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Influence of computational drop representation in LES of a mixing layer with evaporating drops

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ABSTRACT

The objective of this work is to quantify the influence of the number of computational drops and grid spacing on the accuracy of predicted flow statistics and to possibly identify the minimum number, or, if not possible, the optimal number of computational drops that provides minimal error in flow prediction. For this purpose, Large Eddy Simulation (LES) of a mixing layer with evaporating drops has been performed using the dynamic Smagorinsky model and employing various numbers of computational drops. The LES were performed by reducing the number of physical drops by a factor varying from 8 to 128 to obtain the ensemble of computational drops, and by utilizing either a coarse or a fine grid. A set of first order and second order gas-phase statistics as well as drop statistics are extracted from LES predictions and are compared to results obtained by filtering a Direct Numerical Simulation (DNS) database. First order statistics such as Favre averaged streamwise velocity, Favre averaged vapor mass fraction, and the drop streamwise velocity are predicted accurately independent of the number of computational drops and grid spacing. Second order flow statistics depend both on the number of computational drops and on grid spacing. The scalar variance and turbulent vapor flux are predicted accurately by the fine mesh LES only when the computational drop field is reduced by a factor of no more than 32, and by the coarse mesh LES reasonably accurately for all computational drop field values. This is attributed to the fact that when the grid spacing is coarsened, the number of drops in a computational cell must not be significantly lower than that in the DNS.

1. Introduction

Multiphase turbulent flows are encountered in many practical applications including turbine engines or natural phenomena involving particle dispersion. Numerical computations of multiphase turbulent flows are important because they provide a cheaper alternative to performing experiments during an engine design process or because they can provide predictions of pollutant dispersion, etc. For flows with volumetrically dilute particle loading, the most accurate method of numerically simulating the flow is based on Direct Numerical Simulation (DNS) of the governing equations in which all scales of the flow responsible for the overwhelming amount of dissipation are resolved. DNS, however, requires high computational cost and cannot be used in engineering design applications where iterations among several design conditions are necessary or utilized. Large Eddy Simulation (LES) provides a cheaper alternative to numerically simulate multiphase turbulent flows, although it has modeling requirements which do not exist in DNS. In LES only the energy-containing large scales, which are of engineering interest, are resolved and the more universal small scales are modeled thereby minimizing computational costs. The LES equations are obtained by filtering the governing equations. The effect of the filtered small-scale motion on resolved large scale motion appears as Subgrid-Scale (SGS) terms in the LES equation and it depends on the unresolved or "sub-grid" flow field which is unavailable; thus, these terms must be modeled. This modeling is typically done through representing the subgrid scale terms as functions of the large scale flow field.

Another approximation often employed in LES of multiphase turbulent flows is similar in spirit to the reduction in flow scales from DNS to LES and consists in modeling the physical drop field through representing a group of drops by a single "computational" drop [1–4]. This reduction in number of tracked drops leads to a faster simulation but it may also lead to loss of accuracy. Furthermore, there does not seem to be a well-established criterion as to the choice of the reduction factor from the physical drop field. Sankaran and Menon [1] tracked 10^5 computational particles and justified the choice of this number of particles as being large enough to perform meaningful drop statistics. Apte et al. [2] proposed a hybrid method wherein the drops are dynamically tracked but the size and number density of drops produced from drop breakup was determined by the evolution of a PDF in the space of the drop-radius. The method involved following both physical drops and computational drops which were only created if the total number

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of drops in a control volume exceeded a specified threshold. Results showed that the computation was more accurate when an ensemble of 6000 entities consisting of both drops and computational drops were tracked than when only 300 computational drops were followed. Since the number of tracked particles was not the same in the two simulations, the only clear conclusion is that for this relatively small number of tracked particles, it is better to follow a larger than a smaller number of them. Salewski [4] performed LES with 4500, 11,000, 28,000 and 54,000 computational drops and found that "there was no striking difference between the solutions" when the number of drops was increased beyond 11,000. However, Salewski's [4] conclusions were based on examining integral quantities such as the liquid volume fraction and the pdf of the drop size distribution. It is not clear if Salewski's [4] conclusions hold for higher order flow statistics such as Reynolds stresses and scalar fluxes.

To determine the effect of the computational-drop approach on the accuracy of the predicted flow and drop fields, we perform here a series of simulations in which we vary the factor by which we reduce the number of physical drops to the number of computational drops, and we consider the effect of this reduction in conjunction with two different grid spacings. For the purpose of these comparisons, we have created a new DNS database with a much larger number of drops than in the past [3] and with different initial conditions. This DNS database is here used to evaluate the accuracy of the LES predictions.

2. Basic governing equations and LES equations

The situations studied are those in which the volume fraction of the drops in the carrier gas is very small (less than $O(10^{-3})$). Also, the drops are much smaller than the Kolmogorov scale, η_K, and are assumed to be spherical. It is thus legitimate to treat the drops as point sources for the purpose of calculating the contribution of mass, momentum and energy to the gas phase [5]. Consistent with these assumptions, the carrier gas phase is treated in an Eulerian framework, whereas the dispersed liquid drops are tracked in a Lagrangian framework [3].

2.1. Basic governing equations

The compressible continuity, momentum, energy and species conservation equations are solved for the conserved variable vector $\phi = \{\rho, \rho u_i, \rho e_t, \rho Y_V\}$, where ρ is the density, u_i is the velocity in the x_i coordinate, e_t is the total energy and Y_V is the mass fraction of the vapor. The governing equations are

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = S_{mass}, \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_{mom,i}, \tag{2}$$

$$\frac{\partial(\rho e_t)}{\partial t} + \frac{\partial(\rho e_t u_j)}{\partial x_j} = -\frac{\partial(p u_i)}{\partial x_i} + \frac{\partial q_i}{\partial x_i} + \frac{\partial(\sigma_{ij} u_i)}{\partial x_j} + S_{energy}, \tag{3}$$

$$\frac{\partial(\rho Y_V)}{\partial t} + \frac{\partial(\rho Y_V u_j)}{\partial x_j} = -\frac{\partial j_{Vj}}{\partial x_j} + S_{mass}, \tag{4}$$

where t is the time and the source terms (S_{mass},$S_{mom,i}$ and S_{energy}) which appear in Eqs. (1)–(4) describe the exchange of mass, momentum and energy between the two phases. Both carrier gas (mass fraction Y_C) and vapor are assumed to be perfect gases and the perfect gas equation is used to relate the pressure (p) and the temperature (T) through

$$p = \rho R T, \tag{5}$$

where $R = Y_V R_V + Y_C R_C$, $R_V = R_u/m_v$, $R_C = R_u/m_C$, R_u is the universal gas constant, m_C and m_V are the molar masses of the carrier gas and the vapor respectively; $Y_C + Y_V = 1$. The total enthalpy (h) is the sum of the enthalpies of the carrier gas and the vapor

$$h = h_V Y_V + h_C Y_c, \tag{6}$$

where h_C and h_V are the enthalpies of the pure gases.

The temperature is calculated from e_t through

$$e_t = C_v T + h_V^0 Y_V + \frac{1}{2} u_i u_i, \tag{7}$$

where C_v is the heat capacity at constant volume. Considering the small variation of the pressure and temperature observed in the flow, we assume that the specific heat capacities of the gases are constant within this range.

The viscous stresses (σ_{ij}) are computed using

$$\sigma_{ij} = 2\mu\left(S_{ij} - \frac{1}{3} S_{kk}\delta_{ij}\right), \tag{8}$$

where μ is the viscosity coefficient and S_{ij} is the rate of the strain

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \tag{9}$$

The vapor mass flux in Eq. (4) in and heat flux in Eq. (3) has the form

$$j_{Vj} = \rho Y_V V_{Vj} = -\rho Y_V\left[\frac{D}{Y_V}\frac{\partial Y_V}{\partial x_j} + Y_C\left(Y_V + Y_C\frac{m_V}{m_C}\right)\left[\frac{m_C}{m_V} - 1\right]\frac{D}{p}\frac{\partial p}{\partial x_j}\right], \tag{10}$$

$$q_j = -\lambda\frac{\partial T}{\partial x_j} + (h_V - h_C) j_{Vj}, \tag{11}$$

where V_{Vj} is the vapor diffusion velocity, D is the diffusion coefficient and λ is the thermal conductivity. In Eqs. (8), (10) and (11), μ, D and λ are assumed constant, and are related to each other through the Prandtl and Schmidt numbers, $\mathrm{Pr} = \mu C_p/\lambda$ and $Sc = \mu/(\rho D)$.

The governing equations for an individual drop describing the evolution of its position (X_i), velocity (v_i), temperature (T_d) and the mass (m_d) are

$$\frac{dX_i}{dt} = v_i, \tag{12}$$

$$m_d\frac{dv_i}{dt} = F_{drag,i}, \tag{13}$$

$$m_d C_L\frac{dT_d}{dt} = \mathcal{Q} + \frac{dm_d}{dt}L_V, \tag{14}$$

$$\frac{dm_d}{dt} = \dot{m}_d, \tag{15}$$

where $F_{drag,i}$ is the drag force, $\mathcal{Q}$ is the heat flux between gas phase and drop, $\dot{m}_d$ is the evaporation rate, C_L is the heat capacity of the drop liquid and L_V is the latent heat of vaporization. The expressions for the drag, heat flux and the evaporation rate involve the use of the following validated models for the description of a single drop behavior:

$$F_{drag} = \frac{m_d}{\tau_d} f_1(u_i - v_i), \tag{16}$$

$$\mathcal{Q} = \frac{m_d}{\tau_d}\frac{Nu}{3Pr} C_p f_2(T - T_d), \tag{17}$$

$$\dot{m}_d = -\frac{m_d}{\tau_d}\frac{Sh}{3Sc}\ln[1 + B_M], \tag{18}$$

where C_p is the gas heat capacity at constant pressure, $B_M = (Y_{V,s} - Y_{V,f})/(1 - Y_{V,s})$, where $Y_{V,s}$ is calculated directly from the surface vapor mole fraction which is obtained by equating the vapor and liquid fugacities at the surface, $Y_{V,f}$ is vapor mass fraction at the drop location, and τ_d is the drop time constant given by

$$\tau_d = \frac{\rho_l d^2}{18\mu}, \tag{19}$$