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# Numerical assessment of Diffuse-Interface method for air-assisted liquid sheet

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## Abstract

This study presents the implementation and validation of a second-order accurate solver for the 4-equation multi-fluid method in a cell-vertex context, to handle aeronautical air-assisted liquid sheet configurations. Validations include one and two-dimensional shock tube problems, Laplace tests, droplets oscillations, and a two-dimensional configuration reminiscent of an aeronautical airblast injector. Promising results are obtained in the last case, especially when the pressure is increased and the characteristic flow times decreased, a trend observed in recent aeronautical developments, but not necessary in classical academical benchmarks. Being fully compatible of the reactive flow formulation of the cell-vertex solver AVBP, this study paves the way to future monolithic simulations of airblast injectors for aeronautical combustion chambers, including both the multi-phase and the reactive regions.

**Keywords:** Two-phase flow, airblast, diffuse interface, hyperbolic systems

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## 1. Introduction

Liquid injection and atomization are complex processes which are at the heart of many industrial systems. In the context of combustion, these phenomena play a key role as they drive the fuel vapour distribution in a combustion chamber [1, 2], and therefore have a major impact on the flame regime and burner efficiency, as well as pollutant emissions [3]. In addition, fuels are blends of numerous molecules, their exact composition being usually unknown. For example Shastry et al. [4] highlighted the preferential evaporation effect on the structure and propagation speed of spray flames. For these complicated problems numerical simulation represents a convincing approach to supplement experiments. However, atomization is numerically challenging due to the large range of physical scales involved in this multi-physics problem, from the surrounding gas flow to the molecular scale at the interface between liquid and gas phases, considered as a discontinuity for viscosity and density, and consequently requiring specific numerical treatment.

For this reason, a strategy often used in complex industrial systems is to directly inject a train with prescribed droplet velocities and diameter size distribution [5, 6]. Such spray injection models have allowed successful spray flame simulations in both academic and realistic combustion chambers [7–10]. However, they require input parameters which are not always known and they suffer from a lack of physics of atomization, which prevent the spray formation to adapt to the flow.

Several approaches have been proposed in the literature to numerically predict the primary atomization of liquid jets or sheets by modelling the interface between liquid and gaseous phases, which can be split into two main categories: sharp and diffuse interface methods. Sharp interface methods consider the interface between the phases as a discontinuity in a way that flow variables experience a jump in their values. The material interface is tracked by the Front-Tracking methods [11–13] or captured using methods such as the Volume-Of-Fluid (VOF) method [14], or the Level-Set method [15]. These approaches are able to finely predict

the evolution of the interface topology and its primary breakup [16–19]. However they require significant mesh resolution in the interface vicinity [20] which makes them unsuitable for prediction in complex industrial systems. In addition they are usually restricted to incompressible flows, i.e., not directly applicable to

35 combustion. Diffuse interface methods (DIM) do alleviate these issues, with considering the interface as a transition region between the phases instead of a discontinuity, thus relaxing the mesh resolution constraints. To do so, they rely on unified equations of state describing both phases. Two sub-groups of DIM arise from the literature: the Phase-Field (PF) and the Multi-Fluid (MF) methods.

40 PF methods are based on the early works of Van der Waals [21], Korteweg [22] and Cahn and Hilliard [23] to describe the Gibbs potential in the diffuse interface region. The concept is to track the phases with a dedicated field function and to solve each phase independently. Numerous Lattice-Boltzmann numerical formulations rely on this approach, allowing interesting applications

45 for atomization in a incompressible context [24–27]. For compressible finite-volume or finite-element approaches, the second gradient theory [28] recently allowed to handle high density ratio in academic configurations [29]. MF methods rather consider the interface region as a mixture of phases, obeying a single set of equations. Several equilibrium hypotheses have been proposed to reduce

50 the number of equations, from the general 7-equation formulation of Baer and Nunziato [30], to a reduced 5-equation formulation assuming pressure equilibrium [31–34], and down to a so-called homogeneous 4-equation formulation, assuming the mechanical and thermal equilibrium between phases [35]. Because they involve a only set of conservative equations to describe both phases, without

55 tracking the interface, DIM relax the resolution constraint of sharp methods. Convex thermodynamic models [36] are used to close the equation set, such as the Stiffened-Gas [37] or cubic equations of state, as recently proposed in several works [38]. Multi-Fluid methods allow the simulation of compressible, high density ratio industrial configurations at a reasonable computational cost.

60 They were used in liquid rocket engine applications [39] using cubic [38, 40–42] or Stiffened-Gas equations of state [35, 43–45], or in Diesel injection setups with

interesting results [46–48]. Contrary to PF approach, existing MF works have mainly neglected surface tension forces, which play a key role in atomization [49]. Primary and secondary atomization and directly the droplets distribution  
65 in the combustion chamber are a consequence of the surface tension forces.

The present work intends to assess the accuracy and robustness of the homogeneous model (four-equation model [35]) to predict liquid-gas flow dynamics. A Noble-Abel Stiffened-Gas (NASG) equation of state is used to close the system and the Continuum Surface Force formalism [50] extended to a compressible  
70 formulation [51] is considered to account for surface tension forces. As recommended in [52], the vertex-centered HLLC-MUSCL Riemann solver [53] is used for a robust and accurate prediction of the high density ratio faced in the targeted applications. Finally, characteristic boundary conditions which are required for compressible flows, are adapted to NASG thermodynamics. The model is first  
75 validated on a series of academic test cases, and finally applied to liquid film dynamics in an airblast atomizer.

The paper is structured as follows. The transport equations and closure models are presented in Sec. 2, then the numerical scheme is described in Sec. 3. Validations for the characteristic boundary conditions, and the surface  
80 tension implementation are proposed in Sec. 4. Finally, the results for the target application are presented in Sec. 5. Average and instantaneous results are compared to existing correlations, and the effect of pressure injection is investigated.

## 2. Model description

### 85 2.1. The 4-equation model

Initially proposed to simulate evaporating, cavitating and boiling flows [35, 54–56], the homogeneous 4-equation model assumes a mechanical and thermal equilibrium between the phases. Mechanical and thermal equilibria are always true in pure phase media. In a multi-phase mixture, they mean that no slip  
90 velocity exists between phases, both phases have the same temperature. This

implies that the region where both phases coexist is small. Species composing the mixture occupy their own volume and share the same pressure whether they are in liquid or gas phase which is similar to Dalton's law [43]. With this hypotheses, the 4-equation model considers a mono-component liquid ( $k = 1$ ) and a multi-component gas mixture ( $k = [2, \dots, N]$ ), distinguishing the liquid species and its vapour as two different species. The equilibrium leads to the following variable definitions

$$\begin{cases} T &= T_k, \quad \forall k, \\ P &= P_k, \quad \forall k, \\ v &= 1/\rho = \sum_{k=1}^N Y_k v_k, \\ e &= \sum_{k=1}^N Y_k e_k. \end{cases} \quad (1)$$

The resulting 4 equations write

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (2a)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + P \mathbf{I}) = 0, \quad (2b)$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot ((\rho E + P) \mathbf{u}) = 0, \quad (2c)$$

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho Y_k \mathbf{u}) = 0, \quad (2d)$$

where  $Y_k$  represents the mass fraction of species  $k$ ,  $\rho$ ,  $\mathbf{u}$ ,  $P$  and  $E$  respectively denote the mixture density, the velocity, the pressure and the total mixture energy ( $E = e + \mathbf{u}^2/2$ ). The internal energy writes  $e$ . As the 4-equation model governed by Sys. (2) does not contain any non-conservative term, it is fully conservative.

## 2.2. Thermodynamic closure

A consistent Equation of State (EoS) must be used to correctly relate density, temperature and pressure of liquid and gas phases. This EoS should be able to reproduce the thermodynamic behaviour of species on a large range of temperatures and pressures.

As suggested by Le Métayer et al. [37], in the context of the 4-equation model using a convex EoS for each phase allows to preserve the hyperbolicity of

110 the Sys. (2) which simplifies its resolution. The liquid and its vapour are thus  
transported through two distinct equations [35] and mass-transfer between phases  
occurs assuming an instantaneous local thermodynamic equilibrium. When the  
conditions are far from the saturation, no phase change occurs and the local  
thermodynamic equilibrium can be neglected. This is the case in this work, i.e.,  
115 no evaporation/condensation are considered.

### 2.2.1. The Noble-Abel Stiffened-Gas equation of state

Cubic equations of state [57, 58] are good candidates to describe both phases  
but they loose convexity in the spinodal region of the Clapeyron diagram. The  
Noble-Abel Stiffened-Gas (NASG) equation of state [59] extends the popular  
120 Stiffened-Gas formulation which considers covolumes and expresses as for a given  
constituent  $k = [1, \dots, N]$  as

$$P_k = \frac{\rho_k(\gamma_k - 1)C_{v,k}T_k}{1 - \rho_k b_k} - P_{\infty,k}, \quad (3)$$

where  $\gamma_k$ ,  $C_{v,k}$ ,  $b_k$  and  $P_{\infty,k}$  are respectively the Laplace coefficient, the isovolume  
specific heat capacity, the covolume and the constant representing attractive  
effects in liquid phase: the gaseous phase relaxes to the ideal gas EoS with  
125  $P_{\infty,k} = 0$  and  $b_k = 0$ .

Internal energy, enthalpy, entropy and the speed of sound read

$$e_k = \frac{P_k + \gamma_k P_{\infty,k}}{P_k + P_{\infty,k}} C_{v,k} T_k + e_k^0, \quad (4)$$

$$h_k = \gamma_k C_{v,k} T_k + b_k P_k + q_k, \quad (5)$$

$$s_k = C_{v,k} \ln \left( \frac{T_k^{\gamma_k}}{(P_k + P_{\infty,k})^{\gamma_k - 1}} \right) + s_k^0, \quad (6)$$

$$c_k^2 = \frac{\gamma_k (P_k + P_{\infty,k})}{\rho_k (1 - \rho_k b_k)}, \quad (7)$$

where the two added constants  $e_k^0$  and  $s_k^0$  respectively represent the reference  
energy and entropy of species  $k$ . The NASG EoS parameters are determined  
according the methodology proposed in Boivin et al. [60]. In order to avoid small  
time-steps induced by the CFL constraint in the liquid phase, these parameters

130 are derived assuming a modified sound speed in the liquid phase, equal to the one of the gaseous phase [61].

### 2.2.2. Extension of NASG equation of state to multi-component gas mixtures

Extension of Sys. (1) to multi components gas has been proposed in Chiapolino et al. [43], and is reminded here for clarity. Writing Eq. (3) for each  
135 species with  $\rho_k = 1/v_k$ , the mixture temperature is easily retrieved

$$T(v, P, Y_k) = \frac{v - \sum_{k=1}^N Y_k b_k}{\sum_{k=1}^N Y_k \frac{(\gamma_k - 1) C_{v,k}}{P + P_{\infty,k}}}. \quad (8)$$

The mixture pressure is then obtained by rewriting Eq. (8), yielding a quadratic form

$$P = \frac{b + \sqrt{b^2 + 4ac}}{2a}, \quad (9)$$

with

$$\begin{cases} a &= v - Y_1 b_1, \\ b &= \sum_{k=1}^N Y_k (\gamma_k - 1) C_{v,k} T - P_{\infty,1} (v - Y_1 b_1), \\ c &= \sum_{k>1}^N Y_k (\gamma_k - 1) C_{v,k} P_{\infty,1} T. \end{cases} \quad (10)$$

Note that a proof of the pressure positivity was presented by Chiapolino et al.  
140 [43], and that the formula is only valid if a single liquid component is present (here,  $k = 1$ ).

Finally density and internal energy are computed through Eqs. (3) and (4) according to Sys. (1)

$$\frac{1}{\rho} = \sum_{k=1}^N Y_k \left( \frac{(\gamma_k - 1) C_{v,k} T}{P + P_{\infty,k}} + b_k \right), \quad (11)$$

$$e = \sum_{k=1}^N Y_k \left( \frac{P + \gamma_k P_{\infty,k}}{P + \gamma_k P_{\infty,k}} C_{v,k} T + e_k^0 \right). \quad (12)$$

### 2.3. Jacobian flux matrix & boundary conditions

Characteristic boundary conditions [62] are required in a compressible context to be consistent with the system of waves travelling inside the computational domain. The Locally One-Dimensional Inviscid flow (LODI) hypothesis introduced by Thompson [63] is considered. Following Okong'o and Bellan [64],



characteristic formulations must be adapted when using non-perfect equation of state. Pelletier et al. [38] have derived the characteristic formulation for a 4-equation model, closed with a cubic equation of state. A similar exercise is conducted here, for the NASG equation of state. The computation of coefficients  $\Lambda$  and  $\Gamma$  involved in the Jacobian fluxes matrix as well as the speed of sound are detailed in Appendix A,

$$\Lambda = \left. \frac{\partial P}{\partial \rho e} \right|_{\rho Y_k} = \frac{1}{\frac{\rho \bar{C}_p \beta}{\alpha} - \alpha T}, \quad (13)$$

$$\Gamma = \left. \frac{\partial \rho e}{\partial \rho Y_k} \right|_{P, Y_{i \neq k}} = h_k - \frac{\rho \bar{C}_p}{\alpha \rho_k}, \quad (14)$$

with  $\alpha$  and  $\beta$  respectively the isobaric dilatation and isotherm compressibility coefficients. The mean isobaric heat capacity is defined as  $\bar{C}_p = \sum_k Y_k C_{p_k}$ .

#### 145 2.4. Additional terms: surface tension & viscous term

Surface tension is accounted for following the methodology proposed by Brackbill et al. [50], taking the liquid volume fraction  $\alpha_l$  as the continuous color function. The resulting force  $\mathbf{F}_\sigma$  yields

$$\mathbf{F}_\sigma = \sigma \kappa \nabla \alpha_l, \quad (15)$$

with  $\sigma$  the surface tension coefficient and  $\kappa$  the local curvature defined as

$$\kappa = -\nabla \cdot \left( \frac{\nabla \alpha_l}{|\nabla \alpha_l|} \right). \quad (16)$$

The viscous stress tensor and the energy flux read

$$\bar{\bar{\tau}} = -\frac{2}{3} \nabla \cdot (\mathbf{u}) \mathbf{I} + 2 \bar{\bar{S}}, \quad (17)$$

$$\mathbf{q} = -\lambda \nabla T, \quad (18)$$

with  $\bar{\bar{S}} = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^t)$ . The mixture dynamic viscosity  $\mu$  and the thermal diffusion coefficient  $\lambda$  are defined as in Deng and Boivin [45]. Using this formulation, coefficients continuity is conserved across the interface,

$$\mu = \alpha_l \mu_l + \alpha_v \mu_v, \quad (19)$$

$$\lambda = \alpha_l \lambda_l + \alpha_v \lambda_v, \quad (20)$$

150 where  $\mu_l$  and  $\lambda_l$  are the dynamic viscosity coefficient and the thermal diffusion  
coefficient of the liquid phase and  $\mu_g$  and  $\lambda_g$  are the ones of vapour phase. The  
volume fractions are defined as  $\alpha_k = \rho Y_k / \rho_k$ . In this study since only one  
liquid species and a multicomponent gas mixture are considered,  $\alpha_l = \alpha_1$  and  
 $\alpha_g = \sum_{k=2}^N \alpha_k$ . In Eqs. (19) and (20),  $\mu_l$  and  $\lambda_l$  are assumed constant and  
155 independent on temperature. The gaseous viscosity  $\mu_g$  depends on temperature  
and its behaviour is modelled with Sutherland's law [65]. The thermal diffusion  
coefficient of gaseous phase is computed through the Prandtl number  $Pr$ ,  $\mu_g$   
and the mean gaseous mass specific calorific capacity  $\bar{C}_{p,g}$ ,

$$\lambda_g = \frac{\mu_g \bar{C}_{p,g}}{Pr}, \quad (21)$$

with

$$\bar{C}_{p,g} = \frac{\sum_{k=2}^N Y_k C_{p,k}}{\sum_{k=2}^N Y_k}. \quad (22)$$

The complete system of equations with non-Euler terms, taking the surface  
tension force following [51], reads

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (23a)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + P \mathbf{I}) = \mathbf{F}_\sigma + \nabla \cdot (\mu \bar{\bar{\tau}}), \quad (23b)$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot ((\rho E + P) \mathbf{u}) = \mathbf{u} \cdot \mathbf{F}_\sigma + \nabla \cdot (\mu \bar{\bar{\tau}} \cdot \mathbf{u}) - \nabla \cdot \mathbf{q}, \quad (23c)$$

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho Y_k \mathbf{u}) = 0. \quad (23d)$$

### 160 3. Numerical scheme

A vertex-centered Riemann solver scheme has been developed at CERFACS  
[53], and added in the compressible, massively parallel and unstructured Large-  
Eddy-Simulation (LES) solver AVBP [66, 67], to numerically handle with ro-  
bustness high density gradients. Initially intended for plasma applications, it  
165 is adapted here to solve the Sys. (2), in conjunction with the NASG equation  
of state. Appendix B presents the numerical solver HLLC [68] along with the  
second order MUSCL reconstruction. The Sweeby [69] slope limiter is used for

the MUSCL procedure. The temporal integration is performed with a three-step Runge-Kutta (RK) algorithm, as in [70]. The non-Euler terms from Sys. (23) are computed with specific methodologies. In the capillary term the divergence is computed with a  $4\Delta$  methodology presented in [70, 71]. The viscous terms are computed with a Finite Element  $2\Delta$  operator [70, 71] to dissipate small wavelength diagonal modes that could appear. The validation of the Eulerian part of Sys. (2) is presented in appendix Appendix B.3.

#### 4. Canonical validations

In the following, we successively validate:

- the surface tension implementation,
- boundary conditions.

##### 4.1. Surface tension validation

###### 4.1.1. Laplace law

Surface tension, taken into account thanks to Eq. (15), is validated in this subsection thanks to several test cases. The Laplace law is first assessed, considering a  $\text{H}_2\text{O}$  liquid droplet of radius 5 mm, in an atmosphere of a gaseous  $\text{O}_2\text{--N}_2$  mixture. The domain is a square of 50 mm side. The mesh consists in a  $500 \times 500$  grid cells, and the surface tension coefficient is  $\sigma = 73 \times 10^{-3} \text{ N.m}^{-1}$ . The theoretical pressure drop across the interface predicted by the Laplace law is

$$P_l - P_v = \Delta P = \frac{\sigma}{r} = 14.6 \text{ Pa.} \quad (24)$$

Azimuthally averaged pressure drop measured in our simulation is shown in Fig. 1, and leads to a 0.7 % relative error to the theoretical value.

###### 4.1.2. Oscillating droplet test case

The oscillation of an elliptic viscous droplet is then considered, as shown in Fig. 2. An elliptic shape droplet of radius  $a = 1.7 \text{ mm}$  and  $b = 1 \text{ mm}$  is initialized in a  $10 \times 10 \text{ mm}$  domain of air ( $\text{O}_2\text{--N}_2$ ) at rest. Simulations have been

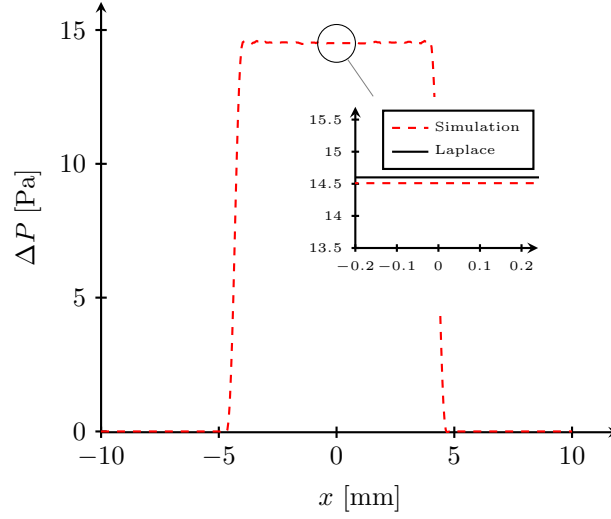


Figure 1: Pressure difference profiles for simulation (red dashed line) and Laplace (black solid line).

performed on a  $750 \times 750$  cells grid. The thermodynamic coefficients are given in Tab. 1. Thermodynamic features are  $P = 1$  bar,  $T = 293$  K and the surface tension coefficient is  $\sigma = 73 \times 10^{-3}$  N.m $^{-1}$ . The liquid and gaseous dynamic viscosities are respectively  $\mu_l = 0.854 \times 10^{-3}$  Pa.s and  $\mu_g = 1.72 \times 10^{-5}$  Pa.s. The initial species profiles are given by

$$Y_{O_2}(x) = Y_{O_2,\min} + (Y_{O_2,\max} - Y_{O_2,\min}) \Phi(x), \quad (25a)$$

$$Y_{N_2}(x) = Y_{N_2,\min} + (Y_{N_2,\max} - Y_{N_2,\min}) \Phi(x), \quad (25b)$$

$$Y_{H_2O}(x) = 1 - Y_{N_2}(x) - Y_{O_2}, \quad (25c)$$

with

$$\Phi(x, y) = \frac{1}{2} \left[ 1 + \tanh \left( \frac{\phi(x, y)}{2\epsilon} \right) \right], \quad (25d)$$

$$\phi(x, y) = 1 - \frac{x^2}{a^2} - \frac{y^2}{b^2}, \quad (25e)$$

where  $2a$  and  $2b$  are respectively the ellipse width and height, and  $\epsilon$  is the interface width.

Table 1: NASG thermodynamic coefficients for  $\text{H}_2\text{O}$  (liquid),  $\text{O}_2$ ,  $\text{N}_2$  species. Determined with NIST reference [72] with Boivin et al. [60] methodology.

Coefficients	$\text{H}_2\text{O}$ (liquid)	$\text{O}_2$	$\text{N}_2$
$C_{p,k}$ [ $\text{J.kg}^{-1}.\text{K}^{-1}$ ]	4185	919	1045
$C_{v,k}$ [ $\text{J.kg}^{-1}.\text{K}^{-1}$ ]	4180	650	742
$P_{\infty,k}$ [Pa]	$1.026 \times 10^7$	0	0
$q_k$ [ $\text{J.kg}^{-1}$ ]	$-7.8998 \times 10^5$	$-2.104 \times 10^3$	$-2.355 \times 10^3$
$b_k$ [ $\text{m}^3.\text{kg}^{-1}$ ]	$9.2 \times 10^{-4}$	0	0

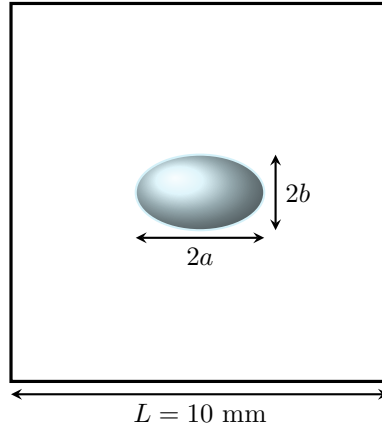


Figure 2: Oscillating droplet test case initialization. Dimensions  $2a$  and  $2b$  are respectively equal to 1.7 mm and 1 mm.

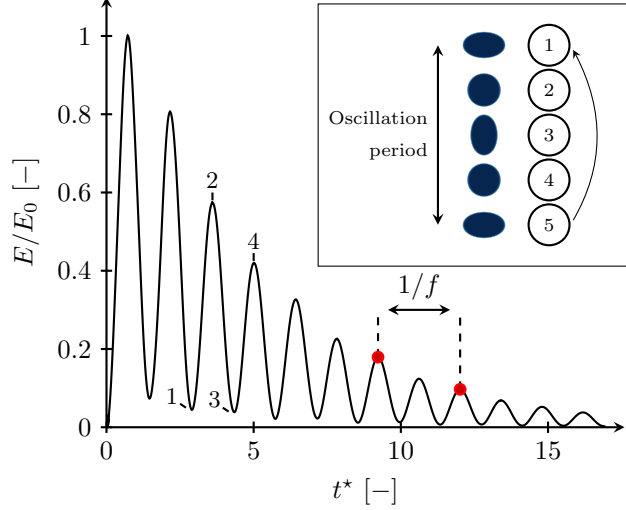


Figure 3: Time evolution of the kinetic energy in the domain and the corresponding droplet shapes from the simulation (density field).

The evolution of kinetic energy in the domain is shown in Fig. 3, evidencing its periodic evolution, damped by viscous forces. The normalized time  $t^*$  is defined as

$$t^* = \frac{t}{\sqrt{\frac{\rho_l r_{\text{eq}}^3}{\sigma}}}. \quad (26)$$

195 Theoretical studies have been proposed to predict the expected frequency of a 2D oscillating droplet. The work by Rayleigh [73], extended by Fyfe et al. [74] to account for surface tension predicts a pulsation

$$\omega^2 = (n^3 - n) \frac{\sigma}{(\rho_l + \rho_g) r_{\text{eq}}^3}, \quad (27)$$

where  $n = 2$  is the most unstable mode. The frequency reads

$$f = \frac{\omega}{2\pi}, \quad (28)$$

200 where  $r_{\text{eq}}$  is the equilibrium droplet radius. The numerical frequency is 73.03 Hz while the theoretical one computed with Eq. (28) is 71.61 Hz, resulting in 2 % relative error and falls in the range of previously reported simulations [51, 75].

#### 4.2. Boundary conditions validation

The Navier-Stokes Characteristic Boundary Condition (NSCBC) formalism for this two-phase framework is first assessed on the evacuation of an acoustic wave, superimposed to an  $\text{H}_2\text{O}-\text{O}_2$  mixture at rest, with  $Y_{\text{H}_2\text{O}} = 1 - Y_{\text{O}_2} = 0.98$ , which results in a liquid volume fraction  $\alpha_l = 7.55\%$ . Thermodynamic conditions are  $P_0 = 1$  atm and  $T_0 = 300$  K, and no artificial stabilization is applied. Gaussian forward and backward acoustic waves are superimposed. The left and right boundary conditions are outlet non-reflecting characteristic conditions [62]. Both HLLC-MUSCL [53] and a Two-step Taylor Galerkin (TTGC) scheme [76] are applied with CFL number 0.7. The use of the TTGC scheme is another validation as its formulation includes the Jacobian matrix and thus the thermodynamic specific terms, see Appendix A. Results are shown in Fig. 4, and evidence the fact that characteristic boundary conditions are able to properly handle acoustics without any reflection in this two-phase context.

The evacuation of a purely gaseous bubble from a pure liquid domain is also considered. This corresponds to the exit of an entropic wave. The test case consists in a pure  $\text{N}_2-\text{O}_2$  bubble, initialized in a pure  $\text{H}_2\text{O}^l$  domain of 1 m long, discretized by 100 mesh nodes, with an initial velocity  $\mathbf{u}_0 = 10 \text{ m.s}^{-1}$ . The thermodynamic conditions are  $P_0 = 1$  atm,  $T_0 = 300$  K. The initial profile of species across the interface follows Eq. (25) but the  $\Phi$  function is modified and reads

$$\Phi(x) = \frac{1}{2} \frac{1 + \tanh(\sqrt{6}(x + 0.3))}{4\Delta x} - \frac{1}{2} \frac{1 + \tanh(\sqrt{6}(x + 0.1))}{4\Delta x}, \quad (29)$$

where  $\Delta x$  is the cell size.

As shown in Fig. 5, the considered characteristic boundary condition allows to correctly evacuate the gaseous bubble from the liquid domain without reflecting waves.

##### 4.2.1. Water droplet advection to non-reflecting boundary condition

This section focuses on the convection of a two-dimensional droplet and aims to investigate the interaction between a curved interface and the outlet

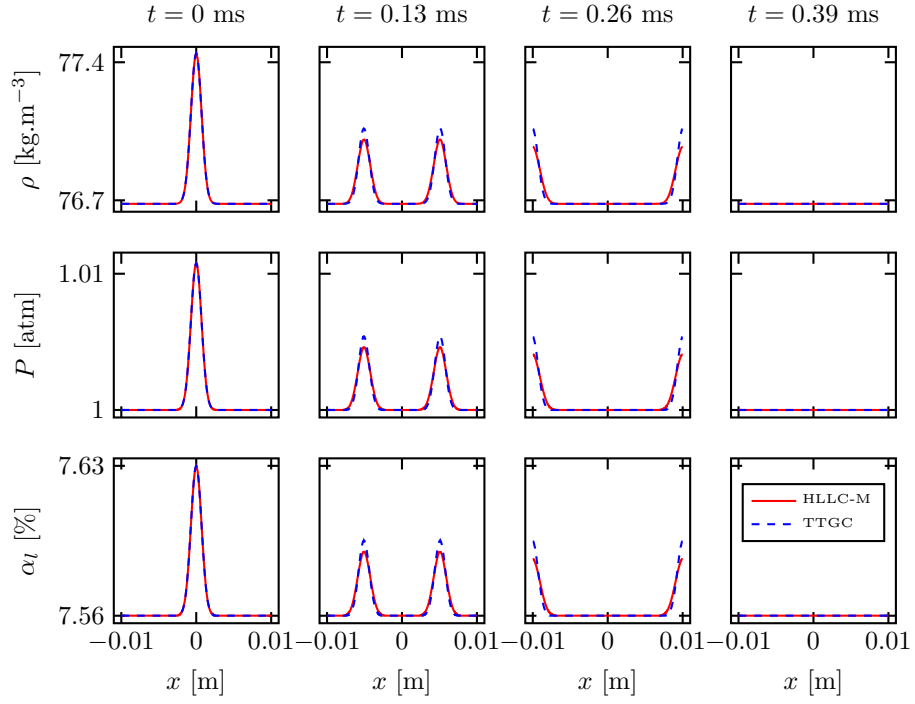


Figure 4: Superimposed backward and forward acoustic waves with fully non-reflecting boundary conditions. Red solid line: HLLC-MUSCL RK3 scheme [53], blue dashed line: TTGC scheme [76].



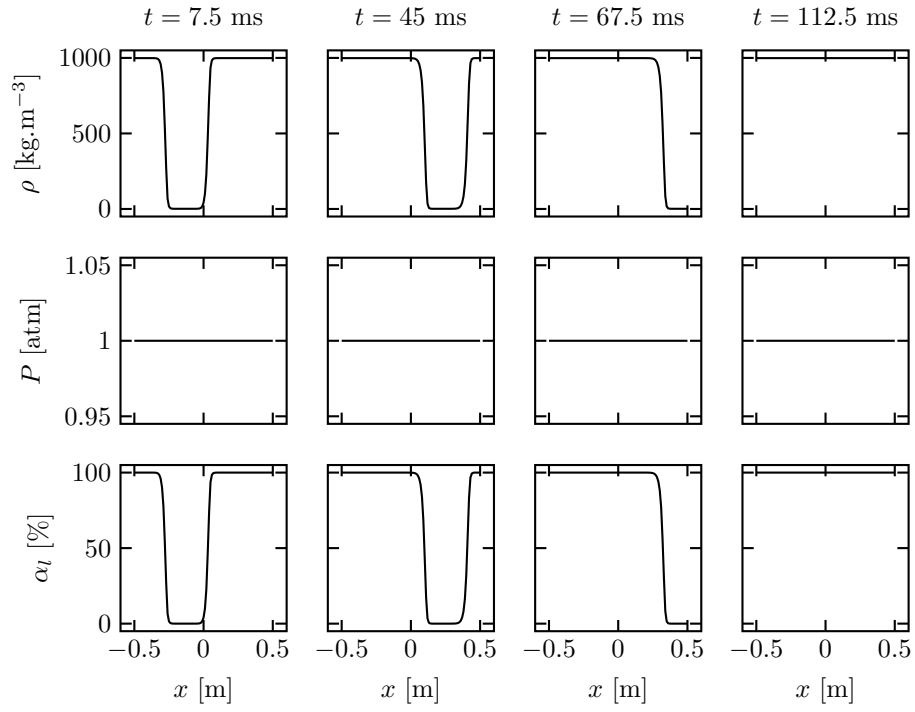


Figure 5: Air bubble in a liquid H<sub>2</sub>O environment transport to the outlet boundary condition.

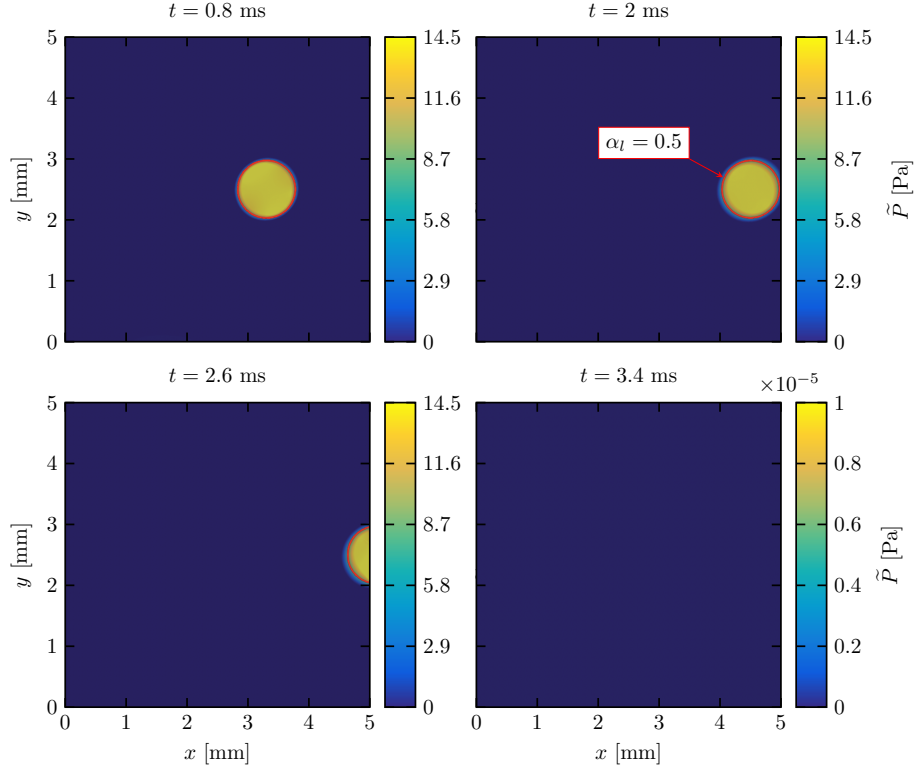
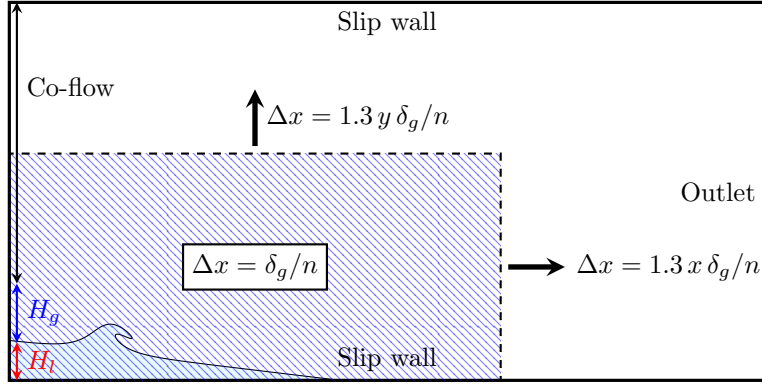


Figure 6: 2D liquid H<sub>2</sub>O droplet advection to the outlet boundary condition with.  $\tilde{P} = P - P_0$ . The red circle is  $\alpha_l = 0.5$  isocontour. Note that the colorbar is rescaled for the last instant.

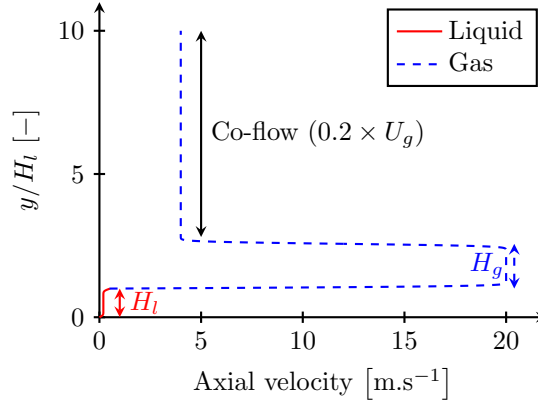
230 boundary condition. A pure liquid H<sub>2</sub>O droplet, initially traveling at a velocity  
of  $\mathbf{u}_0 = 10 \text{ m.s}^{-1}$ , is placed in a pure N<sub>2</sub>–O<sub>2</sub> domain, with thermodynamic  
conditions set to  $P_0 = 1 \text{ bar}$  and  $T_0 = 293 \text{ K}$ . The surface tension coefficient for  
this system is  $\sigma = 73 \times 10^{-3} \text{ N.m}^{-1}$ . The domain is a square of 50 mm side.  
The mesh consists in a  $1000 \times 1000$  grid cells.  
235 The results presented in Fig. 6 demonstrate that the droplet is evacuated without  
producing any reflecting waves.

## 5. Application: 2D Airblast atomizer

The intent of this section is to assess the implemented methodology on a  
practical configuration of interest for aircraft engines. Airblast atomization



(a) Sketch and mesh discretization of the configuration.



(b) Inlet velocity profile. The blue dashed curve represents the gaseous flow while the solid red curve represents the liquid flow.

Figure 7: 2D Airblast configuration.

consists in a low-velocity liquid jet sheared by a faster gaseous co-flow. Such a configuration leads to the development of liquid ligaments which break into droplets [77]. It is of particular interest since liquid atomization is a key parameter for combustion quality in aeronautical or automotive applications. For this study, a configuration experimentally studied at the LEGI lab [78–83] is considered, where a liquid film injected at low velocity along a horizontal wall is sheared by a high-speed air stream.

Experimental and theoretical works [78–81] have shown that a primary instability develops due to a Kelvin-Helmholtz instability between the liquid and

the gas, while a transverse Rayleigh-Taylor instability leads to the development  
 250 of liquid ligaments. A linear stability analysis allows to predict the dominant  
 axial wavelength  $\lambda_{\text{axi}}$  for the primary instability [77, 78, 80, 81] as

$$\lambda_{\text{axi}} = C_{\text{axi}} \sqrt{\frac{\rho_l}{\rho_g}} \delta_g, \quad (30)$$

where  $C_{\text{axi}}$  is a constant,  $\rho_l$  and  $\rho_g$  are respectively liquid and gas densities.  
 The gas vorticity thickness  $\delta_g$  is computed using the experimental correlation  
 established in [81]

$$\delta_g = \frac{6H_g}{\sqrt{Re_g}}, \quad (31)$$

255 where  $Re_g$  is the gaseous flow Reynolds number defined as

$$Re_g = \frac{\rho_g U_g H_g}{\mu_g}. \quad (32)$$

The velocity of the axial instability can be computed thanks to the Dimotakis  
 velocity  $U_c$  [84] which has shown to be in very good agreement with measured  
 wave velocities [78, 80]

$$U_c = \frac{\sqrt{\rho_g} U_g + \sqrt{\rho_l} U_l}{\sqrt{\rho_g} + \sqrt{\rho_l}}, \quad (33)$$

and finally the dominant axial frequency is

$$f_{\text{axi}} = \frac{U_c}{\lambda_{\text{axi}}}. \quad (34)$$

260 Several numerical studies have investigated this experimental configuration,  
 relying on incompressible VOF methods in 2D [85–89] and in 3D [90]. Transversal  
 instabilities are not taken into account in 2D simulations, but results showed a  
 good quantitative agreement with experiments.

The computational domain considered in the present study consists in a  
 265  $20 H_l \times 10 H_l$  rectangular box, sketched in Fig. 7a. The numerical domain is  
 discretized with a cell size equal to  $\delta_g/n$  (with  $n = 2, 4$  and  $8$ ) near the injection  
 and shear zone ( $13 H_l \times 6 H_l$ ), and the mesh is stretched in both vertical and  
 axial directions outside of these regions. The geometric parameters considered in  
 our numerical simulation are the same as in the numerical work of Fuster et al.  
 270 [86], i.e., liquid and gas enter in the domain from left with heights respectively

equal to  $H_l = 6.4$  mm and  $H_g = 10$  mm, as shown in Fig. 7a. The considered species are liquid water  $\text{H}_2\text{O}^l$  for liquid flow and respectively 22 % and 78 % in mass of oxygen  $\text{O}_2^v$  and nitrogen  $\text{N}_2^v$  for the gaseous flow, and the surface tension coefficient is  $\sigma = 69 \times 10^{-3}$  N.m<sup>-1</sup>. Following Bozonnet et al. [89], no  
 275 splitter separating plate is considered and continuous profiles are imposed at the inlet, as illustrated in Fig. 7b. The inlet velocity profile is given by Eqs. (35) to (37):

$$u(y) = \left[ U_l \operatorname{erf} \left( \frac{H_l - y}{\delta_l} \right) + U_i \left( 1 + \operatorname{erf} \left( \frac{y - H_l}{\delta_l} \right) \right) \right] \times \operatorname{erf} \left( \frac{y}{\delta_l} \right), \quad (35)$$

for  $y \leq H_l$ .

$$u(y) = \left[ U_g \operatorname{erf} \left( \frac{y - H_l}{\delta_g} \right) + U_i \left( 1 - \operatorname{erf} \left( \frac{y - H_l}{\delta_l} \right) \right) \right] \times \operatorname{erf} \left( \frac{H_g + H_l - y}{\delta_g} \right) + U_{sm} \left( 1 + \operatorname{erf} \left( \frac{y - (H_g + H_l)}{\delta_g} \right) \right), \quad (36)$$

for  $H_l < y \leq H_g + H_l$ .

$$u(y) = U_{sm} \left( 1 - \operatorname{erf} \left( \frac{y - (H_g + H_l)}{\delta_g} \right) \right) + U_{cf} \operatorname{erf} \left( \frac{y - (H_g + H_l)}{\delta_g} \right), \quad (37)$$

280 for  $y > H_g + H_l$ ,

where  $\delta_g$  is the gas vorticity thickness,  $\delta_l$  the liquid vorticity thickness,  $U_i = \delta_l (U_g \mu_g / \delta_g + U_l \mu_l / \delta_l) / (\mu_l + \mu_g)$  is the interfacial velocity defined in [91],  $U_{cf} = 0.2 U_g$  is the co-flow velocity and  $U_{sm} = (U_{cf} + U_g) / 2$  is the gaseous phase mixing layer velocity. Liquid and gaseous dynamic viscosities are respectively denoted  
 285  $\mu_l$  and  $\mu_g$ .

At the initial state the domain is at rest with temperature  $T = 300$  K. The air flow is fixed at  $U_g = 20$  m.s<sup>-1</sup> and liquid velocity is computed to reach a dynamic pressure ratio  $M = (\rho_g U_g^2) / (\rho_l U_l^2) = 16$  resulting in  $U_l = 0.1735$  m.s<sup>-1</sup> at  $P = 1$  bar. The simulation parameters are given in Tab. 2, and species  
 290 properties are the ones considered in the validation test-cases Tab. 1, for which the liquid water species has a modified sound speed, resulting in a slightly modified density ( $\rho_l = 939$  kg.m<sup>-3</sup> at 1 bar). Imposed inlet velocity values are kept constant in the study. An air co-flow is added on top of the high-speed air

Table 2: Simulation parameters:  $U$  is the velocity,  $\mu$  is the dynamic viscosity and  $\sigma$  is the surface tension coefficient.

Phase	$U$ [m.s <sup>-1</sup> ]	$\mu$ [Pa.s]	$\sigma$ [N.m <sup>-1</sup> ]
Liquid	0.1735	$1 \times 10^{-3}$	$69 \times 10^{-3}$
Gas	20	$1.8 \times 10^{-5}$	–

stream similarly as [90], to limit gaseous recirculations in this region. Inlet and  
 295 outlet boundary conditions are characteristic non-reflecting boundary conditions,  
 validated above in Sec. 4.2 for the current framework.

An instantaneous density field is shown in Fig. 8a, evidencing the development  
 of liquid ligaments. In order to quantitatively assess the results, the liquid core  
 length predicted by the correlation of Raynal [78] is reported with a thick orange  
 300 line. This correlation provides the intact liquid core length  $L$  thanks to Eq. (38),

$$L = \frac{12 H_l}{\sqrt{M}}, \quad (38)$$

and is retrieved from previous numerical works relying on sharp interface methods  
 [75, 87, 88]. Mean profiles of liquid volume fraction  $\alpha_l = 0.1$ , 0.5 and 0.9 are  
 given in Fig. 8b for the three mesh resolutions ( $n = 2$ , 4 and 8). The intact  
 liquid core more likely corresponds to the iso-contour  $\alpha_l = 0.9$ , and Fig. 8b  
 305 shows that increasing mesh resolution allows to obtain a fair agreement with  
 the experimental correlation of Raynal Eq. (38). Figure 8c shows the  $\alpha_l = 0.5$   
 isocontour evolution for the resolution  $n = 8$  during 400 ms, corresponding to  
 the passage of approximately 10 waves. The liquid sheet oscillates above the  
 experimental correlation of Raynal [78] and the film height decreases following  
 310 the slope of Eq. (38) given by the thick black line. The accurate prediction of  
 this liquid core length shows the ability of the diffuse interface method to predict  
 the liquid entrainment within the two-phase mixing layer.

The normalized amplitude spectrograms ( $\mathcal{A}^*$ ) of the interface height for  
 $P = 1$  bar with different mesh resolutions are given in Fig. 9a ( $\Delta x = \delta_g/n$  with  
 315  $n$  given on Fig. 9a), at position  $x = 2 H_l$ . These spectra have been obtained  
 with the Welch method [92] to extract the most amplified frequency. The signal

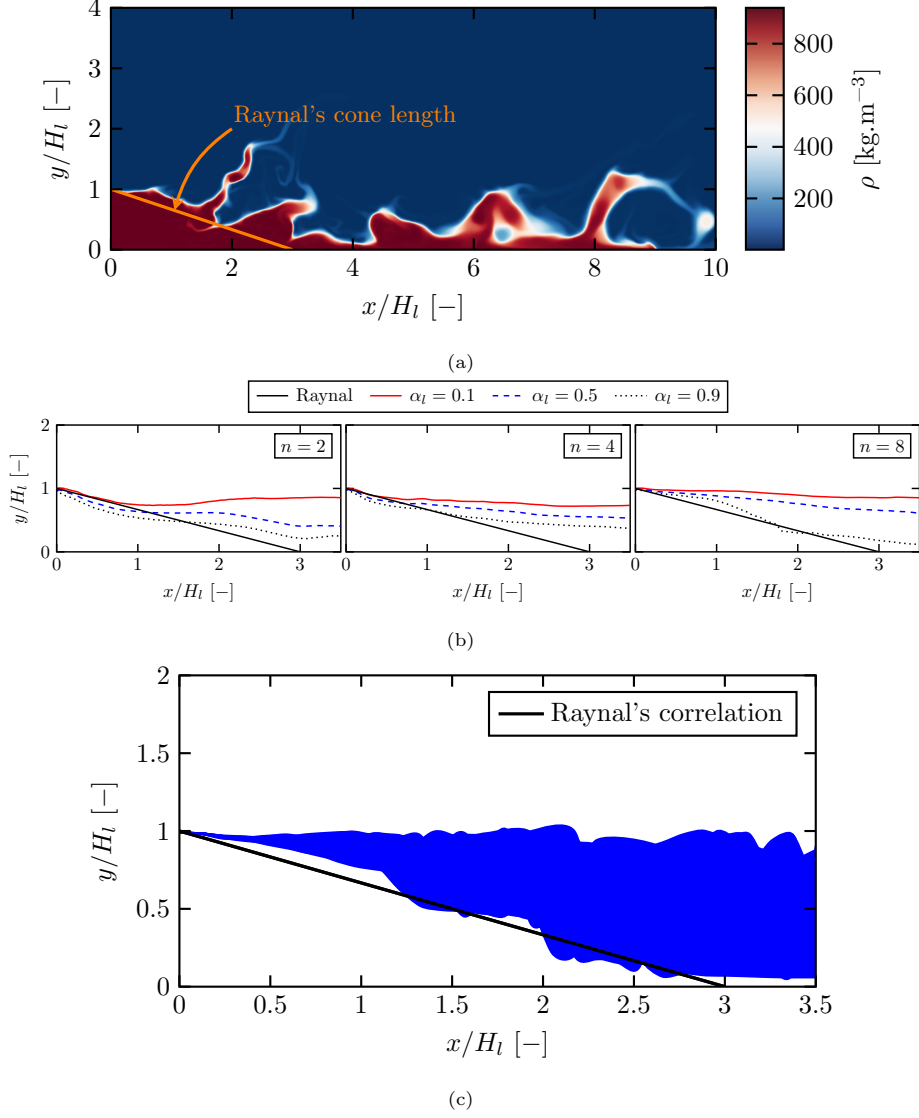


Figure 8: (a) Instantaneous density field. The thick orange line represents the intact cone length of Raynal [78]. (b) Liquid volume fraction mean profiles ( $\alpha_l = 0.1$ , 0.5 and 0.9) for the three resolutions used ( $n = 2$ , 4 and 8) compared to the correlation of Raynal Eq. (38) (black solid line). (c) Comparison of the liquid cone length at  $P = 1$  bar. The thick black line represents the the correlation length of Eq. (38). The blue area represents 40 filled isocontour of  $\alpha_l = 0.5$  over 400 ms with  $n = 8$  resolution.

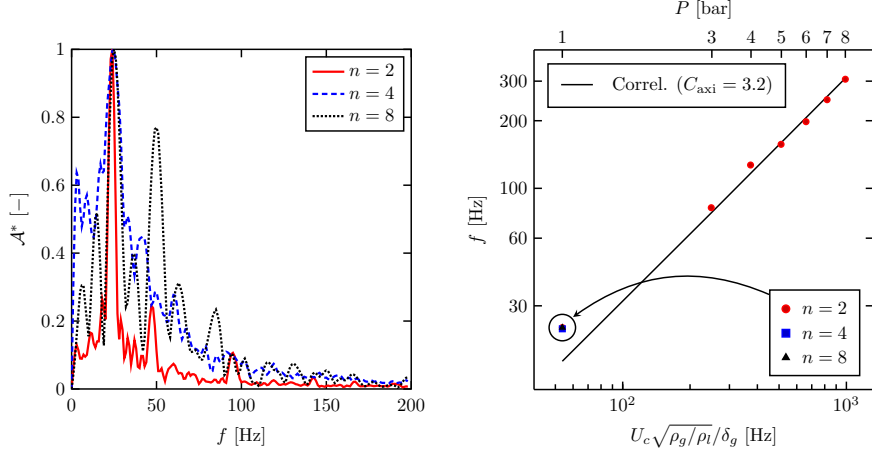
Table 3: Comparison of previous experimental and numerical values of Strouhal numbers with the present study for the case  $M = 16$  and  $P = 1$  bar.

	Strouhal ( $\times 10^{-4}$ )
Raynal [78]	6
Marmottant and Villiermaux [77]	7.5
Ben Rayana [80]	7.6
Matas et al. [81]	5
Fuster et al. [86] (VOF simulation – exp.)	8 – 5
Agbaglah et al. [87] (VOF simulation)	5.3
Present study	6.5

is divided into ten segments with a 60 % overlap as in Bozonnet et al. [89], and the liquid volume fraction is integrated across vertical lines to determine the liquid height. This process is repeated for multiple axial positions ranging from  
320 0 to 13 times the liquid injection height  $H_l$ . Afterwards, the signals undergo Fast Fourier Transform (FFT), and the results are averaged. Despite an increase of numerical noise the main frequency remains the same for the three meshes, meaning that independence from mesh resolution is reached. The signal is processed for a time  $t$  so that the number of generated waves is larger than 30  
325 ( $\tau = f\Delta t$ ). Bozonnet et al. [89] showed that even  $\tau \approx 10$  is enough to obtain a good estimate of the frequency. The value found is  $f = 24$  Hz which is equivalent to a Strouhal number  $St = f\delta_g/U_g = 6.5 \times 10^{-4}$ . The value is compared in Tab. 3 with previous studies at the same operating point and falls in the range of reported Strouhal numbers meaning that the essential instability mechanisms  
330 are captured by the method.

The resolution  $n = 2$  is adopted for the rest of the study to keep reasonable computational costs. Further simulations are finally conducted to investigate new operating ranges, hardly reachable with both experiments and incompressible solvers. Simulations are performed with various density ratios by adapting the  
335 pressure imposed at the outlet. The densities for each pressure are given in Tab. 4.





(a) Normalized amplitudes  $\mathcal{A}^*$  for  $P = 1$  bar. (b) Main frequency as a function of the pressure and the quantity  $U_c \sqrt{\rho_g / \rho_l} / \delta_g$ .

Figure 9: Results of the spectral analysis. (a) Normalized amplitude  $\mathcal{A}^*$  of the Fast Fourier Transform (FFT) at  $P = 1$  bar for different mesh resolutions at position  $x = 2 H_l$  and  $\tau \geq 30$ . (b) Main frequency evolution with pressure. The solid line represents the frequencies obtained with correlations Eqs. (30) and (34).

The gas vorticity thickness  $\delta_g$  is adapted to the operating points in Eqs. (36) and (37) according to Eq. (31). Simulation parameters in Tab. 2 are kept constant. Results for the main frequency at various pressures are given in Fig. 9b and are compared to the one obtained from correlation Eq. (34) (black solid line) where a prefactor  $C_{\text{axi}} = 3.2$  is considered. The same methodology as in Fig. 9a has been used, however for  $P = 7$  and 8 bar raw FFT are considered because of a gas recirculation at the end of the liquid cone length. This phenomenon has also been experimentally observed by Raynal [78], Ben Rayana [80] for large momentum ratios, typically  $M > 100$ . Note that several values for  $C_{\text{axi}}$  can be found in literature. Raynal [78] proposed  $C_{\text{axi}} = 4$ , Ben Rayana [80] proposed  $C_{\text{axi}} = 1.5$  to 1.8. It has been shown that the different methodologies considered to experimentally measure the frequency can be a reason for these different values of  $C_{\text{axi}}$  [81]. Despite this uncertainty, linear stability analysis [78] predicts a linear relation between  $f$  and  $U_c \sqrt{\rho_g / \rho_l} / \delta_g$ , that is perfectly found in our

Table 4: Liquid and vapour densities for each pressure and the associated momentum ratio  $M$ .

Pressure [bar]	3	4	5	6	7	8
Liquid density $\rho_l$ [kg.m <sup>-3</sup> ]	941.6	942.8	943.9	945.1	946.2	947.3
Vapour density $\rho_g$ [kg.m <sup>-3</sup> ]	3.4	4.5	5.7	6.8	7.9	9.1
Momentum ratio $M$ [-]	48	64	80	95	111	127

simulations as pressure increases (Fig. 9b). It is to the authors' knowledge a rare confirmation of this theoretical prediction on a practical case.

Normalized amplitude spectrograms over a distance  $x/H_l = 8$  are given in Fig. 10. For each operating pressure point the main axial frequency is clearly visible near the injection. The frequency decreases downstream of a length approximately equal to the intact liquid cone length given by Eq. (38) highlighted with a solid black line in Fig. 10.

This finally shows that the sheared liquid-gas interface dynamics is well reproduced by the present method. The intact liquid core length is correctly retrieved, and the frequency evolution with pressure theoretically predicted by linear stability analysis is confirmed by our numerical approach. This methodology can therefore be considered with confidence for pressurized airblast configurations in future studies.

## 6. Conclusions

This paper presents first a validation of implemented methods for handling two-phase flow configurations in a fully compressible vertex-centered framework, utilizing a diffuse-interface Multi-Fluid method and a 4-equation model closed with a Noble-Abel Stiffened-Gas equation of state.

The vertex-centered HLLC-MUSCL numerical scheme has been implemented and validated on a number of academic test cases, demonstrating its ability to properly handle contact lines, shocks, and rarefaction waves. Additionally, the method effectively handles acoustics in the context of two-phase flow. Jacobian fluxes have been properly derived to allow the use of non-reflecting characteristic

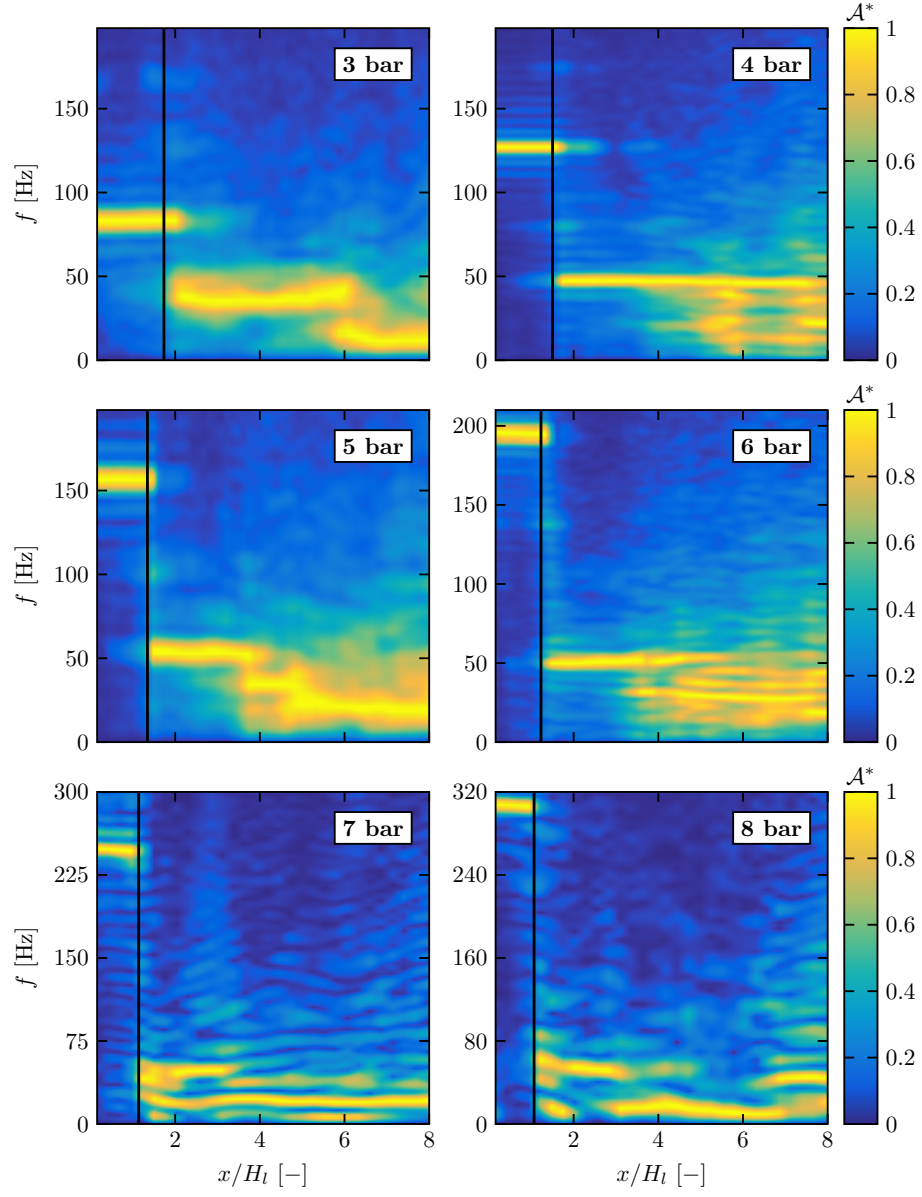


Figure 10: Amplitude normalized spectrograms ( $\mathcal{A}^*$ ) of interface height for  $P = 3$  to 8 bar over a distance  $x/H_l = 8$ . The solid black line represents the intact cone length from Eq. (38).

boundary conditions in conjunction with the NASG EoS. The non-reflectivity is assessed for both 1D and 2D two-phase test-cases. Capillary terms associated  
375 with the liquid-gas interface have been validated on simple configurations, with satisfactory results.

The methodology is then assessed on an air-assisted atomization configuration, for which experimental, theoretical, and numerical results can be found in the literature. Our results show the ability of the diffuse interface method to predict  
380 the intact liquid core length, as well as the interface dynamics. Furthermore, the methodology allows to investigate new operating ranges, and the effect of pressure increase on the primary interfacial wave frequency is studied. Our results show a very good agreement with the theoretical prediction of Raynal [78].

This allows to bridge the gap between usually incompressible methods consid-  
385 ered for primary atomization, and compressible methods considered for prediction of combustion. Future work will be devoted to the development of a phase-change methodology, along with temperature-variable heat capacities, to properly handle reactive conditions. In addition, a coupling with a disperse spray Lagrangian  
390 model will be investigated, to allow a proper spray prediction in a realistic pressurized and reactive environment.

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## Appendix A. Characteristic boundary conditions

Well applied boundary conditions are of major interest in compressible flows in  
order to avoid for example pressure drift and acoustic waves in the computational  
domain. A proper derivation of the coefficients from the Jacobian matrix is  
690 essential as is the speed of sound.

One can recall the one-dimensional 4-equation model

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial x} = 0, \quad (\text{A.1})$$

where  $\mathbf{U} = [\rho, \rho \mathbf{u}, \rho E, \rho Y_k]^t$  and  $\mathbf{F} = [\rho \mathbf{u}, \rho \mathbf{u} \otimes \mathbf{u} + P, (\rho E + P)\mathbf{u}, \rho Y_k \mathbf{u}]^t$ .

Jacobian matrix reads

$$A_x(\mathbf{U}) = \frac{\partial \mathbf{F}(\mathbf{U})}{\partial \mathbf{U}} = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ -\mathbf{u}^2 & \mathbf{u}(2 - \Lambda) & \Lambda & -\Lambda(\Gamma_1 - e_c) & \cdots & -\Lambda(\Gamma_N - e_c) \\ -\mathbf{u}H & H - \Lambda\mathbf{u}^2 & \mathbf{u}(1 + \Lambda) & -\mathbf{u}\Lambda(\Gamma_1 - e_c) & \cdots & -\mathbf{u}\Lambda(\Gamma_N - e_c) \\ -\mathbf{u}Y_1 & Y_1 & 0 & \mathbf{u} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\mathbf{u}Y_N & Y_N & 0 & 0 & \cdots & \mathbf{u} \end{bmatrix}, \quad (\text{A.2})$$

with  $H = E + P/\rho$ ,  $\Lambda = \left. \frac{\partial P}{\partial \rho e} \right|_{\rho Y_k}$  and  $\Gamma = \left. \frac{\partial \rho e}{\partial \rho Y_k} \right|_{P, \rho Y_{i \neq k}}$ .

#### Appendix A.1. Jacobian terms

695 This section proposes the derivation of the  $\Gamma$  and  $\Lambda$  coefficient involved in the jacobian matrix (Eq. (A.2)).

From the mixture laws one can write

$$e = \sum_{k=1}^N Y_k e_k, \quad (\text{A.3})$$

$$v = \sum_{k=1}^N Y_k v_k. \quad (\text{A.4})$$

Derivatives of previous expressions read

$$de = \sum_{k=1}^N Y_k de_k + \sum_{k=1}^N e_k dY_k, \quad (\text{A.5})$$

$$dv = \sum_{k=1}^N Y_k dv_k + \sum_{k=1}^N v_k dY_k. \quad (\text{A.6})$$

Species energy and volume derivatives can be written as

$$\begin{aligned} de_k &= \left. \frac{\partial e_k}{\partial P} \right|_T dP + \left. \frac{\partial e_k}{\partial T} \right|_P dT, \\ &= \frac{P\beta - T\alpha}{\rho} dP + \left( \bar{C}_p - \frac{P\alpha}{\rho} \right) dT, \end{aligned} \quad (\text{A.7})$$

$$\begin{aligned} dv_k &= \left. \frac{\partial v_k}{\partial P} \right|_T dP + \left. \frac{\partial v_k}{\partial T} \right|_P dT, \\ &= -v\beta dP + v\alpha dT, \end{aligned} \quad (\text{A.8})$$



where  $\alpha$  and  $\beta$  are defined in appendix Appendix A.2.

So Eqs. (A.5) and (A.6) can be rewritten as

$$de = \sum_{k=1}^N Y_k \left( \frac{P\beta - T\alpha}{\rho} dP + \left( \bar{C}_p - \frac{P\alpha}{\rho} \right) dT \right) + \sum_{k=1}^N e_k dY_k, \quad (\text{A.9})$$

$$dv = \sum_{k=1}^N Y_k (-v\beta dP + v\alpha dT) + \sum_{k=1}^N v_k dY_k. \quad (\text{A.10})$$

With Eq. (A.10) one can write

$$dT = -\frac{1}{\rho\alpha} d\rho + \frac{\beta}{\alpha} dP - \frac{\rho}{\alpha} \sum_{k=1}^N v_k dY_k. \quad (\text{A.11})$$

So Eq. (A.5) becomes

$$\begin{aligned} de = & \frac{1}{\rho} \left( \frac{\rho\bar{C}_p\beta}{\alpha} - \alpha T \right) dP + \frac{1}{\rho^2} \left( P - \frac{\rho\bar{C}_p}{\alpha} \right) d\rho \\ & - \frac{\rho\bar{C}_p}{\alpha} \sum_{k=1}^N v_k dY_k + \sum_{k=1}^N h_k dY_k. \end{aligned} \quad (\text{A.12})$$

700 Knowing that  $d(\rho e) = \rho de + e d\rho$ ,

$$d(\rho e) = \left( \frac{\rho\bar{C}_p\beta}{\alpha} - \alpha T \right) dP + \sum_{k=1}^N \left( h_k - \frac{\rho\bar{C}_p}{\alpha\rho_k} \right) d(\rho Y_k). \quad (\text{A.13})$$

Finally one can write

$$\Lambda = \frac{\partial P}{\partial \rho e} \Big|_{\rho Y_k} = \frac{1}{\frac{\rho\bar{C}_p\beta}{\alpha} - \alpha T}, \quad (\text{A.14})$$

$$\Gamma = \frac{\partial \rho e}{\partial \rho Y_k} \Big|_{P, Y_{i \neq k}} = h_k - \frac{\rho\bar{C}_p}{\alpha\rho_k}. \quad (\text{A.15})$$

#### Appendix A.2. Isobaric dilatation and isotherm compressibility coefficients

The Isobaric dilatation  $\alpha$  and isothermal compressibility  $\beta$  coefficients respectively read

$$\alpha = \frac{1}{v} \frac{\partial v}{\partial T} \Big|_{P, \mathbf{Y}} = -\frac{1}{\rho} \frac{\partial \rho}{\partial T} \Big|_{P, \mathbf{Y}}, \quad (\text{A.16})$$

$$\beta = -\frac{1}{v} \frac{\partial v}{\partial P} \Big|_{T, \mathbf{Y}} = \frac{1}{\rho} \frac{\partial \rho}{\partial P} \Big|_{T, \mathbf{Y}}. \quad (\text{A.17})$$

In a multicomponent NASG framework the mass-specific volume reads

$$v(T, P, Y_k) = \sum_{k=1}^N Y_k \left( \frac{(\gamma_k - 1)C_{v,k}T}{P + P_{\infty,k}} + b_k \right), \quad (\text{A.18})$$

so that the mixture mass-specific volume derivative at constant composition reads

$$dv = \sum_{k=1}^N Y_k \left( \frac{(\gamma_k - 1)C_{v,k}(P + P_{\infty,k})dT - (\gamma_k - 1)C_{v,k}TdP}{(P + P_{\infty,k})^2} \right). \quad (\text{A.19})$$

705 The mass volume is related to density through

$$\rho = \frac{1}{v}, \quad \text{and} \quad d\rho = -\rho^2 dv. \quad (\text{A.20})$$

So the density derivative reads

$$d\rho = -\rho^2 \sum_{k=1}^N \left( \frac{(\gamma_k - 1)C_{v,k}(P + P_{\infty,k})(Y_k dT + T dY_k) - Y_k(\gamma_k - 1)C_{v,k}TdP}{(P + P_{\infty,k})^2} \right). \quad (\text{A.21})$$

Finally one can write

$$\alpha = \rho \sum_{k=1}^N Y_k \left( \frac{(\gamma_k - 1)C_{v,k}}{P + P_{\infty,k}} \right), \quad (\text{A.22})$$

$$\beta = \rho \sum_{k=1}^N Y_k \left( \frac{(\gamma_k - 1)C_{v,k}T}{(P + P_{\infty,k})^2} \right). \quad (\text{A.23})$$

### Appendix A.3. Speed of sound

The hyperbolic sound speed reads

$$c^2 = \left. \frac{\partial P}{\partial \rho} \right|_{s, \mathbf{Y}}, \quad (\text{A.24})$$

with composition  $\mathbf{Y} = [Y_1, \dots, Y_N]^t$ .

The differential of the mixture mass-specific volume at constant composition

710 can be written as

$$\begin{aligned} dv &= \left. \frac{\partial v}{\partial T} \right|_{P, \mathbf{Y}} dT + \left. \frac{\partial v}{\partial P} \right|_{T, \mathbf{Y}} dP, \\ &= v\alpha dT - v\beta dP, \end{aligned} \quad (\text{A.25})$$

so that

$$dT = -\frac{1}{\rho\alpha}d\rho + \frac{\beta}{\alpha}dP. \quad (\text{A.26})$$

The mixture mass specific entropy reads

$$\begin{aligned} s(P, T, Y_k) &= \sum_{k=1}^N Y_k s_k(P, T), \\ &= \sum_{k=1}^N Y_k \left( C_{v,k} \ln \left( \frac{T^{\gamma_k}}{(P + P_{\infty,k})^{\gamma_k-1}} \right) + s_k^0 \right), \end{aligned} \quad (\text{A.27})$$

where  $C_{v,k}$ ,  $s_k^0$ ,  $P_{\infty,k}$  are specific constants of the NASG thermodynamics framework. The mixture mass specific entropy differential at constant composition

715 reads

$$\begin{aligned} ds &= \left. \frac{\partial s}{\partial T} \right|_{P, \mathbf{Y}} dT + \left. \frac{\partial s}{\partial P} \right|_{T, \mathbf{Y}} dP, \\ &= \frac{\bar{C}_p}{T} dT - \frac{\alpha}{\rho} dP. \end{aligned} \quad (\text{A.28})$$

Casting Eq. (A.26) into Eq. (A.28) yields

$$ds = -\frac{1}{\rho\alpha} \frac{\bar{C}_p}{T} d\rho + \left( -\frac{\alpha}{\rho} + \frac{\bar{C}_p}{T} \frac{\beta}{\alpha} \right) dP. \quad (\text{A.29})$$

Finally, the hyperbolic 4-equation system sound speed reads

$$c^2 = \frac{\bar{C}_p}{\rho\beta\bar{C}_p - \alpha^2 T}, \quad (\text{A.30})$$

with  $\bar{C}_p = \sum_{k=1}^N Y_k C_{p,k}$ .

## Appendix B. A Vertex-centered HLLC-MUSCL scheme

### 720 Appendix B.1. Scheme implementation in a Vertex-Centered framework

Godunov numerical schemes [93] are usually implemented using a cell-centered framework. Fluxes are estimated on cell faces and conservative variables stored at the cell centre. The AVBP solver features a cell-vertex architecture, which offers an efficient way of handling numerical schemes like Lax-Wendroff or Taylor-  
725 Galerkin schemes [76, 94]. The Godunov scheme implemented in this work relies therefore on a node-centered formalism.

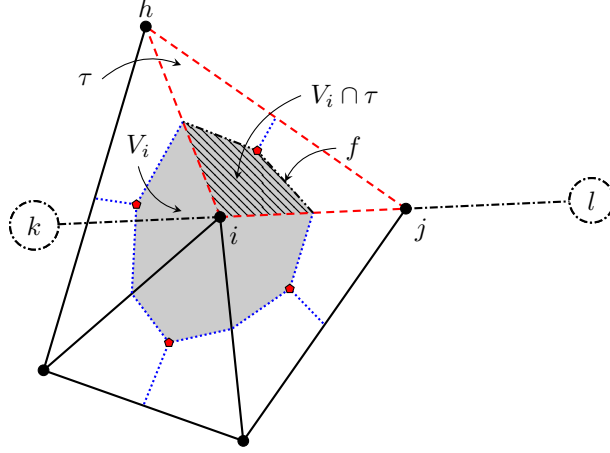


Figure B.11: Discretization at all the cell nodes. The grey area represents the nodal volume  $V_i$ . The hatched area is the intersection of a cell  $\tau$  containing node  $i$  with the nodal volume  $V_i$ . The edges of  $V_i$  ( $f$ ) are defined from the center of cell  $\tau$  and the middle of its edges with node  $i$  ( $j$  and  $h$ ). The virtual nodes  $k$  and  $l$  are used for the MUSCL procedure.

It considers the integral form of the transport equations, written in the compact form as

$$\frac{\partial}{\partial t} \int_V \mathbf{U} \, dV + \oint_{\partial V} \mathbf{F} \cdot \mathbf{n} \, dS = 0. \quad (\text{B.1})$$

The integration is made on the nodal volume  $V_i$  associated to node  $i$ , illustrated  
730 by the grey area in Fig. B.11. Fluxes are computed at all nodal volume faces, determined from the intersection of  $V_i$  surface with all cells  $\tau$  containing the node  $i$ , and noted  $E(i)$

$$\frac{\partial}{\partial t} \mathbf{U}_i + \sum_{\tau \in E(i)} \sum_{f \in V_i \cap \tau} \int_f \mathbf{F} \cdot \mathbf{n} \, dS = 0. \quad (\text{B.2})$$

In Eq. (B.2), the first sum corresponds to a loop over all cells containing a given  
735 volume  $V_i$ .

Surfaces integrals are computed by projecting the flux into the local basis of the edge as it is less computationally expensive than splitting the flux in 3 components in a fixed basis dimension and solving 3 Riemann problems ([95], Ch. 16).

740 *Appendix B.2. MUSCL reconstruction procedure*

A HLLC Riemann solver [68] is considered in this work with a MUSCL reconstruction of variables to compute fluxes at edges. This procedure uses piecewise linear functions to ensure second order accuracy. Cell boundary values are computed as  $\mathbf{U}_i^L = \mathbf{U}_i^n - \Delta\mathbf{U}_i^n/2$  and  $\mathbf{U}_i^R = \mathbf{U}_i^n + \Delta\mathbf{U}_i^n/2$  respectively on  
 745 the left and on the right sides of node  $i$  along a given direction. For stability  $\Delta\mathbf{U}_i^n$  is computed with the limited approach of Sweby [69]:

$$\Delta\mathbf{U}_i^n = \begin{cases} \begin{cases} \max\left[0, \min\left(\beta\Delta\mathbf{U}_{i-1/2}^n, \Delta\mathbf{U}_{i+1/2}^n\right), \right. \\ \left. \min\left(\Delta\mathbf{U}_{i-1/2}^n, \beta\Delta\mathbf{U}_{i+1/2}^n\right)\right], & \text{if } \Delta\mathbf{U}_{i+1/2}^n > 0, \\ \min\left[0, \max\left(\beta\Delta\mathbf{U}_{i-1/2}^n, \Delta\mathbf{U}_{i+1/2}^n\right), \right. \\ \left. \max\left(\Delta\mathbf{U}_{i-1/2}^n, \beta\Delta\mathbf{U}_{i+1/2}^n\right)\right], & \text{if } \Delta\mathbf{U}_{i+1/2}^n < 0, \end{cases} \end{cases} \quad (\text{B.3})$$

where  $\beta \in [1, 2]$  is a limiter parameter.

The  $\Delta\mathbf{U}_{i-1/2}^n$  and  $\Delta\mathbf{U}_{i+1/2}^n$  values correspond respectively to  $\Delta_{ki}$  and  $\Delta_{ij}$  for the node  $i$  and  $\Delta_{ij}$  and  $\Delta_{jl}$  for the node  $j$  as shown in Fig. B.11. In the case  
 750 of irregular meshes in Fig. B.11 virtual nodes are retrieved (dash-dotted circles):  $k$  and  $l$  are respectively at a distance  $\mathbf{ij}$  of  $i$  and  $j$ .

*Appendix B.3. Hyperbolic solver validation*

*Appendix B.3.1. One dimensional shock-tube*

The solver is first validated on a two-phase shock tube configuration without  
 755 surface tension (Sys. (2)). The present study considers a shock tube that is 1 m long and comprised of two chambers, which are separated by an interface located at  $x = 0.7$  m. The left side is filled with liquid water at  $P = 1$  GPa and  $\rho = 1000$  kg.m<sup>-3</sup>. The right side is composed of air at  $P = 1 \times 10^5$  Pa and  $\rho = 10$  kg.m<sup>-3</sup>. The left chamber contains a small amount of air  $Y_{\text{air}} = 1 \times 10^{-8}$ .  
 760 The right chamber has a reversed composition. Thermodynamic properties are displayed in Tab. B.5. The covolume for species H<sub>2</sub>O is zero to retrieve the Stiffened-Gas (SG) EoS. The 1D computational domain is divided into 2000 uniform elements.

Table B.5: SG thermodynamic coefficients for H<sub>2</sub>O (liquid) and Air species.

Coefficients	H <sub>2</sub> O (liquid)	Air
$C_{p,k}$ [J.kg <sup>-1</sup> .K <sup>-1</sup> ]	4400	1001
$C_{v,k}$ [J.kg <sup>-1</sup> .K <sup>-1</sup> ]	1000	715
$P_{\infty,k}$ [Pa]	6×10 <sup>8</sup>	0
$q_k$ [J.kg <sup>-1</sup> ]	0	0
$b_k$ [m <sup>3</sup> .kg <sup>-1</sup> ]	0	0

Results are shown in Fig. B.12, where plots of pressure, density, velocity and  
765 liquid volume fraction are depicted at  $t = 220 \mu\text{s}$ , and compared to the exact  
solution. Agreement is seen to be excellent. Consistently with the literature  
[34, 96], no overshoot is obtained, and Hugoniot relationships are satisfied.

#### Appendix B.3.2. Two dimensional Riemann test case

Two dimensional Riemann ideal gas test-cases are then considered. The  
770 geometry is a  $[-0.5, -0.5] \times [0.5, 0.5]$  meter square with a  $600 \times 600$  regular grid.  
Specific calorific capacities ratio is constant and equal to  $\gamma = 1.4$ . The initial  
condition consists in four quadrants with different initial conditions [97]:

$$(\rho_0, \mathbf{u}_0, \mathbf{v}_0, P_0) = \begin{cases} (3.0, 0.75, 0.5, 1.0) & x \leq 0, y \geq 0, \\ (1.0, -0.75, 0.5, 1.0) & x \leq 0, y \leq 0, \\ (1.0, 0.75, -0.5, 1.0) & x \geq 0, y \geq 0, \\ (2.0, -0.75, -0.5, 1.0) & x \geq 0, y \leq 0. \end{cases} \quad (\text{B.4})$$

Results obtained at CFL = 0.7 and for a  $\beta$ -Sweeby parameter equal to 1.5  
are shown in Fig. B.13a. It evidences the fact that the numerical solver is able  
775 to capture and transport stiff gradients with robustness and accuracy.

Other test-cases from Lax and Liu [97], Kurganov and Tadmor [98] are  
conducted, introducing rarefaction and shock waves in addition to the contact  
discontinuity. The initial states are defined thanks to Eqs. (B.5) and (B.6), and  
results are presented in Figs. B.13b and B.13c. Results are again very satisfying.

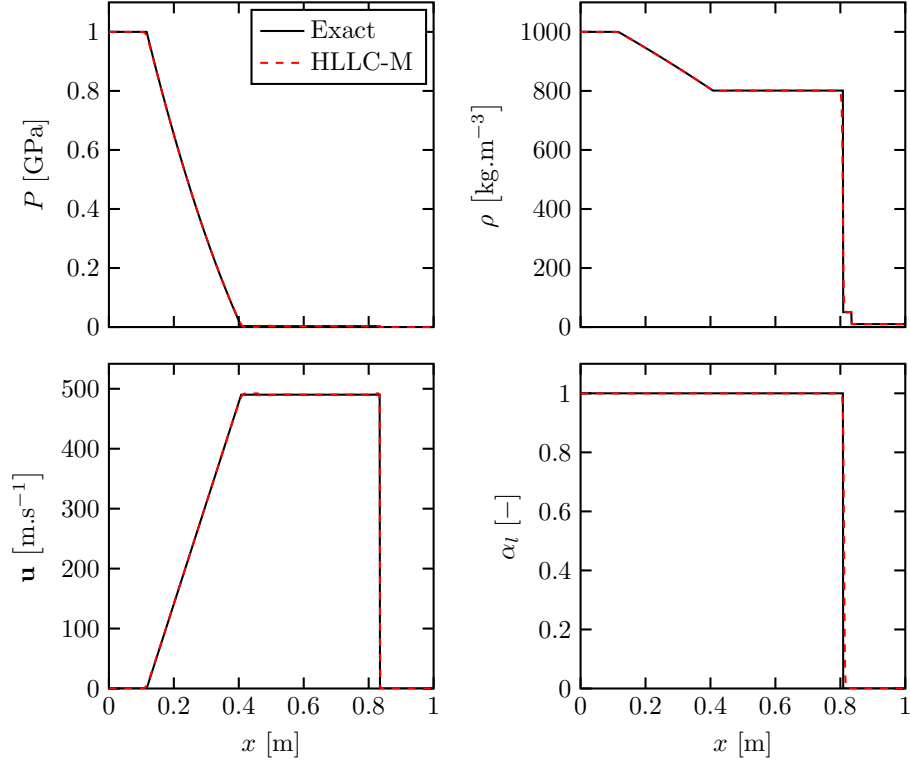
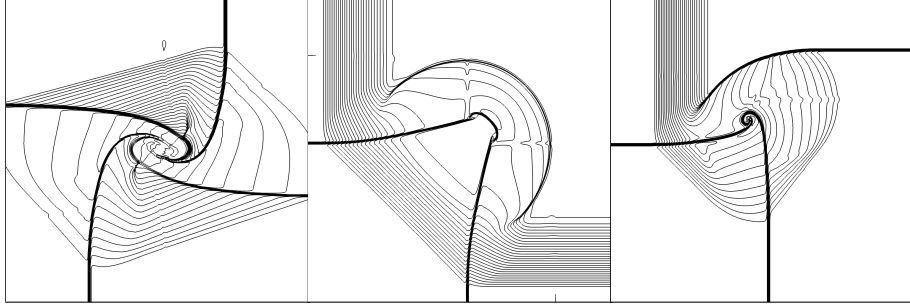


Figure B.12: Liquid-gas shock tube results at  $t = 220 \mu\text{s}$  at  $\text{CFL} = 0.5$ .



(a) Configuration of Eq. (B.4). (b) Configuration of Eq. (B.5). (c) Configuration of Eq. (B.6).

Figure B.13: Density isocontours (60 lines) on a  $600 \times 600$  grid at (a)  $t = 0.3 \text{ s}$ , (b)  $t = 0.25 \text{ s}$ , (c)  $t = 0.2 \text{ s}$ . The numerical scheme is HLLC-M RK3 with  $\text{CFL} = 0.7$ . The wave configurations are the following: (a) 4 contact discontinuities, (b) 2 contact discontinuities, 2 rarefaction waves, (c) 1 shock wave, 1 rarefaction wave, 2 contact discontinuities.

$$(\rho_0, \mathbf{u}_0, \mathbf{v}_0, P_0) = \begin{cases} (3.0, -0.6259, 0.1, 1.0) & x \leq 0, y \geq 0, \\ (0.8, 0.1, 0.1, 1.0) & x \leq 0, y \leq 0, \\ (0.5197, 0.1, 0.1, 0.4) & x \geq 0, y \geq 0, \\ (1.0, 0.1, -0.6259, 1.0) & x \geq 0, y \leq 0. \end{cases} \quad (\text{B.5})$$

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$$(\rho_0, \mathbf{u}_0, \mathbf{v}_0, P_0) = \begin{cases} (1.0, -0.6179, 0.1, 1.0) & x \leq 0, y \geq 0, \\ (0.8, 0.1, 0.1, 0.4) & x \leq 0, y \leq 0, \\ (0.5313, 0.1, 0.1, 1.0) & x \geq 0, y \geq 0, \\ (1.0, 0.1, 0.8276, 1.0) & x \geq 0, y \leq 0. \end{cases} \quad (\text{B.6})$$

### Appendix B.3.3. Order of accuracy

The order of accuracy of the scheme is next assessed thanks to the convection of an isentropic Gaussian vortex, defined with the following functions

$$v'_r = 0, \quad v'_\theta = \frac{\Gamma r}{R_c^2} \exp\left(-\frac{r^2}{2R_c^2}\right), \quad (\text{B.7})$$

while the temperature writes

$$T' = -\frac{\Gamma^2}{2C_p R_c^2} \exp\left(-\frac{r^2}{R_c^2}\right), \quad (\text{B.8})$$

785 where  $r = \sqrt{x^2 + y^2}$ . The pressure finally results from

$$P = P_\infty \left(\frac{T}{T_\infty}\right)^{\frac{\gamma}{\gamma-1}}. \quad (\text{B.9})$$

Tests are conducted on a  $[0, 0] \times [0.1, 0.1]$  meter square domain, filled with air, with periodic boundary conditions. Pressure and temperature are set to 101325 Pa and 300 K. The mean velocity is  $100 \text{ m.s}^{-1}$  while the vortex is characterized by a  $R_c = 1 \text{ cm}$  radius and a  $\Gamma = 1 \text{ m}^2.\text{s}^{-1}$  strength.

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The different profiles of density after one convective time depending on the limiter parameter  $\beta$  are shown in Fig. B.14. The MUSCL reconstruction allows to recover a correct solution without excessive diffusion.

A mesh convergence study is conducted to assess the spatial order accuracy of the scheme from  $32 \times 32$  to  $2048 \times 2048$  cells grids.  $\mathcal{L}^2$ -error for the density,



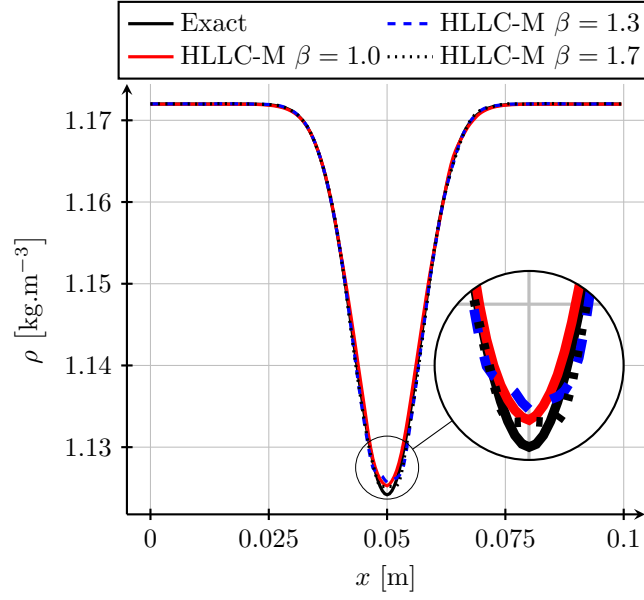


Figure B.14: Comparison of the schemes after one convective time with  $256 \times 256$  resolution.

795 where the  $\mathcal{L}^2$ -error is defined as

$$\mathcal{L}^2(\varepsilon_\rho) = \sqrt{\frac{\sum_i V_i (\tilde{\rho}_i - \rho_i)^2}{\sum_i V_i}}, \quad (\text{B.10})$$

with  $\tilde{\rho}$  the exact solution and  $V_i$  the node volumes, is shown in Fig. B.15 at  $\text{CFL} = 0.7$  for HLLC-MUSCL. A second-order accuracy is recovered, with the slope limiter parameter  $\beta$  having an influence only for coarse meshes.

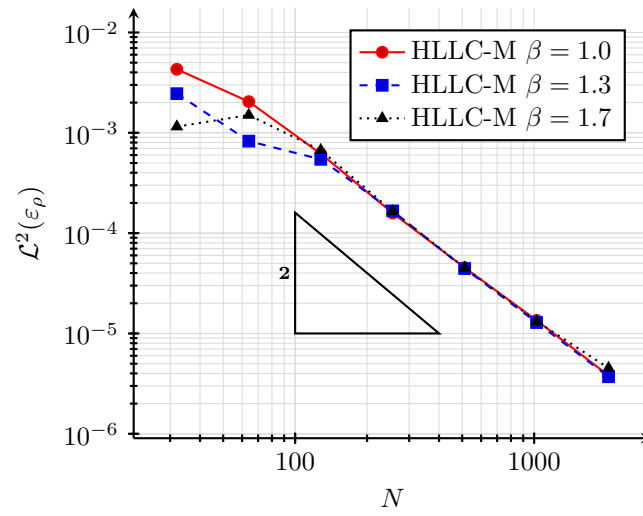


Figure B.15: Order of the schemes on the vortex test case after one convective time.