A priori and a posteriori Analysis of Turbulent Sprays

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Abstract
We are interested in the modeling and simulation of turbulent multiphase flows. These flows are of great research interest because of their presence in a variety of engineering problems. The difficulties in solving these types of problems lie in the complexity of the highly non-linear governing equation and in resolving the highly dynamic, small length-scale phenomena associated with surface and interface dynamics. In this work we adopt a coupled level-set and volume-of-fluid (CLSVOF) approach to capture the liquid-gas dynamics in an Eulerian framework. Direct numerical simulation (DNS) is a promising tool but too compute-intensive to be used as a research and design tool. The more practical approach is to perform large eddy simulation (LES), instead of DNS. LES is accomplished via the use of subgrid-scale (SGS) models to capture the small-scale dynamics, while the large-scale dynamics are resolved explicitly. Besides the traditional and familiar SGS terms arising from the single-phase turbulent flow problem, there are terms that comes from the multiphase and interface effects. Modeling of these terms is our ultimate goal. In this work, we have performed a preliminary study on the SGS terms, by first performing a decomposition of the flow quantities into resolved and unresolved components. Only a few literature results can be found on the SGS analysis for such system and no validated SGS model has been set up yet. Our ultimate goal is to set up the SGS models for the interface dynamics terms, and being able to set up validated LES models. In addition to evaluating the large/resolved-scale and the SGS components, we will show some preliminary work assessing the performance of the simulations via comparison to physical data from experiments performed at The Dow Chemical Company.

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Introduction
Drift control in agricultural spray has been extensively studied in the past few decades [1]. Small droplets formed in the spray, which typically have a diameter of 100 micron or less, are easily drifted and travel a long distance in air before settling down to the ground [2], thus causing damage to the non-target crops, water, animal or humans. Many techniques have been employed to control the droplet size and reduce the small droplets from forming, including application of different nozzle designs, addition of adjuvants, and so on. Our particular interest is to investigate the effect of the adjuvants addition on the spray formation and breakup pattern, as well as evaluating the efficiency of different adjuvants in reducing the amount of small droplets being formed in spray.

Despite of its wide applications in industries and agriculture, turbulent spray and atomization are not well understood. It is recognized as a complicated process with a variety of phenomena present and coupled, including turbulent mixing, primary and secondary breakup as well as droplet coalescence. Due to the limitation of experimental techniques to capture and resolve such high frequency and small-scale structure in multiphase flow, numerical simulation is becoming a more and more promising way to investigate such flow. Direct numerical simulation (DNS) is a promising tool for obtaining information in the dense zone of the spray, where nearly no experimental data are available. Numerical techniques for multiphase flow have been developed and employed in the past decade, dividing into Lagrangian methods such as front-tracking [3], and Eulerian methods such as level set, volume of fluid [4][5][6], aiming to help people understanding the physical mechanism of multiphase flow and being able to model the complicated flow numerically. One of the most effective way is the coupled level set and volume of fluid (CLSVOF) [6][7], where one can take advantage of the method of level set's ability to capture geometry and curvature of interfaces in multiphase flow accurately, meanwhile conserving mass due to the mass preserving nature of volume of fluid method. We will adopt a similar methodology in our research.

Despite the accuracy of results from DNS, it is highly computationally expensive, and hence difficult to be employed in industry. The more feasible way in practical use is large eddy simulation (LES), which gives the time dependent fluctuating field, unlike the time averaged result using RANS, as well as reducing the computational cost by using the subgrid model for modeling the unresolved scales. To build the bridge from DNS to LES, subgrid models are needed. The traditional and familiar turbulent subgrid stress are presented, as well as the lesser studied surface tension subgrid term. This term is brought about by the small scale interface structures and surface tension in a multiphase turbulent flow, as well as the trans- port term present the level set and volume of fluid convection equation. Recently, there have been a few investigations on the subgrid effect of the surface tension terms in turbulent multiphase flow [8][9], but no validated SGS model has been presented yet. The goal of this paper is to perform a preliminary subgrid scale analysis on the DNS data from the two-phase planar jet in order to help us understand the effect of the new subgrid scale surface tension term physically. This is a necessary step to achieve our ultimate goal of building subgrid models for the turbulent spray problem and extending such analysis to Non-Newtonian fluid with the rheology modifier, thereby further enabling the LES study on the spray problem.

Formulation
LES is used to achieve affordable computations by solving the transport of the filtered variables. Filtering is performed to remove the small scales, which has the effect of reducing the required resolution. However, models for the small or sub-grid scales (SGS) need to be introduced as these interactions/dynamics are not explicitly captured. LES is performed by solving the filtered equations. The filtered mass equation is

\[
\frac{\partial \langle u \rangle}{\partial t} + \frac{\partial \langle u \rangle \langle u \rangle}{\partial x_j} = 0,
\]

where \( \langle u \rangle \) is the filtered velocity in the \( \langle x \rangle \) direction.

The filtered momentum equation is given by

\[
\frac{\partial \langle u \rangle}{\partial t} + \frac{\partial \langle u \rangle \langle u \rangle}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_j} + \frac{\mu}{\rho} \frac{\partial^2 \langle u \rangle}{\partial x_i \partial x_j} - \frac{1}{\rho} \gamma \kappa^F \frac{\partial H}{\partial x_i} \frac{\partial \tau_{ij}}{\partial x_j} + M_i,
\]

where \( \tau_{ij} \) is the SGS Reynolds stress given by

\[
\tau_{ij} = \langle u_i u_j \rangle - \langle u_i \rangle \langle u_j \rangle,
\]

and \( \kappa^F \) is the curvature obtained using the filtered level-set,

\[
\kappa^F = \frac{\partial^2 \langle \phi \rangle}{\partial x_i \partial x_j} \frac{\partial \langle \phi \rangle}{\partial x_j} \frac{\partial \langle \phi \rangle}{\partial x_i}.
\]
neglected subgrid surface tension on the coarser mesh, introducing the subgrid term to affect the dynamics of the interface curvature to affect the dynamics of the liquid surface. This could have significant effects on the dynamics of droplet formation, since the pinch-off mechanism driven by surface tension might be reduced and thus tend to produce less droplets in the flow. This effect, brought on by filtering, is taken care of by introducing the subgrid term $M_i$ which models the neglected subgrid surface tension on the coarser mesh, in an effort to capture the correct droplet forming mechanism.

The transport equation of the filtered or resolved level-set is given by

$$\frac{\partial \langle \phi \rangle}{\partial t} + \frac{\partial \langle u_i \rangle}{\partial x_i} = \frac{\partial \Phi_j}{\partial x_j}, \quad (14)$$

where $\Phi_j = \langle \phi u_i \rangle - \langle \phi \rangle \langle u_i \rangle$ is the SGS turbulent level set flux. The SGS level-set-level-set interactions represent the effect of small-scale fluctuations and how they interact with the surface tension and the interface curvature to affect the dynamics of the liquid surface.

The transport equation for the filtered volume of fluid is given by

$$\frac{\partial \langle F \rangle}{\partial t} + \frac{\partial \langle u_i \rangle}{\partial x_i} = \frac{\partial \Theta_j}{\partial x_j}, \quad (15)$$

where $\Theta_j = \langle F u_i \rangle - \langle F \rangle \langle u_i \rangle$ is the SGS volume of fluid flux. The SGS volume of fluid flux is similar to the SGS level set flux, representing the small-scale fluctuations of volume of fluid due to turbulent mixing.

From above, the new subgrid terms introduced in CLSVOF method are $M_i$, $\Phi_j$ and $\Theta_j$ in the momentum, level set and volume of fluid equations, respectively. These terms are important for correctly capture the liquid-gas interface dynamics and crucial for predicting droplet forming, thus requires accurate modeling.

**Results**

We have utilized the DNS code to simulate a 2D planar jet. The goal is to show the effects of the aforementioned small-scale interactions on jet breakdown. Namely, given the exact hydrodynamic field we calculate the surface tension term in the y-momentum equation. We also calculate this term using the filtered quantities. The difference between the two captures the SGS effects on the surface tension force. For the 2D planar jet, the Reynolds number based on the jet is 3500, Weber number based on jet is 50, density ratio of the jet to the coflow is 2:1. Figure 1 shows the surface tension term calculated from the filtered level set, one can see that the small scale details are smoothed out due to averaging. Figure 2 shows the SGS surface tension term $M_i$, which contains all the small scale information that are smoothed out in the filtering operation. While the fine structures in Figure 2 cannot be explicitly captured in a coarser mesh as being used in LES, by correctly modeling the subgrid surface tension term shown in Figure 2, one is able to reproduce the small scale structures and make correction on surface tension term shown in Fig. 1 using the coarser mesh. In turn we are able to capture the small scale surface dynamics such as forming of small droplets accurately, which is of specific interest of our future research.

To show this more clearly, a close up view of the exact surface tension force is shown in Fig. 3(a) while the SGS component is shown in Fig. 3(b). The data shows that the magnitude of the SGS component is the same as that of the total force, suggesting that the small-scale fluctuations may be significant. One can see that the SGS term has both positive and negative component close to the interface and is acting in a complicated way, which keeps the liquid column from breaking up in some places, and accelerates the break up at other places.

**References**


Figure 1. A prior result from DNS on a planar jet. Color contour shows surface tension term calculated from filtered level. The details are smoothed out and need correction using SGS term.

Figure 2. A priori analysis of the surface tension force in a planar jet. The contours represent the SGS surface tension force.

Figure 3. A close up view of the surface tension force in a planar jet. The contours on the left represent the exact force while the contour on the right represents the SGS surface tension force. The latter needs to be modeled in LES.