International Journal of Heat and Fluid Flow 31 (2010) 93–100

Contents lists available at ScienceDirect

International Journal of Heat and Fluid Flow

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

Large Eddy simulation of a droplet laden turbulent mixing layer

W.P. Jones *, S. Lyra, A.J. Marquis

Department of Mechanical Engineering, Imperial College London, Exhibition Road, London SW7 2AZ, UK

ARTICLE INFO

Article history:
Received 19 December 2008
Received in revised form 15 July 2009
Accepted 3 October 2009
Available online 6 November 2009

Keywords:
LES
Mixing layer
Two-phase flows
Self-similarity
Preferential particle concentration

ABSTRACT

Large Eddy simulation (LES) is applied to a droplet laden turbulent mixing layer and the influence of shear, on the transport and preferential concentration of the dispersed phase is discussed. A Lagrangian formulation has been adopted for the particle dispersion coupled with an Eulerian description for the carrier gas. A stochastic model has been used to account for influence of the sub-grid scale motions of the continuous phase on the particle motion. Simulations conducted neglecting this sub-grid dispersion model show that the liquid dispersion is under predicted. However, when the sub-grid model is included the results show good agreement when compared with the experimental findings, demonstrating that the characteristics of the flow are well captured. A sensitivity analysis on the effect of the dispersion constants has been conducted, suggesting that increasing the contribution of the stochastic term, leads to a higher accumulation of smaller particles at the edge of the mixing layer.

1. Introduction

Two-phase flows are encountered in many practical systems with industrial, environmental and biomedical applications. Examples of such flows include the dispersion of pollutants in the atmosphere, the transport of liquid spray droplets in internal combustion engines and jet engine combustors, the dilution of medicines by blood through the vessels and dust inhalation into human lungs. Industrial and aircraft gas turbines in particular, are fuelled by liquid hydrocarbons making spray atomisation and evaporation crucial phenomena in the analysis of combustion dynamics.

Over the past decades, extensive experimental and theoretical studies have been performed to determine the response of particles (solid or liquid) in shear flows and the modification of turbulent characteristics, in a number of different geometrical configurations such as turbulent jets, boundary layers and mixing layers, Chung and Troutt (1988), Kulick et al. (1994). Mixing layers in particular, are characterised by the presence of large-scale stream and spanwise vortical structures, with size comparable to the transverse length scale of the flow, that play a dominant role in the particulate dispersion process and whose interaction causes the growth of the mixing region, Brown and Roshko (1974). The effects of these structures on solid particle dispersion has been studied by Chein and Chung (1987), Lazaro and Lasheras (1992) concluding that the dispersion phenomena are strongly dependent on the size of the particulate phase. Squires and Eaton (1991a) investigated the preferential concentration of solid particles in high strain regions, in terms of the Stokes number while Kiger and Lasheras (1997) examined the additional dissipation of the kinetic energy occurring due to interphase energy transfer in dilute particle laden shear flows. Despite the numerous experimental efforts, several aspects governing the interaction of liquid droplets or solid particles on a carrier gas phase remain unsolved as it is often difficult to isolate the momentum exchange between particles and gas from the production and dissipation mechanisms in a turbulent flow.

Consequently, numerical simulations for the prediction of the interactions between particles and turbulence and the modulation of turbulence due to the particles' motion have received increasing attention. Direct numerical simulation (DNS) of particle transport in homogeneous isotropic stationary, Squires and Eaton (1990, 1994), or decaying, Elghobashi and Truesdell (1993), turbulence with two-way coupling between the gaseous and the discrete phase suggests that the presence of particles increases the turbulent kinetic energy at high wave numbers and decreases it at low wave numbers and that the distortion of the turbulence energy spectrum depends on parameters such as the particle relaxation time. Later studies, Squires and Eaton (1991b), focused on the particle dispersion, turbulence modulation and preferential concentration of solid particles or liquid droplets and demonstrated that the mixing of particles by turbulence depends strongly on the relative timescales of the two phases.

Despite the fact that DNS studies can provide a detailed description of two-phase flows, they are still very expensive computationally, even when a moderate number of particles is considered. Large Eddy simulation (LES) is a promising tool for the prediction

* Corresponding author. Tel.: +44 0207594 7037.
E-mail address: w.jones@imperial.ac.uk (W.P. Jones).

0142-727X/$ - see front matter © 2009 Elsevier Inc. All rights reserved.
doi:10.1016/j.ijheatfluidflow.2009.10.001

of turbulent flows as it is less computationally demanding and has proved able to provide an accurate description of turbulent mixing. In LES, direct simulation techniques are applied to determine precisely the contribution of the large-scale flow features, which are assumed to be the most important with respect to momentum and energy transport in turbulent flows. A spatial filter is applied to the governing equations, in order to eliminate the need to solve the contribution of the scales smaller than the filter width, Piomelli (1999). The LES equations that describe two-phase flows include terms that represent the sub-grid fluctuations of the continuous phase and the filtered source terms arising from the contribution of the dispersed phase. Several LES studies, Wang and Squires (1996), Uijttewaal and Oliemans (1996), Wang and Squires (1998), Yeh and Lei (1991a,b), have been conducted taking into account only the effects of the resolved scales and neglecting the influence of the unresolved scales on the particle motion, under the assumption that the trajectories of the heavy particles ($\mathrm{St} \gg 1$) are not affected by the smaller turbulent scales due to their inertia, despite the fact that in these simulations small particles ($St \sim 1$), were also considered. Fundamental studies, Miller and Bellan (2000), have shown that the sub-grid effects on the droplet transport in turbulent shear flows cannot be neglected as significant errors are introduced in the prediction of the droplet drag force and evaporation rates if they are omitted. As a consequence for small droplets the interactions between turbulence, spray dispersion, vapour micro-mixing and combustion that occur at scales much smaller than the filter width can be significant and models are thus required for sub-grid scale effects on droplet break-up, dispersion and evaporation.

The present study aims to investigate numerically, by the use of LES, a spatially evolving, turbulent, droplet laden mixing layer and focuses on the influence of shear, on the transport and preferential concentration of the dispersed phase. The liquid phase is tracked in a Lagrangian reference frame, whereas the gas phase flow variables are solved in an Eulerian reference frame. A stochastic model has been used for the representation of the effects of the unresolved scales on the droplet motion.

The model involves a Weiner process in which the diffusion coefficient is a function of the sub-grid turbulence kinetic energy and a particle 'Eddy-interaction' timescale. This timescale is dependent on the sub-grid timescale and the particle relaxation time and involves two constants, C_o which is of the order of unity and α which has been assigned a value 0.8. Previous studies, Bini and Jones (2008), have discussed the effect of the stochastic term on the normalised liquid concentration in similar shear flows, concluding that if it is neglected the particle diffusion is underestimated. In addition, the influence of the 'Eddy- interaction' timescale has been investigated, where it was demonstrated to have a significant effect on the particle acceleration probability density function, *pdf*. Moreover, Bini and Jones (2007), suggested that for particles transported in isotropic turbulence a value of $\alpha = 0.8$ reproduces accurately the heavy tailed *pdfs* observed experimentally. The present work builds upon previous findings and aims to investigate the effect of the sub-grid dispersion model on the quantities that characterise a turbulent droplet laden mixing layer and in particular, focuses on the sensitivity of the results to the values of the constants, α and C_o. The dispersed phase is composed of discrete spherical droplets, has a relatively small volume fraction and as a consequence droplet collisions, breakup and coalescence effects are negligible.

The structure of this paper is as follows. The mathematical formulation and the assumptions involved in the modelling of the particle dispersion in a turbulent gas carrier phase as well as the *pdf* approach for the dispersed phase are presented in the next section. The experimental apparatus used in the test case examined, the computational details of the simulations, the predictions of the calculations and the comparison with the experimental data are presented and discussed in the third section. The conclusions of the study are summarised in the final section.

2. Modelling

2.1. Filtered Navier–Stokes equations

In LES, a spatial filter is applied to the Navier–Stokes equations. The filtering operation is defined as

$$\bar{f}(\mathbf{x},t) = \int_{\Omega} G(\mathbf{x}-\mathbf{x}';\Delta(\mathbf{x}))f(\mathbf{x}',t)d\mathbf{x}', \tag{1}$$

where G is the filter function and Δ is the filter width assigned as the cube root of the local cell volume, Germano et al. (1991). In flows where large density fluctuations occur, the introduction of density filter quantities is essential and are defined as: $\tilde{f} = \overline{\rho f}/\bar{\rho}$.

The density weighted filtered Navier–Stokes equations with the contribution of the dispersed phase, as point sources of mass momentum and energy can be written as:

$$\frac{\partial\bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial x_i} = \bar{S}_{mass}. \tag{2}$$

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial\bar{p}}{\partial x_i} + \frac{\partial\bar{\sigma}_{ij}}{\partial x_j} + \tilde{\tau}_{ij} + \bar{\rho}g_i + \bar{S}_{mom,i}. \tag{3}$$

The Smagorinsky (1963) model is used for the sub-grid scale tensor: $\tau^d_{ij} = -2\mu_{sgs}\widetilde{S}_{ij}$, where τ^d_{ij} is the deviatoric *sgs* stress with $\mu_{sgs} = \bar{\rho}(C_s\Delta^2)\|\widetilde{S}_{ij}\|$. C_s is the Smagorinsky constant equal to 0.07 and $\|\widetilde{S}_{ij}\|$ is the Frobenius norm $\|\widetilde{S}_{ij}\| = \sqrt{2\widetilde{S}_{ij}\widetilde{S}_{ij}}$ of the filtered strain tensor, $\widetilde{S}_{ij} = 0.5\left(\frac{\partial\widetilde{U}_i}{\partial x_j} + \frac{\partial\widetilde{U}_j}{\partial x_i}\right)$. Dynamic versions of the Smagorinsky model, Germano (1992), Piomelli and Liu (1995), allow the value of the parameter C_s to be determined as a function of time and position. However, there is little to be gained by the use of more complex *sgs* models in the case of high Reynolds number free flows of the type considered. As is clear from the results presented below the standard Smagorinsky model gives good results for mixing layer flows.

The source terms appearing in the gas phase equations can be evaluated as: $\bar{S} = \frac{1}{\Delta^3}\sum_{i=1}^{n} S^{(\alpha)}$, where the summation is over the number of the droplets present in the cell volume under consideration and S^{α} is the source term arising from the α-th droplet which can be written as:

$$S^{\alpha}_{mass} = -\frac{dm^{(\alpha)}}{dt}, \tag{4}$$

$$S^{\alpha}_{mom,i} = -\frac{d}{dt}(mu_i)^{(\alpha)}. \tag{5}$$

The source term in the momentum equation accounts for two-way coupling between the gas and liquid phase. In dilute flows, such as that presently considered, the effects of this coupling are negligible and the term could almost certainly be omitted without loss. It is however, retained for completeness.

2.2. PDF modelling of fuel sprays

Following Bini and Jones (2008) the dispersed phase is described through a set of independent macroscopic variables, the droplet radius r, the droplet number n, the droplet velocity $\mathbf{v}$ and the droplet temperature θ. The Weber number is presumed small enough, $We < 20$, so the droplets have a spherical shape. The evolution of the filtered joint *pdf* $\bar{P}(R,N,\mathbf{V};\mathbf{x},t)$ is derived using the fine-grained probability density function approach, Lundgren (1967), *i.e.*: