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Exploring different approaches for the simulation of multi-scale atomization process

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Abstract

A big effort has been made in the last decades to try to numerically simulate multiphase flows and specifically the atomization process. This has become a key topic for aeronautical application, as the combustion process must be optimized in order to reduce pollutant emission. Despite this effort, there is not a global approach capable of simulating the entire atomization process, starting from the nozzle up to the disperse phase region. The first part of this work deals with the design of a simple configuration able to reproduce high Weber and Reynolds numbers of industrial interest, on which DNS computation can be performed. The second part introduces the comparison of the DNS experiments results with the ones of simulations performed with two reduced order models. The comparison addresses the topology (liquid core length, penetration study), the first and the second order statistics in the diffuse interface zone, in order to have for the first time a common test case to evaluate advantages and effects of different modelling strategies.

Introduction

More and more aggressive objectives have been imposed by ICAO on the reduction of NO_x emission leading to extensive effort in trying to simulate the atomization process. The nature of an atomized flow is extremely complex, due to its multi-scale nature. Near the nozzle outlet, coherent structures of liquid are separated from the gas phase and this region is commonly called separated phase zone. In a transition zone instabilities decompose the elongated structures in lignaments of liquid and downstream they end up in a polydisperse spray. In the literature it is possible to find different attempt to model the process starting from the nozzle up to the polydisperse spray. DNS simulation has been widely used to try to solve all the dynamics. The two phases are solved separately using interface reconstruction methods like VOF (Hirt and Nichols 1981), level-set (Osher and Fedkiw 2001) or a coupling of them (Ménard, Tanguy, and Berlemont 2007). The important computational and time effort at high Reynolds and Weber numbers and the limited opportunity to use complex geometries, has led to the development of reduced order models. Some research groups developed coupling strategies with the interface-capturing approach for the separated phase zone and with the Lagrangian approach for the disperse phase zone (Anez et al. 2018). Others have dedicated their effort on finding an unified description between the two zones, by progressing in the diffuse interface modelling (Drui et al. 2016) and in reducing the phase space in the disperse phase area (Essadki et al. 2018). By looking at the global picture, it is not clear which are the advantages of each model. One of the cause is that only few DNS computations have been done on the same configurations used as a benchmark for the validation of the different reduced order models, due to their complexity. Furthermore experimental results in the separated phase zone are challenging, due to the difficulty of optical techniques in capturing the dynamic of the flow in this zone. The purpose of this work is firstly to design a simple but at the same time industrially meaningful configuration on which DNS computation can be performed. Then the results can be compared with two reduced order models computations. A second objective is to evaluate the advantages of each model in terms of interface reconstruction and dynamics capturing, through qualitative and quantitative analysis.

The numerical configuration

The testing configuration is an air assisted planar liquid sheet simulated using ARCHER code (Ménard, Tanguy, and Berlemont 2007) developed in CORIA (fig. 1). In This DNS code is implemented the advanced CLSVOF interface reconstruction method, with Ghost Fluid used to keep the transition between the two phases in only one cell. This is a classical configuration used in literature (e.g. the review Dumouchel 2008) because it is manageable to obtain the entire multi-scale atomization process and it is possible to replicate high Reynolds and Weber numbers of industrial interest. In fact, at a defined density ratio the only governing parameter for this kind of flow is the momentum ratio $J = \frac{\rho_g U_g^2}{\rho_l U_l^2}$. The smaller the magnitude is, the wider the liquid core is and the further away from the nozzle will happen the atomization process (as detailed in Carvalho, Heitor, and Santos 2002). In order to have an extended liquid core together with a fast atomization, different configurations with different momentum ratio have been tested .

Figure 1: Surface of the liquid-gas interface and mid-plane of velocity contours for a DNS simulation of the numerical configuration. $n_x \times n_y \times n_z = 64 \times$ $256\times256.$

Numerical models and comparison strategy

In this work, two codes are used to simulate the test case described in the previous section. The diffuse interface strategy tested is implemented in the CanoP code. A thermodynamically and mathematically consistent model has been derived (Drui et al. 2016) and the diffusion at the interface between the liquid and the gas is managed through the use of high order numerical methods and Adaptive Mesh Refinement. The second strategy tested is an interface capturing model is based on an approach implemented in OpenFOAM (Rusche 2002). In this case the jump between the two phases and the diffusion is managed through the model, introducing a numerical flux opposite to the diffusion direction.

The comparison strategy covers four different points. First of all, topological features of the flow, such as penetration study and the length of the liquid core will be addressed. A second point of the comparison covers the time averaged velocity field, liquid volume fraction and density. These quantities

should give a general statistical characterization of the flow. The third point is to study the second order statistics (e.g Reynolds tensor \overline{uu} , correlation between velocity and liquid volume fraction $\overline{u\alpha}$, correlation between density and velocity $\overline{\rho u}$). These quantities are crucial in order to extend the study to a possible turbulence modelling strategy and to understand influence of the model on the correlations of different quantities. Correlations unified with the conditionally averaged quantities and the computation of curvatures (Di Battista et al. 2018) extend the study to the management of the transition from the separated phase zone to the disperse phase zone.

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