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# A Compressible Σ-Y Two-Fluid Atomization Model with Dynamic Interface Sharpening based on Flow Topology Detection

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**Abstract**

Liquid fuel atomization is characterized by multi-scale flow features and the coexistence of different flow regimes which complicate the simulation of an atomizing spray under realistic operating conditions. The present work introduces an atomization model dealing with such multi-scale complexities. The proposed model is compressible, so it can capture the density variations that affect spray penetration and atomization mechanisms. It is developed within a multi-phase Eulerian-Eulerian framework that considers slip velocity effects between the phases and introduces an additional transport equation for the surface area (Σ); the latter aims to model the unresolved sub-grid scale surface area variation. Moreover, a flow topology detection algorithm is applied in the flow field aiming to distinguish between different flow regimes; finally, the numerical algorithm applies appropriate closure relations for the interfacial source terms of the two-fluid model. The interfacial structures are also treated differently depending on the flow topology; a VOF method is applied in dense spray regions for resolving the interface fully and a non-sharp interface model is imposed in dilute spray regions, where sub-grid scale models are implemented for the modelling of relevant phenomena. The efficient coupling between the two-fluid model and the VOF method is examined via a standard interface capturing validation case of a rising bubble in a stagnant liquid. For the validation of the dynamic switching between different model formulations based on local topology and the numerical stability under the coexistence of various flow regimes, a Rayleigh-Taylor instability case is simulated and tested with the proposed model.

Keywords: two-fluid model, Eulerian-Eulerian framework, interface sharpening, flow topology, atomization, OpenFOAM®

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## Introduction

Liquid fuel atomization is a complex multi-scale phenomenon in space and time which has been extensively studied over the years, as it is a key factor in reducing pollutant emissions in combustion engines through the design of more efficient fuel injection systems. The numerical modelling of spray atomization concerns various mathematical methodologies aiming to the precise description of this complicated and computationally demanding problem. In the Discrete Droplet Method [1], the spray is represented within a Lagrangian framework in which each computational droplet represents a number of similar physical droplets and Eulerian equations are solved for the continuous gaseous phase. Source terms are introduced in the Eulerian equations to account for the interactions between the two phases. Nevertheless, the Lagrangian model is generally valid only in highly homogeneously distributed flows and introduces statistical error. The Σ-Y model [2] is a fully Eulerian model in which the liquid/gas mixture is treated as a pseudo-fluid with a single velocity field. Based on the single-continuum hypothesis, the source terms are eliminated from the governing equations and interfacial interactions are taken into account in the transport equation for the mean liquid mass fraction (Y). Moreover, the extent of the atomization process is computed from an equation for the interface density surface area (Σ) and then it is not required to presume any particular shape for liquid fragments, which are not necessarily spherical droplets in the atomization region. The ELSA model [3] is a coupled multi-phase solver which uses a fully Eulerian method for modelling the liquid in the near nozzle dense spray region additionally with a transport equation for Σ, all combined to a Lagrangian method for zones far away from the nozzle exit where the spray is sufficiently diluted, taking advantage of the benefits of each approach in specific flow regions. The Two-Fluid model [4] is a fully Eulerian model with the two phases being treated as inter-penetrating continua. A set of conservation equations is solved for each phase with additional source terms to consider the contribution of interfacial interactions and usually semi-empirical closure correlations which are highly dependent on the flow regime and introduce uncertainty in the model.

Each of the aforementioned atomization models provide accurate capturing of the flow phenomena under specific flow conditions. However, different mechanisms and flow regimes are dominant and affect spray penetration and atomization in different regions of the flow field, imposing the necessity of considering the multi-scale flow character in an accurate atomization model. Specifically, in the primary break-up zone intense surface tension effects are present and the flow regime can be considered mainly as a stratified flow with large-scale ligaments to be dominant, while aerodynamic forces and sub-grid scale phenomena dominate the dilute secondary break-up

zone far away from the nozzle exit. The present work introduces an atomization model which considers basic principles of the currently used models respecting the spatially and temporary changes of flow regimes and the need for the continuously changing flow topology to be treated accordingly within a single model framework. Validation cases of the various formulations of the proposed model are following.

**Numerical Method**

The proposed *Compressible Σ-Y Two-Fluid model* is taking advantage of the basic principles of the Two-Fluid model [4], the Σ-Y model [2] and a newly developed flow topology detection algorithm, which provides the flexibility of distinguishing dynamically between different flow regimes, namely a sharp and a diffusive interface regime, treating the interfacial structures accordingly and applying appropriate closure relations for the interfacial source terms based on the respective flow region and the local characteristics of the flow field. The model is developed in OpenFOAM using the compressible fully-Eulerian twoPhaseEulerFoam solver.

The governing equations of the atomization model consist of:

**i.** a set of continuity, momentum and energy conservation equations for each phase k

$$\frac{\partial}{\partial t}(a_k\rho_k) + \nabla\cdot(a_k\rho_k u_k) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(a_k\rho_k u_k) + \nabla\cdot(a_k\rho_k u_k u_k) = -a_k\nabla p + \nabla\cdot\left(a_k\tau_k^{eff}\right) + a_k\rho_k g + \sum_{\substack{l=1\\ l\neq k}}^{2} M_{kl} \tag{2}$$

$$\frac{\partial}{\partial t}(a_k\rho_k h_k) + \nabla\cdot(a_k\rho_k u_k h_k) + \frac{\partial}{\partial t}(a_k\rho_k k_k) + \nabla\cdot(a_k\rho_k k_k u_k) = -\nabla\left(a_k q_k^{eff}\right) + a_k\frac{\partial p}{\partial t} + a_k\rho_k g\cdot u_k + \sum_{\substack{l=1\\ l\neq k}}^{2} H_{kl} \tag{3}$$

In the momentum equation (2) the interfacial source term $M_{kl}$ depends on local flow topology.

- In the sharp interface regime, the surface tension is dominant against the aerodynamic forces and thus, its contribution is taken into account using the continuum surface tension force model of Brackbill et al. [5].
- In the diffusive interface regime, the aerodynamic forces and particularly the drag force acting on the dispersed fluid structures is the dominant factor in interfacial momentum exchange between the liquid and gaseous phases and is calculated using a characteristic length proportional to the liquid density surface area (Σ). Different drag models [6] are implemented depending on the flow regime.

In the energy equation (3) the interfacial source term $H_{kl}$ is modelled via a standard heat transfer model [7] irrespectively of the flow region.

**ii.** a transport equation for the liquid volume fraction

$$\frac{\partial a_1}{\partial t} + \nabla\cdot(a_1 u) + \nabla\cdot\left(u_c a_1(1-a_1)\right) = (1-v_{topo}) * \left[-\nabla\cdot[a_1(1-a_1)(u_1-u_2)] + \nabla\left(\frac{v_t}{Sc_t}\nabla a_1\right)\right] \tag{4}$$

where the artificial compression velocity is given by [8]: $u_c = C_a|u|\frac{\nabla a_1}{|\nabla a_1|}$

- In the sharp interface regime ($v_{topo}$=1), the compression coefficient $C_a$ is set equal to 1 for a sharp interface to be imposed. The liquid volume fraction equation is solved without the sub-grid scale terms of the RHS, so that the equation has the typical form of a phase fraction transport equation used in a VOF interface sharpening method and being solved with MULES solver in OpenFOAM [8].
- In the diffusive interface regime ($v_{topo}$=0), the compression coefficient $C_a$ is set equal to 0 and in the RHS appears a model for the turbulent liquid flux which captures the effect of the relative velocity between the two phases. The slip velocity contribution [9] is able to be modelled directly due to the two-fluid formulation, where for the drift velocity contribution a standard first order closure [10] with the properties of the liquid/gas mixture is implemented.

**iii.** a transport equation for the liquid density surface area

$$\frac{\partial \Sigma'}{\partial t} + \nabla\cdot(u\Sigma') = (1-v_{topo}) * \left[-\nabla\cdot\left[a_1(1-a_1)(u_1-u_2)\frac{\Sigma'}{a_1}\right] + \nabla\left(\frac{v_t}{Sc_t}\nabla\Sigma'\right) + \frac{\Sigma}{\tau_t}\left(1-\frac{\Sigma}{\Sigma^*}\right)\right] \tag{5}$$

where the simultaneous existence of liquid and gas implies the presence of a minimum interface area $\Sigma_{min}$ [11] and $\Sigma = \Sigma' + \Sigma_{min}$.

The source terms in the RHS of equation (5) represent the production and destruction of the surface density by mean shear, turbulence and liquid structure interactions. The sub-grid scale information is taken into consideration only in the diffusive interface regime ($v_{topo}$=0). Under the assumption of a dense zone, turbulence is the dominant mechanism for liquid break-up and coalescence and thus, $\tau_t$ is the turbulent time-scale [11].

The flow topology detection method uses two different switching criteria depending on the interfacial treatment of the currently examined cell in the previous iteration of the solution algorithm:

**i.** switching on the sharp interface

Based on the interface density, the mean Sauter droplet/bubble diameter ($d_\Sigma$) is calculated in each diffusive cell as following: $d_\Sigma = \frac{6a_1(1-a_1)}{\Sigma}$ [11]. When the mean Sauter diameter is larger than the cell size, then the previously diffusive flow features can no longer be treated as mesh unresolvable structures and a switch to a sharpened interface state is required.

$$d_\Sigma > min(d_{cell}) \tag{6}$$

**ii.** switching on the diffusive interface

In a previously sharply treated cell, based on the curvature (κ) of the sharp interface, a diameter of an equivalent spherical structure with the respective curvature can be calculated as: $d_{curv} = \frac{2}{\kappa}$ [12]. Assuming that approximately 3 cells are needed for the adequate capture of a spherical structure, when the following criterion is not satisfied, a diffusive interface should be imposed.

$$d_{curv} < 3 * max(d_{cell}) \tag{7}$$

## Results and Discussion

### *Rising Bubble*

The introduction of a sharpened interface within a two-fluid framework, as it is applied under the sharp interface regime of the proposed model, is a contradictory procedure. In the limit of a sharp interface, the velocities on either side of the interface must be equal in order to eliminate the relative velocity and meet a no-slip interface condition, while at the same time basic principle of the Two-Fluid model is the presence of two different velocity fields. In the Compressible Σ-Y Two-Fluid model an "artificial drag" term, as a function of relative velocity and time-step, is introduced in the momentum equations, similar to the approach presented by Strubelj et al. [13], so as to ensure instantaneous equalizing of the velocities near the resolved interface:

$$F_{Da} = F(u_r)\frac{\tau_r}{\Delta t} \tag{8}$$

where $F(u_r)$ is an expression proportional to the relative velocity $u_r$ between the two phases, Δt the time-step and $\tau_r$ a relaxation factor which needs to be calibrated in each case in order to meet a no-slip interface condition.

The effective coupling between the Two-Fluid model and a VOF method is examined against the benchmark case of an initially circular gas rising bubble in a stagnant liquid with density and viscosity ratios equal to 10, as proposed by Hysing et al. [14]. The two-dimensional simulation was conducted with the initial and boundary conditions of Figure 1 in a computational mesh of 320×640 cells. The gravity in the system is g=-0.98m/s$^2$ and the surface tension between the two fluids is σ=24.5N/m.

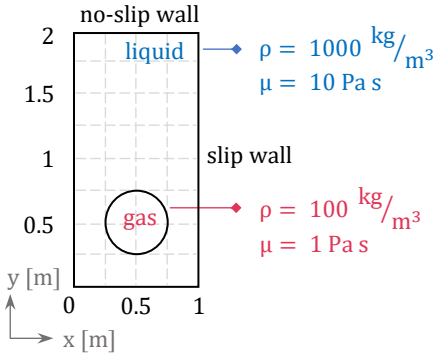


**Figure 1** Initial configuration and physical properties of a circular gas rising bubble in a stagnant liquid.

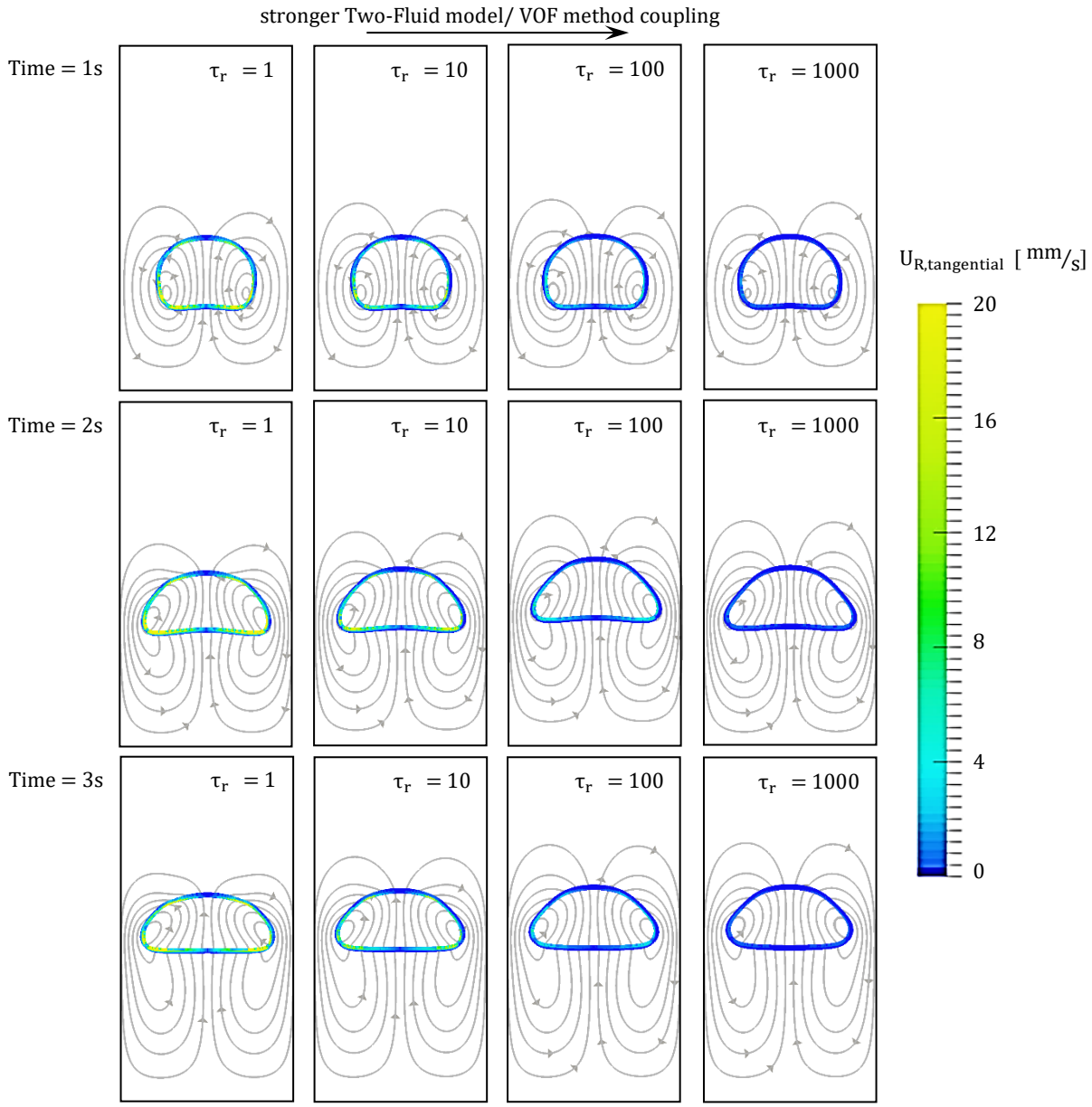


**Figure 2** Tangential relative velocity distribution at the interface of a rising bubble and gas/liquid mixture velocity vectors at successive times under the effect of different relaxation factors $\tau_r$.

As observed in Figure 2, a stronger coupling between the Two-Fluid model and the VOF method is achieved by maximizing the relaxation factor $\tau_r$ in the artificial drag force in equation (8). This "numerical trick" overcomes the two-fluid principle of the mathematical model which imposes different velocity fields for each phase and approaches a pure VOF method in which all phases share a single momentum equation. The increase of the relaxation factor apart from the gradual elimination of the relative velocity in the interfacial region of the bubble also affects the macroscopic characteristics of the interface evolution, such as the bubble shape development. Examining the benchmark quantities of bubble evolution in Figure 3, namely the mass centre position, the rise velocity and the circularity and comparing with the results presented by Strubelj et al. [15] using a similar concept of coupling the Two-Fluid model with an interface capturing method, it is verified that a stronger Two-Fluid model/VOF coupling using the maximum value for the relaxation factor provides an evolution of the rising bubble closer to the expected behaviour. Specifically, the final position of the bubble centre of mass with the optimum relaxation factor $\tau_r=10^3$ differs 1.22% from the reference solution, the maximum rise velocity is observed at 0.92s and deviates by 2.58% from Strubelj results, while the minimum bubble circularity occurs at 1.98s, approximately 0.1s later than in Strubelj results but with respect to the trend of circularity evolution in time and a quantitative error of 1.7%. Additionally, the shape of the bubble at its final position at 3s calculated with minimum and maximum $\tau_r$ values show the significant effect of an effective coupling in bubble shape development with regard to the results of Strubelj [15] and Hysing [14].

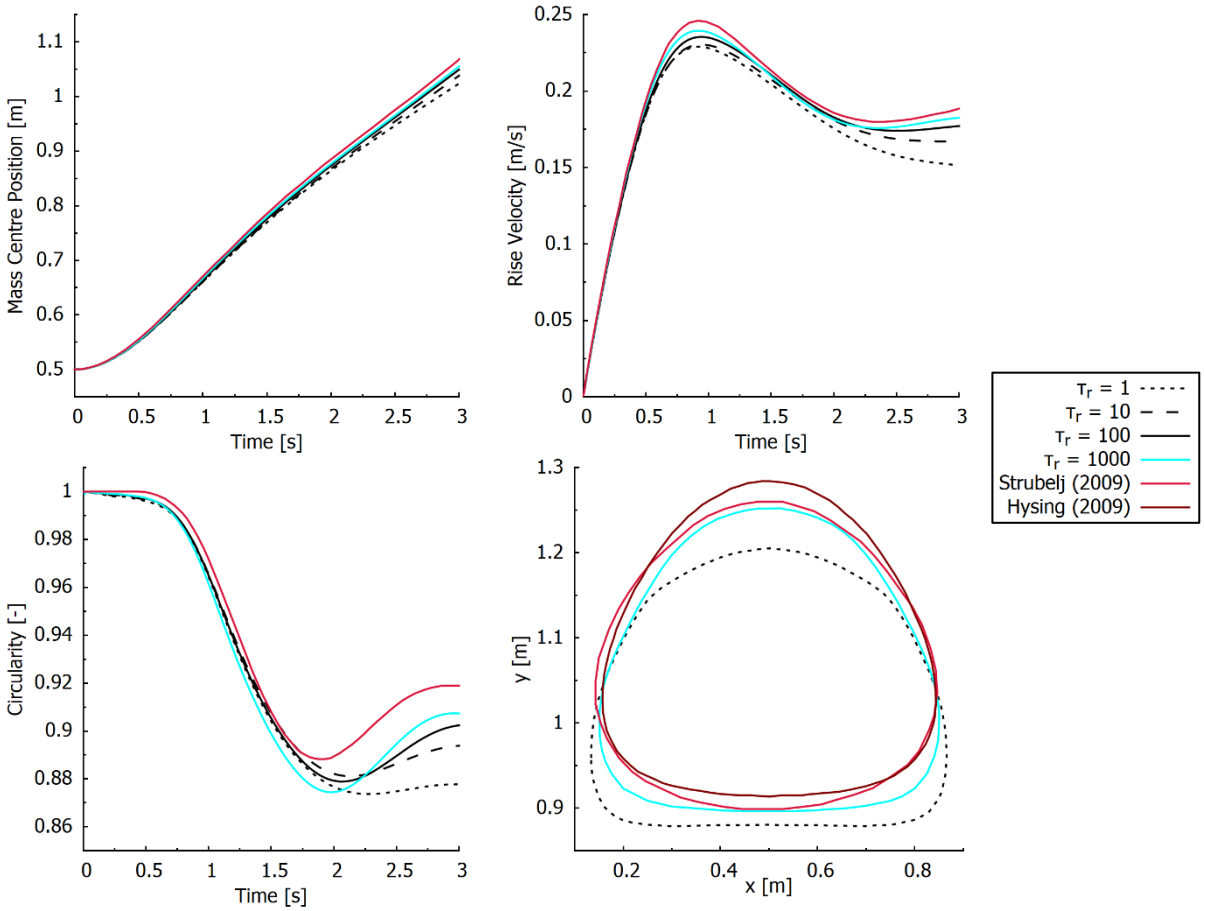


**Figure 3** Bubble benchmark quantities, i.e. mass centre position, rise velocity and circularity, evolution in time under the effect of different relaxation factors $\tau_r$ and in simulation performed by Strubelj et al. [15]. Bubble shape at its final position at 3s computed with minimum and maximum $\tau_r$ values and the models of Strubelj et al. [15] and Hysing et al. [14].

***Rayleigh-Taylor instability***

The Rayleigh-Taylor instability, being present in numerous natural and industrial systems, has been examined as a validation case for the proposed numerical model, so as to test the switching algorithm between the sharp and the diffusive interface regime and the model accuracy when operating under the classical Two-Fluid model and the Two-Fluid model/VOF coupling formulation simultaneously at the flow field with spatial and temporal switching between the two [13], [16]. The evolution of the instability starting from a stratified flow regime with significant surface tension effects and gradually developing to flow regions under the dispersed flow regime, makes it a suitable case to show the capabilities of the proposed model.

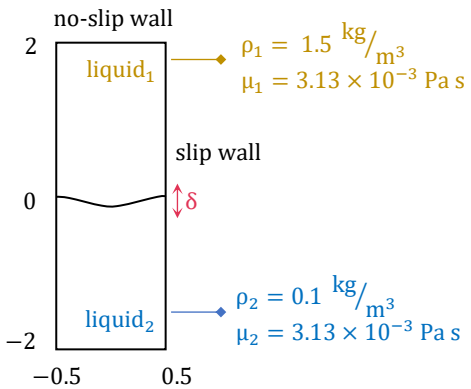


**Figure 4** Initial configuration and physical properties for the simulation of Rayleigh-Taylor instability.

Two immiscible isothermal fluids at ambient pressure and temperature with a density ratio 15 are located in a closed box with the higher density liquid to lie initially above the liquid with the lower density, as depicted in Figure 4. The gravitational forces in the system with gravity acceleration set to g=-9.8m/s$^2$ act to destabilize the interface between the two liquids and the higher density liquid starts to move below. On the other hand, the surface tension forces have an opposite effect on the system, trying to stabilize the interfacial disturbances. The surface tension coefficient between the two liquids is set to σ=0.01N/m. Two-dimensional simulations have been conducted with the initial configuration of Figure 4 in a coarse and a fine computational mesh of 64×256 cells and 128×512 cells respectively. An initial weak cosine disturbance is applied in the interface between the liquids at the initial state, as used in the simulations of Bilger et al. [17]:

$$y = -0.05cos(2\pi x) \tag{9}$$

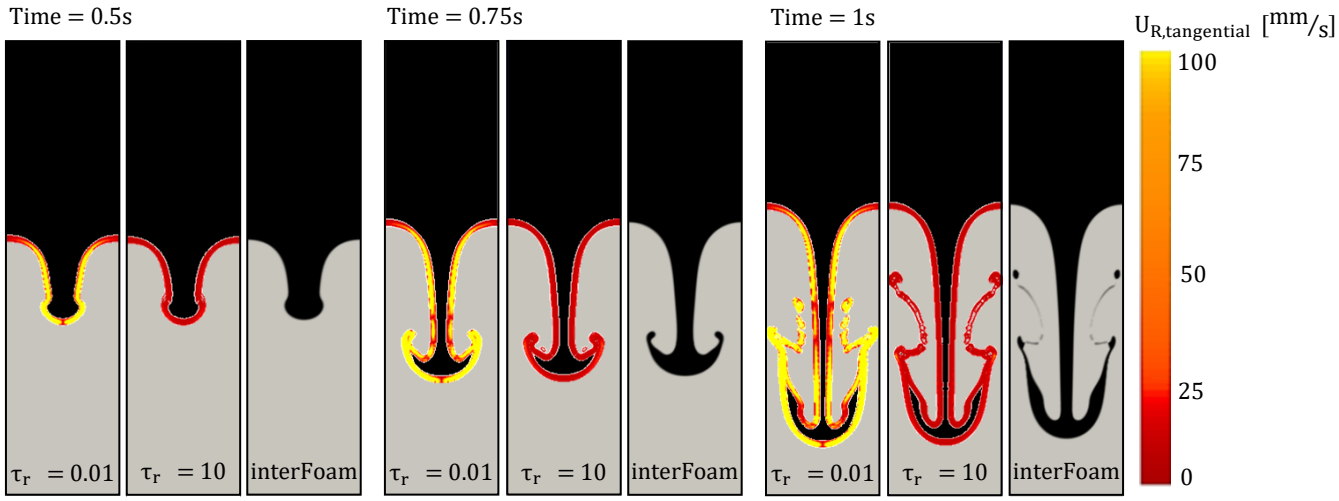


**Figure 5** Rayleigh-Taylor instability development and tangential relative velocity distribution at the interface at successive times under the effect of the suboptimal and the optimal relaxation factor $\tau_r$ and in simulation performed with interFoam solver.

At an initial state, Rayleigh-Taylor instability has been simulated with the fine mesh using exclusively the sharp interface regime formulation of the model under different $\tau_r$ values, so as to calibrate the optimum relaxation factor for an effective Two-Fluid model/VOF coupling. As depicted in Figure 5, the required relative velocity reduction at the interfacial region is performed successfully. Comparing the instability development with the solution obtained from interFoam, an OpenFOAM VOF solver with the implementation of MULES algorithm [8], it is noticeable that a non-adequate Two-Fluid model/VOF coupling leads to a non-physical evolution of the instability, as observed at 1s with $\tau_r$=0.01.

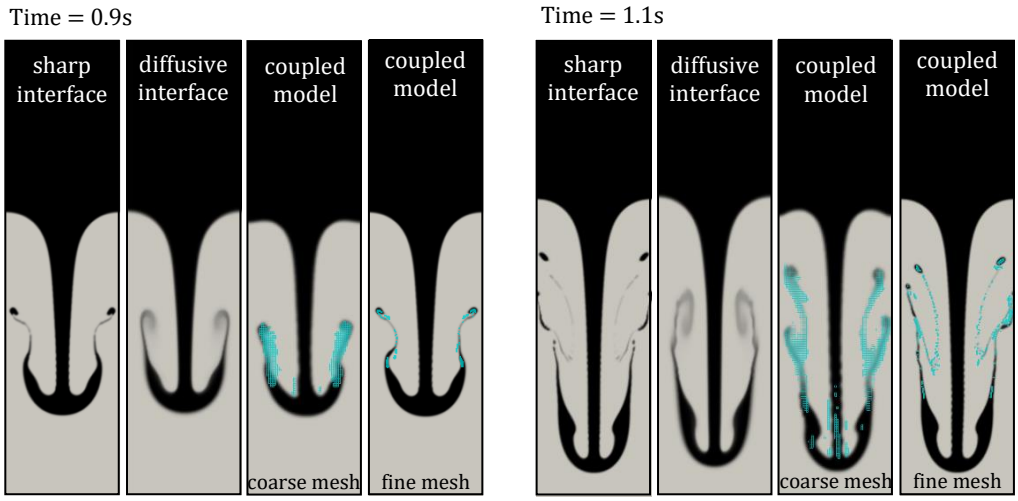


**Figure 6** Rayleigh-Taylor instability development at successive times obtained after simulations with different formulations of the atomization model. With blue colour in the coupled model results are marked the cells which are subject to a diffusive interface regime.

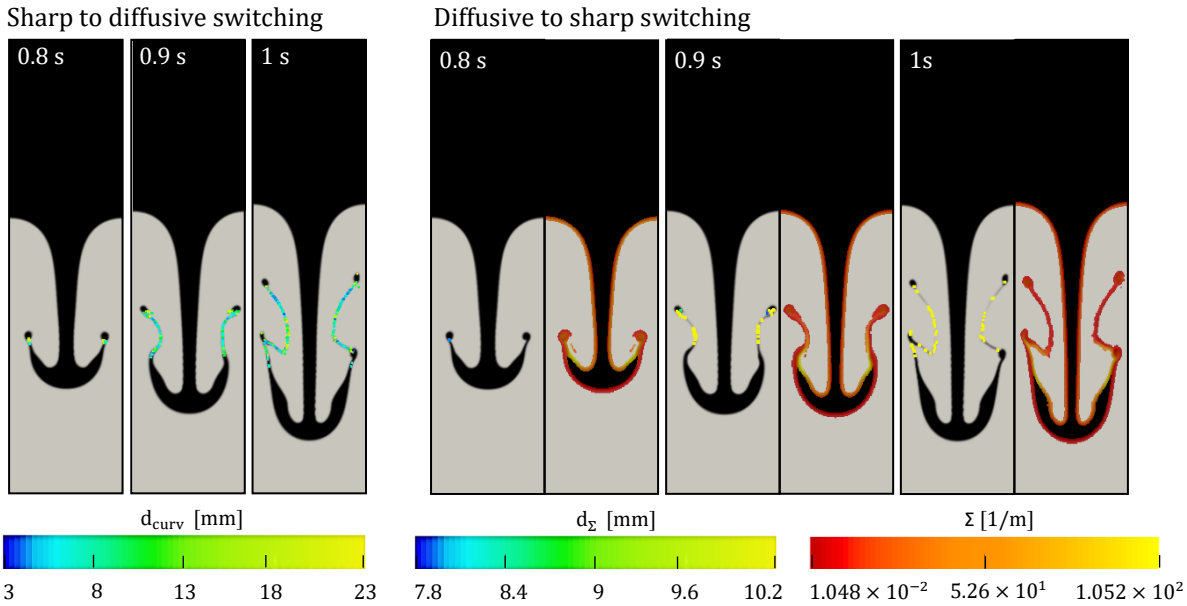


**Figure 7** Flow topology detection algorithm application and the characteristic diameter values based on which a regime switching is performed, i.e. the curvature equivalent diameter for a sharp to diffusive switching and the mean Σ Sauter diameter for a diffusive to sharp switching. The simulations have been conducted with a fine mesh.

As presented in Figure 6, Rayleigh-Taylor instability has been simulated under different formulations of the numerical model, namely only sharp interface regime, only diffusive interface regime and as a coupled model switching between the respective modes based on local flow topology. It can be observed that the finer the mesh, the closer the coupled model gets to the only sharp interface formulation with an instability development similar to the VOF results and most of the computational cells operating in the sharp regime. Nevertheless, even with the coupled model and a coarse mesh, the results of the computationally expensive VOF simulation are adequately captured and with a significant accuracy comparing to the exclusively diffusive solution. Thus, the coupled model methodology allows effectively the modelling of flow structures and phenomena which fall below the grid scale and avoids the use of a very fine computational mesh to capture the sub-grid scale information.

In Figure 7, there are marked at successive times the cells which exceed the bound of the quantitative criteria for flow topology regime switching as described in equations (6) and (7) and as a result in the following iteration of the solver will be treated within a different interface framework. The lower bound of the curvature equivalent diameter ($d_{curv}$) below which a flow structure can no longer be accurately resolved with a VOF method and should turn into a diffusive formulation is approximately 23.34mm. For switching on the sharp interface regime, the upper bound of the mean Σ Sauter diameter ($d_\Sigma$) calculated from the interface density (Σ) is the minimum cell diameter, namely 7.8mm for the uniform fine mesh. As depicted in the results, the coexistence of stratified and dispersed flow regimes during the evolution of Rayleigh-Taylor instability in time, allow the simultaneous switching between the sharp and the diffusive interface regime in different flow regions, increasing the complexity of the phenomenon and the computational challenge of the stability of the solution.

**Summary and Conclusions**

A Compressible Σ-Y Two-Fluid model has been developed and implemented in OpenFOAM aiming to simulate highly compressible flows with significant slip effects and multiscale complexities using a single solver, which detects dynamically the different flow regimes and operates under the appropriate formulation. The computationally challenging coupling of a Two-Fluid model with an interface sharpening method has been extensively examined and validated against a benchmark case of a rising bubble, obtaining useful results on how eliminating the relative velocity at the interfacial region to achieve an effective coupling. The model dynamic switching formulation based on local flow topology has been tested in a Rayleigh-Taylor instability case, where the initially stratified flow regime and the large-scale flow structures gradually develop to a dispersed flow regime with flow structures which fall below the grid scale. Comparing the results with different formulations of the model, it appears that Compressible Σ-Y Two-Fluid model is numerically stable under the coexistence and simultaneous switching between different flow regimes and has a decreased computational cost with regard to a VOF method due to the modelling of sub-grid scale phenomena and the avoidance of very fine meshes. Subject of the ongoing research is the implementation of high-speed liquid spray simulations using the proposed model capabilities.

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