International Journal of Multiphase Flow 85 (2016) 326–335

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

journal homepage: www.elsevier.com/locate/ijmultiphaseflow

DNS analysis of small-scale turbulence-scalar interactions in evaporating two-phase flows

Zakaria Bouali[a], Benjamin Duret[b], François-Xavier Demoulin[b], Arnaud Mura[a,*]

[a] Institut Pprime, UPR3346 CNRS - ENSMA and University of Poitiers, BP40109, 86961 Chasseneuil, France
[b] UMR6614-CORIA, Technopôle du Madrillet, BP 12, Saint-Etienne-du-Rouvray Cedex 76801, France

ARTICLE INFO

Article history:
Received 16 November 2015
Revised 2 June 2016
Accepted 25 June 2016
Available online 1 July 2016

Keywords:
Turbulent flows
turbulence-scalar interaction
Two-phase flows with vaporization
Scalar dissipation rate

ABSTRACT

Scalar dissipation rate (SDR) is a key quantity in turbulent flow modeling since it measures the scalar mixing intensity. It is well known that turbulence-scalar interaction (TSI) processes play an essential role in turbulent scalar mixing and drive to a large extent the SDR evolution. These processes are characterized by the tensor inner product between the scalar gradient vector and the strain-rate tensor. Direct numerical simulations are conducted to analyze the physics of this interaction in vaporizing turbulent two-phase flows. The well known alignment of the scalar gradient with the most compressive principal direction of the strain-rate tensor – resulting in production of the scalar gradient by turbulence – is recovered in statistics collected sufficiently far from the liquid–gas interface. By contrast, the action of the turbulence-scalar interaction is progressively attenuated as we approach this interface, where the scalar gradient tends to have a direction intermediate between the extensive and the compressive directions. This result questions the validity of passive-scalar turbulence concepts and closures that are commonly used for to tackle the modeling of scalar behavior in vaporizing two-phase flows featuring (or not) subsequent chemical reactions.

1. Introduction

It is commonly admitted that the scalar dissipation rate (SDR), which is defined as the product of the scalar diffusivity with the squared scalar gradient, provides a good measure of the molecular mixing efficiency (Bilger, 2004). This quantity indeed settles the equivalence ratio probability density function (PDF) the importance of which is crucial for combustion ignition. The consideration of its transport equation shows that, in gaseous conditions, it is mainly driven by two terms: (i) a dissipation contribution and (ii) the third-order correlation between the velocity gradient tensor and the small-scale scalar anisotropy tensor. The scalar mixing efficiency thus appears to be controlled by the latter quantity, which is often denoted as the turbulence-scalar interaction (TSI) term. It can be shown that only the symmetric part (rate of strain) of the velocity gradient tensor contributes to this term; the antisymmetric part indeed modifies the orientation of the scalar gradient but not its magnitude. Then the classical approach is to analyze this contribution in the eigenframe of the rate of strain tensor (Betchov, 1956; Tsinober, 2009). Such analyses show that, in homogeneous isotropic turbulence (HIT), the scalar gradient tends to align with the most compressive direction, thus leading to SDR production. However, the presence of a density jump with mass exchange at the interface is expected to modify this classical picture. For instance, it has been recently established that propagating premixed flames may change the sign of this specific contribution with SDR production ensured by other terms in the SDR budget (Chakraborty et al., 2011; Chakraborty and Swaminathan, 2007; Mura et al., 2008). Clearly, the presence of an interface with mass exchange is thus expected to promote similar changes in turbulent flows with vaporization. The influence of vaporization on mixture fraction statistics, i.e. scalar PDF, has been early anticipated by Borghi (1996) and recently analyzed in detail by Duret et al. (2012a). Considering the close relation that exists between the one-point one-time scalar PDF and micro-mixing term (Chen et al., 1989), we expect that the vaporization effects will also affect the SDR dynamics. To the best of the authors' knowledge this issue has never been addressed in the scientific literature and this is the objective of the present study to scrutinize this influence.

The present manuscript is organized as follows: the next section introduces the numerical methodology that is used to construct a Direct Numerical Simulation (DNS) database of turbulent two-phase flows with vaporization. The derivation of the scalar dissipation rate transport equation is then discussed in

* Corresponding author. Fax: +33 549 498 176.
E-mail address: arnaud.mura@ensma.fr (A. Mura).

http://dx.doi.org/10.1016/j.ijmultiphaseflow.2016.06.020
0301-9322/

Section 3 within the framework of the two-phase flow conditions that are presently investigated. The core of the present study follows in Section 4, which offers a detailed investigation of the TSI contribution. It is based on a classical orientation analysis, which is performed in the eigenframe of the strain-rate tensor. Finally, the manuscript ends with a brief section of conclusions where some perspectives for future works are also presented.

2. Numerical methods

2.1. Navier–Stokes solver and interface tracking method

A detailed presentation of the computational method may be found elsewhere (Duret et al., 2012a), and only its salient ingredients will be recalled below. The computations make use of a joint level-set volume-of-fluid method, which is coupled to an incompressible flow projection algorithm. The corresponding solver is used to perform the direct numerical simulation of incompressible flows described by the Navier–Stokes equations:

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

where p is the fluid pressure, $\boldsymbol{V}$ is the velocity vector, $\mu = \rho\nu$ is the dynamic viscosity, and $\boldsymbol{D}$ is the viscous deformation tensor. At the interface, the surface tension force is taken into account: the quantity σ denotes the surface tension, $\boldsymbol{n} = \nabla G/|\nabla G|$ is the normal unit vector pointing towards the liquid phase, and $\kappa(G) = \nabla.\boldsymbol{n}$ is the curvature evaluated from the level set function G. To compute the spatial derivatives, a fifth-order WENO scheme is used for convective terms (Shu, 1997), while a second-order central finite difference scheme is employed for diffusive terms. A forcing method is required to maintain the turbulent kinetic energy at a prescribed level. This is achieved through the source term $\boldsymbol{f}$ in the righ-hand side of Eq. (1), which induces a linear forcing (Rosales and Meneveau, 2005), and results in $\boldsymbol{f} = A\boldsymbol{v}'$ where A is the forcing coefficient, and $\boldsymbol{v}'$ denotes velocity fluctuations. In the present study, the operator $\overline{(\cdot)}$ refers to volume averaging and a Reynolds decomposition is applied to the velocity field $\boldsymbol{V} = \overline{\boldsymbol{v}} + \boldsymbol{v}'$ with $\overline{\boldsymbol{v}}$ being the mean flow velocity.

A brief overview of the interface tracking method and treatment of discontinuities is now provided. The level set method uses a continuous function to describe the interface (Osher and Fedkiw, 2001; Sethian, 1996). This function is defined as the signed distance between any points of the domain and the interface. The zero level curve ($G = 0$) therefore provides the interface location. The transport equation that describes the motion of the interface reads:

$$\frac{\partial G}{\partial t} + \boldsymbol{V}.\nabla G = 0. \tag{2}$$

Equation (2) is the hyperbolic type, and its discretization must combine a high convergence order and robustness. Thus, a fifth-order WENO scheme (Shu, 1997) is used to discretize the convective term in the above equation. Unfortunately the level set G no longer remains a distance function when solving Eq. (2) numerically, and a renormalization algorithm is thus applied to keep it as the signed distance to the interface (Sussman et al., 1998). However, even if combined with such a redistancing algorithm, the numerical resolution may induce a loss of mass in under-resolved regions. Therefore, many extensions of the method have been proposed (Enright et al., 2002; Olsson and Kreiss, 2005; Sussman and Puckett, 2000). The coupled level-set/volume-of-fluid method (CLSVOF), see Sussman and Puckett (2000), was found to be well-suited to capture atomization processes (Lebas et al., 2009; Menard et al., 2007). The main concept behind the CLSVOF method is to take benefit from the advantage of both level-set and VOF strategies: mass loss is limited through the VOF method, and a detailed description of interface properties is ensured with the level-set framework.

Fluid dynamics equations are solved within the low Mach number framework, based on a projection method for the direct numerical simulation of incompressible Navier–Stokes equations (Tanguy and Berlemont, 2005). Density and viscosity depend on the sign of the level set function according to each phase (liquid and gas). Jump conditions across the interface are taken into account with the ghost fluid (GF) method. In the GF method, ghost cells are defined on each side of the interface (Kang et al., 2000; Liu et al., 2000), which prolongs the description of each phase beyond the interface location so as to allow smooth derivatives computations in the vicinity of the interface. As defined above, the interface is characterized through the distance function, and jump conditions are extrapolated on a few nodes on each side of the interface. Further details on the implementation of the GF method to solve the Poisson equation with discontinuous coefficients can be found in Liu et al. (2000) and Tanguy and Berlemont (2005).

2.2. Scalar transport equation

2.2.1. Evolution equation

The choice of the passive scalar is representative of an evaporation process occurring at low temperature levels at the interface, inducing a low saturation pressure of vapor at the interface. In such a case, assuming local thermodynamic equilibrium at the liquid–gas interface, an evaluation of the saturation level of the vapor mass fraction Y_{vs} can be made by means of the Clausius–Clapeyron equation. In this study, the considered scalar ξ is the normalized form of the vapor mass fraction: $\xi = Y_v/Y_{vs}$. The scalar is thus equal to unity at the liquid–gas interface, and it evolves in the gas phase due to convection and diffusion. Following our previous investigation (Duret et al., 2012a), it is considered herein that the amount of mass transferred from the liquid into the gas phase is small enough to be neglected if the saturation equilibrium is reached rapidly, which is the case. Therefore, the mass of liquid in the domain remains approximately constant while the vapor phase evolution is considered and analyzed. This assumption leads to no significant phase change, but it is of practical interest to the study of scalar mixing induced by vaporization when turbulence velocity fluctuations are greater than the Stephan flow velocity. Moreover, as emphasized in our recent DNS studies on evaporating two-phase flows (Duret et al., 2013a; 2014), considering the whole process of vaporization requires additional equations, such as energy and species equations, as well as additional jump conditions. Using such a formalism would undoubtedly improve the description of the vaporization process but it is not yet adapted for the present HIT configuration because of the confinement effect due to periodic boundary conditions.

The evolution equation of the inert scalar ξ may be written:

$$\frac{\partial \xi}{\partial t} + \boldsymbol{V}.\nabla\xi = \nabla.(\mathcal{D}\nabla\xi), \tag{3}$$

where $\mathcal{D}$ is the molecular diffusivity, which is evaluated from the viscosity values without any specific account of non-unity Schmidt number effects, i.e. $\mathcal{D} = \nu_g$.

From the numerical point of view, a fifth-order WENO scheme is used to compute the convective terms, while for molecular contributions, a second-order central finite difference scheme is used. Finally, as stated above, the time integration is performed by using a third-order Runge–Kutta scheme.

2.2.2. Interface boundary condition

As far as reactive flows are concerned it is standard to consider a transport equation similar to Eq. (3), but featuring a source term $\dot{\omega}_\xi$ associated to the influence of vaporization on the concentration