ICLASS 2009, 11th Triennial International Annual Conference on Liquid Atomization and Spray Systems, Vail, Colorado USA, July 2009

A Large Eddy Simulation Subgrid Model for Turbulent Phase Interface Dynamics

M. Herrmann*
Department of Mechanical and Aerospace Engineering, Arizona State University
Tempe, Arizona 85287,USA

M. Gorokhovski
Laboratoire de Mecanique des Fluides et Acoustique
Ecole Central de Lyon, France

Abstract

In this paper we report on the outline of a Large Eddy Simulation subgrid model for liquid/gas phase interface dynamics. A key feature of the proposed model is to take the subgrid phase interface dynamics fully into account by employing a dual-scale approach. Instead of modeling the LES subgrid phase interface geometry, we fully resolve it on an auxillary grid using the Refined Level Set Grid approach (Herrmann 2008). We then propose to model the LES subgrid velocity on the auxillary grid needed to move the fully resolved phase interface, by solving a dedicated PDE for its evolution near the phase interface. This PDE contains three different contributions. First, the subfilter turbulent eddies are taken into account by modeling the subfilter acceleration in lines of Oboukhovs log-normality conjecture on the stochastic field of ε. The second term, a velocity increment due to the relative motion between the two phases is modeled deriving renormalized velocity boundary condition at the phase interface. The final term, due to subfilter surface tension induced subfilter velocities is modeled following a Taylor analogy. Knowing the fully resolved phase interface geometry, all previously unclosed terms in the filtered Navier-Stokes equations can be directly closed using explicit filtering.

Introduction

Atomization processes are characterized by a vast range of length and time scales. Performing detailed simulations aiming to resolve all relevant scales is a daunting task even with today's computational resources [1]. Detailed simulations are thus limited to research oriented tasks and not a viable approach for engineering design work. Models, simplifying the atomization process by pre-assuming certain types of atomization mechanisms, on the other hand, lack the ability to reliably predict atomization, especially in novel atomizer configurations. Simulation approaches in between detailed simulations and model simulations that do not presume the atomization mechanism are thus desirable. It has been shown in the past that for single phase flows involving mixing processes with complexity comparable to two-phase atomizing flows, Large Eddy Simulation (LES) approaches yield superior results as compared to RANS simulations [2]. However, introducing spatial filtering into the governing equations results in several unclosed terms. These include the subfilter contribution of the stress tensor, the subfilter surface tension term, and a subfilter transport term for liquid volume fraction. Previous LES approaches [3–8] have modeled the subfilter contribution of the stress tensor using a single phase formulation and have simply neglected the latter two terms on the faulty premise that they either cancel each other, or that they are not important on the subfilter scale. However, especially the subfilter surface tension term can be dominant and must not be neglected, since surface tension forces are inversely proportional to the length scales of local surface corrugations and topology changes always involve small scales. The purpose of this paper is to propose a novel LES modeling approach for phase interface dynamics that incorporates all the previously neglected terms.

Governing equations

The equations governing the fully resolved motion of an unsteady, incompressible, immiscible, two-fluid system are the Navier-Stokes equations

*Corresponding Author: marcus.herrmann@asu.edu

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla \cdot \left(\mu \left(\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u}\right)\right) + \frac{1}{\rho}\boldsymbol{T}_\sigma \,, \tag{1}$$

where $\boldsymbol{u}$ is the velocity, ρ the density, p a Lagrange multiplier, μ the dynamic viscosity, and $\boldsymbol{T}_\sigma$ the surface tension force, non-zero only at the location of the phase interface $\boldsymbol{x}_f$. Furthermore, the continuity equation results in a divergence-free constraint on the velocity field, $\nabla \cdot \boldsymbol{u} = 0$. The phase interface location $\boldsymbol{x}_f$ between the two fluids can be described by a level set scalar G, with $G(\boldsymbol{x}_f, t) = 0$ at the interface, $G(\boldsymbol{x}, t) > 0$ in fluid 1, and $G(\boldsymbol{x}, t) < 0$ in fluid 2. Differentiating with respect to time yields the level set equation,

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

Assuming ρ and μ are constant in each fluid, density and viscosity at any point $\boldsymbol{x}$ can be calculated from

$$\rho(\boldsymbol{x}) = H(G)\rho_l + (1 - H(G))\rho_g \,, \quad \mu(\boldsymbol{x}) = H(G)\mu_l + (1 - H(G))\mu_g \,, \tag{3}$$

where indices l and g denote values in liquid and gas, respectively, and H is the Heaviside function. From the definition of the level set scalar it follows that $\delta(\boldsymbol{x} - \boldsymbol{x}_f) = \delta(G)|\nabla G|$, with δ the Dirac delta function. Furthermore, the interface normal vector $\boldsymbol{n}$ and the interface curvature κ can be expressed in terms of the level set scalar, resulting in $\boldsymbol{n} = \nabla G/|\nabla G|$, $\kappa = \nabla \cdot \boldsymbol{n}$, and

$$\boldsymbol{T}_\sigma(\boldsymbol{x}) = \sigma\kappa\delta(\boldsymbol{x} - \boldsymbol{x}_f)\boldsymbol{n} = \sigma\kappa\delta(G)|\nabla G|\boldsymbol{n} \tag{4}$$

for the surface tension force $\boldsymbol{T}_\sigma$, with σ the constant surface tension coefficient.

Filtered governing equations

Introducing a spatial filter function $\mathcal{G}$, the filtered governing equations can be derived,

$$\frac{\partial \widetilde{\boldsymbol{u}}}{\partial t} + \widetilde{\boldsymbol{u}} \cdot \nabla \widetilde{\boldsymbol{u}} = -\frac{1}{\overline{\rho}}\nabla p + \frac{1}{\overline{\rho}}\nabla \cdot \left(\overline{\boldsymbol{\tau}} + \boldsymbol{\tau}^{SGS}\right) + \frac{1}{\overline{\rho}}\overline{\boldsymbol{T}_\sigma} \,, \tag{5}$$

and $\nabla \cdot \widetilde{\boldsymbol{u}} = 0$, where $\widetilde{\ }$ denotes Favre filtering, $\widetilde{f} = \overline{\rho f}/\overline{\rho}$, $\overline{\ }$ indicates spatial filtering, p is a Lagrange multiplier, $\overline{\boldsymbol{\tau}}$ is the stress tensor calculated using filtered velocities, and $\boldsymbol{\tau}^{SGS}$ is the subfilter contribution of the stress tensor. Four terms in the above governing equations are unclosed and require modeling: the filtered density $\overline{\rho}$, the filtered viscosity $\overline{\mu}$ contained in $\overline{\boldsymbol{\tau}}$, the subgrid scale stress tensor $\boldsymbol{\tau}^{SGS}$, and the filtered surface tension term $\overline{\boldsymbol{T}_\sigma}$. Using (3), the filtered density and viscosity are

$$\overline{\rho} = \rho_l\overline{\psi} + \rho_g(1 - \overline{\psi}) \qquad \overline{\mu} = \mu_l\overline{\psi} + \mu_g(1 - \overline{\psi}) \,, \tag{6}$$

where

$$\overline{\psi} = \int \mathcal{G}(\boldsymbol{x})H(G)d\boldsymbol{x} \tag{7}$$

requires a model. The filtered surface tension term is

$$\overline{\boldsymbol{T}_\sigma} = \overline{\sigma\kappa\delta(\boldsymbol{x} - \boldsymbol{x}_f)\boldsymbol{n}} \,. \tag{8}$$

In summary, three terms remain to be modeled to describe the phase interface dynamics of a liquid/gas phase interface on the filtered scale: $\overline{\psi}$, $\boldsymbol{\tau}^{SGS}$, and $\overline{\boldsymbol{T}_\sigma}$.

Previous LES modeling attempts

Several attempts have been made in the past to develop a LES model for the phase interface dynamics of turbulent liquid/gas flows [3–8]. These attempts typically use the strategy outlined in the following.

To determine $\overline{\psi}$, $\overline{\psi}$ is identified as a filtered marker function, ranging from 0 in the gas to 1 in the liquid (in essence a liquid volume fraction). Filtering the fully resolved liquid volume fraction transport equation, $\partial\psi/\partial t + \boldsymbol{u} \cdot \nabla\psi = 0$, results in

$$\frac{\partial \overline{\psi}}{\partial t} + \overline{\boldsymbol{u}} \cdot \nabla\overline{\psi} + \nabla \cdot \overline{\boldsymbol{u}'\psi'} = 0 \,, \tag{9}$$

where $\overline{\boldsymbol{u}'\psi'}$ is unclosed and requires modeling. However, this term is usually simply neglected, following an argument outlined below, resulting in

$$\frac{\partial \overline{\psi}}{\partial t} + \overline{\boldsymbol{u}} \cdot \nabla\overline{\psi} = 0 \,. \tag{10}$$

The subfilter contribution of the stress tensor, $\boldsymbol{\tau}^{SGS}$, is calculated using a single phase approach, either by solving an SGS turbulent energy transport equation [3–5, 8] or by a Smagorinsky-type model [6, 7]. The filtered surface tension $\overline{\boldsymbol{T}_\sigma}$ can be expressed as the sum of a resolved term, depending only on quantities larger or equal to the filter size, and a subfilter term, i.e.,

$$\overline{\boldsymbol{T}_\sigma} = \sigma\overline{\kappa}\delta(\boldsymbol{x}-\overline{\boldsymbol{x}_f})\overline{\boldsymbol{n}} + \sigma\left(\overline{\kappa\delta(\boldsymbol{x}-\boldsymbol{x}_f)\boldsymbol{n}} - \overline{\kappa}\delta(\boldsymbol{x}-\overline{\boldsymbol{x}_f})\overline{\boldsymbol{n}}\right). \quad (11)$$

In the cited LES papers, the subfilter part of the filtered surface tension term is then neglected, based on the faulty premise that subfilter surface tension forces are small for large Weber number flows. Using a Continuum Surface Force (CSF) approach [9], this then results in $\overline{\boldsymbol{T}_\sigma} = \sigma\overline{\kappa}\nabla\overline{\psi}$, where $\overline{\kappa}$ is calculated from $\overline{\psi}$ and is therefore not the filtered curvature, but instead the curvature associated with $\overline{\psi}$. However, even in large Weber number flows, the subfilter part of the surface tension term should not be neglected since it is proportional to surface curvature, which increases with decreasing length scales. Surface tension forces are thus dominant on small scales.

Another argument for neglecting the subfilter surface tension term is that it is restorative, i.e., decreasing surface fluctuations on the subfilter scale, whereas the neglected subfilter contribution in Eq. (10) would increase surface fluctuations. The two contributions would thus cancel each other. However, this assumption would only be valid in 2-D flows, since only there is the surface tension force always restorative. In three dimensions, surface tension can actually increase surface fluctuation, as the simple example of a capillary instability (Rayleigh-instability) demonstrates.

We thus argue that both the subfilter surface tension term as well as the subfilter contribution to Eq. (9) cannot be neglected and should be included in any LES model of the phase interface dynamics.

The dual-scale approach to modeling subfilter phase interface dynamics

From a conceptual point of view, classical LES modeling approaches assume the existence of a cascade process. This implies that the physical processes on the subfilter scale can be inferred from the resolved physical processes on the filtered scale. Can such a procedure be followed to model $\overline{\boldsymbol{u}'\psi'}$ and the subfilter surface tension term? Recent evidence from high-resolution simulations of atomizing Diesel jets seem to indicate that the atomization process is not a cascade process [10]. The primary atomization of the jet does not occur by first breaking up into large-scale structures that then continuously break up into ever smaller drops. Instead, very small-scale drops can be ripped out of the liquid directly via ligament-formation processes, bypassing any cascade process for the phase interface geometry [10].

In this paper, we propose an alternative modeling strategy. Imagine that one would be able to maintain a fully resolved realization of the phase interface geometry at all times, expressed, for example, in terms of a level set scalar G. Then $\overline{\psi}$ could be calculated exactly by explicit filtering of $H(G)$ using Eq. (7). This in turn would give $\overline{\rho}$ and $\overline{\mu}$ exactly using Eq. (6). Since no transport equation for $\overline{\psi}$ would need to be solved on the filter scale, the unclosed subgrid scale term of Eq. (9) , $\overline{\boldsymbol{u}'\psi'}$, does not arise. The only term left to close is the filtered surface tension term $\overline{\boldsymbol{T}_\sigma}$. However, using Eq. (8) and realizing that κ, $\boldsymbol{x}_f$, and $\boldsymbol{n}$ are simply functions of G and thus available as a fully resolved realization, $\overline{\boldsymbol{T}_\sigma}$ can be calculated exactly by simple application of the spatial filter function,

$$\overline{\boldsymbol{T}_\sigma} = \int \mathcal{G}(\boldsymbol{x})\sigma\kappa\delta(\boldsymbol{x}-\boldsymbol{x}_f)\boldsymbol{n}d\boldsymbol{x}\,. \quad (12)$$

Although this is an exact closure, the problem of modeling is of course simply shifted to the problem of maintaining a fully resolved realization of the phase interface geometry. This entails in essence two challenges. The first is to describe the fully resolved motion of the phase interface. Since $\boldsymbol{u} = \overline{\boldsymbol{u}} + \boldsymbol{u}_{sg}$, this results in

$$\frac{\partial G}{\partial t} + (\overline{\boldsymbol{u}} + \boldsymbol{u}_{sg})\cdot\nabla G = 0\,, \quad (13)$$

where the only term requiring modeling is $\boldsymbol{u}_{sg}$. The second challenge is to address the feasibility from a computational cost perspective of solving Eq. (13) on a fully resolved scale.

At first glance, it is doubtful whether an efficient LES model can be constructed that needs to solve Eq. (13) on the fully resolved scale, after all, the entire purpose of resorting to an LES approach is to avoid having to resolve all scales. However, we need not solve the full set of Navier-Stokes equations on the fully resolved scale, only a simple advection equation. Furthermore, and most importantly, the level set advection equation need not be solved in the whole computational domain, it need only be solved in the vicinity of the phase interface due to the definition of the level set scalar. Total resolution requirement does therefore not scale with N^3, i.e. $\mathrm{Re}^{9/4}$ [11], but instead scales with only N^2, i.e. $\mathrm{Re}^{3/2}$, where N is the number of grid nodes in each spatial direction. To efficiently solve Eq. (13), we propose the use of the recently introduced Refined Level Set Grid (RLSG) method [12]. By design, it solves the level set equation on a separate, highly resolved Cartesian G-grid, independent of the underlying flow solver grid, using a dual narrow-band approach. The numerical approach is optimized for massively parallel computer systems and allows for significantly refined

G-grids at low cost compared to the flow solver [12]. Coupling to a finite volume flow solver is achieved by explicitly evaluating the definition of a control volume quantity ϕ_{cv},

$$\phi_{cv} = \int_{V_{cv}} \phi(\boldsymbol{x}) d\boldsymbol{x} \,, \tag{14}$$

using ϕ defined on the G-grid. This is in fact equivalent to applying a filter $\mathcal{G}$ of size equal to the local control volume to the fully resolved equation. Thus, explicit filtering of $\overline{\boldsymbol{T}_\sigma}$ results in

$$\overline{\boldsymbol{T}_\sigma} = \int_{V_{cv}} \sigma\kappa(\boldsymbol{x})\delta(\boldsymbol{x}-\boldsymbol{x}_f)\boldsymbol{n}(\boldsymbol{x}) d\boldsymbol{x} \,, \tag{15}$$

where κ and $\boldsymbol{n}$ are functions of the fully resolved G, see Eq. (4), evaluated on the G-grid.

Finally, for the subgrid scale stress tensor $\boldsymbol{\tau}^{SGS}$ we propose to use a single-phase formulation, for example, a dynamic Smagorinsky approach. While this is certainly valid in the single-phase regions of the flow away from the phase interface, it does require more scrutiny and validation near the phase interface, when the spatial filter function $\mathcal{G}$ incorporates significant fractions of both fluids.

A new model for the subfilter velocity

As described in the previous section, the only term that requires modeling in the proposed LES model is the fully resolved subfilter velocity vector $\boldsymbol{u}_{sg}$ at the phase interface. We propose to model $\boldsymbol{u}_{sg}$ as the sum of three different subfilter velocities,

$$\boldsymbol{u}_{sg} = \boldsymbol{u}' + \delta\boldsymbol{u} + \boldsymbol{u}_\sigma \,, \tag{16}$$

where $\boldsymbol{u}'$ is due to subfilter turbulent eddies, $\delta\boldsymbol{u}$ is attributed to the interface velocity increment due to relative subfilter motion between the two phases, and $\boldsymbol{u}_\sigma$ is due to subfilter velocities induced by subfilter surface tension forces. All three terms require modeling.

We propose to model $\boldsymbol{u}'$ based on the recently proposed LES-Stochastic Subgrid Acceleration Model (SSAM) [13, 14]. The key idea here is to not model $\boldsymbol{u}'$ directly, but instead its acceleration, $d\boldsymbol{u}'/dt$. This is motivated by the experimental observation that at small length/time scales, the Lagrangian particle acceleration exhibits strong intermittency [15]. Although the Lagrangian acceleration rapidly decorrelates with increasing time lag, the norm of the Lagrangian acceleration exhibits a long memory on the order of a few integral times. Thus, we propose to follow [13, 14] and model the subfilter acceleration due to subfilter turbulence by solving

$$\frac{d\boldsymbol{u}'}{dt} = \boldsymbol{a}' = a'\boldsymbol{e} \tag{17}$$

on the G-grid, where $\boldsymbol{e}$ is a random unit vector. The solution to Eq. (17) is subject to the condition $\int_{G=0} \boldsymbol{u}' \cdot \boldsymbol{n}\, d\boldsymbol{x} = 0$ to preserve liquid volume. The norm of the subgrid acceleration in Eq. (17) is calculated in line with Oboukhov's log-normality conjecture on the stochastic field of ε. Namely, applying the Ito transformation [16] to the stochastic equation for ε in homogeneous stationary turbulence, [13, 14] obtained the following stochastic equation for the norm of the acceleration a',

$$da' = -a'\left(\ln\frac{a'}{a_\eta} - \frac{3}{16}\sigma_\chi^2\right)T_\chi^{-1}dt + \frac{3}{4}a'\sqrt{2\sigma_\chi^2 T_\chi^{-1}}dW(t) \,, \tag{18}$$

where $dW(t)$ is the increment of a standard Brownian process, $a_\eta = (\varepsilon_\Delta^3/\nu)^{1/4}$ is the Kolmogorov acceleration, $T_\chi = \nu_{tur}/\Delta^2$, $\sigma_\chi^2 = A + m\ln \mathrm{Re}_\Delta^{3/4}$, $\mathrm{Re}_\Delta = \nu_{tur}/\nu$, $A \approx -0.863$, and $m \approx 0.25$ [17].

For $\delta\boldsymbol{u}$ we propose the following approach. Let a regular LES flow solver cell of size Δ be subdivided into a number of small cells of size Δ_G, as for example in our case, the G-grid subdivides the flow solver grid. The G-grid thus constitutes a subfilter, or SGS mesh. In the following, we will consider Gaussian filtering denoted by $\langle . \rangle_\alpha$ only, where α is the employed filter scale

Now consider a Δ_G-cell, in which the liquid/gas interface is located. In this cell, the two phases are fluctuating simultaneously. The relative motion between phases generates a force on the liquid surface, which causes motion of the interface and induces its curvature. Such a force per unit mass contained in the cell may be written in the following form,

$$\boldsymbol{F}_{gl} = -\nabla\left(\frac{\rho_g}{\rho_l+\rho_g}\left(\boldsymbol{u}-\boldsymbol{u}_G\right)^2\right) \,, \tag{19}$$

where $\boldsymbol{u}_G$ is the interface velocity. Hence the main problem in the modelling of subgrid motion of the interface is to evaluate the velocity increment on the interface $\langle \boldsymbol{u}-\boldsymbol{u}_G\rangle_{\Delta_G}$, and then $\delta\boldsymbol{u} = \langle \boldsymbol{F}_{gl}\rangle_{\Delta_G} dt$.

The required model for $\langle \boldsymbol{u}-\boldsymbol{u}_G\rangle_{\Delta_G}$ can be derived from this as follows [18]. Let us introduce the vector $\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{x}_f$ characterizing the position relatively to the interface. In each Δ_G-cell, containing the interface,

$0 \le z \le \Delta_G$. We formulate the boundary condition on the interface as $\langle \delta(\boldsymbol{z})\,[\boldsymbol{u}(\boldsymbol{z}) - \boldsymbol{u}_G]\rangle_{\Delta_G} = 0$, where $\boldsymbol{u}(\boldsymbol{z})$ and $\boldsymbol{u}_G$ are the fully resolved instantaneous velocities of the gas and the interface, respectively, and $\delta(\boldsymbol{z})$ is the Dirac delta function. Using the Leonard expansion [19], this can be written as

$$\sum_{n=0}^{\infty} \frac{\Delta_G^{2n}}{n!} \nabla^n \langle \delta \rangle_{\Delta_G}(\boldsymbol{z}) \nabla^n \langle \boldsymbol{u} - \boldsymbol{u}_G \rangle_{\Delta_G}(\boldsymbol{z}) = 0\,. \tag{20}$$

From this expression, up to the second order terms, one can obtain

$$\langle \boldsymbol{u} - \boldsymbol{u}_G \rangle_{\Delta_G} = z \frac{d\langle \boldsymbol{u} \rangle_{\Delta_G}}{dz} + \frac{1}{2}\left(\Delta_G^2 - z^2\right) \frac{d^2 \langle \boldsymbol{u} \rangle_{\Delta_G}}{dz^2}\,. \tag{21}$$

The first and the second derivatives in Eq. (21) are unknown on the SGS mesh and need to be modeled. According to [20], the typical turbulent acceleration on the Δ_G-scale can be estimated as $a_{\Delta_G} = \langle \varepsilon \rangle_{\Delta_G} / \Delta_G^{1/3}$, where $\langle \varepsilon \rangle_{\Delta_G}$ is the viscous dissipation. Meanwhile, the typical acceleration on the resolved scales Δ can be written as $a_\Delta = \langle \varepsilon \rangle_\Delta / \Delta^{1/3}$ and consequently, $a_{\Delta_G} = a_\Delta (\Delta/\Delta_G)^{1/3}$. Defining the acceleration on the resolved scales by $a_\Delta = \Delta |S_{ijk}|^2$, we have for the subgrid acceleration $a_{\Delta_G} = |S_{ijk}|^2 \Delta^{4/3} / \Delta_G^{1/3}$. It is natural to assume that close to the interface, this acceleration is of order of the viscous force $d^2 \langle \boldsymbol{u} \rangle_{\Delta_G} / dz^2 = \boldsymbol{a}_{\Delta_G} / \nu$. Integrating this gives

$$\frac{d\langle \boldsymbol{u} \rangle_{\Delta_G}}{dz} = \frac{\boldsymbol{a}_{\Delta_G}}{\nu} z + const. \tag{22}$$

When $z \to 0$, the velocity gradient is controlled by vortical structures of order of Kolmogorov's scale, which are attached to the interface [21]. Hence one may write $const = (\langle \varepsilon \rangle_\Delta / \nu)^{1/2}$, and finally, Eq. (21) becomes

$$\langle \boldsymbol{u} - \boldsymbol{u}_G \rangle_{\Delta_G} = z \left(\frac{\langle \varepsilon \rangle_\Delta}{\nu} \right)^{1/2} \boldsymbol{e}_1(t) + \frac{1}{2}\left(\Delta_G^2 + z^2\right) |S_{ijk}|^2 \frac{\Delta^{4/3}}{\nu \Delta_G^{1/3}} \boldsymbol{e}_2(t)\,, \tag{23}$$

where $\boldsymbol{e}_1(t)$ is a unit vector in a random direction tangential to the interface and $\boldsymbol{e}_2(t)$ is a unit vector normal to the interface, pointing randomly in the liquid or gas direction in such a way that $\int_{G=0} \langle \boldsymbol{u} - \boldsymbol{u}_G \rangle_{\Delta_G} \cdot \boldsymbol{n}\, d\boldsymbol{x} = 0$ to preserve liquid volume.

The need for the third term in Eq. (16), the subfilter surface tension induced subfilter velocity $\boldsymbol{u}_\sigma$, is best illustrated by the following example. Imagine a detached, small thin ligament of liquid. Surface tension forces at the tips of the ligament will induce large velocities there, pulling the end tips toward the center. If the ligament is well-resolved by the flow solver, this behavior will be well-reproduced by the governing equations solved by the flow solver. Now imagine reducing the flow solver resolution, i.e., introducing implicit filtering, to such a level that the complete ligament will reside within a single flow solver cell. Note that the ligament geometry can still be fully resolved by the fine G-grid. However, explicit filtering of the surface tension force will result in a zero net force for the control volume containing the ligament. Thus, the flow solver cannot generate the physical velocities at the tips of the ligament, and the shape of the ligament will not change. This is not an incorrect behavior of the flow solver, it just illustrates that all induced velocities are on the subfilter scale and have to be included thus directly into the equation for $\boldsymbol{u}_{sg}$.

We propose to model $\boldsymbol{u}_\sigma$ by following in essence the Taylor analogy,

$$\frac{d\boldsymbol{u}_\sigma}{dt} = c_\sigma \sigma (\kappa - \overline{\kappa}) \boldsymbol{n} \delta - c_\mu \frac{\nu^*}{L^2} \boldsymbol{u}_\sigma\,, \tag{24}$$

where $\overline{\kappa}$ is the explicitly filtered fully resolved curvature, L is a characteristic length scale, ν^* is a kinematic viscosity defined below, and c_σ and c_μ are two yet to be determined constants. The first term in Eq. (24), containing the surface tension, acts in essence as a spring. To illustrate this, consider the fully resolved phase interface geometry Γ_κ and the phase interface geometry $\Gamma_{\overline{\kappa}}$ that is associated with the filtered curvature $\overline{\kappa}$. Figure 1 depicts two such geometries. In the first case, a stretched out ligament, i.e. an ellipsoid, is fully contained within a single flow solver grid cell, whereas the second case consists of a cylindrical element with a small indentation contained entirely in a single flow solver grid cell. On the filtered scale, the first case results in a constant $\overline{\kappa}$, equivalent to a sphere, thereby not generating any flow on the filtered scale, whereas $\overline{\kappa}$ in the second case will result in a small variation, that severely under-predicts the fully resolved curvature variation, and thereby strongly under-predicts the resulting flow field. In the first case, the subfilter surface tension force should act in a stabilizing manner, in the second case it should destabilize the phase interface due to the Rayleigh instability. This is precisely the result the first term of Eq. (24) yields. If the fully resolved local curvature κ is larger than the filtered value $\overline{\kappa}$, the term acts as an acceleration in the direction of $\boldsymbol{n}$, i.e. in the direction of the liquid, if it is smaller, the direction is reversed. This results in the acceleration directions indicated by the arrows in Fig. 1, consistent with the physical picture just outlined.

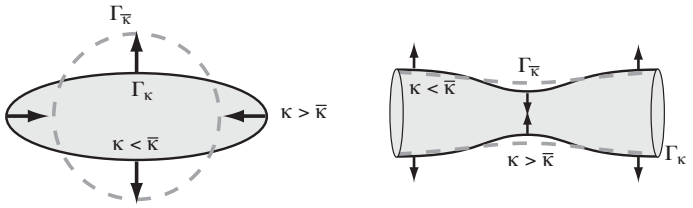

Figure 1. Direction of surface tension induced subfilter acceleration of Eq. (24) for a subfilter ellipsoid (left) and dented cylinder (right). Solid line denotes fully resolved phase interface geometry Γ_κ with local curvature κ, dashed line shows phase interface geometry $\Gamma_{\overline{\kappa}}$ corresponding to filtered curvature $\overline{\kappa}$.

The second term in Eq. (24), containing the viscosity, acts as a damper since on the small scales considered here, viscous forces are important. The length scale L contained in the viscous term exists for dimensional reasons, its modeling is not yet clear. However it might be incorporated into the coefficient c_μ. The viscosity ν^* should be evaluated at the phase interface. It is thus an average quantity of the liquid and gas viscosities. Here, we propose to use a density weighted average, $\nu^* = (\rho_l\nu_l+\rho_g\nu_g)/(\rho_l+\rho_g)$, since it naturally encompasses the limit of the gaseous phase being a vacuum. Equation (24) has to be solved on the G-grid, but only for cells directly adjacent to the phase interface, setting $\nabla(\boldsymbol{u}_\sigma \cdot \boldsymbol{n}) \cdot \nabla G = 0$ in the remaining narrow band cells.

Conclusions

In this paper we have presented an outline for a novel LES subgrid model for phase interface dynamics of liquid/gas phase interfaces. It follows a dual-scale approach by aiming to maintain a fully resolved representation of the phase interface geometry on a separate high-resolution grid using the RLSG method. All previously unclosed terms in the filtered Navier-Stokes equations relating to the phase interface can then be closed exactly by explicitly filtering the fully resolved phase interface geometry. To maintain a realistic realization of the fully resolved phase interface geometry, we propose to model the phase interface propagation velocity by simulating the subfilter flow structure and accounting for subfilter surface tension forces. How well the proposed approach works in reality, remains to be seen. Implementation, verification, and validation will be conducted in the future.

Acknowledgments

This work was initiated at the 2008 CTR Summer Program at Stanford University.

References

[1] Gorokhovski, M. and Herrmann, M. *Annual Review of Fluid Mechanics* 40(1):343–366, 2008.
[2] Akselvoll, K. and Moin, P. *J. Fluid Mech.* 315:387, 1996.
[3] Ishimoto, J., Hoshina, H., et al. *Interdisciplinary Information Sciences* 13(1):7–16, 2007.
[4] Ishimoto, J., Ohira, K., et al. *Cryogenics* 48(5-6):238–247, 2008.
[5] Srinivasan, V., Salazar, A.J., et al. *Atom. Sprays* 7:571–617, 2008.
[6] Bianchi, G.M., Pelloni, P., et al. Technical Report 2005-24-089, SAE, 2005.
[7] Bianchi, G.M., Pelloni, P., et al. *SAE Tech. Pap.* (2007-01-0244), 2007.
[8] de Villiers, E., Gosman, A.D., et al. Technical Report 2004-01-0100, SAE, 2004.
[9] Brackbill, J.U., Kothe, D.B., et al. *J. Comput. Phys.* 100:335–354, 1992.
[10] Herrmann, M. In *ILASS Americas 21st Annual Conf.*. Orlando, FL, 2008.
[11] Pope, S.B. *Turbulent Flows*. Cambridge University Press, Cambridge, UK, 2000.
[12] Herrmann, M. *J. Comput. Phys.* 227(4):2674–2706, 2008.
[13] Sabel'nikov, V., Chtab, A., et al. *Advances in Turbulence XI*, p. 209–211. Springer, 2007.
[14] Sabel'nikov, V., Chtab, A., et al. *Notes on Num. Fluid Mech. and Multidis. Design*, 97(299–304), 2008.
[15] Mordant, N., Lévêque, E., et al. *New Journal of Physics* (116), 2004.
[16] Pope, S.B. and Chen, Y.L. *Phys. Fluids A* 2(1437–1449), 1990.
[17] Lamorgese, A.G., S. B. Pope, P.K.Y., et al. *J. Fluid Mech.* 582:423–448, 2007.
[18] Gorokhovski, M. private communication. CTR Summer Program, 2008.
[19] Saveliev, V.L. and Gorokhovski, M.A. *Phys. Rev. E* 72(016302), 2005.
[20] Monin, A.S. and Yaglom, A.M. *Statistical Fluid Mechanics: Mechanics of Turbulence*. MIT Press, 1981.
[21] Townsend, A.A. *The structure of turbulent shear flow*. Combridge University Press, 1981.