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A-priori assessment of subgrid scale models for large-eddy simulation of multiphase primary breakup

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ABSTRACT

While Large-Eddy Simulation (LES) of single phase flows is well established in computational fluid dynamics, LES of multiphase flow is at an early development stage. The presence of the phase interface causes additional subgrid scale (SGS) terms to appear in the LES formalism. Not only turbulent structures but also interfacial deformations need to be captured by SGS models. The fidelity of multiphase LES depends on the complex interaction between turbulence and the phase interface at the unresolved scale. A variety of traditional and more recent SGS models of eddy viscosity or scale similarity type is suggested for the SGS terms in multiphase LES. Two new models for the SGS stress and for the SGS scalar flux are proposed. The first is based on a Taylor series expansion of the convolution filter, the latter is inspired by flamelet theory of turbulent premixed combustion. The closure models are a-priori assessed with respect to explicitly filtered direct numerical simulation (DNS) data of primary breakup of a liquid jet. The model performance is evaluated based on a correlation analysis and an order of magnitude study. Model accuracy is discussed depending on the filter size and the flow region. Promising candidates for a-posteriori analysis are identified.

1. Introduction

Atomization describes the disintegration of a liquid core into a large number of droplets and is a fundamental process in numerous industrial applications. Pollutant emissions in power generation or combustion performance rely on the evaporation and homogeneity of the air/fuel mixture which is controlled by the preceding atomization. In order to improve the design of industrial devices, predictive computational methods for atomization are strived for. Whereas models for secondary atomization (drops or small liquid structures collapsing into smaller drops) are well established [37,43], primary breakup remains the major deficiency of predicting atomization by numerical tools [11]. The liquid breakup includes potentially large density ratios, strong capillary forces and is dominated by turbulence which results in a complex multiscale problem. In the last two decades, progress in numerical methods allowed DNS computations of primary breakup at least for academic cases at moderate Reynolds and Weber numbers. Especially in the vicinity of the liquid core, where experimental access is limited due to the surrounding dense spray [11,40], detailed numerical simulations can help to gain insights in the mechanisms of turbulent liquid breakup. However, DNS of jet atomization for industrial devices which are often characterized by high Reynolds and Weber numbers will remain out of scope in the near future. The wide range of time and length scales results in excessive computational costs. LES provides a good compromise between statistically averaged RANS and DNS simulations in terms of accuracy and computational effort. Following Liovic and Lakehal [31] multiphase LES may be also called Large Eddy and Interface Simulation (LEIS) because the large scales of turbulence and the large deformations of the interface are explicitly captured. LES for multiphase flows including a sharp interface remains as of this day a relatively unexplored area. Because of the lack of spatial resolution in LES, not only turbulent but also interfacial structures remain subgrid. Labourasse et al. [24], Liovic and Lakehal [30–32], Toutant et al. [44,45] provided the mathematical background for LES in multiphase flows. The presence of the interface and the resulting filtering across the discontinuity cause additional SGS terms in the LES formalism. These terms contain the complex coupling between turbulence and the interface at the unresolved scale and the fidelity of multiphase LES strongly depends on their modeling. While fluctuating energy decreases with decreasing turbulence scales, small liquid structures can carry a lot of momentum and small scale phenomena can significantly influence large scale structures [11].

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A-priori investigations, estimating the order of magnitude of the SGS terms in academic test cases [26,31,45,47] and primary atomization, demonstrated their importance for the accuracy of multiphase LES [7]. Also a-posteriori LES of primary breakup, where the effect of filtering variables across the phase interface was neglected, underlined their significance [4,6,10]. Without accounting for the small scale instabilities and the unresolved turbulence-interface interaction, primary breakup in a-posteriori LES strongly depends on the mesh since only the resolved large scale instabilities can contribute to the destabilization of the jet [4,6,10]. Incorporating interfacial SGS deformations revealed the potential of improving the prediction of jet destabilization by means of LES [8]. Beneficial effects are also expected by SGS capillary forces [16]. Hence, the inclusion of SGS turbulent and interfacial effects is expected to be of crucial importance in order to predict the correct flow behavior in multiphase LES.

Little progress has been made so far to accurately model the SGS terms in multiphase LES. The additional modeling complexity arises from the fact that models should account for the unresolved interaction of turbulent eddies with the interface. The presence of the interface and its fluctuations generate and modulate the turbulence [47]. Classical subgrid models are based on the assumption that subgrid fluctuations ultimately originate from large scale structures generated by mean flow gradients [39]. Fluctuations emerging from interface interaction are not accounted for and specific models need to be developed to take this into account. It has been shown that eddy viscosity models are not appropriate in the vicinity of the interface [7,24] and require a damping towards the phase boundary [31]. Furthermore, opposed to Kolmogorov theory of turbulence, interfacial structures may not pass a cascade process [15,16,27]. Since liquid structures are not necessarily produced on large scales [11], the importance of small liquid scales complicates SGS modeling [11]. Only few models have been developed for the SGS surface tension force [1,3,16,32,41]. None of these models has been studied in a-priori analysis so far. Tryggvason et al. [46] stated that the development of next generation models for large scale, or averaged multiphase flows is one of the most urgent challenges.

The future overall modeling strategy to predict atomization by means of LES is an Eulerian-Lagrangian approach. Whereas large scale primary breakup is resolved in an Eulerian framework, small interfacial strucutures and secondary breakup unresolved by the LES mesh will be captured using Lagrangian droplets. This work is devoted to an a-priori assessment of SGS models for multiphase LES of the Eulerian phase. First, a variety of models for the different SGS terms is proposed. These include traditional SGS models established in single phase flow or combustion, as well as SGS models proposed for multiphase LES. Further, two new models for the SGS stress term and the interfacial SGS term are derived. The first one is based on a Taylor series expansion of the convolution filter, the second one is inspired by flamelet theory used in turbulent premixed combustion. The accuracy of the SGS models is evaluated with respect to explicitly filtered DNS data of primary breakup. The model performance is evaluated based on a correlation analysis and an order of magnitude study. Model accuracy is discussed depending on the filter size and the flow region relative to the interface.

The rest of the paper is organized as follows. A DNS of a round diesel jet injected into stagnant air at moderate Reynolds and Weber numbers is presented first, which provides detailed data for a-priori evaluations. The derivation of the governing LES conservation equations with its unclosed SGS terms is briefly summarized in Section 3. Various SGS closures for the dominating SGS terms are suggested in Section 5 and details in regards to the a-priori analysis are given in Section 4. Finally, the SGS model accuracy is evaluated and discussed in Section 6.

2. Direct numerical simulation database

The a-priori assessment of subgrid scale models for multiphase LES is based on a fully resolved DNS flow field. The dynamics of the two phase flow are described by the one-fluid formulation of the incompressible Navier–Stokes equations. In the single field representation, the two phases are locally identified by a Heavyside function [31] defined as

$$H(x,t) = \begin{cases} 1 & \text{if } x \text{ is in fluid,} \\ 0 & \text{if } x \text{ is in gas.} \end{cases} \tag{1}$$

The material properties change abruptly across the interface such that the local density ρ and viscosity μ are weighted as

$$\rho = H\rho_l + (1-H)\rho_g, \quad \mu = H\mu_l + (1-H)\mu_g \tag{2}$$

where ρ_l, μ_l and ρ_g, μ_g are the density and viscosity of the liquid and gas respectively. The interface is transported by the advection equation for incompressible flows

$$\frac{\partial H}{\partial t} + \frac{\partial}{\partial x_i}(H u_i) = 0, \tag{3}$$

where u_i describes the local fluid velocity. The incompressibility constraint and the single field momentum equation read

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{4}$$

$$\rho\left(\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j}\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \sigma\, n_i\, \kappa\, \delta_S \tag{5}$$

where p denotes the pressure field. The curvature is described by κ and σ denotes the surface tension. The normal vector of the interface is represented by n_i. The Dirac distribution δ_S restricts the presence of the surface tension term to the vicinity of the interface.

The DNS is conducted with the open-source code PARIS-Simulator [29]. A projection method including a second-order predictor-corrector technique for time integration solves the Navier–Stokes Eqs. (4)–(5). Spatial discretization is realized by the finite-volume approach on a regular, cubic staggered grid. A second-order centered difference scheme explicitly treats the viscous term. The advection term is discretized by the third-order QUICK scheme. The elliptic equation for the pressure is solved by a BiCGSTAB solver in the projection step. Numerically, the interface is treated by a volume of fluid (VOF) method. The volume fraction indicator function or volume of fluid quantity α is the discrete version of H. The interface advection Eq. (3) consists of a Mixed Young-Centered piecewise linear interface reconstruction and a Lagrangian explicit direction split advection. Momentum advection at the interface is conducted in a consistent manner with the VOF advection. A balanced Continuous-Surface-Force method computes the surface tension force. Local interface curvatures are calculated by the height-function method [36].

Fig. 1 shows the primary breakup of a round jet injected into air. The jet is characterized by moderate Reynolds and Weber numbers of $Re = \rho_l U_0 D/\mu_l = 5000$ and $We = \rho_l U_0^2 D/\sigma = 2000$ in order to allow for a DNS computation. D denotes the jet diameter at the inlet with the injection velocity U_0. The density and viscosity ratios take the values $\rho_l/\rho_g = \mu_l/\mu_g = 40$ which imitates a diesel injection at a pressure and temperature of around 5.2 MPa and 900 K. The computational domain is a rectangular box which extends 15D downstream of the injector and $5D \times 5D$ in vertical and horizontal direction. The configuration is resolved with 1920 $\times$ 640 $\times$ 640 $\approx$ 786 Mio cubic cells which gives a resolution of