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DNS analysis of turbulent mixing in two-phase flows

B. Duret, G. Luret, J. Reveillon, T. Menard, A. Berlemont, F.X. Demoulin *

UMR6614-CORIA, Technopôle du Madrillet, BP 12, Avenue de l'Université, 76801 Saint-Etienne-du-Rouvray Cedex, France

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ABSTRACT

This study focuses on the evaporation and mixing process in turbulent two-phase flows with a direct resolution of the flow near the interface. A first approach, using a passive scalar to represent the evaporation and mixing process in a two-phase dense turbulent flow, has been developed and applied in a homogeneous isotropic turbulence over a large range of liquid volume fractions. This model is restricted to low vaporization rates, thus the interface is barely affected by the evaporation process. A statistical analysis of the vapor field is performed. Obtained results suggest that the beta PDF, frequently used in combustion modeling, are not adequate to represent the state of scalar mixing when interfaces are taken into account.

A spectral analysis of the velocity and the scalar field is carried out simultaneously in both phases as well as in each phase separately. A procedure using the liquid volume fraction field is employed to separate the contribution of each phase. The evaporation process does not affect the spectrum shape of the scalar, but it has a direct influence on the energy level of the scalar.

1. Introduction

The combustion of fuel issued from the evaporation of a liquid phase remains one of the major sources of energy, especially in the transport industry. Liquid injection in a combustion chamber is a critical step in fuel–air mixture preparation and its induced combustion. Hence, numerous studies have been devoted to the description and understanding of the injection process and its influence on vaporization and mixing. However, experiments are difficult, in particular in the vicinity of the dense zone of the spray. Numerical simulations could be of significant use if adapted methods are carefully developed following two main axes: the interface tracking ability and the phase change capture. These are sketched in Fig. 1 along with several major liquid/gas interactions to be captured.

The last decade has seen the apparition of various numerical methods devoted to two-phase flow simulations with an accurate description of the interface position and evolution. Volume of Fluid (Hirt and Nichols, 1981), Level Set (Sussman et al., 1994) and Front-tracking (Unverdi and Tryggvason, 1992) are the most common interface tracking methods developed to carry out direct numerical simulations of two-phase flows. In such simulations, discontinuities at the interface have to be treated carefully. With this aim, numerical methods such as the delta function method (Brackbill et al., 1992) and the ghost fluid method (Fedkiw et al., 1999) have been developed. The latter allows for applying sharp jump conditions at the interface and new works have proved it possible to accurately describe the primary atomization of liquid jets (Ménard et al., 2007; Desjardins et al., 2008; Shinjo and Umemura, 2010).

In the framework of combustion chamber modeling, interface tracking has to be coupled with an evaporation process. Such studies are relatively recent because of the complexity of multiple interactions between the various physical phenomena that prove to cover a wide range of different space and time scales (Tryggvason et al., 2005, 2010). Solving phase change requires the resolution of the Navier–Stokes equations, but energy and species equations have to be considered with appropriate jump conditions at the interface. The interface velocity is also affected by the phase change, as are mass and energy transfers (Fig. 1). All of these constraints lead to numerous problems, in particular the difficulty to estimate the local vaporization rate, which depends on the species and temperature gradients at the interface. Recently developed numerical methods to study these flows are expensive, and only basic configurations can be considered so far. One of the first tentative attempts was dedicated to bubbly flows with a two dimensional moving mesh (Welch, 1995). The mesh, which prevented wide deformations of the interface, limited this study. Moreover, computational costs were prohibitively expensive. Thereafter, Calimez (1998) made a major step forward by coupling phase change with the VOF method to study droplet group combustion in two-dimensions. Strong thermodynamic hypothesis were made to reduce computational cost and complexity. The same year, Juric and Tryggvason (1998) associated phase change with a front tracking method to simulate bubbly flows in two-dimensions. But this method was

* Corresponding author. Tel.: +33 232 953 674; fax: +33 232 910 485.
E-mail address: demoulin@coria.fr (F.X. Demoulin).

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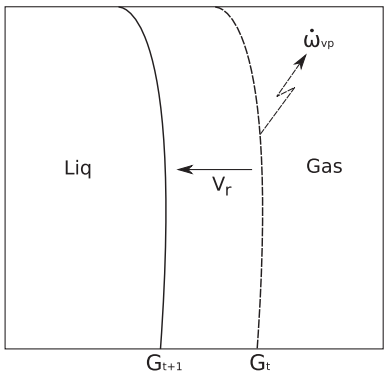

Fig. 1. Phase change phenomena at the interface. V_r is the regressing velocity, $\dot{\omega}_{vp}$ is the local vaporization rate, G is the Level Set function.

unable, at the time, to manage significantly deformed interfaces. More recently, Tomar et al. (2005) studied phase change with a coupled Level Set VOF method but found it was necessary to smooth discontinuities across the interface. By using the Ghost Fluid method coupled with the Level Set method in two dimensional simulations, Tanguy et al. (2007) and Gibou et al. (2007) subsequently proposed a model to determine interface velocities aimed at solving continuity equations even including evaporation source terms. Strotos et al. (2008) analyzed droplet vaporization on a heated wall thanks to adaptive mesh refinement and the coupling between evaporation models and the VOF method. Schlottke and Weigand (2008) also developed a model to calculate velocities at the interface for deformed droplet vaporization in three dimensions with the VOF method.

All of the above mentioned methods are very promising. However, their complexity prevents them from being used in practical geometries. In this work, we propose to simplify the interactions between the various physical phenomena while focusing on the capture of an accurate vapor field. Saturation conditions at the interface are assumed to be constant, particularly the vapor pressure. No energy equation is resolved, and the liquid's vapor evolution is characterized by an inert scalar. Because the flow remains inert, the vapor mass fraction is equivalent to the mixture fraction, which defines the level of mixing between vapor and air. The saturation level of vapor in the domain can normalize this mixture fraction. It leads to the variable Z, which is thus bounded between 0 (no fuel vapor) and 1 (saturated fuel vapor). Z is an inert scalar, the evolution of which is driven by a standard convection/ diffusion equation in the gas phase. Z is bounded by 1 at all interface positions. A sketch to illustrate the simplified evaporation process is shown in Fig. 2. This is the first step towards a simultaneous

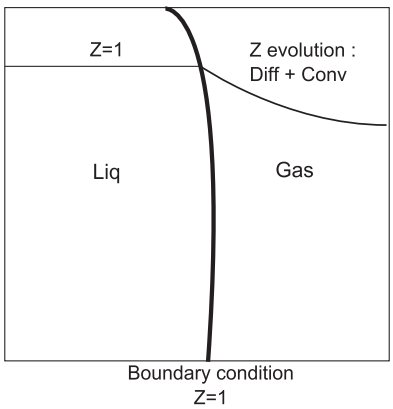

Fig. 2. Phase change modeling at the interface in the present work.

understanding of atomization, vaporization and mixing processes in dense sprays. As a preliminary work, since the mixing characteristic time is very short compared to the evaporation delay, interface regression is not considered. We focus on the properties of Z when the flow is shifting from very dense towards dispersed liquid presence, which mimics the liquid spatial evolution of an atomization process. To accurately control the various inputs of the simulation, a three-dimensional forced homogeneous turbulence of a gas/ liquid flow is considered with a liquid volume fraction ranging from 1% to 99%. Both phases will be resolved in DNS with the ARCHER code (Ménard et al., 2007); the interface tracking method that has been used is a coupled Level Set/VOF method. A high-density ratio between the two phases is chosen to simulate realistic engine conditions. Both quantitative and qualitative aspects are analyzed.

In the following part of this work, the constitutive equations and numerical procedures are first described. The flow geometry is then depicted along with the various prescribed parameters. Next, a statistical analysis of the mixture fraction is carried out by studying the evolution of the probability density function of Z. Finally, an original spectral analysis is proposed, giving rise to the discussion of the links between droplet dispersion, the evaporation process and the final topology of vapor of liquid.

2. Numerical considerations

2.1. Navier–Stokes and scalar equations

The joint Level Set/VOF method is coupled with a projection method to carry out the direct numerical simulation of incompressible Navier–Stokes equations:

$$\frac{\partial \boldsymbol{V}}{\partial t} + (\boldsymbol{V}.\nabla)\boldsymbol{V} = -\frac{\nabla p}{\rho} + \frac{1}{\rho}\nabla.(2\mu \boldsymbol{D}) + \boldsymbol{g} + \boldsymbol{f} + \frac{1}{\rho}\sigma\kappa\delta(G)\boldsymbol{n} \tag{1}$$

where p is the fluid pressure, $\boldsymbol{V}$ the velocity vector, $\boldsymbol{g}$ the gravity vector, μ the dynamic viscosity, and $\boldsymbol{D}$ the viscous deformation tensor. At the interface, the surface tension force can be considered based on the Dirac function $\delta(G)$: σ is the surface tension, $\boldsymbol{n}$ the normal unit vector, κ is the curvature computed from the Level Set function G (definition of κ, $\boldsymbol{n}$ and G are given in Section 2.2). The gravity term is neglected in this study. To solve the derivatives, a fifth-order scheme, WENO 5 (Shu, 1997), is used for convective terms, and a second-order central finite difference scheme is chosen for diffusive terms. (See Ménard et al. (2007) for further details concerning the numerical procedure.) A forcing method is necessary to maintain the turbulent kinetic energy at a prescribed level. This is achieved through the source term $\boldsymbol{f}$, which induces linear forcing (Rosales and Meneveau, 2005). It results in $\boldsymbol{f} = A\boldsymbol{v}'$, where A is the forcing coefficient, $\boldsymbol{v}'$ represents velocity fluctuations, and $\bar{\boldsymbol{v}}$ is the mean flow velocity. In this paper, $\overline{(\cdot)}$ refers to volume averaging. A Reynolds decomposition has been applied to the velocity field $\boldsymbol{V}$. The evolution equation of the turbulent kinetic energy $k = \frac{1}{2}\overline{\boldsymbol{v}'^2}$ may be written:

$$\frac{\partial k}{\partial t} + \nabla \cdot (\bar{\boldsymbol{v}} k) = C_k + 2Ak \tag{2}$$

where C_k regroups the typical energetic contributions (i.e. without forcing) for the sake of clarity. The estimation of C_k involves a phase change and a liquid–gas interface. It is therefore complex to estimate A directly from Eq. (2), thus, the following two-stage procedure has been set up:

Stage 1. Estimation of C_k^{n-1} based on the A^{n-1} constant value:

$$C_k^{n-1} = \frac{k^n - k^{n-1}}{\Delta t} - 2A^{n-1}k^{n-1} \tag{3}$$