compare the solutions computed by both approaches (multidimensional interface model and one-dimensional two-layer shallow water one), the test configuration schematically depicted in Fig. 4.15 is used with data summarized in Table 4.2.

Test	h_1 (m)	h_1' (m)	h_2 (m)	$\rho_1 \; (\mathrm{kg.m}^{-3})$	$\rho_2 \; (\mathrm{kg.m^{-3}})$	γ_1	γ_2
$1\mathrm{D}/2\mathrm{D}$	10^{-6}	1	10	3.506	1.29	1.67	1.4

Table 4.2: Initial conditions of the test problem comparing the multidimensional interface approach and the one-dimensional two-layer shallow water model. γ_k represents the thermodynamic polytropic coefficient of fluid k used in the compressible two-phase flow model.



Figure 4.15: Schematic representation of the test problem comparing the multidimensional interface approach and the one-dimensional two-layer shallow water model. A fluid layer with a Heaviside profile is set to motion under gravity effects and interacts with the lighter fluid initially above.

Krypton and air are considered at rest and at atmospheric conditions initially. The flow is set to motion by the gravity acceleration $|g| = 10 \text{ m.s}^{-2}$ and consists of two ideal gases evolving at low Mach number. Due to symmetric boundary conditions, only half of the domain is computed with the multidimensional approach. This latter uses an unstructured mesh made of about 510,000 triangular elements with spatial discretization varying from about 1.5 cm in the zone of interest (\cong 480,000 elements located between y = 0 m and y = 1 m) to about 1 m in the upper far field. The numerical boundaries are considered as atmospheric outflows except for the left side (symmetric condition) and bottom one (flat ground) considered as walls.

The accurate capture of interfaces in multidimensional computations is improved with a secondorder numerical method. The MUSCL-type method with "Overbee" limiter at interfaces is used as detailed in [17] (Chapter 1). The very same second-order method is used with the two-layer shallow water system, computed on a 1000-cell mesh with van Leer's limiter [62]. Non-reflecting boundary conditions are used for the shallow water computations.

Results are shown in Fig. 4.16 at times t = 5 s and t = 8 s. The computed averaged height and averaged velocity of the multidimensional computation are determined by the integration on the two-dimensional numerical domain as,

$$h_1 = \int_0^{h_2} \alpha_1 dy, \tag{4.5.1}$$

and

$$u_x = \frac{\int_0^{h_2} (\alpha_1 \rho_1 u_x) \, dy}{\int_0^{h_2} (\alpha_1 \rho_1) \, dy},\tag{4.5.2}$$

where α_1 denotes the volume fraction of krypton and u_x denotes the averaged velocity of the two-phase mixture in the x-axis direction. The one-fluid shallow water solution is shown as well in Fig. 4.16 for comparison.



Figure 4.16: Comparison of the one-dimensional solution (thin lines and symbols) of the present twolayer shallow water model (HLL-type solver, $\theta_k = 2$) versus the two-dimensional computation of the diffuse interface model of Saurel et al. (2009) [27] (thick lines). The exact solution of the one-layer Saint-Venant equations is plotted (dotted lines) as well for comparison. The dashed lines represent the initial conditions. For the sake of clarity, 50 symbols are plotted for the two-layer solution. The column at left shows the results at time t = 5 s and the column at right shows the same results at time t = 8s. For symmetry reasons, only half of the numerical domain is computed with the two-dimensional simulation. Both computations (two-layer and diffuse interface systems) use CFL = 0.8.

As expected, the two-layer model provides better results than the one-fluid model. The density ratio $r = \frac{\rho_2}{\rho_1} = \frac{1.29}{3.506} \simeq 0.37$ being moderate, the interaction between the two fluids is meant to be significant. The results of the two-layer shallow water system present a large zone where the agreement with the two-dimensional simulation is very good. Beyond this zone, the results computed by the multidimensional interface model present oscillations. These oscillations are due to the presence of Kelvin-Helmholtz instabilities as seen for example in Fig. 4.17 showing the 2D results at time t = 2 s.

Indeed, the multidimensional solution involves hydrodynamic instabilities that cannot be accounted for with the present two-layer shallow water model. The overall qualitative behavior of the onedimensional approach is correct but the krypton is spread too far ahead with the two-layer model.

To improve agreement between 1D and 2D computations, drag effects are added in the two-layer



Figure 4.17: Kelvin-Helmholtz instabilities observed during the descent of krypton due to gravity effects, $g = -10 \text{ m.s}^{-2}$. The figure presents krypton volume fraction contours. The black rectangle represents the initial position of the gas. The results are shown at time t = 2 s and are computed with the diffuse interface model of Saurel et al. (2009) [27] on an unstructured mesh made of about 510,000 triangular elements. MUSCL-type method is used with the "sharpening-interface" method of Chiapolino et al. (2017) [17] (Chapter 1) and CFL = 0.8. For symmetry reasons, only half of the numerical domain is computed.

formulation. Pressure (or "acoustic") drag is considered only and is modeled through the velocity relaxation terms that appear in the right-hand side of the momentum equations,

$$\begin{cases}
\frac{\partial (h_1 \rho_1 u_1)}{\partial t} + \frac{\partial (h_1 \rho_1 u_1^2 + h_1 p_1(\rho_1) + \frac{1}{2} \rho_1 g h_1^2 + g \rho_2 h_1 h_2)}{\partial x} = \rho_2 g h_2 \frac{\partial h_1}{\partial x} + p_0 \frac{\partial h_1}{\partial x} + \frac{Z_1 Z_2}{Z_1 + Z_2} A_I(u_2 - u_1) \\
\frac{\partial (h_2 \rho_2 u_2)}{\partial t} + \frac{\partial (h_2 \rho_2 u_2^2 + h_2 p_2(\rho_2) + \frac{1}{2} \rho_2 g h_2^2)}{\partial x} = -\rho_2 g h_2 \frac{\partial h_1}{\partial x} + p_0 \frac{\partial h_2}{\partial x} - \frac{Z_1 Z_2}{Z_1 + Z_2} A_I(u_2 - u_1).
\end{cases}$$
(4.5.3)

 $Z_k = \rho_k c_k$ denotes the acoustic impedance of fluid k and A_I denotes the specific interfacial area. $\rho_1 = 3.506 \text{ kg.m}^{-3}$, $c_1 = 218 \text{ m.s}^{-1}$ for krypton and $\rho_2 = 1.29 \text{ kg.m}^{-3}$, $c_2 = 340 \text{ m.s}^{-1}$ for air are used in this work. This acoustic drag effect modeling was developed in Saurel et al. (2003) [102] and Chinnayya et al. (2004) [114], pages 504 and 510. It is obtained by local interfacial pressure integration over the surface of a piece of interface. The interfacial pressure is estimated through an approximate Riemann solver for the Euler equations of gas dynamics. Let us mention that upon integration over height, as done in Eqs. (4.5.1) and (4.5.2), the specific interfacial area A_I becomes dimensionless.

As shown in Figs. 4.18 and 4.19, computed results are significantly improved when drag effects are considered. The two figures show the solutions with respectively $A_I = 0.0003$ and $A_I = 0.00015$. A comparison of the different results at time t = 8 s is presented in Fig. 4.20, showing the influence of the A_I parameter.

Indeed, the overall solution presents very good agreement with the 2D simulation using the diffuse interface two-phase flow model. The results show the ability of the new two-layer shallow water model to predict the spreading and dispersal of two gases evolving at low Mach number. The numerical advantages of this system are significant. In addition to its simple resolution through the HLL-type Riemann solver (Section 4.3), computational time saving is tremendous. For instance, the computation of the preceding test problem required about 30 hours for the two-dimensional simulation (computing only half of the domain) with a parallel code (MPI) running on 64 cores, while the one-dimensional computation needed only a couple of seconds in sequential implementation.



Figure 4.18: Comparison of the one-dimensional solution (thin lines and symbols) of the present twolayer shallow water model (HLL-type solver, $\theta_k = 2$) versus the two-dimensional computation of the diffuse interface model of Saurel et al. (2009) [27] (thick lines). Drag effects are included in the shallow water system with $A_I = 0.0003$. For the sake of clarity, 50 symbols are plotted for the twolayer solution. The column at left shows the results at time t = 5 s and the column at right shows the same results at time t = 8 s. For symmetry reasons, only half of the numerical domain is computed with the two-dimensional simulation. Both computations (two-layer and diffuse interface systems) use CFL = 0.8.



Figure 4.19: Comparison of the one-dimensional solution (thin lines and symbols) of the present twolayer shallow water model (HLL-type solver, $\theta_k = 2$) versus the two-dimensional computation of the diffuse interface model of Saurel et al. (2009) [27] (thick lines). Drag effects are included in the shallow water system with $A_I = 0.00015$. For the sake of clarity, 50 symbols are plotted for the two-layer solution. The column at left shows the results at time t = 5 s and the column at right shows the same results at time t = 8 s. For symmetry reasons, only half of the numerical domain is computed with the two-dimensional simulation. Both computations (two-layer and diffuse interface systems) use CFL = 0.8.



Figure 4.20: Influence of the interfacial area in drag force between the two layers. The solutions of the present one-dimensional two-layer shallow water system (HLL-type solver, $\theta_k = 2$) are displayed in thin lines and symbols. The solution of the two-dimensional computation of the diffuse interface model of Saurel et al. (2009) [27] is shown in thick lines. Drag effects are included in the shallow water system with various values of the specific interfacial area A_I . For the sake of clarity, 50 symbols are plotted for the two-layer solution. The results are shown at time t = 8 s. For symmetry reasons, only half of the numerical domain is computed with the two-dimensional simulation. Both computations (two-layer and diffuse interface systems) use CFL = 0.8. 1D and 2D computations are in good agreement with $A_I = 0.0002$.

4.6 Conclusion

A pressure relaxation model with 6 equations has been built, especially devoted to two-layer shallow water flows. The mathematical structure of the new formulation is well-posed and results in a strictly hyperbolic model. The system considers weak compressibility of the fluids, which is responsible for its hyperbolic behavior, and is shown to tend to the conventional, but conditionally hyperbolic, two-layer shallow water model in the stiff pressure relaxation limit.

A simple, efficient and robust HLL-type Riemann solver has been derived to solve the corresponding non-conservative system. Computational examples have shown capabilities of the present formulation.

Compared to multi-D computations of gravity-driven interfacial flows, the new model offers tremendous numerical advantages and computational savings. This is done at the price of a single parameter in the drag force model.

This research work can be continued in many directions. Among them, the consideration of variable topography, friction with the ground and interfacial area creation through turbulence modeling seem important.

Acknowledgements

The authors are very grateful to Dr. Jeaniffer Vides for participating in multiple valuable discussions that definitely helped to improve the quality of this work.

Part of this work has been carried out in the framework of the Labex MEC (ANR-10-LABX-0092) and of the A*MIDEX project (ANR-11-IDEX-0001-02) funded by ANR.

Support from CEA Gramat and especially Emmanuel Lapébie are particularly acknowledged.

General conclusion

A fundamental and applied research work has been developed in this manuscript. The present scientific topics are highly linked to a continued need of scientific expertises destined to industries of space, energy and the safety community as well. In this context, efforts have been done regarding the theoretical modeling and the numerical treatment of compressible two-phase flows.

Sharpening diffuse material interfaces and contact waves for compressible fluid models has been reconsidered in Chapter 1, in the frame of diffuse interface models. A numerical method, relying on a new flux limiter named "Overbee", has been developed and allows to reduce significantly the interface capture zone at the price of slight but subtle code modifications. The proposed method can be adapted to multiple situations. For example, solid-fluid interaction considered through a Level-Set-type characteristic function has been considered in Carmouze et al. (2018) [115] with the help of the new "Overbee" limiter, yielding efficient and simple computations. The sharpening method developed in Chapter 1 is expected to appeal to CFD practitioners working on two-phase flows presenting multiple interfaces. Indeed, in addition to its simplicity, the ability of the sharpening method to deal with both structured and unstructured meshes and an arbitrary number of fluids is also in favor of the present algorithm. In future work, the sharpening method is expected to be coupled with a mixture model involving phase transition as well.

Mass transfer computation has also been addressed in this manuscript through a stiff thermochemical relaxation solver. Stiffness assumes mass exchanges between liquid and vapor phases to happen instantaneously. Such relaxation solver can be used when the topology of the flow is unknown, insufficiently documented or unnecessary. In Chapter 2, a new instantaneous thermochemical relaxation solver has been developed. The new method relies on the basis of simple estimates resulting in efficient, fast and robust computations. Hereby, many industrial situations involving severe thermodynamic conditions and complex geometries can be treated with the proposed method. The design of this latter is in agreement with the physics brought into play in such instantaneous phase change phenomena. In future work, the theoretical modeling and the numerical treatment of situations involving several liquids seem important. The specific case of mixture of several liquids is of particular interest and requires a consequent theoretical and applied research work.

Moreover, equations of state used to describe the thermodynamic behavior of different phases have their own ranges of validity. In specific contexts, it is necessary to extend these ranges of validity. Consequently, the extension of the "Noble-Abel-Stiffened-Gas" (NASG) equation of state (EOS) has been considered in Chapter 3, as future industrial applications intend to consider fluids transitioning to supercritical state. The ENASG equation of state has been developed in this manuscript ("E" stands for "Extended"). It is a well-posed formulation that seems able to deal with a liquid evolving in the whole liquid phase domain. Besides, the transition from pure liquid to supercritical state seems to be possible and accurate with the ENASG EOS. Its particular interest dwells in variable attractive and repulsive effects. For the sake of convexity and simplicity, the formulation reduces to the ideal gas description for vapor and supercritical phases. Thereby, the saturated vapor phase necessarily lacks of accuracy near the critical point. This drawback constitutes nonetheless a great incentive for future works. Water and oxygen have been considered in Chapter 3. Those two fluids present respectively a triatomic and diatomic molecular structure, but future applications may require to address different families of fluids as well.

In another framework, Chapter 4 deals with dense fluid dispersal at both large time and space scales. Many situations may involve fluid dispersal in large urban or natural places during an important period of time. These large time and space scales motivated the design of a new, strictly hyperbolic, two-layer shallow water type model in the direction of dense-gas-dispersion computations. Indeed, the shallow water strategy allows to address 2D simulations to mimic 3D results. The gain in CPU time compared to conventional multi-fluid models is expected to be tremendous. Besides, this research work may appeal to CFD practitioners working with shallow water systems used in oceanic flows or weather predictions for example. Indeed, the extension of the proposed model to multiple layers while keeping the hyperbolic property of the mathematical system seems possible with the new formulation that is well-posed as a consequence of pressure disequilibrium and compressible character of the fluids. In future works, the consideration of variable topographies, friction with the ground and interfacial area creation through turbulence modeling seem important in addition to 2D computations.

The overall content of this manuscript is meant to provide fundamental and applied tools in the interest to the computational fluid dynamics community. The different projects mentioned in this manuscript already use these contributions routinely.

Bibliography

- A. Chiapolino, P. Boivin, R. Saurel, A simple phase transition relaxation solver for liquid-vapor flows, International Journal for Numerical Methods in Fluids 83 (7) (2017) 583–605.
- [2] C. Hirt, B. Nichols, Volume of fluid (VOF) method for the dynamics of free boundaries, Journal of Computational Physics 39 (1) (1981) 201–225.
- [3] R. Saurel, R. Abgrall, A multiphase Godunov method for compressible multifluid and multiphase flows, Journal of Computational Physics 150 (2) (1999) 425–467.
- [4] R. Saurel, R. Abgrall, A simple method for compressible multifluid flows, SIAM Journal on Scientific Computing 21 (3) (1999) 1115–1145.
- [5] A. Kapila, R. Menikoff, J. Bdzil, S. Son, D. Stewart, Two-phase modeling of deflagration-todetonation transition in granular materials: Reduced equations, Physics of Fluids 13 (10) (2001) 3002–3024.
- [6] R. Saurel, O. Le Métayer, A multiphase model for compressible flows with interfaces, shocks, detonation waves and cavitation, Journal of Fluid Mechanics 431 (2001) 239–271.
- [7] F. Petitpas, R. Saurel, E. Franquet, A. Chinnayya, Modelling detonation waves in condensed energetic materials: Multiphase CJ conditions and multidimensional computations, Shock Waves 19 (5) (2009) 377–401.
- [8] R. Saurel, P. Boivin, O. Le Métayer, A general formulation for cavitating, boiling and evaporating flows, Computers and Fluids 128 (2016) 53–64.
- [9] G. Perigaud, R. Saurel, A compressible flow model with capillary effects, Journal of Computational Physics 209 (1) (2005) 139–178.
- [10] N. Favrie, S. Gavrilyuk, R. Saurel, Solid-fluid diffuse interface model in cases of extreme deformations, Journal of Computational Physics 228 (16) (2009) 6037–6077.

- [11] S. Ndanou, N. Favrie, S. Gavrilyuk, Multi-solid and multi-fluid diffuse interface model: Applications to dynamic fracture and fragmentation, Journal of Computational Physics 295 (2015) 523–555.
- [12] K. Shyue, F. Xiao, An Eulerian interface sharpening algorithm for compressible two-phase flow: The algebraic THINC approach, Journal of Computational Physics 268 (2014) 326–354.
- [13] G. Allaire, S. Clerc, S. Kokh, A five-equation model for the simulation of interfaces between compressible fluids, Journal of Computational Physics 181 (2) (2002) 577–616.
- [14] A. Harten, High resolution schemes for hyperbolic conservation laws, Journal of Computational Physics 49 (3) (1983) 357–393.
- [15] P. Sweby, High resolution schemes using flux limiters for hyperbolic conservation laws, SIAM Journal on Numerical Analysis 21 (5) (1984) 995–1011.
- [16] P. Roe, Some contributions to the modelling of discontinuous flows, in: Large-scale computations in fluid mechanics, 1985, pp. 163–193.
- [17] A. Chiapolino, R. Saurel, B. Nkonga, Sharpening diffuse interfaces with compressible fluids on unstructured meshes, Journal of Computational Physics 340 (2017) 389–417.
- [18] R. Saurel, F. Petitpas, R. Abgrall, Modelling phase transition in metastable liquids: application to cavitating and flashing flows, Journal of Fluid Mechanics 607 (2008) 313–350.
- [19] A. Chiapolino, P. Boivin, R. Saurel, A simple and fast phase transition relaxation solver for compressible multicomponent two-phase flows, Computers & Fluids 150 (2017) 31–45.
- [20] O. Le Métayer, Modélisation et résolution de la propagation de fronts perméables, application aux fronts d'évaporation et de détonation, Ph.D. thesis, Université de Provence (2003).
- [21] O. Le Métayer, Modélisation et élaboration d'outils de simulations dédiés aux écoulements multiphasiques compressibles réactifs, Aix Marseille Université, H.D.R (2013).
- [22] O. Le Métayer, R. Saurel, The Noble-Abel Stiffened-Gas equation of state, Physics of Fluids 28 (4) (2016) 046102.
- [23] A. Chiapolino, R. Saurel, Extended Noble-Abel Stiffened-Gas Equation of State for Sub-and-Supercritical Liquid-Gas Systems Far from the Critical point, Fluids 3 (48) (2018).
- [24] S. Hank, R. Saurel, O. Le Métayer, E. Lapébie, Modeling blast waves, gas and particles dispersion in urban and hilly ground areas, Journal of hazardous materials 280 (2014) 436–449.

- [25] S. Hank, Modélisation et Simulation de la Dispersion de Fluide en Milieu Fortement Hétérogène, Ph.D. thesis, Aix Marseille Université (2012).
- [26] A. Chiapolino, R. Saurel, Models and methods for two-layer shallow water flows, Journal of Computational Physics 371 (2018) 1043–1066.
- [27] R. Saurel, F. Petitpas, R. Berry, Simple and efficient relaxation methods for interfaces separating compressible fluids, cavitating flows and shocks in multiphase mixtures, Journal of Computational Physics 228 (5) (2009) 1678–1712.
- [28] J. VonNeumann, R. Richtmyer, A method for the numerical calculation of hydrodynamic shocks, Journal of Applied Physics 21 (3) (1950) 232–237.
- [29] C. Hirt, A. Anthony, J. Cook, An arbitrary Lagrangian-Eulerian computing method for all flow speeds, Journal of Computational Physics 14 (3) (1974) 227–253.
- [30] E. Caramana, M. Shashkov, Elimination of artificial grid distortion and hourglass-type motions by means of Lagrangian subzonal masses and pressures, Journal of Computational Physics 142 (2) (1998) 521–561.
- [31] J. Glimm, J. Grove, X. Li, K. Shyue, Y. Zeng, Q. Zhang, Three-dimensional front tracking, SIAM Journal on Scientific Computing 19 (3) (1998) 703–727.
- [32] A. Dervieux, F. Thomasset, A finite element method for the simulation of a Rayleigh-Taylor instability, in: Approximation methods for Navier-Stokes problems, Springer, 1980, pp. 145–158.
- [33] R. Fedkiw, T. Aslam, B. Merriman, S. Osher, A non-oscillatory Eulerian approach to interfaces in multimaterial flows (the Ghost Fluid Method), Journal of Computational Physics 152 (2) (1999) 457–492.
- [34] J. Cahn, J. Hilliard, Free energy of a nonuniform system. I. Interfacial free energy, The Journal of Chemical Physics 28 (2) (1958) 258–267.
- [35] H. Lund, A hierarchy of relaxation models for two-phase flow, SIAM Journal on Applied Mathematics 72 (6) (2012) 1713–1741.
- [36] R. Abgrall, How to prevent pressure oscillations in multicomponent flow calculations: A quasi conservative approach, Journal of Computational Physics 125 (1) (1996) 150–160.
- [37] K. Shyue, An efficient shock-capturing algorithm for compressible multicomponent problems, Journal of Computational Physics 142 (1) (1998) 208–242.

- [38] J. Massoni, R. Saurel, B. Nkonga, R. Abgrall, Proposition de méthodes et modèles Eulériens pour les problèmes à interfaces entre fluides compressibles en présence de transfert de chaleur: Some models and Eulerian methods for interface problems between compressible fluids with heat transfer, International Journal of Heat and Mass Transfer 45 (6) (2002) 1287–1307.
- [39] A. Murrone, H. Guillard, A five equation reduced model for compressible two phase flow problems, Journal of Computational Physics 202 (2) (2005) 664–698.
- [40] M. Pelanti, K. Shyue, A mixture-energy-consistent six-equation two-phase numerical model for fluids with interfaces, cavitation and evaporation waves, Journal of Computational Physics 259 (2014) 331–357.
- [41] R. Shukla, C. Pantano, J. Freund, An interface capturing method for the simulation of multiphase compressible flows, Journal of Computational Physics 229 (19) (2010) 7411–7439.
- [42] A. Tiwari, J. Freund, C. Pantano, A diffuse interface model with immiscibility preservation, Journal of Computational Physics 252 (2013) 290–309.
- [43] R. Loubere, M. Dumbser, S. Diot, A new family of high order unstructured MOOD and ADER finite volume schemes for multidimensional systems of hyperbolic conservation laws, Communications in Computational Physics 16 (3) (2014) 718–763.
- [44] K. Shyue, A wave-propagation based volume tracking method for compressible multicomponent flow in two space dimensions, Journal of Computational Physics 215 (1) (2006) 219–244.
- [45] D. Youngs, Time-dependent multi-material flow with large fluid distortion, Numerical Methods for Fluid Dynamics 24 (2) (1982) 273–285.
- [46] E. Olsson, G. Kreiss, A conservative level set method for two phase flow, Journal of Computational Physics 210 (1) (2005) 225–246.
- [47] S. Kokh, F. Lagoutiere, An anti-diffusive numerical scheme for the simulation of interfaces between compressible fluids by means of a five-equation model, Journal of Computational Physics 229 (8) (2010) 2773–2809.
- [48] B. van Leer, Towards the ultimate conservative difference scheme. V. A second-order sequel to Godunov's method, Journal of Computational Physics 32 (1) (1979) 101–136.
- [49] M. Baer, J. Nunziato, A two-phase mixture theory for the deflagration-to-detonation transition (DDT) in reactive granular materials, International Journal of Multiphase Flow 12 (6) (1986) 861–889.

- [50] R. Saurel, O. Le Métayer, J. Massoni, S. Gavrilyuk, Shock jump relations for multiphase mixtures with stiff mechanical relaxation, Shock Waves 16 (3) (2007) 209–232.
- [51] F. Petitpas, E. Franquet, R. Saurel, O. Le Métayer, A relaxation-projection method for compressible flows. part II: Artificial heat exchanges for multiphase shocks, Journal of Computational Physics 225 (2) (2007) 2214–2248.
- [52] S. Schoch, N. Nikiforakis, B. Lee, R. Saurel, Multi-phase simulation of ammonium nitrate emulsion detonations, Combustion and Flame 160 (9) (2013) 1883–1899.
- [53] O. Le Métayer, J. Massoni, R. Saurel, Elaborating equations of state of a liquid and its vapor for two-phase flow models; élaboration des lois d'état d'un liquide et de sa vapeur pour les modèles d'écoulements diphasiques, International Journal of Thermal Sciences 43 (3) (2004) 265–276.
- [54] E. Toro, M. Spruce, W. Spears, Restoration of the contact surface in the HLL-Riemann solver, Shock Waves 4 (1) (1994) 25–34.
- [55] T. Barth, D. Jespersen, The design and application of upwind schemes on unstructured meshes, Proceedings of the AIAA 27th Aerospace Science Meeting (Reno, Nevada), (1989).
- [56] P. Sweby, M. Baines, Convergence of Roe's scheme for the general non-linear scalar wave equation, University of Reading. Department of Mathematics, 1981.
- [57] B. Leonard, The ULTIMATE conservative difference scheme applied to unsteady onedimensional advection, Computer methods in applied mechanics and engineering 88 (1) (1991) 17–74.
- [58] E. Toro, Riemann solvers and numerical methods for fluid dynamics: A practical introduction, Springer Science & Business Media, 1997.
- [59] D. Sidilkover, P. Roe, Unification of some advection schemes in two dimensions, NASA Contractor Report 195044, (1995).
- [60] R. LeVeque, Finite volume methods for hyperbolic problems, Vol. 31, Cambridge University Press, 2002.
- [61] A. Harten, On a class of high resolution total-variation-stable finite-difference schemes, SIAM Journal on Numerical Analysis 21 (1) (1984) 1–23.
- [62] B. van Leer, Towards the ultimate conservative difference scheme. II. Monotonicity and conservation combined in a second-order scheme, Journal of Computational Physics 14 (4) (1974) 361–370.

- [63] E. Tadmor, Convenient total variation diminishing conditions for nonlinear difference schemes, SIAM Journal on Numerical Analysis 25 (5) (1988) 1002–1014.
- [64] P. Lax, B. Wendroff, Systems of conservation laws, Communications on Pure and Applied Mathematics 13 (2) (1960) 217–237.
- [65] R. Warming, R. Beam, Upwind second-order difference schemes and applications in aerodynamic flows, AIAA Journal 14 (9) (1976) 1241–1249.
- [66] R. LeVeque, Numerical methods for conservation laws, Vol. 132, Springer, 1992.
- [67] R. Richtmyer, Taylor instability in shock acceleration of compressible fluids, Communications on Pure and Applied Mathematics 13 (2) (1960) 297–319.
- [68] E. Meshkov, Instability of the interface of two gases accelerated by a shock wave, Fluid Dynamics 4 (5) (1969) 101–104.
- [69] G. Layes, O. Le Métayer, Quantitative numerical and experimental studies of the shock accelerated heterogeneous bubbles motion, Physics of Fluids 19 (4) (2007) 042105.
- [70] M. Holt, Underwater explosions, Annual Review of Fluid Mechanics 9 (1) (1977) 187–214.
- [71] J. Grove, R. Menikoff, Anomalous reflection of a shock wave at a fluid interface, Journal of Fluid Mechanics 219 (1990) 313–336.
- [72] O. Le Métayer, J. Massoni, R. Saurel, Dynamic relaxation processes in compressible multiphase flows. Application to evaporation phenomena, in: ESAIM: Proceedings, Vol. 40, EDP Sciences, 2013, pp. 103–123.
- [73] B. Abramzon, W. Sirignano, Droplet vaporization model for spray combustion calculations, International Journal of Heat and Mass Transfer 32 (9) (1989) 1605–1618.
- [74] M. Jacobson, Fundamentals of atmospheric modeling, Cambridge University Press, 2005.
- [75] D. Furfaro, R. Saurel, Modeling droplet phase change in the presence of a multi-component gas mixture, Applied Mathematics and Computation 272 (2016) 518–541.
- [76] S. Le Martelot, B. Nkonga, R. Saurel, Liquid and liquid-gas flows at all speeds, Journal of Computational Physics 255 (2013) 53–82.
- [77] P. Downar-Zapolski, Z. Bilicki, L. Bolle, J. Franco, The non-equilibrium relaxation model for one-dimensional flashing liquid flow, International Journal of Multiphase Flow 22 (3) (1996) 473–483.

- [78] M. Barret, E. Faucher, J. Hérard, Schemes to compute unsteady flashing flows, AIAA Journal 40 (5) (2002) 905–913.
- [79] H. Lund, A hierarchy of relaxation models for two-phase flow, SIAM Journal on Applied Mathematics 72 (6) (2012) 1713–1741.
- [80] A. Singhal, M. Athavale, H. Li, Y. Jiang, Mathematical basis and validation of the full cavitation model, Journal of Fluids Engineering 124 (3) (2002) 617–624.
- [81] F. Petitpas, J. Massoni, R. Saurel, E. Lapébie, L. Munier, Diffuse interface model for high speed cavitating underwater systems, International Journal of Multiphase Flow 35 (8) (2009) 747–759.
- [82] S. Le Martelot, R. Saurel, B. Nkonga, Towards the direct numerical simulation of nucleate boiling flows, International Journal of Multiphase Flow 66 (2014) 62–78.
- [83] H. Orbey, S. Sandler, Modeling vapor-liquid equilibria: Cubic equations of state and their mixing rules, Vol. 1, Cambridge University Press, 1998.
- [84] G. Allaire, G. Faccanoni, S. Kokh, A strictly hyperbolic equilibrium phase transition model, Comptes Rendus Mathematique 344 (2) (2007) 135–140.
- [85] G. Faccanoni, S. Kokh, G. Allaire, Modelling and simulation of liquid-vapor phase transition in compressible flows based on thermodynamical equilibrium, ESAIM : Mathematical Modelling and Numerical Analysis 46 (05) (2012) 1029–1054.
- [86] M. Lallemand, R. Saurel, Pressure relaxation procedures for multiphase compressible flows, Tech. rep., INRIA Report (2000).
- [87] A. Wood, A textbook of sound, G. Bell and Sons Ltd., London, 1930.
- [88] D. Furfaro, R. Saurel, A simple HLLC-type Riemann solver for compressible non-equilibrium two-phase flows, Computers and Fluids 111 (2015) 159–178.
- [89] D. Youngs, An interface tracking method for a 3D Eulerian hydrodynamics code, Atomic Weapons Research Establishment (AWRE) Technical Report (44/92) (1984) 35.
- [90] S. Kokh, F. Lagoutiere, An anti-diffusive numerical scheme for the simulation of interfaces between compressible fluids by means of a five-equation model, Journal of Computational Physics 229 (8) (2010) 2773–2809.
- [91] R. Saurel, C. Pantano, Diffuse Interfaces and Capturing Methods in Compressible Two-Phase Flows, Annual Review of Fluid Mechanics 50 105–130.

- [92] R. Saurel, A. Chinnayya, Q. Carmouze, Modelling compressible dense and dilute two-phase flows, Physics of Fluids 29 (6) (2017) 063301.
- [93] B. Plohr, Shockless acceleration of thin plates modeled by a tracked random choice method, AIAA journal 26 (4) (1988) 470–478.
- [94] R. Menikoff, B. Plohr, The Riemann problem for fluid flow of real materials, Reviews of modern physics 61 (1) (1989) 75.
- [95] J. Cocchi, R. Saurel, A Riemann problem based method for the resolution of compressible multimaterial flows, Journal of Computational Physics 137 (2) (1997) 265–298.
- [96] B. McBride, S. Gordon, M. Reno, Coefficients for Calculating Thermodynamic and transport Properties of Individual Species, Tech. rep., NASA Technical Memorandum 4513 (1993).
- [97] J. van der Waals, J. Rowlinson, J.D van der Waals: On the Continuity of the Gaseous and Liquid States, Vol. 14, North Holland, 1988.
- [98] G. Soave, Equilibrium constants from a modified Redlich-Kwong equation of state, Chemical Engineering Science 27 (6) (1972) 1197–1203.
- [99] Y. Wei, R. Sadus, Equations of state for the calculation of fluid-phase equilibria, AIChE Journal 46 (1) (2000) 169–196.
- [100] F. Marble, Dynamics of a gas containing small solid particles, Combustion and Propulsion (5th AGARD Colloquium) (1963) 175–213.
- [101] A. Forestier, J. Hérard, X. Louis, Solveur de type Godunov pour simuler les écoulements turbulents compressibles, Comptes Rendus de l'Académie des Sciences. Paris Série 1, Mathématique 324 (8) (1997) 919–926.
- [102] R. Saurel, S. Gavrilyuk, F. Renaud, A multiphase model with internal degrees of freedom: Application to shock-bubble interaction, Journal of Fluid Mechanics 495 (2003) 283–321.
- [103] D. Lhuillier, C. Chang, T. Theofanous, On the quest for a hyperbolic effective-field model of disperse flows, Journal of Fluid Mechanics 731 (2013) 184–194.
- [104] G. Richard, S. Gavrilyuk, A new model of roll waves: comparison with Brock's experiments, Journal of Fluid Mechanics 698 (2012) 374–405.
- [105] S. Gavrilyuk, V. Liapidevskii, A. Chesnokov, Spilling breakers in shallow water: Applications to Favre waves and to the shoaling and breaking of solitary waves, Journal of Fluid Mechanics 808 (2016) 441–468.

- [106] R. Abgrall, S. Karni, Two-layer shallow water system: A relaxation approach, SIAM Journal on Scientific Computing 31 (3) (2009) 1603–1627.
- [107] T. Gallouet, J. Masella, Un schéma de Godunov approché, Comptes Rendus de l'Académie des Sciences. Paris Série 1, Mathématique 323 (1) (1996) 77–84.
- [108] L. Ovsyannikov, Two-layer "shallow water" model, Journal of Applied Mechanics and Technical Physics 20 (2) (1979) 127–135.
- [109] A. Kurganov, G. Petrova, Central-upwind schemes for two-layer shallow water equations, SIAM Journal on Scientific Computing 31 (3) (2009) 1742–1773.
- [110] R. Monjarret, Local well-posedness of the two-layer shallow water model with free surface, SIAM Journal on Applied Mathematics 75 (5) (2015) 2311–2332.
- [111] A. Harten, P. Lax, B. van Leer, On Upstream Differencing and Godunov-Type Schemes for Hyperbolic Conservation Laws, SIAM Review 25 (1) (1983) 35–61.
- [112] E. Toro, Riemann solvers and numerical methods for fluid dynamics: A practical introduction, Springer Science & Business Media, 2013.
- [113] S. Davis, Simplified second-order Godunov-type methods, SIAM Journal on Scientific and Statistical Computing 9 (3) (1988) 445–473.
- [114] A. Chinnayya, E. Daniel, R. Saurel, Modelling detonation waves in heterogeneous energetic materials, Journal of Computational Physics 196 (2) (2004) 490–538.
- [115] Q. Carmouze, F. Fraysse, R. Saurel, B. Nkonga, Coupling rigid bodies motion with single phase and two-phase compressible flows and unstructured meshes, Journal of Computational Physics 375 (2018) 1314–1338.
- [116] S. Godunov, A. Zabrodine, M. Ivanov, A. Kraïko, G. Prokopov, V. Platonov, Résolution numérique des problèmes multidimensionnels de la dynamique des gaz, Éditions Mir (Moscou), 1979.
- [117] H. B. Callen, THERMODYNAMICS, an introduction to the physical theories of equilibrium thermostatics and irreversible thermodynamics, John Wiley & Sons, Inc, 1960.
- [118] B. Lee, M. Kesler, A generalized thermodynamic correlation based on three-parameter corresponding states, AIChE Journal 21 (3) (1975) 510–527.
- [119] R. Reid, J. Prausnitz, B. Poling, The properties of gases and liquids, 4th Edition, McGraw-Hill, 1987.

- [120] O. Redlich, J. Kwong, On the Thermodynamics of Solutions. V. An Equation of State. Fugacities of Gaseous Solutions, Chemical reviews 44 (1) (1949) 233–244.
- [121] D. Peng, D. Robinson, A new two-constant equation of state, Industrial & Engineering Chemistry Fundamentals 15 (1) (1976) 59–64.
- [122] F. Harlow, A. Amsden, Fluid dynamics. monograph LA-4700, Tech. rep., Los Alamos National Laboratory, NM (1971).

Appendix A

Material interfaces

A.1 Sharpening contact discontinuities in single-phase flows

This appendix follows the conclusion given in Chapter 1 where a very simple and dramatically efficient sharpening method is developed and wisely used in the context of two-phase flows.

It is interesting to examine the capabilities of the new "Overbee" limiter to sharpen contact discontinuities in single-phase flows. The Euler equations (A.1.1) are thus considered with the ideal gas equation of state (A.1.2),

$$\begin{cases} \frac{\partial \rho}{\partial t} + div(\rho \mathbf{u}) = 0, \\ \frac{\partial(\rho \mathbf{u})}{\partial t} + div(\rho \mathbf{u} \otimes \mathbf{u} + p\underline{I}) = 0, \\ \frac{\partial(\rho E)}{\partial t} + div([\rho E + p]\mathbf{u}) = 0, \end{cases}$$
(A.1.1)
$$p(\rho, e) = (\gamma - 1)\rho e.$$
(A.1.2)

The new limiter is unable to compute shocks and smooth profiles, such as expansion waves. The main issue is thus to detect contact discontinuities only. This is done with the following filter (A.1.3):

$$\begin{cases} \frac{|\rho^{n+1} - \rho^n|}{\rho^n} \ge \epsilon, \\ \frac{|p^{n+1} - p^n|}{p^n} < \epsilon, \end{cases}$$
(A.1.3)

where n and n + 1 denote two successive time steps. This "contact discontinuity detection" can be done with the predicted variables of the MUSCL-type scheme. When the contact discontinuity is detected, the second-order process is repeated on the cells of interest with zero gradients for variables u and p while the density gradient is limited by "Overbee".

A typical computational example is shown in Fig. A.1 with a 1D shock tube. The small parameter

is set to $\epsilon = 10^{-3}$ leading to three contact-surface cells detected between x = 0.58 m and x = 0.60 m.



Figure A.1: Air shock tube computation with and without contact-surface sharpening. The dashed lines represent the initial conditions: $p^{left} = 2$ bar, $p^{right} = 1$ bar, $\rho^{left} = 2$ kg.m⁻³, $\rho^{right} = 1$ kg.m⁻³, $u^{left} = u^{right} = 0$ m.s⁻¹. The full circle symbols • on the left graph represent the solution with Superbee limiter. The full circle symbols • on the right graph represent the solution when contact-surface sharpening is used in addition. The full lines represent the exact solution. Final time: $t \approx 1$ ms. Mesh: 100 cells. CFL = 0.8.

Appendix B

Stiff phase transition phenomena

B.1 Summary of the iterative algorithm computing phase transition between a liquid and a multicomponent gas phase

This section summarizes the iterative procedure that computes phase changes in the context of a liquid in equilibrium with a multicomponent gas phase. Only the liquid and vapor species react through phase transition as the other components of the gas phase are considered non-condensable. The solutions of the iterative algorithm are compared to the ones computed with the simple thermochemical relaxation solver developed in Chapter 2.

The algebraic system to be solved is,

$$\begin{cases} v = Y_1^* v_1(p^*, T^*) + Y_2^* v_2(p^*, T^*) + \sum_{k \ge 3} Y_k v_k(p^*, T^*), \\ e = Y_1^* e_1(p^*, T^*) + Y_2^* e_2(p^*, T^*) + \sum_{k \ge 3} Y_k e_k(p^*, T^*), \\ p_{sat}(T^*) = \left(\frac{\frac{Y_2^*}{W_2}}{\frac{Y_2^*}{W_2} + \sum_{k \ge 3} \frac{Y_k}{W_k}}\right) p^*, \end{cases}$$
(B.1.1)

where the superscript * denotes the thermodynamic equilibrium state. Since $Y_1 = 1 - Y_2 - \sum_{k \ge 3} Y_k$, the algebraic system reads,

$$\begin{cases} f_1(p^*, T^*, Y_2^*) = v - \left(1 - Y_2^* - \sum_{k \ge 3} Y_k\right) v_1(p^*, T^*) - Y_2^* v_2(p^*, T^*) - \sum_{k \ge 3} Y_k v_k(p^*, T^*), \\ f_2(p^*, T^*, Y_2^*) = e - \left(1 - Y_2^* - \sum_{k \ge 3} Y_k\right) e_1(p^*, T^*) - Y_2^* e_2(p^*, T^*) - \sum_{k \ge 3} Y_k e_k(p^*, T^*), \\ f_3(p^*, p_{sat}^*, Y_2^*) = p_{sat}^* - \left(\frac{\frac{Y_2^*}{W_2}}{\frac{Y_p^*}{W_2} + \sum_{k \ge 3} \frac{Y_k}{W_k}}\right) p^*. \end{cases}$$
(B.1.2)

However the relation between $p_{sat}(T^*)$ and T^* ,

$$\ln(p_{sat} + p_{\infty,v}) = A + \frac{B + E \, p_{sat}}{T_{sat}} + C \ln(T_{sat}) + D \ln(p_{sat} + p_{\infty,l}), \qquad (B.1.3)$$

is non-linear and no analytical relation can be found. An additional equation is consequently added to System (B.1.2).

It is convenient to use a reference state defined with the other NASG or SG coefficients that have been determined via theoretical equations and experimental data (see Le Métayer et al. (2004) [53], Le Métayer and Saurel (2016) [22]). Let us define,

$$\begin{cases} T_{ref} = \frac{q_1 - q_2}{C_{p,2} - C_{p,1}} = \frac{B}{C}, \\ p_{ref} = \frac{(C_{p,2} - C_{v,2}) p_{\infty,1} - (C_{p,1} - C_{v,1}) p_{\infty,2}}{(C_{p,1} - C_{v,1}) - (C_{p,2} - C_{v,2})} = \frac{p_{\infty,1} - Dp_{\infty,2}}{D - 1}. \end{cases}$$
(B.1.4)

Equation (B.1.3) is now written with the built reference state p_{ref}, T_{ref} ,

$$\ln\left(p_{ref} + p_{\infty,2}\right) = A + \frac{B + E \, p_{ref}}{T_{ref}} + C \ln\left(T_{ref}\right) + D \ln\left(p_{ref} + p_{\infty,1}\right). \tag{B.1.5}$$

Subtracting Eq. (B.1.5) to Eq. (B.1.3), it is straightforward to find another formulation connecting the saturation pressure and temperature,

$$\frac{p_{sat} + p_{\infty,2}}{p_{ref} + p_{\infty,2}} = \exp\left\{C\left[\frac{T_{ref}}{T_{sat}} + \ln\left(\frac{T_{sat}}{T_{ref}}\right) - 1\right]\right\} \left(\frac{p_{sat} + p_{\infty,1}}{p_{ref} + p_{\infty,1}}\right)^D \exp\left\{E\left(\frac{p_{sat}}{T_{sat}} - \frac{p_{ref}}{T_{ref}}\right)\right\}.$$
 (B.1.6)

The algebraic system thus reads,

$$\begin{cases} f_1(p^*, T^*, Y_2^*) = v - \left(1 - Y_2^* - \sum_{k \ge 3} Y_k\right) v_1(p^*, T^*) - Y_2^* v_2(p^*, T^*) - \sum_{k \ge 3} Y_k v_k(p^*, T^*), \\ f_2(p^*, T^*, Y_2^*) = e - \left(1 - Y_2^* - \sum_{k \ge 3} Y_k\right) e_1(p^*, T^*) - Y_2^* e_2(p^*, T^*) - \sum_{k \ge 3} Y_k e_k(p^*, T^*), \\ f_3(p^*, p_{sat}^*, Y_2^*) = p_{sat}^* - \left(\frac{Y_2^*}{\frac{Y_2^*}{W_2}} + \sum_{k \ge 3} \frac{Y_k}{W_k}\right) p^*, \\ f_4(p_{sat}^*, T^*) = \frac{p_{sat}^* + p_{\infty, 2}}{p_{ref} + p_{\infty, 2}} - \exp\left\{C\left[\frac{T_{ref}}{T^*} + \ln\left(\frac{T^*}{T_{ref}}\right) - 1\right]\right\} \left(\frac{p_{sat}^* + p_{\infty, 1}}{p_{ref} + p_{\infty, 1}}\right)^D \exp\left\{E\left(\frac{p_{sat}^*}{T^*} - \frac{p_{ref}}{T_{ref}}\right)\right\}. \\ (B.1.7) \end{cases}$$

Four variables are unknown, p^* , T^* , Y_2^* , p_{sat}^* and System (B.1.7) is non-linear calling for an iterative

method. Let us then denote,

$$X = \begin{pmatrix} p^* \\ T^* \\ Y_2^* \\ p_{sat}^* \end{pmatrix}, \quad F(X) = \begin{pmatrix} f_1(p^*, T^*, Y_2^*) \\ f_2(p^*, T^*, Y_2^*) \\ f_3(p^*, p_{sat}^*, Y_2^*) \\ f_4(p_{sat}^*, T^*) \end{pmatrix}.$$
 (B.1.8)

The system F(X) = 0 has to be resolved. Its solution is given by,

$$X^{n} = X^{n-1} - J \left\{ F(X^{n-1}) \right\}^{-1} F(X^{n-1}),$$
(B.1.9)

with n denoting the current iteration and $J\left\{F(X^{n-1})\right\}^{-1}$ the inverse of the Jacobian matrix,

$$J(f_{1}, f_{2}, f_{3}, f_{4}) = \begin{pmatrix} \frac{\partial f_{1}(p^{*}, T^{*}, Y_{2}^{*})}{\partial p^{*}} & \frac{\partial f_{1}(p^{*}, T^{*}, Y_{2}^{*})}{\partial T^{*}} & \frac{\partial f_{1}(p^{*}, T^{*}, Y_{2}^{*})}{\partial Y_{2}^{*}} & \frac{\partial f_{1}(p^{*}, T^{*}, Y_{2}^{*})}{\partial p^{*}_{sat}} \\ \frac{\partial f_{2}(p^{*}, T^{*}, Y_{2}^{*})}{\partial p^{*}} & \frac{\partial f_{2}(p^{*}, T^{*}, Y_{2}^{*})}{\partial T^{*}} & \frac{\partial f_{2}(p^{*}, T^{*}, Y_{2}^{*})}{\partial Y_{2}^{*}} & \frac{\partial f_{2}(p^{*}, T^{*}, Y_{2}^{*})}{\partial p^{*}_{sat}} \\ \frac{\partial f_{3}(p^{*}, p_{sat}^{*}, Y_{2}^{*})}{\partial p^{*}} & \frac{\partial f_{3}(p^{*}, p_{sat}^{*}, Y_{2}^{*})}{\partial T^{*}} & \frac{\partial f_{3}(p^{*}, p_{sat}^{*}, Y_{2}^{*})}{\partial Y_{2}^{*}} & \frac{\partial f_{3}(p^{*}, p_{sat}^{*}, Y_{2}^{*})}{\partial p^{*}_{sat}} \\ \frac{\partial f_{4}(p_{sat}^{*}, T^{*})}{\partial p^{*}} & \frac{\partial f_{4}(p_{sat}^{*}, T^{*})}{\partial T^{*}} & \frac{\partial f_{4}(p_{sat}^{*}, T^{*})}{\partial Y_{v}^{*}} & \frac{\partial f_{4}(p_{sat}^{*}, T^{*})}{\partial p^{*}_{sat}} \end{pmatrix} \right).$$
(B.1.10)

In order to gain accuracy and robustness, it is convenient to write Eq. (B.1.9) as,

$$\begin{cases} J(F(X^{n-1})) \triangle X = -F(X^{n-1}), \\ \triangle X = X^n - X^{n-1}. \end{cases}$$
(B.1.11)

Thereby, for a given X, a linear system is found and the variation ΔX is determined via the Gauss elimination method. The variables are then updated as,

$$X^n = \triangle X + X^{n-1}. \tag{B.1.12}$$

A solution is obtained when $\Delta X < \epsilon$ or alternatively when $|f_1| < \epsilon$, $|f_2| < \epsilon$, $|f_3| < \epsilon$, $|f_4| < \epsilon$, with $\epsilon \to 0$.

This procedure is robust and accurate. It is used in all test problems of Section 2.12.

Appendix C

Equations of state

This appendix is related to the Extended-Noble-Abel-Stiffened-Gas (ENASG) equation of state developed in Chapter 3.

C.1 Convexity of the ENASG formulation

The convexity of the equation of state requires five different conditions to be fulfilled (Godunov et al. (1979) [116], Menikoff and Plohr (1989) [94]. Those are analyzed hereafter,

$$a) \quad \left(\frac{\partial^{2}e}{\partial v^{2}}\right)_{s} > 0, \quad b) \quad \left(\frac{\partial^{2}e}{\partial s^{2}}\right)_{v} > 0, \quad c) \quad \left(\frac{\partial}{\partial s}\left(\frac{\partial e}{\partial v}\right)_{s}\right)_{v} < 0,$$

$$d) \quad \left(\frac{\partial^{2}e}{\partial s^{2}}\right)_{v}\left(\frac{\partial^{2}e}{\partial v^{2}}\right)_{s} - \left[\left(\frac{\partial}{\partial s}\left(\frac{\partial e}{\partial v}\right)_{s}\right)_{v}\right]^{2} > 0, \quad e) \quad \left(\frac{\partial^{3}e}{\partial v^{3}}\right)_{s} < 0.$$
(C.1.1)

Combining Eqs. (3.2.20), (3.2.21) and (3.2.40), the internal energy expresses as,

$$e(v,s) = q + \frac{(\gamma - 1)C_v\gamma p_{\infty,0}[v - b(v)]}{(\gamma - b_1)[(\gamma - 1)C_v - \gamma p_{\infty,1}[v - b(v)]]} - \frac{\gamma^2 p_{\infty,1} p_{\infty,0}[v - b(v)]^2}{(\gamma - b_1)[(\gamma - 1)C_v - \gamma p_{\infty,1}[v - b(v)]]} + \frac{C_v \exp\left(\frac{s - q''}{C_v}\right) \exp\left(\frac{\gamma p_{\infty,1}[v - b(v)]}{C_v(1 - b_1)}\right)}{[v - b(v)]^{\frac{\gamma - b_1}{1 - b_1}}}.$$
(C.1.2)

After some algebraic manipulations, the first partial derivative reads,

$$\left(\frac{\partial e}{\partial v}\right)_{s} = \frac{\exp\left(\frac{s-q''}{C_{v}}\right)\exp\left(\frac{\gamma p_{\infty,1}\left[v-b(v)\right]}{C_{v}(1-b_{1})}\right)\left[-(\gamma-1)C_{v}+\gamma p_{\infty,1}\left[v-b(v)\right]\right]}{\left[v-b(v)\right]^{\frac{\gamma-b_{1}}{1-b_{1}}}} + \frac{\gamma p_{\infty,0}(1-b_{1})}{\gamma-b_{1}}.$$
(C.1.3)

Analyzing Eqs. (3.2.40) and (C.1.3), it appears that the thermodynamic definition of the pressure is satisfied, $p = -\left(\frac{\partial e}{\partial v}\right)_s$. Continuing the calculations, the second derivative reads,

$$\frac{\left(\frac{\partial^2 e}{\partial v^2}\right)_s}{\exp\left(\frac{s-q''}{C_v}\right)} = (\gamma - b_1)(\gamma - 1)C_v \left[v - b(v)\right]^{\frac{-\gamma - 1 + 2b_1}{1 - b_1}} \exp\left(\frac{\gamma p_{\infty,1} \left[v - b(v)\right]}{C_v (1 - b_1)}\right) \\
+ \frac{(\gamma p_{\infty,1})^2}{C_v} \exp\left(\frac{\gamma p_{\infty,1} \left[v - b(v)\right]}{C_v (1 - b_1)}\right) \left[v - b(v)\right]^{\frac{1 - \gamma}{1 - b_1}} \\
- 2\gamma p_{\infty,1} (\gamma - 1) \left[v - b(v)\right]^{\frac{-\gamma + b_1}{1 - b_1}} \exp\left(\frac{\gamma p_{\infty,1} \left[v - b(v)\right]}{C_v (1 - b_1)}\right).$$
(C.1.4)

Analyzing Eq. (C.1.4), it appears that condition (C.1.1) (a) is satisfied unambiguously if $p_{\infty,1} \leq 0$ and $b_1 < \gamma$. Equation (C.1.2) is now used and yields the following partial derivative,

$$\left(\frac{\partial e}{\partial s}\right)_{v} = \frac{\exp\left(\frac{s-q''}{C_{v}}\right)\exp\left(\frac{\gamma p_{\infty,1}\left[v-b(v)\right]}{C_{v}(1-b_{1})}\right)}{\left[v-b(v)\right]^{\frac{\gamma-1}{1-b_{1}}}}.$$
(C.1.5)

Furthermore, manipulating Eq. (3.2.33), the liquid temperature can be expressed as,

$$T(v,s) = \frac{\exp\left(\frac{s-q''}{C_v}\right)\exp\left(\frac{\gamma p_{\infty,1}\left[v-b(v)\right]}{C_v(1-b_1)}\right)}{\left[v-b(v)\right]^{\frac{\gamma-1}{1-b_1}}}.$$
 (C.1.6)

Analyzing Eqs. (C.1.5) and (C.1.6), it appears that the thermodynamic definition of the temperature is satisfied, $T = \left(\frac{\partial e}{\partial s}\right)_v$. With the help of (C.1.5), the second partial derivative is expressed as,

$$\left(\frac{\partial^2 e}{\partial s^2}\right)_v = \frac{\exp\left(\frac{s-q''}{C_v}\right)\exp\left(\frac{\gamma p_{\infty,1}\left[v-b(v)\right]}{C_v(1-b_1)}\right)}{C_v\left[v-b(v)\right]^{\frac{\gamma-1}{1-b_1}}}.$$
(C.1.7)

Condition (C.1.1) (b) is then satisfied $\forall p_{\infty,1}$ and $b_1 \neq 1$. Also, from Eq. (C.1.3), relation (C.1.1) (c) transforms to,

$$\left(\frac{\partial}{\partial s}\left(\frac{\partial e}{\partial v}\right)_{s}\right)_{v} = \frac{\exp\left(\frac{s-q''}{C_{v}}\right)\exp\left(\frac{\gamma p_{\infty,1}\left[v-b(v)\right]}{C_{v}(1-b_{1})}\right)\left[\gamma p_{\infty,1}\left[v-b(v)\right]-(\gamma-1)C_{v}\right]}{C_{v}\left[v-b(v)\right]^{\frac{\gamma-b_{1}}{1-b_{1}}}}.$$
 (C.1.8)

Condition (C.1.1) (c) is then unambiguously satisfied and defined if $p_{\infty,1} \leq 0$ and $b_1 \neq 1$. Besides, combining Eqs. (C.1.4), (C.1.7) and (C.1.8) leads to the next relation,

$$\left(\frac{\partial^2 e}{\partial s^2}\right)_v \left(\frac{\partial^2 e}{\partial v^2}\right)_s - \left[\left(\frac{\partial}{\partial s}\left(\frac{\partial e}{\partial v}\right)_s\right)_v\right]^2 = \left[\exp\left(\frac{s-q''}{C_v}\right)\right]^2 \left[\exp\left(\frac{\gamma p_{\infty,1}\left[v-b(v)\right]}{C_v(1-b_1)}\right)\right]^2$$

$$\left((1-b_1)(\gamma-1)\left[v-b(v)\right]^{\frac{-2\gamma+2b_1}{1-b_1}}\right).$$

$$(C.1.9)$$

Condition (C.1.1) (d) is then satisfied as well if $b_1 < 1$. Finally, from Eq. (C.1.4), relation (C.1.1) (e) reads,

$$\frac{\left(\frac{\partial^{3}e}{\partial v^{3}}\right)_{s}}{\exp\left(\frac{s-q''}{C_{v}}\right)} = \left[\frac{\gamma p_{\infty,1}}{C_{v}}\exp\left(\frac{\gamma p_{\infty,1}[v-b(v)]}{C_{v}(1-b_{1})}\right)\right] \left[(\gamma-b_{1})(\gamma-1)C_{v}[v-b(v)]^{\frac{-\gamma-1+2b_{1}}{1-b_{1}}} + \frac{(\gamma p_{\infty,1})^{2}}{C_{v}}[v-b(v)]^{\frac{1-\gamma}{1-b_{1}}} - 2\gamma p_{\infty,1}(\gamma-1)[v-b(v)]^{\frac{-\gamma+b_{1}}{1-b_{1}}}\right] + \exp\left(\frac{\gamma p_{\infty,1}[v-b(v)]}{C_{v}(1-b_{1})}\right) \left[(\gamma-b_{1})(\gamma-1)C_{v}(-\gamma-1+2b_{1})[v-b(v)]^{\frac{-\gamma-2+3b_{1}}{1-b_{1}}} - (\gamma-1)\frac{(\gamma p_{\infty,1})^{2}}{C_{v}}[v-b(v)]^{\frac{-\gamma+b_{1}}{1-b_{1}}} + 2\gamma p_{\infty,1}(\gamma-1)(\gamma-b_{1})[v-b(v)]^{\frac{-\gamma-1+2b_{1}}{1-b_{1}}}\right].$$
(C.1.10)

Analyzing Eq. (C.1.10), condition (C.1.1) (e) is satisfied unambiguously if $p_{\infty,1} \leq 0, b_1 < \gamma$ and $b_1 < \frac{1}{2} + \frac{\gamma}{2}$. As $\gamma > 1$, the most restrictive condition regarding the covolume remains $b_1 < 1$.

The present formulation is then unambiguously convex if,

$$p_{\infty,1} \le 0, \quad p_{\infty,0} \ge 0 \quad \text{and} \quad b_1 < 1.$$
 (C.1.11)

C.2 Maxwell's relations

Maxwell's relations arise from the equality of the mixed partial derivatives of the fundamental thermodynamic relations [117]. The different functions of common use read,

a)
$$\left(\frac{\partial s}{\partial p}\right)_{T} = -\left(\frac{\partial v}{\partial T}\right)_{p},$$
 b) $\left(\frac{\partial p}{\partial T}\right)_{v} = \left(\frac{\partial s}{\partial v}\right)_{T},$
c) $\left(\frac{\partial T}{\partial v}\right)_{s} = -\left(\frac{\partial p}{\partial s}\right)_{v},$ d) $\left(\frac{\partial T}{\partial p}\right)_{s} = \left(\frac{\partial v}{\partial s}\right)_{p}.$ (C.2.1)

This section aims at verifying that those fundamental relations are satisfied with the ENASG formulation. Using Eqs. (3.2.18) and (3.2.38), the next relation directly arises,

$$\left(\frac{\partial s}{\partial p}\right)_T = -\frac{(\gamma - 1)C_v}{(1 - b_1)\left[p + p'_{\infty}(T)\right]} + \frac{\gamma p_{\infty,1}(\gamma - 1)C_vT}{(1 - b_1)\left[p + p'_{\infty}(T)\right]^2} = -\left(\frac{\partial v}{\partial T}\right)_p.$$
 (C.2.2)

It is then clear that Maxwell's relation (C.2.1) (a) is satisfied. Equations (3.2.18) and (3.2.33) are now used and lead to,

$$\left(\frac{\partial p}{\partial T}\right)_{v} = \frac{(\gamma - 1)C_{v}}{v - b(v)} - \gamma p_{\infty,1} = \left(\frac{\partial s}{\partial v}\right)_{T}.$$
(C.2.3)

Consequently, Maxwell's relation (C.2.1) (b) is also satisfied. This is not surprising as these two equations, (C.2.1) (a)-(b), are precisely Eqs. (3.2.23) and (3.2.4), which are the basis of the theoretical derivations. Equations (C.1.6) and (3.2.40) being now considered, the following partial derivatives are obtained,

$$\left(\frac{\partial T}{\partial v}\right)_{s} = \exp\left(\frac{s-q''}{C_{v}}\right) \exp\left(\frac{\gamma p_{\infty,1}\left[v-b(v)\right]}{C_{v}(1-b_{1})}\right) \left[-(\gamma-1)\left[v-b(v)\right]^{\frac{-\gamma+b_{1}}{1-b_{1}}} + \frac{\gamma p_{\infty,1}}{C_{v}}\left[v-b(v)\right]^{\frac{-\gamma+1}{1-b_{1}}}\right] = -\left(\frac{\partial p}{\partial s}\right)_{v} \left[(C.2.4)\right]^{\frac{-\gamma+b_{1}}{1-b_{1}}} + \frac{\gamma p_{\infty,1}}{C_{v}}\left[v-b(v)\right]^{\frac{-\gamma+b_{1}}{1-b_{1}}} = -\left(\frac{\partial p}{\partial s}\right)_{v}$$

showing that Maxwell's relation (C.2.1) (c) is satisfied as well.

Let us then analyze the fourth relation. Considering Eq. (3.2.40), it is noted that v(s, p) cannot be directly formulated unless $p_{\infty,1} = 0$, that reduces the formulation to the NASG equation of state with a variable covolume. However, the partial derivatives can be directly formulated. Indeed, as the left-hand side of Eq. (C.2.1) (d) considers constant entropy, the following relation can be used,

$$ds = \left(\frac{\partial s}{\partial p}\right)_T dp + \left(\frac{\partial s}{\partial T}\right)_p dT = 0.$$

Consequently, the partial derivative is found as,

$$\frac{dT}{dp} = \left(\frac{\partial T}{\partial p}\right)_s = -\frac{\left(\frac{\partial s}{\partial p}\right)_T}{\left(\frac{\partial s}{\partial T}\right)_p}.$$
(C.2.5)

The same reasoning is repeated for $\left(\frac{\partial v}{\partial s}\right)_p$ yielding,

$$\frac{dv}{ds} = \left(\frac{\partial v}{\partial s}\right)_p = -\frac{\left(\frac{\partial p}{\partial s}\right)_v}{\left(\frac{\partial p}{\partial v}\right)_s}.$$
(C.2.6)

 $\left(\frac{\partial s}{\partial p}\right)_T$ and $\left(\frac{\partial s}{\partial T}\right)_p$ have been determined previously, Eqs. (C.2.2) and (3.2.35). Equation (C.2.5) then

reads after calculations,

$$\left(\frac{\partial T}{\partial p}\right)_{s} = -\frac{-(\gamma - 1)C_{v}\left[p + p_{\infty}'(T)\right] + \gamma p_{\infty,1}(\gamma - 1)C_{v}T}{\frac{C_{v}}{T}(\gamma - b_{1})\left[p + p_{\infty}'(T)\right]^{2} - \left[\gamma p_{\infty,1}(\gamma - 1)C_{v}\right]\left(2p + \gamma p_{\infty,1}T + \frac{2\gamma p_{\infty,0}(1 - b_{1})}{\gamma - b_{1}}\right)}.$$
 (C.2.7)

 $\left(\frac{\partial p}{\partial s}\right)_v$ has also been determined previously (Eq. (C.2.4)) and thanks to relation (3.2.40), the next derivative arises after some algebraic manipulations,

$$\left(\frac{\partial p}{\partial v}\right)_{s} = \exp\left(\frac{s-q''}{C_{v}}\right) \exp\left(\frac{\gamma p_{\infty,1}\left[v-b(v)\right]}{C_{v}(1-b_{1})}\right)$$

$$\left[-(\gamma-b_{1})(\gamma-1)C_{v}\left[v-b(v)\right]^{\frac{-\gamma-1+2b_{1}}{1-b_{1}}} + 2(\gamma-1)\gamma p_{\infty,1}\left[v-b(v)\right]^{\frac{-\gamma+b_{1}}{1-b_{1}}} - \frac{(\gamma p_{\infty,1})^{2}}{C_{v}}\left[v-b(v)\right]^{\frac{1-\gamma}{1-b_{1}}}\right].$$

$$(C.2.8)$$

Equation (C.2.6) then reads after calculations,

$$\left(\frac{\partial v}{\partial s}\right)_{p} = -\frac{(\gamma - 1)C_{v} - \gamma p_{\infty,1}[v - b(v)]}{-C_{v}^{2}(\gamma - 1)(\gamma - b_{1})[v - b(v)]^{-1} + 2\gamma p_{\infty,1}(\gamma - 1)C_{v} - (\gamma p_{\infty,1})^{2}[v - b(v)]}.$$
 (C.2.9)

Inserting Eq. (3.2.18) into Eq. (C.2.9), the following result is obtained after some algebraic manipulations,

$$\left(\frac{\partial v}{\partial s}\right)_{p} = -\frac{-(\gamma - 1)C_{v}\left[p + p'_{\infty}(T)\right] + \gamma p_{\infty,1}(\gamma - 1)C_{v}T}{\frac{C_{v}}{T}(\gamma - b_{1})\left[p + p'_{\infty}(T)\right]^{2} - \left[\gamma p_{\infty,1}(\gamma - 1)C_{v}\right]\left(2p + \gamma p_{\infty,1}T + \frac{2\gamma p_{\infty,0}(1 - b_{1})}{\gamma - b_{1}}\right)}.$$
 (C.2.10)

Analyzing Eqs. (C.2.7) and (C.2.10), the last Maxwell's relation (C.2.1) (d) is satisfied.

C.3 Methodology to determine the various Extended NASG (ENASG) parameters

This section details the procedure used in this work to determine the different ENASG parameters for liquid and gas phases. Depending on the studied application, the determination of the corresponding parameters can be different, but the use of the experimental curves is mandatory.

Liquid phase

In this section, let us introduce,

$$A_{l} = \gamma_{l} p_{\infty,1,l}, \quad B_{l} = \frac{b_{0,l}}{1 - b_{1,l}}, \quad C_{l} = \frac{\gamma_{l} p_{\infty,0,l} (1 - b_{1,l})}{\gamma_{l} - b_{1,l}}.$$
 (C.3.1)

In the calculations that follow, these coefficients will be considered as known. Their numerical values will be addressed later. The liquid coefficients are determined with the help of experimental saturation data. In the following, the least squares method is used with the specific volume, Eq. (3.2.18). Searching the optimum γ_l coefficient, the next relation appears after some algebraic manipulations,

$$S_{v1} - (\gamma_l - 1)C_{v,l}S_{v2} = 0,$$

$$S_{v1} = \sum_{i=1}^{N} \left(\frac{(v_{exp,l,i} - B_l)T_{exp,l,i}}{(1 - b_{1,l})(p_{exp,l,i} + A_l T_{exp,l,i} + C_l)} \right),$$

$$S_{v2} = \sum_{i=1}^{N} \left(\frac{T_{exp,l,i}^2}{(1 - b_{1,l})^2(p_{exp,l,i} + A_l T_{exp,l,i} + C_l)^2} \right).$$
(C.3.2)

In this section, let us introduce the following convention: $_{exp}$ denotes the experimental values and N the number of experimental points considered. The experimental values of the internal energy are now used. Combining Eqs. (3.2.18), (3.2.20) and (3.2.21), the internal energy reads,

$$\begin{cases} e_l(p,T) &= C_{v,l} \frac{p + \gamma_l D_l(p,T) + E_l(p,T)}{F_l(p,T)} + q_l, \\ D_l(p,T) &= \frac{C_l(p + C_l)}{(1 - b_{1,l})(p + A_l T + C_l)}, \\ E_l(p,T) &= -\frac{C_l b_{1,l}}{1 - b_{1,l}} + \frac{A_l C_l T}{(1 - b_{1,l})(p + A_l T + C_l)}, \\ F_l(p,T) &= \frac{p + A_l T + C_l}{T} - A_l. \end{cases}$$
(C.3.3)

A reference state $_{ref}$ is now used to express the liquid reference energy q_l . Using (C.3.3), the next relation arises,

$$q_{l} = e_{ref,l} - C_{v,l} \frac{p_{ref,l} + \gamma_{l} D_{l}(p_{ref,l}, T_{ref,l}) + E_{l}(p_{ref,l}, T_{ref,l})}{F_{l}(p_{ref,l}, T_{ref,l})}.$$
(C.3.4)

Inserting Eq. (C.3.4) into (C.3.3), the internal energy transforms to,

$$e_{l}(p,T) = e_{ref,l} + C_{v,l} \left(\frac{p + \gamma_{l} D_{l}(p,T) + E_{l}(p,T)}{F_{l}(p,T)} - \frac{p_{ref,l} + \gamma_{l} D_{l}(p_{ref,l},T_{ref,l}) + E_{l}(p_{ref,l},T_{ref,l})}{F_{l}(p_{ref,l},T_{ref,l})} \right).$$
(C.3.5)

The least squares method is now applied to Eq. (C.3.5). Searching the optimum $C_{v,l}$ coefficient, the following relation appears after some algebraic manipulations,

$$\begin{cases} S_{e1} - C_{v,l}S_{e2} + \gamma S_{e3} - \gamma_l C_v S_{e4} - \gamma_l^2 C_{v,l}S_{e5} = 0, \\ S_{e1} = \sum_{i=1}^{N} \left((e_{exp,l,i} - e_{ref,l}) \left(\frac{p_{exp,l,i} + E_l(p_{exp,l,i}, T_{exp,l,i})}{F_l(p_{exp,l,i}, T_{exp,l,i})} \right) - \frac{(e_{exp,l,i} - e_{ref,l})(p_{ref,l}, T_{ref,l})}{F_l(p_{ref,l}, T_{ref,l})} \right) \right), \\ S_{e2} = \sum_{i=1}^{N} \left(\left[\frac{p_{exp,l,i} + E_l(p_{exp,l,i}, T_{exp,l,i})}{F_l(p_{exp,l,i}, T_{exp,l,i})} - \frac{p_{ref,l} + E_l(p_{ref,l}, T_{ref,l})}{F_l(p_{ref,l}, T_{ref,l})} \right]^2 \right), \\ S_{e3} = \sum_{i=1}^{N} \left(\frac{(e_{exp,l,i} - e_{ref,l})D_l(p_{exp,l,i}, T_{exp,l,i})}{F_l(p_{exp,l,i}, T_{exp,l,i})} - \frac{(e_{exp,l,i} - e_{ref,l})D_l(p_{ref,l}, T_{ref,l})}{F_l(p_{ref,l}, T_{ref,l})} \right), \\ S_{e4} = \sum_{i=1}^{N} \left[\frac{2D_l(p_{exp,l,i}, T_{exp,l,i})}{F_l^2(p_{exp,l,i}, T_{exp,l,i})} - \frac{e_{exp,l,i} - e_{ref,l})D_l(p_{exp,l,i}, T_{exp,l,i})}{F_l(p_{exp,l,i}, T_{exp,l,i})} \right) - \frac{2\left[\left[p_{exp,l,i}, F_{exp,l,i} \right] D_l(p_{ref,l}, T_{exp,l,i})}{F_l^2(p_{exp,l,i}, T_{exp,l,i})} \right] \right], \\ S_{e5} = \sum_{i=1}^{N} \left(\left[\frac{D_l(p_{exp,l,i}, T_{exp,l,i})}{F_l^2(p_{exp,l,i}, T_{exp,l,i})} - \frac{D_l(p_{ref,l}, T_{ref,l})}{F_l(p_{ref,l}, T_{ref,l})} \right]^2 \right).$$

$$(C.3.6)$$

Equations (C.3.2) and (C.3.6) then create a two-unknown equation system whose solution provides γ_l and $C_{v,l}$. An analytical solution is available and reads,

$$\gamma_{l} = \frac{-S_{v2}S_{e1} + S_{v2}S_{e3} + S_{v1}S_{e4} \pm \sqrt{\left[S_{v2}(S_{e1} - S_{e3}) - S_{v1}S_{e4}\right]^{2} + 4(S_{v2}S_{e1} + S_{v1}S_{e2})(S_{v2}S_{e3} - S_{v1}S_{e5})}{2S_{v2}S_{e3} - 2S_{v1}S_{e5}}$$
(C.3.7)

$$C_{v,l} = \frac{S_{v1}}{(\gamma_l - 1)S_{v2}}.$$
(C.3.8)

The expressions of γ_l and $C_{v,l}$ are now available. Their numerical values will be determined with the help of the parameters A_l, B_l, C_l and $b_{0,l}, b_{1,l}$. Those are addressed hereafter. From Eq. (3.2.17), the coefficient A_l is estimated as, $A_l = \frac{p'_{\infty,c} - C_l}{T_c}$. In this relation, the critical point is used via T_c and $p'_{\infty,c}$ that will be given arbitrary as $p'_{\infty,c} \to 0$. However, the coefficients $b_{0,l}$ and $b_{1,l}$ are included in B_l and C_l . Those are estimated as, $b_{1,l} = \frac{b_c - b_{ref,l}}{v_c - v_{ref,l}}$ and $b_{0,l} = b_{ref,l} - b_{1,l}v_{ref,l}$. The reference $_{ref}$ and critical $_c$ states are considered known either by an experimental point or arbitrary.

The coefficient B_l is then known through $b_{0,l}$, $b_{1,l}$. The parameter A_l depending only on C_l , the coefficients γ_l and $C_{v,l}$ become consequently, $\gamma_l = \gamma_l(C_l)$ and $C_{v,l} = C_{v,l}(C_l)$. The coefficient C_l is then the only unknown at this point. To determine this latter, the speed of sound is used with another reference state denoted $_0$ (atmospheric conditions). With the help of Eq. (3.2.42), the next relation

arises,

$$f(C_l) = -c_{0,l}^2 - \frac{A_l(C_l)v_{0,l}^2(p_0 + C_l)}{C_{v,l}(C_l)} - v_{0,l}^2 \left(\frac{p_0 + C_l}{\left[\gamma_l(C_l) - 1\right]C_{v,l}(C_l) - A_l(C_l)\left[v_{0,l} - b(v_{0,l})\right]}\right) \times \left(A_l(C_l)\left[\gamma(C_l) - 1\right] - \frac{\left[\gamma_l(C_l) - b_{1,l}\right]\left[\gamma_l(C_l) - 1\right]C_{v,l}(C_l)}{v_{0,l} - b(v_{0,l})}\right),$$
(C.3.9)

and can be solved with an iterative method. $p_{\infty,0,l}$ and $p_{\infty,1,l}$ are then determined via Eq. (C.3.1), and the reference internal energy is computed with Eq. (C.3.4). The reference entropy is the only unknown value at this point. The least squares method is used one more time with Eq. (3.2.38). Searching the optimum q'_l coefficient, the following relation appears after some algebraic manipulations,

$$q_{l}' = \frac{1}{N} \sum_{i=1}^{N} \left[s_{exp,l,i} - C_{v,l} \ln \left(\frac{T_{exp,l,i}^{\frac{\gamma_{l} - b_{1,l}}{1 - b_{1,l}}}}{\left[p_{exp,l,i} + p_{\infty}'(T_{exp,l,i}) \right]^{\frac{\gamma_{l} - 1}{1 - b_{1,l}}}} \right) + \frac{\gamma_{l} p_{\infty,1,l}(\gamma_{l} - 1) C_{v,l} T_{exp,l,i}}{\left[1 - b_{1,l} \right] \left[p_{exp,l,i} + p_{\infty}'(T_{exp,l,i}) \right]} \right].$$
(C.3.10)

The different reference state values used for the calculation of the liquid ENASG coefficients are summarized in Tables C.1 and C.2. In this work, all experimental data come from $NIST^1$ website. For the liquid phase, the saturation (boiling) curve is considered.

Fluid	Ν	T_c (K)	p_c (bar)	$v_c \; (\mathrm{m}^3/\mathrm{kg})$	$p'_{\infty,c}$ (Pa)	$b_c \ ({\rm m}^3/{\rm kg})$	$c_0 ({\rm m/s})$	p_0 (bar)	$v_0 \ (\mathrm{m}^3/\mathrm{kg})$
H_2O	374	646.16	221	0.0025101	100	10^{-6}	1552.1	1	0.0010182
O_2	101	154.36	50	0.0019522	100	10^{-6}	1065.7	1	0.00080871

Table C.1: Reference state values used for the determination of liquid ENASG coefficients.

Fluid	T_{ref} (K)	p_{ref} (Pa)	$v_{ref} \ (\mathrm{m^3/kg})$	$e_{ref}~({\rm kJ/kg})$	$b_{ref} \ (\mathrm{m}^3/\mathrm{kg})$
H_2O	300.16	3570.2	0.0010035	113.23	0.0009125
O_2	70.631	6684.7	0.00080952	-166.823	0.000769

Table C.2: Reference state values used for the determination of liquid ENASG coefficients (continued).

Gas phase

In the present formulation (3.4.2), the gas phase is considered as ideal and the different parameters are determined regardless of the saturation conditions. Only four parameters are required for the gas phase, C_v , γ , q and q'. The atmospheric conditions are used in this work via the experimental isobar

¹http://webbook.nist.gov/chemistry/

 $p_0 = 1$ bar. According to the experimental data of water and oxygen at such low pressure, there exists a significant temperature range where the heat capacity (C_v) is quite constant. The parameter C_v is thereby chosen as a constant, representative of the present thermodynamic conditions.

The parameter γ is then determined as $\gamma = \frac{C_p}{C_v}$ with $C_p - C_v = \hat{R}/W$ according to Mayer's relation. In the previous relation, \hat{R} denotes the universal gas constant and W the molar mass. The values reported in Tables 3.1 and 3.2 are consequently close to the expected triatomic (H₂O) and diatomic (O₂) predictions for ideal gases ($\gamma = 1.3079 \simeq 9/7$ and $C_v = 1500 \text{ J/kg/K} \simeq (7/2)R$ for water and $\gamma = 1.3985 \simeq 1.4$ and $C_v = 652 \text{ J/kg/K} \simeq (5/2)R$ for oxygen).

A reference point on the present isobar $p_0 = 1$ bar is used to determine the coefficient q,

$$q = e_0 - C_v T_0. (C.3.11)$$

In this work $T_0 = 393.38$ K and $e_0 = 2537.7$ kJ/kg are used for water and $T_0 = 100.07$ K and $e_0 = 63.657$ kJ/kg for oxygen.

The last coefficient q'_g is finally determined with the least squares method, corresponding to the ideal gas reduction of Eq. (C.3.10). The isobar $p_0 = 1$ bar is used one more time with N = 542 points for water corresponding to the temperature range $T_{exp} \in [372.76 - 1275]$ K and $N_{exp} = 579$ points, $T_{exp} \in [90.062 - 1000]$ K for oxygen.

Note that for the VdW and SRK EOSs, the specific internal energy, enthalpy and entropy require $C_v^{(0)}$, q and q' as well for practical computations. In the present work $C_{v,H_2O}^{(0)} = 1750 \text{ J/kg/K}$, $C_{v,O_2}^{(0)} = 652 \text{ J/kg/K}$ both for VdW and SRK EOSs. $q_{H_2O} = 1799218 \text{ J/kg}$, $q_{O_2} = 17918 \text{ J/kg}$, $q'_{H_2O} = -3360 \text{ J/kg/K}$, $q'_{O_2} = 2793 \text{ J/kg/K}$ for the VdW EOS and $q_{H_2O} = 1799885 \text{ J/kg}$, $q_{O_2} = -682 \text{ J/kg}$, $q'_{H_2O} = -3360 \text{ J/kg/K}$, $q'_{O_2} = 2793 \text{ J/kg/K}$ for the SRK EOS.

C.4 Connection temperature between the ENASG EOS and ideal gas formulation

The different parameters of the quadratic equation (3.6.4) are provided hereafter for the specific volume (v), internal energy (e) and enthalpy (h). The solution of Eq. (3.6.4) provides the connection temperature between the ENASG EOS and ideal gas formulation during the liquid-to-supercritical
state transition,

$$\begin{cases} a_{v} = \frac{(1-b_{1,l})\gamma_{l}p_{\infty,1,l}(\gamma_{g}-1)C_{v,g}}{p}, \\ b_{v} = (1-b_{1,l})\left(p + \frac{\gamma_{l}p_{\infty,0,l}(1-b_{1,l})}{(\gamma_{l}-b_{1,l})}\right)\frac{(\gamma_{g}-1)C_{v,g}}{p} - (\gamma_{l}-1)C_{v,l} - \gamma_{l}p_{\infty,1,l}b_{0,l}, \\ c_{v} = -b_{0,l}\left(p + \frac{\gamma_{l}p_{\infty,0,l}(1-b_{1,l})}{(\gamma_{l}-b_{1,l})}\right), \end{cases}$$
(C.4.1)

$$\begin{cases} a_e = \gamma_l p_{\infty,1,l} (C_{v,l} - C_{v,g}), \\ b_e = C_{v,l} (p + \gamma_l p_{\infty,0,l}) + \gamma_l p_{\infty,1,l} (q_l - q_g) - C_{v,g} \left(p + \frac{\gamma_l p_{\infty,0,l} (1 - b_{1,l})}{\gamma_l - b_{1,l}} \right), \\ c_e = (q_l - q_g) \left(p + \frac{\gamma_l p_{\infty,0,l} (1 - b_{1,l})}{\gamma_l - b_{1,l}} \right), \end{cases}$$
(C.4.2)

$$\begin{cases} a_{h} = (1 - b_{1,l})\gamma_{l}p_{\infty,1,l}(C_{v,l} - \gamma_{g}C_{v,g}), \\ b_{h} = \gamma_{l}C_{v,l}p + C_{v,l}\left[\gamma_{l}p_{\infty,0,l}(1 - b_{1,l}) - pb_{1}\right] + \gamma_{l}p_{\infty,1,l}b_{0,l}p + \gamma_{l}p_{\infty,1,l}(1 - b_{1,l})(q_{l} - q_{g}) \\ - \gamma_{g}C_{v,g}(1 - b_{1,l})\left(p + \frac{\gamma_{l}p_{\infty,0,l}(1 - b_{1,l})}{\gamma_{l} - b_{1,l}}\right), \\ c_{h} = \left(p + \frac{\gamma_{l}p_{\infty,0,l}(1 - b_{1,l})}{\gamma_{l} - b_{1,l}}\right)\left[pb_{0,l} + (1 - b_{1,l})(q_{l} - q_{g})\right]. \end{cases}$$
(C.4.3)

The subscripts l and g denote the liquid and gas phases respectively. Note that the determination of connection temperature for the entropy requires an iterative method because of the logarithmic function present in Eq. (3.4.1).

C.5 Towards the critical point

Near the critical point, the vapor phase necessarily lacks of accuracy with the present ENASG EOS that is reduced to the ideal gas expression. The reason is linked to the absence of gas attractive effects. However, the introduction of those latter ones results in conditional convexity. They are thereby removed in this work. Nevertheless, they also result in much better agreement with experimental data as illustrated in the following.

Equation (3.2.16), recalled hereafter, does consider an attractive term via the parameter d,

$$p(v,T) = \frac{(\gamma - 1)C_vT}{v - b(v)} - p'_{\infty}(T) - \frac{d}{\left[v - b(v)\right]^{\frac{\gamma - b_1}{1 - b_1}}}.$$
(C.5.1)

Previously the coefficient d was set to zero for the sake of convexity and simplicity. This $d/[v-b(v)]^{\frac{\gamma-b_1}{1-b_1}}$ extra term is reminiscent of cubic EOSs but seems nonetheless essential to describe dense gases near

the critical point. With this parameter, the attractive pressures $p_{\infty}(T)$ and $p'_{\infty}(T)$ are no longer required for the gas phase and the thermal equation of state reads,

$$p_v(v,T) = \frac{(\gamma_v - 1)C_{v,v}T}{v - b_{0,v}} - \frac{d_v}{(v - b_{0,v})^{\gamma_v}}.$$
(C.5.2)

Equation (C.5.2) does not provide an explicit formulation of the specific volume v(p, T). Cubic EOSs present the same flaw. Note that $b(v) = b_0 = cst$ is accurate enough when dealing with gases. Following a mathematical procedure based on Maxwell's relations, similar to the derivations detailed in the previous sections, the present "alternative" formulation yields,

$$\begin{cases} p_{v}(e,v) = \frac{(\gamma_{v}-1)(e-q_{v})}{v-b_{0,v}}, \\ e_{v}(p,T) = C_{v,v}T - \frac{d_{v}}{(\gamma_{v}-1)\left[v(p,T)-b_{0,v}\right]^{\gamma_{v}-1}} + q_{v}, \\ h_{v}(p,T) = \frac{p\left[v(p,T)-b_{0,v}\right]}{\gamma_{v}-1} + pv(p,T) + q_{v}, \\ s_{v}(p,T) = C_{v,v}\ln(T) + (\gamma_{v}-1)C_{v,v}\ln\left[v(p,T)-b_{0,v}\right] + q'_{v}, \\ g_{v}(p,T) = \frac{p\left[v(p,T)-b_{0,v}\right]}{\gamma_{v}-1} + pv(p,T) + q_{v} - C_{v,v}T\left[(\gamma_{v}-1)\ln\left[v(p,T)-b_{0,v}\right] + \ln(T) + \frac{q'_{v}}{C_{v,v}}\right], \\ c_{v}^{2}(p,v) = \frac{\gamma_{v}v^{2}p}{v-b_{0,v}}, \\ C_{p,v}(p,T) = \frac{\gamma_{v}C_{v,v}\left[(\gamma_{v}-1)C_{v,v}T\left[v(p,T)-b_{0,v}\right]^{\gamma_{v}-1} - d_{v}\right]}{(\gamma_{v}-1)C_{v,v}T\left[v(p,T)-b_{0,v}\right]^{\gamma_{v}-1} - \gamma_{v}d_{v}}. \end{cases}$$
(C.5.3)

The $_{v}$ subscript denotes here the vapor phase. For the sake of space, the details of calculations are omitted. This "alternative" formulation respects Maxwell's relations and is thermodynamically consistent and convex under condition,

$$d_v < \frac{(\gamma_v - 1)C_{v,v}T(v - b_{0,v})^{\gamma_v - 1}}{\gamma_v}.$$
 (C.5.4)

To represent correctly the physics of attractive terms, $d_v > 0$ must be chosen and condition (C.5.4) becomes restrictive. The same observation holds for cubic EOSs. It is worth mentioning that despite this conditional convexity, the speed of sound remains unambiguously positive unlike cubic EOSs and corresponds to the Noble-Abel (NA) sound speed. Table C.3 provides the associated parameters of this "alternative" but conditionally convex formulation (C.5.3) for water and oxygen. Figures C.1 and C.2 display the corresponding results at saturation.

As seen in Figs. C.1 and C.2 the theoretical saturation pressure, liquid enthalpy, liquid and vapor specific densities are in very good agreement with experimental saturation data from the lowest



Figure C.1: Comparison between experimental and theoretical saturation curves for liquid l and vapor v water. Symbols represent experimental data. The thick lines represent the theoretical saturation curves obtained with the liquid Extended NASG EOS (ENASG) Eq. (3.4.1) and its "alternative" but conditionally convex formulation for the vapor phase, Eq. (C.5.3). The thin solid lines represent the theoretical saturation curves obtained with the ENASG EOS reducing to the ideal gas description for the vapor species (Chapter 3, Table 3.1). The dotted lines represent the theoretical saturation curves obtained with the NASG EOS (Chapter 3, Table 3.1). p_{sat} denotes the saturation pressure, L_v the latent heat, h the specific enthalpy and ρ the density.



Figure C.2: Comparison between experimental and theoretical saturation curves for liquid l and vapor v oxygen. Symbols represent experimental data. The thick lines represent the theoretical saturation curves obtained with the liquid Extended NASG EOS (ENASG) Eq. (3.4.1) and its "alternative" but conditionally convex formulation for the vapor phase, Eq. (C.5.3). The thin solid lines represent the theoretical saturation curves obtained with the ENASG EOS reducing to the ideal gas description for the vapor species (Chapter 3, Table 3.2). The dotted lines represent the theoretical saturation curves obtained with the NASG EOS (Chapter 3, Table 3.2). p_{sat} denotes the saturation pressure, L_v the latent heat, h the specific enthalpy and ρ the density.

Coefficients	$\mathrm{ENASG}_{H_2O, Liq}$	$\mathrm{ENASG}_{H_2O, vap}$	$\mathrm{ENASG}_{O_2, Liq}$	$\mathrm{ENASG}_{O_2, vap}$
γ	1.0178	1.3189	1.033	1.3875
$C_v ~({ m J/kg/K})$	3848	1719	1451	779
b_1	-0.5934	0	-0.6661	0
$b_0~({ m m}^3/{ m kg})$	1.4905×10^{-3}	3.3514×10^{-4}	1.3013×10^{-3}	0
$p_{\infty,1} (\mathrm{Pa/K})$	-607195	0	-405133	0
$p_{\infty,0}$ (Pa)	396642530	0	63642939	0
$q~({ m J/kg})$	-1065948	1975421	-272675	-1597
$q'~({ m J/kg/K})$	-20985	-3131	-3277	2224
$d (\operatorname{Pa} \mathrm{m}^{3\gamma}/\mathrm{kg}^{\gamma})$	0	41200	0	2950

Table C.3: Coefficients for water and oxygen for the "alternative" ENASG EOS whose formulation is summarized in Eq. (C.5.3). With such description, the gas attractive effects are taken into account via the parameter d but result in conditional convexity, Eq. (C.5.4). The liquid ENASG EOS is unchanged, Eq. (3.4.1).

available temperature to the critical one. Yet, the vapor enthalpy seems to present lesser agreement. It is interesting to note that vapor enthalpy is the only thermodynamic variable that presents a nonmonotonic behavior. However, analyzing the range of variation, it seems that the theoretical order of magnitude is satisfied. The latent heat, very important during phase transition $(L_v = h_v - h_l)$ is also in very good agreement with experimental data. The introduction of the coefficient *d* involves a conditional convexity (Eq. (C.5.4)) but does illustrate the significance of the gas attractive effects.

Appendix D

Fluid dispersal at large scales

D.1 Extended formulation with variable external pressure

When dealing with liquids and large hydrostatic effects, the two-layer shallow water model developed in Chapter 4 can be reformulated with extra pressure terms as a function of heights of the fluid layers, and does not cause extra fundamental issues than those already addressed in the previous chapter.

To account for variable external pressure, System (4.2.3) is generalized as,

$$\begin{pmatrix}
\frac{\partial h_1}{\partial t} + u_1 \frac{\partial h_1}{\partial x} = \frac{\mu(p_1 - p_0 - \rho_2 g h_2)}{\rho_1 c_1^2}, \\
\frac{\partial(h_1 \rho_1)}{\partial t} + \frac{\partial(h_1 \rho_1 u_1)}{\partial x} = 0, \\
\frac{\partial(h_1 \rho_1 u_1)}{\partial t} + \frac{\partial(h_1 \rho_1 u_1^2 + h_1 p_1(\rho_1, \rho_2, h_2) + \frac{1}{2} \rho_1 g h_1^2)}{\partial x} = \rho_2 g h_2 \frac{\partial h_1}{\partial x} + p_0 \frac{\partial h_1}{\partial x}, \\
\frac{\partial h_2}{\partial t} + u_2 \frac{\partial h_2}{\partial x} = \frac{\mu(p_2 - p_0)}{\rho_2 c_2^2}, \\
\frac{\partial(h_2 \rho_2)}{\partial t} + \frac{\partial(h_2 \rho_2 u_2)}{\partial x} = 0, \\
\frac{\partial(h_2 \rho_2 u_2)}{\partial t} + \frac{\partial(h_2 \rho_2 u_2^2 + h_2 p_2(\rho_2) + \frac{1}{2} \rho_2 g h_2^2)}{\partial x} = -\rho_2 g h_2 \frac{\partial h_1}{\partial x} + p_0 \frac{\partial h_2}{\partial x}.
\end{cases}$$
(D.1.1)

With this formulation, the equation of state of the first (heaviest) fluid transforms to,

$$p_1 = p_0 + \rho_2 g h_2 + c_1^2 \left(\rho_1 - \rho_1^{(0)} \right), \qquad (D.1.2)$$

while it is unchanged for the upper layer,

$$p_2 = p_0 + c_2^2 \left(\rho_2 - \rho_2^{(0)} \right). \tag{D.1.3}$$

The $g\rho_2 h_1 h_2$ flux term present in System (4.2.3) is now considered in the equation of state of the first

fluid. The hydrostatic pressure of the first fluid has been consequently reformulated in the relaxation term of the height equation as well. It is important to check that the hyperbolicity of the reformulated system is still valid. Also, the stiff pressure relaxation limit is meant to recover Ovsyannikov's [108] system (Eq. (4.2.1)). These points are examined hereafter.

System (D.1.1) is expressed in primitive-variable formulation (without source terms) as,

$$\frac{\partial W}{\partial t} + A(W)\frac{\partial W}{\partial x} = 0, \tag{D.1.4}$$

with

$$W = \begin{pmatrix} h_1 \\ h_2 \\ \rho_1 \\ \rho_2 \\ u_1 \\ u_2 \end{pmatrix}, \quad A(W) = \begin{pmatrix} u_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & u_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & u_1 & 0 & \rho_1 & 0 \\ 0 & 0 & 0 & u_2 & 0 & \rho_2 \\ \frac{p_1 - p_0 - \rho_2 g h_2}{h_1 \rho_1} + g & 0 & \frac{c_1^2 + \frac{1}{2} g h_1}{\rho_1} & 0 & u_1 & 0 \\ g & \frac{p_2 - p_0}{h_2 \rho_2} + g & 0 & \frac{c_2^2 + \frac{1}{2} g h_2}{\rho_2} & 0 & u_2 \end{pmatrix}. \quad (D.1.5)$$

The wave speeds are solutions of det $(A(W) - \lambda \underline{I}) = 0$ resulting in,

$$(u_1 - \lambda)(u_2 - \lambda)\left[(u_2 - \lambda)^2 - \left(c_2^2 + \frac{1}{2}gh_2\right)\right]\left[(u_1 - \lambda)^2 - \left(c_1^2 + \frac{1}{2}gh_1\right)\right] = 0.$$
(D.1.6)

The six real and distinct eigenvalues of System (4.2.3) are recovered,

$$\begin{cases} \lambda_1 = u_1, \quad \lambda_2 = u_1 + \sqrt{c_1^2 + \frac{1}{2}gh_1}, \quad \lambda_3 = u_1 - \sqrt{c_1^2 + \frac{1}{2}gh_1}, \\ \lambda_4 = u_2, \quad \lambda_5 = u_2 + \sqrt{c_2^2 + \frac{1}{2}gh_2}, \quad \lambda_6 = u_2 - \sqrt{c_2^2 + \frac{1}{2}gh_2}. \end{cases}$$
(D.1.7)

System (D.1.1), like System (4.2.3), is therefore strictly hyperbolic.

Asymptotic limit

Let us now consider the following expansion,

$$\begin{cases} p_1 = p_1^{(0)} + \epsilon p_1^{(1)} + \dots, \\ p_0 + h_2 \rho_2 g = (p_0 + h_2 \rho_2 g)^{(0)} + \epsilon (p_0 + h_2 \rho_2 g)^{(1)} + \dots, \end{cases}$$
(D.1.8)

with $\epsilon = \frac{1}{\mu}$. The first equation of System (D.1.1) becomes,

$$\frac{\partial h_1}{\partial t} + u_1 \frac{\partial h_1}{\partial x} = \frac{1}{\epsilon} \frac{p_1^{(0)} - (p_0 + \rho_2 g h_2)^{(0)}}{\rho_1 c_1^2} + \frac{p_1^{(1)} - (p_0 + \rho_2 g h_2)^{(1)}}{\rho_1 c_1^2}.$$
 (D.1.9)

Hence, at leading order,

$$p_1^{(0)} = (p_0 + h_2 \rho_2 g)^{(0)} . (D.1.10)$$

This last result is introduced in the momentum equation of the first fluid of System (D.1.1) and yields,

$$\frac{\partial \left(h_1 \rho_1 u_1\right)}{\partial t} + \frac{\partial \left(h_1 \rho_1 u_1^2 + \frac{1}{2} \rho_1 g h_1^2 + g \rho_2 h_1 h_2\right)}{\partial x} = \rho_2 g h_2 \frac{\partial h_1}{\partial x}.$$
 (D.1.11)

The momentum equation of System (4.2.1) is thus recovered. Similar manipulations on the second layer momentum equation of the present model lead to,

$$\frac{\partial \left(h_2 \rho_2 u_2\right)}{\partial t} + \frac{\partial \left(h_2 \rho_2 u_2^2 + \frac{1}{2} \rho_2 g h_2^2\right)}{\partial x} = -\rho_2 g h_2 \frac{\partial h_1}{\partial x}.$$
 (D.1.12)

The second momentum equation of System (4.2.1) is recovered as well. The present formulation thus tends in the limit of stiff pressure relaxation to the conventional two-layer Saint-Venant model. Thereby, System (D.1.1) allows to compute solutions of the non-hyperbolic model [108] with a hyperbolic step using the preceding wave speeds (Eq. (D.1.7)) followed by a correction step regarding the heights.

This latter is supposed to be isentropic. The equation of state (EOS) for the second fluid (lightest) reads: $p_2 = p_0 + c_2^2 \left(\rho_2 - \rho_2^{(0)}\right)$. At the end of the relaxation step, $p_2^* = p_0$ and implies $\rho_2^* = \rho_2^{(0)}$. As the mass quantity is known from the hyperbolic evolution and is constant during the relaxation process, $m_2 = h_2\rho_2 = h_2^*\rho_2^*$, the relaxation step just consists in reseting the height: $h_2^* = \frac{h_2\rho_2}{\rho_2^{(0)}}$.

For the first fluid, the EOS now reads: $p_1 = p_0 + \rho_2^* g h_2^* + c_1^2 \left(\rho_1 - \rho_1^{(0)}\right)$. At the end of the relaxation process, the pressure reads $p_1^* = p_0 + \rho_2^* g h_2^*$. Consequently, $\rho_1^* = \rho_1^{(0)}$ and the relaxation step reduces to $h_1^* = \frac{h_1 \rho_1}{\rho_1^{(0)}}$ as before with System (4.2.3). The only difference is that $\rho_1^{(0)}$ no longer represents the density of fluid 1 at atmospheric pressure p_0 but is corrected by hydrostatic effects as $\rho_1^{(0)} = \rho_1^{(0)} + \frac{\rho_2^* g h_2^*}{c_1^2}$, where $\rho_1^{(00)}$ represents the density of fluid 1 at atmospheric pressure.

System (D.1.1) is then an extended formulation of System (4.2.3). Formulation (D.1.1) provides another interpretation of the flux term $g\rho_2h_1h_2$ that is now expressed through the equation of state of the first layer (heaviest). Besides, this extended formulation seems more attractive for a multi-layer extension of the present model.

At the discrete level this model does not cause extra computational difficulties. It has been coded and tested on the example of Fig. 4.15 showing excellent agreement with results of Fig. 4.20.

Appendix E

Summary

E.1 Résumé

Depuis maintenant plusieurs décennies, les écoulements diphasiques suscitent un intérêt croissant au sein de la communauté scientifique ainsi que dans la communauté industrielle. Plusieurs raisons expliquent cet engouement. La première est liée au fort potentiel de développement quant à la richesse de la physique que les modèles multiphasiques peuvent prendre en compte. D'autre part, dans le contexte économique actuel, les besoins industriels devenant de plus en plus spécifiques, les modèles théoriques développés par le passé nécessitent aujourd'hui d'importantes extensions et adaptations. De plus, les capacités informatiques étant simultanément en plein essor, il devient maintenant envisageable d'effectuer des simulations numériques de ces écoulements de plus en plus massives et précises. Enfin, les écoulements diphasiques sont omniprésents dans l'industrie mais aussi dans la nature. C'est dans ce contexte que cette thèse de doctorat porte sur la modélisation et la simulation numérique des écoulements diphasiques compressibles.

Les travaux de recherche présentés dans ce manuscrit sont fortement liés à un besoin constant d'expertises scientifiques à destination des industriels notamment dans les domaines de l'Espace, de l'Énergie, des Risques et de la Sûreté. Ceux-ci possèdent en effet de nombreuses applications faisant intervenir une large gamme de phénomènes physiques fortement transitoires où la compressibilité des milieux joue un rôle déterminant. Dans ce contexte, une recherche fondamentale et appliquée a été développée au cours de cette thèse. Les problématiques abordées dans cet ouvrage concernent:

- La dynamique des interfaces ainsi que leurs instabilités,
- Les phénomènes d'évaporation et de condensation fortement dynamiques,
- Les équations d'état pour des systèmes liquide-gaz sous et supercritiques,
- La dispersion de fluides non-miscibles.

Ce type de problématique est effectivement présent dans de nombreuses situations industrielles. La connaissance des phénomènes physiques mis en jeu est essentielle autant d'un point de vue sécuritaire que pour le bon fonctionnement de systèmes industriels. Dans ce cadre, cette thèse porte sur l'élaboration de modèles et d'outils de simulation afin d'appréhender des phénomènes physiques se produisant dans des systèmes industriels de plus en plus sophistiqués.

Dans le domaine de l'Espace, les travaux présentés dans ce manuscrit sont fortement liés au dimensionnement des chambres de combustion et des systèmes d'injection du moteur cryotechnique du lanceur spatial d'Ariane 6. Il s'agira du premier moteur de l'histoire capable de se rallumer dans l'espace à des fins commerciales, à savoir permettre le changement d'orbite pour la dépose d'autres satellites. D'intenses phénomènes de changement de phase sont à prévoir dans de telles chambres de combustion où le fluide est attendu d'atteindre son état supercritique suite à la combustion des gaz résultants. Cependant, les aspects relatifs à la combustion ne sont pas étudiés dans ce travail de thèse.

Le projet Ariane 6 implique trois des thématiques de recherche mentionnées ci-dessus. En effet, avant que le moteur n' atteigne les conditions supercritiques, l'écoulement consiste en un jet d'oxygène liquide encerclé d'un écoulement d'hydrogène à grande vitesse. L'entrée du jet liquide dans la chambre de combustion implique naturellement la dynamique d'interfaces matérielles qui doivent être capturées correctement par une méthode numérique appropriée. Dans de telles circonstances, ces interfaces sont sujettes à l'évaporation et ce changement de phase joue un rôle essentiel au sein de l'écoulement diphasique. Enfin les thermodynamiques des phases pures ainsi que celle du mélange sont décrites par des équations d'état appropriées dont l'importance est capitale et constitue également une grande motivation pour ce travail de thèse.

Chapitre 1: Réduction de la diffusion numérique dans la capture des interfaces

Une partie de ce manuscrit porte sur l'extension d'une théorie partiellement initiée par le directeur de cette thèse, Professeur Richard Saurel, en ce qui concerne le traitement des interfaces entre fluides et entre milieux continus.

Aussitôt que le domaine numérique implique plus d'un fluide ou matériau, une difficulté fondamentale apparaît. En effet, dans de telles situations un type supplémentaire de discontinuité est présent en plus des ondes de chocs et des discontinuités de contact présentes dans les écoulements monophasiques. Une interface sépare deux matériaux, éventuellement gouvernés par le même jeu d'équations (par exemple les interfaces séparant de l'air et de l'eau liquide) mais comportant des comportements thermodynamiques différents. Aussitôt que l'interface arrive dans une maille de calcul, cette dernière devient une maille de mélange et la détermination de l'état thermodynamique devient problématique. Les fluides ont différentes densités et énergies internes, ces dernières étant également différentes de la densité et de l'énergie interne du mélange dans la maille de calcul. Il n'est pas possible de déterminer la thermodynamique de la cellule de calcul et en particulier la pression sans informations supplémentaires. Dans ce contexte, plusieurs approches ont été développées au cours de ces dernières décennies.

La première classe de méthodes a pour principe d'éviter l'apparition de mailles de mélange en maintenant des profils d'interface raides. Les méthodes Lagrangienne [28] et "Arbitrary Lagrangian Eulerian" (ALE) [29] traquent ces interfaces mais sont limitées par des distorsions de maillage d'amplitudes arbitraires [30]. La méthode de Front Tracking [31] tente de réduire ces distorsions en considérant des maillages fixes et des interfaces mobiles, traquées par des marqueurs Lagrangiens. Ceci est réalisé aux prix de limitations telle que la gestion de plusieurs solveurs d'écoulement, ou la distorsion des interfaces impliquant des singularités géométriques, résultant en d'importantes difficultés numériques.

Pour progresser dans la direction de la simplicité et de la généralité, la méthode Level-Set [32] a été adaptée aux fluides compressibles et la méthode Ghost Fluid [33] a été utilisée pour déterminer un état thermodynamique approché dans les mailles de mélange, en particulier la pression. Pour éviter les complexités liées à la gestion du maillage avec les méthodes précédentes, l'interface est suivie implicitement via une fonction Eulérienne et deux jeux d'équations d'Euler sont utilisés pour stocker et faire évoluer les variables désirées de l'écoulement quand ceci est nécessaire, en particulier dans les mailles de mélange. La méthode Ghost Fluid est utilisée pour transférer les conditions limites aux interfaces. Dans ce contexte, une extrapolation spécifique permet une communication entre les deux jeux d'équations d'Euler. Bien que simple en apparence, cette méthode demande toujours des efforts afin d'améliorer sa robustesse dans des conditions d'écoulements sévères, pour maintenir la conservation et pour considérer une physique supplémentaire.

La seconde famille de méthodes dédiées aux mailles de mélange est appelée "Méthodes des interfaces diffuses" (DIM). Deux sous-classes de DIM sont présentes dans la littérature. La première considère des interfaces physiquement diffuses ayant une structure visco-capillaire [34]. Dans ce contexte, la résolution spatiale doit être plus petite que la largeur de l'interface, *i.e.* quelques nanomètres. De plus, l'équation d'état est prévue pour décrire le changement de phase entre un liquide et sa vapeur à l'aide d'une formulation de type cubique. À la connaissance des auteurs, cette approche n'a jamais montré sa capacité à décrire des interfaces séparant des fluides non-miscibles (eau et air par exemple). Ceci semble restreint aux simulations de changement de phase aux petites échelles.

La seconde classe de DIM considère les mailles de mélange ayant une origine numérique et non physique. Les travaux pionniers dans cette direction ont été faits avec la méthode "Volume of Fluid" (VOF) [2] dans le cadre de fluides incompressibles. Une équation supplémentaire est ajoutée et le modèle adopte une description diphasique de l'écoulement avec des sous-volumes occupés par les phases et plusieurs équations de masse. L'extension de cette approche aux fluides compressibles a été réalisée dans Saurel and Abgrall (1999) [3] et Kapila et al. (2001) [5].

Les mailles de mélange sont inévitables en raison de la diffusion numérique inhérente à toute méthode de capture de discontinuité. Elles sont en particulier responsables de nombreuses difficultés d'ordre numérique pouvant conduire purement et simplement à l'échec des calculs. La stratégie de la méthode des interfaces diffuses cherche à traiter ces "mailles mixtes" comme de véritables mélanges multiphasiques, à l'aide d'une modélisation appropriée. Le système hyperbolique étendu qui en résulte permet la résolution de chaque milieu continu pur ainsi que de la zone interfaciale à l'aide d'un unique système d'équations aux dérivées partielles, résolu en tout point par le même schéma numérique (Saurel and Le Métayer (2001) [6]). Certains avantages résultent de cette approche. Les plus évidents sont la simplicité de mise en œuvre ainsi que la robustesse puisque le même algorithme est employé partout. La conservation est garantie pour le mélange multiphasique alors que les algorithmes classiques garantissent seulement la conservation de la masse dans le meilleur des cas. Les conditions d'interface sont parfaitement respectées, même lors du couplage de milieux complexes en présence d'ondes de choc et de transfert de masse (évaporation, condensation, détonation, ...). En outre, cette approche est la seule capable de décrire l'apparition d'interfaces qui ne seraient pas présentes initialement comme c'est le cas dans les phénomènes de cavitation ou d'écaillage. Il s'agit d'une modélisation de mélange de fluide qui s'avère inconditionnellement hyperbolique où les phases sont séparées. Cela signifie que chaque fluide possède sa propre thermodynamique (donc sa propre loi d'état) et son propre système d'équations.

Contrairement aux chocs, capturés avec l'aide d'une viscosité artificielle, la description de l'interface séparant des matériaux de thermodynamiques différentes n'a pas de régularisation visqueuse. Comme montré dans [3], [5], [35], le calcul de la thermodynamique du mélange peut être réalisé via des effets de relaxation dans les mélanges multiphasiques. Dans ce contexte les milieux purs, loin des interfaces, sont gouvernés par des systèmes hyperboliques (les équations d'Euler ou des modèles plus sophistiqués), il est alors naturel d'utiliser les modèles hyperboliques d'interfaces diffuses.

Le travail de recherche de ce manuscrit se place dans ce contexte. La simplicité de l'implémentation des méthodes d'interfaces diffuses est le point clé pour la simulation d'écoulements complexes, présentant des interfaces altérées, des ondes de choc et leurs interactions. L'insertion de ces méthodes dans les codes de calcul CFD compressibles est en général simple.

Dans ce cadre, Abgrall (1996) [36] considéra des interfaces séparant deux gaz parfaits. Shyue (1998) [37] et Saurel and Abgrall (1999) [4] considérèrent des interfaces liquide-gaz et ajoutèrent des équations d'évolution pour les paramètres de l'équation d'état Stiffened-Gas afin de calculer la thermodynamique des mailles de mélange. Ces méthodes ont été généralisées et rationalisées via la modélisation des écoulements multiphasiques comme celle présentée par exemple dans Kapila et al. (2001) [5].

Dans ces formulations, le but est de "résoudre" les interfaces avec un unique jeu d'équations aux

dérivées partielles (un modèle d'écoulement étendu) avec un solveur hyperbolique unique. Les interfaces sont capturées et non traquées ou reconstruites. Une telle approche est obligatoire pour la plupart des écoulements compressibles où les déformations des interfaces sont arbitrairement complexes.

Ces méthodes sont en permanence améliorées, par exemple pour réduire l'étalement artificiel et raidir les interfaces [12], [41], [42] ou pour augmenter l'ordre d'approximation de la méthode globale [43].

Une extension de la physique a également été prise en compte: réactions chimiques [7], changement de phase [8], tension de surface [9], solide-fluide [10] ou les transformations plastiques [11] pour en citer quelques unes.

La principale limitation de ces méthodes d'interfaces diffuses est liée à leur excessive diffusion numérique, typiquement quatre points et même plus lors des évolutions en temps longs. Dans certains cas, ceci peut devenir pathologique, s'il s'agit par exemple de distinguer la diffusion physique telle que la diffusion de masse avec la dissipation numérique. Ceci n'est pas problématique pour des écoulements rapides et transitoires où les interfaces sont en général maintenues suffisamment raides pendant une durée suffisante, mais cela devient problématique du moins pour les écoulements plus lents. Plusieurs contributions ont été promues pour maintenir ou restaurer des interfaces raides. Shyue (2006) [44] adapta la méthode de reconstruction d'interface de Youngs (1982) [45] à un modèle compressible d'interface diffuse. Pantano et ses collaborateurs (2010, 2013) [41], [42] adaptèrent la méthode de raidissement d'Olsson and Kreiss (2005) [46] à un autre modèle d'interface diffuse. Kokh and Lagoutiere (2010) [47] promurent une autre méthode basée sur un limiteur "downwind" (décentré aval). Shyue and Xiao (2014) [12] examinèrent un autre limiteur, combiné avec une reconstruction de type tangente hyperbolique. Il est clair que ce domaine de recherche est très actif et que des directions variées sont examinées.

Cependant, il n'existe à ce jour aucune méthode simple et efficace permettant de réduire la dissipation numérique sur des maillages non-structurés et pour des écoulements comportant un nombre arbitraire d'interfaces et de fluides. Ces deux derniers points sont pourtant essentiels à la vue des situations industrielles visées. La problématique de la capture des interfaces et ondes de contact pour les modèles de fluides compressibles a en conséquence été reconsidérée dans ce manuscrit. Une nouvelle méthode est développée au Chapitre 1 permettant de réduire considérablement la zone de capture des interfaces moyennant de simples mais subtiles modifications de code de calculs. Cette méthode se place dans le contexte de la méthode MUSCL (Monotonic Upstream-centered Scheme for Conservation Laws), très employée dans les codes de production, et sur maillage non-structuré, cette caractéristique étant très importante pour les applications réelles. La méthode est également indifférente au nombre de fluides présents dans l'écoulement, ce qui constitue un autre atout majeur.

Celle-ci repose sur la théorie des schémas TVD (Total Variation Diminishing) basée sur l'utilisation

de limiteurs de flux. La notion TVD a été historiquement présentée dans les travaux de Harten en 1983 [14] qui proposa ce concept afin de construire des schémas numériques ne présentant pas d'oscillation. Dans ce contexte, l'emploi des limiteurs de flux est essentiel afin de s'assurer que la propriété TVD du schéma soit maintenue et que ce dernier demeure par conséquent stable. Sweby proposa en 1984 [15] une analyse théorique et graphique de la notion TVD et définit ce que l'on dénomme la zone TVD du premier ordre. Dans la même contribution, Sweby compléta la théorie TVD en introduisant la zone d'ordre deux qui est en fait délimitée par la fonction limiteur Superbee développée précédemment par Roe (1981) [16]. Depuis, la majorité des limiteurs de flux reposent dans cette zone TVD d'ordre 2, la zone d'ordre 1 (région supérieure) étant inappropriée pour les champs continus et les ondes de choc.

Cependant, le Chapitre 1 s'intéresse en particulier à la capture numérique d'interfaces. Ces dernières sont représentées par des fonctions discontinues de type Heaviside et nécessitent en conséquence une attention particulière. Dans ce contexte bien précis, la zone TVD d'intérêt est reconsidérée dans ce manuscrit. Il s'avère alors que lorsqu'une discontinuité de type Heaviside comme par exemple une interface est considérée, la zone TVD d'ordre 2 n'est en réalité plus une limite et la zone d'ordre 1 (partie supérieure) devient la véritable restriction. Ceci est examiné au Chapitre 1 de cet ouvrage où un nouveau limiteur de flux dénommé "Overbee" est développé.

Contrairement aux limiteurs conventionnels, la fonction "Overbee" est un limiteur TVD du premier ordre et est la pierre angulaire de la méthode de raidissement d'interface développée dans ce travail de thèse. Dans ce contexte, la fonction limiteur de toutes les variables de l'écoulement est mise à zéro à l'exception de la fraction volumique, discontinue à l'interface, où le nouveau limiteur "Overbee" est utilisé. Cette approche est inhabituelle dans le contexte de la méthode MUSCL où la majorité des limiteurs de gradients appartiennent à la zone TVD d'ordre 2. Le nouveau limiteur va au dela de cette zone d'ordre 2 et est donc inapproprié pour les chocs et les solutions continues. Cependant, il permet d'obtenir d'excellents résultats pour les champs discontinus de type Heaviside comme les fractions volumiques aux interfaces.

La méthode de raidissement d'interface repose ainsi sur l'utilisation d'un nouveau limiteur de flux appartenant à la zone TVD d'ordre 1 (partie supérieure). Cette méthode est particulièrement simple et s'adapte aisément aux maillages non-structurés. De plus, cette dernière peut être utilisée dans d'autres situations impliquant la capture de discontinuités de type Heaviside, tel que le couplage fluide-solide indéformable (Carmouze et al. (2018) [115]).

Ce travail a été publié dans un journal scientifique, Chiapolino et al. (2017) [17]. Dans le futur, l'adaptation de la méthode de raidissement d'interface incluant le changement de phase sera considérée.

Chapitre 2: Solveurs rapides pour la détermination de l'équilibre thermodynamique liquide-gaz

Le transfert de masse résultant en un changement de phase a également été considéré dans cet ouvrage. En effet sous certaines conditions, les interfaces matérielles peuvent être sujettes à des phénomènes de transition de phase. Ceux-ci sont d'une importance fondamentale dans de nombreuses activités industrielles. Leur connaissance et leur prise en compte dans les codes de calcul sont primordiales afin de reproduire les effets souhaités.

Les écoulements dans les moteurs cryotechniques de lanceurs spatiaux sont caractérisés par leurs états multiphasiques, instationnaires et multidimensionnels qui viennent s'ajouter aux phénomènes de changement de phase, jouant un rôle primordial. Dans ce manuscrit, cette thématique est liée à l'étude du remplissage de chambres de combustion par un combustible cryogénique dans le cadre du nouveau lanceur spatial d'Ariane 6. Dans de telles circonstances, il est nécessaire de prédire non seulement l'état du fluide mais également les conditions thermodynamiques régnant au sein de la chambre de combustion à chaque redémarrage du moteur.

Pendant la phase d'ignition (pour laquelle le moteur n'a pas encore atteint les conditions supercritiques), l'écoulement au sein de la chambre de combustion consiste en un jet d'oxygène liquide (LOX) encerclé d'un écoulement d'hydrogène (H_2) à grande vitesse. L'objectif de cette opération est de produire une réaction de combustion (non considérée dans ce document) au sein de la phase gazeuse (H_2 et O_2). De l'oxygène sous forme gazeuse est alors nécessaire mais est initialement absent de la chambre de combustion. Le changement de phase de l'oxygène liquide en vapeur est alors la seule source d'oxygène sous forme gazeuse.

D'un point de vue physique, la transition de phase s'effectue lorsqu'un fluide atteint un état dit "métastable". Cette terminologie fait référence à un déséquilibre thermodynamique. Ceci peut arriver:

- Soit lorsque le liquide est surchauffé, ce qui peut se produire en raison des échanges de chaleur avec le gaz ou par propagation d'une onde de détente qui diminue la température de saturation du liquide. Dans ce cas le liquide s'évapore en vapeur saturée.
- Soit lorsque la vapeur est sous refroidie, c'est à dire à une température inférieure à la température de saturation à la pression courante. Dans ce cas la vapeur se condense en liquide à saturation. Ceci peut se produire par exemple au travers d'une onde de choc, car la température du liquide varie peu alors que la température de saturation augmente. La condensation peut également apparaître au niveau des parois si celles-ci sont froides.

Lorsqu'une de ces conditions est satisfaite (comparaison de la température du mélange par rapport à la température de saturation) la transition de phase s'opère.

De nombreuses simulations d'écoulements diphasiques sont sujettes à la modélisation des phénomènes de changement de phase. Dans ce contexte, une des difficultés est d'adopter le modèle de transfert de masse approprié à une situation donnée. Certaines approches considèrent des mélanges en déséquilibre des températures et des vitesses. Lorsqu'il est possible de déterminer l'aire interfaciale spécifique séparant les phases liquide et gazeuse, la détermination du taux de transfert de masse peut être réalisée en se basant sur les corrélations de Nusselt et Sherwood. Une telle méthode a été dérivée pour l'évaporation "sprays" dans Ambramzon and Sirignano (1989) [73] et pour les écoulements atmosphériques dans Jacobson (2005) [74]. La généralisation aux "flashing" et "condensing spray" a été réalisée dans Furfaro and Saurel (2016) [75].

Cependant, la détermination de l'aire interfaciale spécifique dans un mélange diphasique est seulement possible pour des écoulements à bulles ou comportant des gouttes. Quand la topologie est arbitraire, seule l'étude de cas limites est possible, en supposant par exemple l'absence de transfert de masse si l'aire interfaciale est supposée très petite, ou au contraire un transfert de masse instantané (équilibre thermodynamique local) si l'aire interfaciale est supposée très grande. Lorsqu'une telle hypothèse est faite, un solveur d'équilibre approprié est requis.

La Chapitre 2 de ce manuscrit entreprend la construction d'un tel solveur à destination de modèles hyperboliques hors équilibres comme celui de Baer and Nunziato (1986) [49]. Toutefois, la méthode proposée n'est pas restreinte à ce modèle seul mais est aussi valide pour des modèles réduits tels que le modèle à 5 équations de Kapila et al. (2001) [5] et son extension aux écoulements cavitants, Saurel et al. (2008) [18], Le Martelot et al. (2013) [76]. Les modèles HRM (Homogeneous Relaxation Model) et HEM (Homogeneous Equilibrium Model) de Downar-Zapolski et al. (1996) [77] et Barret et al. (2002) [78] sont aussi des versions réduites de ces modèles avec respectivement 4 et 3 équations. Le solveur de changement de phase développé au cours de cette thèse s'applique également à ces formulations.

Le lien théorique entre tous ces modèles a été dérivé sur la base de l'analyse asymptotique de Saurel et al. (2008) [18] et plus systématiquement dans Lund (2012) [79]. Principalement, le solveur de changement de phase peut être utilisé chaque fois que les effets de compressibilité des phases liquide et gazeuse sont considérés. Tous les modèles mentionnés ci-dessus considèrent ces effets et ceux-ci sont responsables de la nature hyperbolique des équations.

Les modèles à 5, 4 et 3 équations sont capables de représenter des mélanges de fluides évoluant respectivement en équilibre mécanique, mécanique et thermique, et en équilibre thermodynamique. Ces derniers impliquent une seule vitesse (le déséquilibre des vitesses est en effet absent) et sont en conséquence restreints principalement pour des applications spécifiques tels que,

Les écoulements cavitants car il apparaît impossible en pratique de déterminer l'aire interfaciale et par conséquent le glissement entre phases. Des simulations de tels écoulements sont données dans Singhal et al. (2002) [80], Petitpas et al. (2009) [81], Le Martelot et al. (2013) [76] et

Saurel et al. (2016) [8].

- Les écoulements de type "flashing and condensing" qui sont des écoulements à grandes vitesses et sujets à une relaxation thermodynamique instantanée.
- Les écoulements présentant des interfaces où les mêmes équations traitent la simulation numérique directe d'écoulements bouillants à des échelles inférieures à celle d'une bulle (Le Martelot et al. (2014) [82], Saurel et al. (2016) [8]).

Le solveur d'équilibre thermodynamique développé au Chapitre 2 est un point essentiel pour les modèles hyperboliques et diphasiques à 7, 5, 4 et 3 équations. En effet ce dernier permet de déterminer l'équilibre thermodynamique local et ainsi le taux d'évaporation maximalement admissible. Dans le contexte des écoulements où seules les phases liquide et vapeur coexistent, la construction d'un tel solveur d'équilibre a été entreprise dans Orbey et al. (1998) [83], Allaire et al. (2007) [84], Faccanoni et al. (2012) [85] et Le Métayer et al. (2013) [72] sur la base d'un système algébrique fortement non-linéaire construit à partir des conditions de saturation, de la masse de mélange et de l'énergie de mélange. Ce système présente des difficultés résultant du caractère non-linéaire des équations notamment pour les limites des phases de liquide pur et de vapeur pure où le problème devient mal posé.

La résolution du système est alors délicate, exigeante en temps de calcul et peut résulter en une solution numérique instable, en particulier lorsque l'état final sort du domaine diphasique pour rejoindre une des phases pures, la difficulté étant la relation non-linéaire liant la température et la pression à saturation. De plus, l'ajout de gaz incondensables dans le système amène des difficultés supplémentaires, cette situation étant cependant incontournable pour la considération d'applications réelles. Dans ce cas, la pression et la température ne sont pas directement sur la courbe de saturation mais sont liées par la pression partielle de l'espèce vapeur présente dans le mélange multi-constituants.

Le moyen le plus direct pour résoudre le système non-linéaire traduisant le changement de phase consiste à utiliser une méthode itérative exigeante en temps de calcul. Cependant cette stratégie s'est avérée néfaste au schéma numérique qui peut devenir instable. Ceci motive l'introduction d'une nouvelle méthode de relaxation où la solution est relaxée graduellement vers la solution exacte au moyen d'estimations successives simples. Cette approche permet d'obtenir une méthode numérique stable, rapide et particulièrement simple à implémenter dans un code de calcul. La raison de son efficacité est liée à sa simplicité. En conséquence, de nombreuses situations industrielles impliquant de sévères conditions thermodynamiques, des géométries complexes et où les phénomènes de changement de phase jouent un rôle majeur peuvent être traitées par la méthode de relaxation introduite au Chapitre 2 de ce manuscrit. Ceci a résulté en deux publications dans des journaux scientifiques, Chiapolino et al. (2017) [1], [19]. Dans un travail futur, les situations impliquant le mélange de plusieurs liquides devront être considérées.

Chapitre 3: Construction d'équations d'état

Au cours d'un phénomène de changement de phase, l'équation d'état doit décrire à la fois le comportement des phases liquide et vapeur mais aussi celui du mélange diphasique comportant la plupart du temps des constituants inertes. Les équations d'état décrivant le comportement thermodynamique des différentes phases ont par ailleurs leurs propres champs de validité. Par rapport aux applications industrielles envisagées, une extension de la thermodynamique des phases est nécessaire.

Plusieurs équations d'état sont disponibles dans la littérature [20], [21]. Chaque forme est plus ou moins complexe et dépend du milieu à représenter et des transformations pouvant se produire. La description complète du diagramme de phase comporte les phases liquide, vapeur et fluide supercritique. Ces trois milieux présentent des comportements thermodynamiques totalement différents. Plusieurs exemples illustrent ce propos. La vitesse du son dans un liquide est généralement plus grande que dans un gaz. La densité standard est également caractéristique d'un fluide, comme par ailleurs sa compressibilité ou encore sa capacité calorifique (à volume ou à pression constante).

L'approche thermodynamique la plus commune repose sur l'utilisation d'équations d'état cubiques. On peut citer par exemple les lois d'état de Lee and Kesler (1975) [118] ou Reid et al. (1987) [119]. Parmi ces équations cubiques, la loi d'état de van der Waals [97], proposée en 1873 fut la première à décrire la coexistence des phases liquide et vapeur.

Plus tard, Redlich and Kwong (1949) [120] tentèrent d'améliorer sa précision en introduisant une dépendance à la température pour les effets attractifs. Soave (1972) [98] et Peng and Robinson (1976) [121] proposèrent ensuite des modifications supplémentaires afin de prédire encore plus précisément le comportement liquide et vapeur d'un fluide. Un revue détaillée sur les équations d'état cubiques peut être trouvée dans Wei and Sadus (2000) [99] par exemple.

Cette description thermodynamique est particulièrement intéressante car elle assemble tous les états de la matière en une formulation unique, en prédisant les transitions d'un état à l'autre. En particulier, les effets attractifs responsables de la cohésion des liquides disparaissent lorsque la densité diminue et devient celle d'un gaz.

La modélisation de systèmes liquide-gaz avec ou sans changement de phase est un sujet de recherche ancien au sein de la communauté de la physique mais est toujours problématique autant du point de vue théorique que numérique. L'approche thermodynamique la plus commune repose sur l'utilisation d'équations d'état cubiques dont le prototype de base est la loi d'état de van der Waals. En effet cette loi d'état rassemble tous les effets moléculaires présents dans la matière, à savoir l'agitation thermique, les effets à courte distance des forces répulsives et les effets attractifs à longue distance. L'équation d'état de van der Waals est donc capable de décrire, du moins qualitativement, un liquide pur, la vapeur pure et un mélange liquide-vapeur.

Cette loi d'état, comme toutes les autres équations cubiques, est utilisée pour clore les modèles d'écoulements basés sur les équations de conservation de la masse de mélange, du mouvement du mélange et de l'énergie de mélange. Les équations d'Euler font partie des options pertinentes comme d'autres plus sophistiquées visant à décrire les effets capillaires, à titre d'exemple: le modèle de Cahn and Hiliard (1958) [34]. Dans ce contexte, l'état thermodynamique est déterminé à partir de deux variables internes seulement, la densité et l'énergie interne du mélange ou alternativement la densité et la température en fonction de la formulation choisie des équations. Cette approche semble en conséquence simple mais implique de sérieuses difficultés et limitations:

- La première et certainement la plus évidente et restrictive est liée à l'incapacité des équations d'état cubiques à décrire un liquide et un gaz incondensable comme par exemple les écoulements présentant des interfaces eau-air. La thermodynamique de ces deux milieux étant considérée comme discontinue, des traitements spécifiques (théoriques et numériques) ont été proposés. Dans ce contexte, les méthodes Arbitrary Lagrangian Eulerian (Hirt et al. (1974) [29], Interface Reconstruction (Youngs (1984) [89]), Front Tracking (Glimm et al. (1998) [31]), Level-Set (Fedkiw et al. (1999) [33]) font partie des options possibles. Une autre approche porte sur l'utilisation de modèles continus avec des variables internes supplémentaires comme les fractions volumiques et massiques et des lois d'état étendues. Le système de Kapila et al. (2001) [5] fait partie de ces modèles tout comme son extension au changement de phase (Saurel et al. (2008) [18]). Avec ces formulations, les mêmes équations sont résolues partout de façon routinière, dans le liquide pur, le gaz pur et à l'interface qui devient une zone diffuse. Ces modèles sont envisagés dans les chapitres qui précèdent. Avec cette approche, les modèles hyperboliques avec relaxation sont considérés et chaque phase évolue dans son propre volume et avec sa propre thermodynamique. En particulier, il n'est pas nécessaire d'utiliser des formulations cubiques. Quand le changement de phase apparaît, ceci se fait par le biais de termes de transfert de masse qui peuvent être caractérisés à taux fini (Saurel et al. (2008) [18], Furfaro and Saurel (2016) [75]), ou supposés instantanés lorsque la connaissance de la cinétique de changement d'état est inconnue, pas assez documentée ou simplement non-nécessaire (Le Métayer et al. (2013) [72], Chiapolino et al. (2017) [1], [19]).
- La seconde limitation des équations d'état cubiques apparaît lorsque l'on s'intéresse à la propagation des ondes dans le dôme de saturation. En effet, ce type de lois d'état présente un vitesse du son imaginaire, traduisant la perte de convexité, à l'intérieur de la zone diphasique et présente donc un comportement inadmissible pour la propagation des ondes lorsque la transition de phase se produit.

- Une autre inconsistance apparaît lorsque l'on s'intéresse à la description du changement d'état.
 Dans la représentation de van der Waals ainsi que toutes autres lois d'état cubiques, la transition de phase apparaît comme un chemin thermodynamique. La notion de retard temporel ou de cinétique d'évaporation est donc absente.
- La quatrième limitation mais peut être pas la dernière est liée au traitement numérique des conditions aux limites. Par exemple, le couplage entre l'enthalpie d'arrêt, l'invariance de l'entropie et les invariants de Riemann permet la modélisation d'entrées ou de sorties subsoniques. Cependant ces derniers sont définis correctement seulement si l'équation d'état est bien posée. La seconde difficulté liée au manque de convexité des équations cubiques réapparaît donc à ce niveau. De plus, les expressions des invariants de Riemann peuvent être inextricables avec ce type de lois d'état.

Cette liste d'arguments motive le travail entrepris au Chapitre 3 de ce manuscrit où une version étendue de l'équation d'état Noble-Abel-Stiffened-Gas (NASG, Le Métayer and Saurel (2016) [22]) est développée afin d':

- Améliorer la représentation de la thermodynamique des phases liquide, vapeur et supercritique.
 La combinaison de la loi d'état du liquide et celle de la vapeur doit représenter aussi précisément que possible la zone diphasique.
- L'équation d'état de chaque phase doit être convexe dans son domaine respectif.
- L'équation d'état doit être aussi simple que possible tout en restant précise afin de simplifier son implémentation.

Il existe une équation convexe, et donc bien posée, liant richesse du point de vue physique et simplicité: la récente loi d'état Noble-Abel-Stiffened-Gas (NASG, Le Métayer ans Saurel (2016) [22]). L'équation d'état NASG est une combinaison de la loi d'état Noble-Abel (NA), aussi appelée équation du covolume, et de la loi d'état Stiffened-Gas (SG), décrite dans Harlow and Amsden (1971) [122]. Cette dernière correspond à une linéarisation d'une loi d'état de type "Mie-Grüneisen" autour d'un point de référence. La combinaison de ces deux lois d'état (NA et SG) permet d'améliorer considérablement les prédictions de la densité d'un liquide en prenant en compte les effets répulsifs au travers du covolume (NA) en complément de ceux déjà présents dans la représentation Stiffened-Gas (attraction et agitation). Les principales forces moléculaires sont alors représentées par la description NASG.

Ses prédictions sont en bon accord avec les données expérimentales mais seulement dans une gamme de température restreinte, [300 - 500] K pour l'eau liquide à saturation par exemple. Cette limitation

est liée aux effets attractifs et répulsifs qui sont considérés constants dans cette représentation. En effet, cette hypothèse n'est plus valable lorsque de larges variations de pression et de température sont considérées. Le Chapitre 3 de cette thèse tente alors d'étendre la loi d'état NASG en considérant des effets attractifs et répulsifs variables afin d'améliorer son champ de validité.

En effet, dans la direction des écoulements supercritiques, de fortes variations en température et en pression sont présentes. La loi d'état NASG est alors intéressante et est une alternative aux équations cubiques. Cependant cette équation d'état, dans sa forme originale, permet seulement de décrire de façon satisfaisante les écoulements diphasiques évoluant dans des conditions sous-critiques et dans une gamme de température réduite.

Une extension est alors nécessaire et est entreprise dans ce manuscrit. Ainsi l'équation d'état ENASG est développée au Chapitre 3 ("E" traduit "Extended"). Il s'agit d'une équation d'état convexe capable de décrire de façon satisfaisante un liquide dans de nombreuses et variées conditions thermodynamiques. Son intérêt repose sur la description des effets attractifs et répulsifs, présents dans les milieux condensés, qui évoluent respectivement avec la température et la densité contrairement à la loi d'état NASG où ces effets demeurent constants. De plus, la transition de la phase liquide en fluide supercritique semble possible et continue avec cette nouvelle formulation.

Les thermodynamiques des phases liquide et vapeur doivent être combinées correctement afin de reproduire le diagramme de phase ainsi que ses propriétés pertinentes comme la chaleur latente de changement de phase par exemple. La détermination des différents paramètres de l'équation d'état est également discutée au Chapitre 3. Ce travail a été publié dans un journal scientifique, Chiapolino and Saurel (2018) [23].

Afin de préserver la convexité de la formulation lors de la description du gaz, la nouvelle loi d'état ENASG est réduite en équation d'état des gaz parfaits. En conséquence, elle présente une description imprécise de la vapeur à l'approche du point critique. Ceci constitue cependant une perspective de recherche pour le futur. La prise en compte des capacités calorifiques variables avec la température est alors aisément considérée, rendant l'équation d'état du gaz capable de décrire le fluide supercritique à des températures élevées.

Chapitre 4: Dispersion de fluides non-miscibles sur de grandes échelles de temps et d'espace

Dans un autre contexte, la problématique de la dispersion de fluides non-miscibles sur de grandes échelles de temps et d'espace a également été abordée dans ce manuscrit. En effet, ceci correspond à une thématique intéressant les communautés industrielles notamment celles des Risques et de la Sûreté. De nombreuses situations impliquant la dispersion de fluides sur de grandes échelles de temps peuvent se produire dans de grands espaces urbains ou naturels. La dispersion de gaz denses est une situation d'un intérêt particulier. Dans de telles circonstances, les gaz denses et potentiellement toxiques peuvent être dispersés sur des kilomètres et entraîner de sévères conséquences. Du point de vue de la modélisation et de la simulation numérique, la difficulté dans ce contexte est d'obtenir des résultats relativement précis pour un temps de calcul raisonnable. Les modèles de type "shallow water" bi-couche sont alors très attractifs. En effet ceux-ci permettent d'obtenir des résultats 2D mais imitant les effets 3D obtenus par un modèle multi-fluide conventionnel. Le gain attendu en temps de calcul dans ce cas est alors considérable.

Les modèles de type "shallow water" bi-couche (ou multi-couche) sont particulièrement intéressants pour certains cas limites d'écoulements multi-fluides à densités variables séparés par des interfaces presque horizontales. Ce type de formulation concerne la dynamique de fluides incompressibles s'écoulant sous l'effet de la gravité. Ces modèles peuvent en outre décrire par exemple:

- Les écoulements d'un même liquide mais à différentes températures résultant en des différences de densités. Une telle situation est typique des écoulements océaniques.
- Les écoulements de deux liquides de différentes densités.
- Les écoulements de deux gaz évoluant à faible nombre de Mach.

L'approche bi-couche est particulièrement intéressante lorsqu'on la compare avec les approches multidimensionnelles qui considèrent le mouvement vertical. En effet des simulations beaucoup plus rapides sont attendues avec la stratégie bi-couche. Cette dernière est également très utile lorsque la hauteur d'une des couches est arbitrairement faible. En effet, il n'est dans ce cas pas nécessaire de "résoudre" spatialement cette couche. La diffusion numérique des interfaces presque horizontales est alors absente et aucune méthode de "tracking" de l'interface est requise. Cependant, il y a bien évidemment des limitations avec cette approche:

- La vitesse verticale est négligée.
- La vitesse est supposée uniforme dans chaque section de chaque couche.

Ce type de modélisation implique également de sérieuses difficultés. En effet, la plupart des modèles ne sont pas hyperboliques. Ce problème amenant de néfastes conséquences pour la description de la propagation des ondes, qui devient mal posée, et pour la construction de schémas numériques associés. Une seconde difficulté apparaît quant à la présence de termes non-conservatifs dans les équations de la conservation du mouvement. Le Chapitre 4 de ce manuscrit entreprend ces problématiques et propose des solutions.

Dans le cadre d'équations moyennées ou homogénéisées en mécanique des fluides, le problème lié à l'hyperbolicité des formulations théoriques apparaît dans différents types de modèles. Les modèles diphasiques en déséquilibre en sont un exemple. Seules quelques formulations semblent bien posées dans ce contexte, le modèle de Marble (1963) [100], Baer and Nunziato (1986) [49], Saurel et al. (2017) [92]. Il existe principalement deux solutions pour s'affranchir de ce problème.

- Considérer les phases comme compressibles et utiliser des procédures de relaxation [86]. Cette approche implique la propagation du son dans les phases et est particulièrement efficace dans de nombreuses situations. Cette stratégie a été adoptée dans les deux dernières références mentionnées ci-dessus.
- Considérer les effets turbulents dans les phases. Ceux-ci résultent en l'apparence d'une vitesse du son "turbulente" (Forestier et al. (1997) [101], Saurel et al. (2003) [102], Lhuillier et al. (2013) [103]. Dans le contexte des modèles "shallow water", ces effets ont été étudiés dans Richard and Gavrilyuk (2012) [104] et Gavrilyuk et al. (2016) [105].

Dans ce manuscrit, la première méthode est adoptée et les fluides sont considérés faiblement compressibles. Ceci résulte en un modèle strictement hyperbolique présenté au Chapitre 4. Dans la limite instantanée de relaxation des pressions, le modèle "shallow water" bi-couche conventionnel mais non-hyperbolique est retrouvé. Cette stratégie est semblable à l'approche développée par Abgrall and Karni (2009) [106] à la différence que des termes supplémentaires en pression sont présents dans la nouvelle formulation. Cette dernière donne également une nouvelle interprétation de l'approche de relaxation qui est maintenant basée sur les effets de compressibilité.

La seconde problématique résidant en la présence de termes non-conservatifs dans les équations de conservation du mouvement est également abordée au Chapitre 4. En analysant la structure du problème de Riemann, il s'avère que des constantes locales apparaissent aux endroits où la dérivée de la fonction Heaviside émerge. En conséquence, les produits non-conservatifs deviennent localement bien définis et une forme conservative locale est obtenue. Cette propriété est exploitée dans un solveur de Riemann de type HLL.

La précision du nouveau solveur de type HLL est vérifiée en comparant ses résultats avec ceux obtenus par Abgrall and Karni (2009) [106] et avec ceux obtenus avec un solveur basé sur la méthode VFRoe de Gallouet and Masella (1996) [107]. Cette dernière est en effet capable de considérer des systèmes conservatifs et non-conservatifs. Comme présenté au Chapitre 4, le nouveau modèle "shalow water" bi-couche et le nouveau solveur de type HLL montrent des résultats de grande précision et sont exempt d'oscillation.

La formulation théorique développée dans ce travail de thèse ainsi que sa résolution numérique constituent alors une stratégie intéressante pour la simulation de la dispersion de gaz denses sur de grandes échelles de temps et d'espace. De plus l'extension à un nombre arbitraire de couches semble possible avec la nouvelle formulation et sera réalisée dans le futur. Ce travail a également résulté en une publication scientifique, Chiapolino and Saurel (2018) [26]. Le modèle est pour le moment restreint au cas 1D mais son extension au cas 2D sera nécessaire. La considération des effets de la topographie, la friction avec le sol et la création d'aire interfaciale au travers de la modélisation de la turbulence font également partie des perspectives futures.

Le contenu global de ce manuscrit apparaît alors intéressant pour la communauté "CFD" travaillant avec les écoulements diphasiques. Les différents projets entrepris au cours de ce travail de recherche utilisent déjà les outils numériques développés dans cette thèse et ce de façon routinière. Au prix de quelques répétitions, chaque chapitre est pratiquement indépendant et possède de nombreuses références. Le lecteur peut alors choisir de commencer à lire cet ouvrage depuis le milieu ou sauter directement au dernier chapitre.

Titre

Quelques contributions à la modélisation et simulation numérique des écoulements diphasiques compressibles

Résumé

Ce manuscrit porte sur la modélisation et la simulation numérique d'écoulements diphasiques compressibles. Dans ce contexte, les méthodes d'interfaces diffuses sont aujourd'hui bien acceptées. Cependant, un progrès est encore attendu en ce qui concerne la précision de la capture numérique de ces interfaces. Une nouvelle méthode est développée et permet de réduire significativement cette zone de capture. Cette méthode se place dans le contexte des méthodes numériques de type "MUSCL", très employées dans les codes de production, et sur maillages non-structurés. Ces interfaces pouvant être le lieu où une transition de phase s'opère, celle-ci est considérée au travers d'un processus de relaxation des énergies libres de Gibbs. Un nouveau solveur de relaxation à thermodynamique rapide est développé et s'avère précis, rapide et robuste y compris lors du passage vers les limites monophasiques. En outre, par rapport aux applications industrielles envisagées, une extension de la thermodynamique des phases et du mélange est nécessaire. Une nouvelle équation d'état est développée en conséquence. La formulation est convexe et est basée sur l'équation d'état "Noble-Abel-Stiffened-Gas". Enfin, sur un autre plan la dispersion de fluides non-miscibles sous l'effet de la gravité est également abordée. Cette problématique fait apparaître de larges échelles de temps et d'espace et motive le développement d'un nouveau modèle multi-fluide de type "shallow water bi-couche". Sa résolution numérique est également traitée.

Mots clés

Écoulements diphasiques, changement de phase, équations d'état, interfaces, systèmes hyperboliques, relaxation, méthodes numériques, solveurs de Riemann, termes non-conservatifs, shallow water bicouche.

Title

Some contributions to the theoretical modeling and numerical simulation of compressible two-phase flows

Abstract

This manuscript addresses the theoretical modeling and numerical simulation of compressible twophase flows. In this context, diffuse interface methods are now well-accepted but progress is still needed at the level of numerical accuracy regarding their capture. A new method is developed in this research work, that allows significant sharpening. This method can be placed in the framework of MUSCL-type schemes, widely used in production codes and on unstructured grids. Phase transition is addressed as well through a relaxation process relying on Gibbs free energies. A new instantaneous relaxation solver is developed and happens to be accurate, fast and robust. Moreover, in view of the intended industrial applications, an extension of the thermodynamics of the phases and of the mixture is necessary. A new equation of state is consequently developed. The formulation is convex and based on the "Noble-Abel-Stiffened-Gas" equation of state. In another context, the dispersion of non-miscible fluids under gravity effects is considered as well. This problematic involves large time and space scales and has motivated the development of a new multi-fluid model for "two-layer shallow water" flows. Its numerical resolution is treated as well.

Keywords

Two-phase flows, phase transition, equations of state, interfaces, hyperbolic systems, relaxation, numerical methods, Riemann solvers, non-conservative terms, two-layer shallow water flows.