Sub-grid scale modelling for the LES of interfacial gas-liquid flows

Modélisation des écoulements avec interface gaz-liquide par simulation des grandes échelles (LES)

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INTRODUCTION

Traditionally, turbulent multi-fluid flows have been simulated as inter-penetrating media, using the averaged two-fluid representation for void fraction distribution and the Reynolds-averaged Navier-Stokes (RANS) framework for turbulence modeling. In terms of interface topology and turbulence modeling, the two-fluid and RANS approximation approaches are equivalent, in that interface and turbulence structures are not directly generated as part of the solution, but rather modeled. Phase averaging in the two-fluid formalism is not ideal for capturing interface-turbulence interactions, because interface jump conditions cannot be included when the phases are mixed. In the case of interfacial multi-fluid flows, the interface location can be tracked only by means of the single-fluid method. Modern interface-tracking techniques are indeed capable of providing accurate solutions for interface dynamics within finite-volume/difference simulations, with the possibility of tackling surface-turbulence interactions in flows involving abrupt topology changes. Turbulent interfacial flows are nowadays within reach of interface tracking methods [Liovic et al., 2001].

In this paper we explore the application of the LES approach for a specific class of turbulent multi-fluid flows, followed by a critical discussion of its usefulness and limitations. The idea behind the method, in this context, relies on the density-based filtered single-fluid Navier-Stokes equations [Lakehal, 2004]. The super-grid interface kinematics...
and turbulence are fully resolved, whereas the unresolved turbulence and interfacial scales are modeled. The strategy amounts to a subtle combination of any robust interface-tracking scheme that is capable of resolving interfacial topology changes down to the grid scale including fragmentation and coalescence with a high degree of conservativeness and symmetry preservation. Only with this type of algorithms can the physics of the flow -including turbulence- be simulated down to the grid-resolved level. In this new LES framework, the grid scale represents the minimum resolvable interfacial radius of curvature, while in turbulence it represents the minimum resolvable eddy length scale. The incorporation of SGS physics is analogous to some extent.

The work initiated by our group represents a first attempt to incorporate explicit SGS modeling for LES into an interface tracking–based finite–volume code for the simulation of interfacial flows. We use the PLIC-VOF method, which has been proven to be a powerful framework for solving flows dominated by massive topological changes [Liovic et al., 2001]. The method has been applied to capturing interface-turbulence interactions in the downward gas injection into a water pool [Liovic et al., 2004], and wave breaking generated turbulence in spilling breakers. In these two applications use was made of the Smagorinsky model for unresolved turbulence scales, which proved highly dissipative, affecting near-interface regions in particular. The dynamic approach of Germano et al. [1991] could not be extended to non-homogeneous flows, where it is difficult to infer a specific direction for space averaging the resolved-field based length scale.

In this paper we present first results obtained with an SGS Smagorinsky-based model using a near-interface treatment. The model has been applied to the stratified air-water flow studied by Fugosi et al. [2003], for which extensive DNS data are available for comparison. The core of the LES approach (SGS modeling) has been incorporated into the pseudo-spectral solver used by Fulgosi, in which the interface deformations are simulated by the Boundary-Fitting method.

II TURBULENCE AND INTERFACIAL SCALES

In modeling turbulent multi-fluid flows, it is important to correctly reproduce the multitude of scales involved in the system and their impact on the inter-phase exchange mechanisms. In the multi-fluid flow context, turbulence is the main agent responsible for scale separation, too, but the presence of moving interfaces is likely to change the energy cascade. The interdependence between turbulence and interface related scales could not be fully understood without the help of DNS and LES. It is likely that in the foreseeable future there will be an incentive to extend the research towards these techniques, the LES in particular. Flows involving immiscible fluids separated by a well-defined continuous interface, such as stratified pipe flows or sea-water waves involve indeed specific turbulence spectra on each side of the interface. Emphasis is then placed on predicting these scales down to the interface level for each phase.

To put interfacial gas-liquid flows in context, we note their implication in scalar exchange problems between turbulent streams separated by deformable interfaces. These sorts of transport mechanisms are notoriously known to play an important role in environmental systems. There has been an intense and renewed interest in the mass transfer subject due to its central role in the uptake of greenhouse gases and release of moisture by terrestrial water bodies. As far as the greenhouse gas uptake problem is concerned, it should be noted that the uncertainty in the correlations used to estimate the mass transfer is still very high [Banerjee & S. MacIntyre, 2004]. A considerable incentive exists today to improve the understanding of scalar exchange phenomena and to reduce such uncertainties. Passive and active gas exchange problems (i.e. direct contact condensation) also occur in energy-conversion settings, and, in particular in thermal-hydraulics systems of nuclear reactors, where it can be of significant safety concern.

II.1 DNS of Turbulence at a Deformable Gas-Liquid Interface

The configuration of the two-phase flow investigated is sketched in figure 1, where the flow in each sub-domain is driven by a constant pressure gradient. Several recent studies have been devoted to this problem, for both standing fixed waves [DeAngelis, 1998] as well as for deformable interfaces [Fulgos et al., 2003]. The reference quantities used throughout for normalization are the effective shear velocity \( u_s \), defined by \( u_s = \sqrt{\tau_{\omega} / \rho} \), where \( \tau_{\omega} \) represents the shear stress at the interface, the half-depth of each computational domain \( h \), and the kinematic viscosity \( \nu \). It is important to note that at the beginning of the simulation, when the interface is still flat, the interfacial shear balances exactly the imposed mean pressure gradient, so that \( u_s \) corresponds to the shear velocity \( u_s \). As the interfacial waves start to develop, part of the energy is transferred into form drag leading to a reduction of the interfacial shear, i.e. \( u_s < u_c \). The shear-based Reynolds number, defined by \( Re_s = u_s 2h/\nu \), with \( u_s \) taken at the initial stage of the simulation, is 171 in both phases. Moreover, the non-dimensional time is defined by \( t^* = t\nu/u_s^2 \) in wall units, or by \( t^* = tU_s/h \) in large-scale units, where \( U_s \) is the mean streamwise velocity. These reference quantities \( (u_s, \nu, U_s, h) \) will serve the non-dimensionalisation of the Navier-Stokes equations for the incompressible, isothermal, Newtonian fluids to be solved in the two sub-domains.

In the absence of mass transfer, the gas and liquid phases are explicitly coupled at the interface by the continuity of velocities and shear stresses, i.e. the interfacial jump conditions, as follows

\[
\begin{align*}
\frac{1}{Re_s} (\sigma_L - \sigma_G) \cdot n \cdot n + p_L - p_G - \frac{1}{We} \cdot \nabla \cdot n - \frac{1}{Fr} f = 0 \\
((\sigma_L - \sigma_G) \cdot n) \cdot t_i = 0, i = 1, 2 \\
-u_G = u_L/R
\end{align*}
\]

where the subscripts \( L \) and \( G \) stand for liquid and gas respectively, \( \sigma \) is the viscous stress tensor, \( f \) measures the vertical displacement of the interface with respect to the mid plane, \( n \) and \( t_i \) are the normal and the two tangential unit vectors, respectively, and \( R = \sqrt{\rho_L/\rho_G} \) is the parameter measur-
ing the density ratio. The Weber and Froude numbers are defined as

\[ We = \frac{\rho_i h u_i^2}{\sigma} \quad \text{and} \quad Fr = \frac{u_i^2 \rho_i g h (\rho_i - \rho_o)}{\sigma} \]  

respectively, where \( \sigma \) stands for the surface tension coefficient. Periodic boundary conditions are applied in the streamwise (x) and spanwise (y) directions.

At the outer boundaries, free-slip boundary conditions are employed in order to avoid turbulence generation other than in the interface region.

The interface motion is simulated by solving an advection equation for the vertical elevation of the interface, denoted by \( f(x, t) \):

\[ \partial_t f + \mathbf{u} \cdot \nabla f = 0 \]  

Since the method relies on solving separately the two phases, it therefore cannot handle strong topological changes of the interface, such as fragmentation and wave breaking. For this reason, the Weber and Froude number were carefully selected (\( We = 4.8 \times 10^{-3} \) and \( Fr = 8.7 \times 10^{-5} \)) so as to limit the wave steepness to the range of capillary waves.

At each time step, the distorted physical domain was mapped onto a rectangular parallelepiped on which the Navier-Stokes equations were solved using a pseudo-spectral technique. Details of the numerical method and the mapping procedure can be found in JFM, 482, 2003. The computational domain for each phase was 1074 \( \times \) 537 \( \times \) 171 wall units in the streamwise, spanwise and normal directions respectively, with a resolution of 64 \( \times \) 64 \( \times \) 65 for the DNS and 32 \( \times \) 32 \( \times \) 32 for the LES. The density ratio between the two phases was such that \( R = 29.9 \), corresponding to air-water flows at atmospheric pressure and at roughly 320 K. The usual 3/2 de-aliasing rule applies for the LES, too. Statistical data analysis was accomplished by averaging the results over the two homogeneous directions (x-y plane average), then over time.

II.2 LES of Turbulence at a Deformable Gas-Liquid Interface

The aforementioned DNS has been successfully performed for various conditions. However, it requires large computational resources, which increase with the Reynolds number. In order to investigate higher Reynolds number flows, it is necessary to adopt the LES approach where only the large-scale motions are directly computed. High Reynolds number flows could thus be within reach of the simulation even on relatively coarse grids (as compared to the DNS requirement), provided the non-resolved scales are appropriately modeled. Despite the simple topology of the flow considered hereafter, its analysis involves many critical aspects, which need to be carefully considered. A key point is that the simulation methodology used should be strictly conservative with regard to all the transported quantities as the interface deforms, and that the SGS model in both phases is capable to restore the main features of the small-scale turbulence near the interface, for example to accommodate the asymptotic behavior of turbulence near the interface. For wall-bounded flow, the usual Smagorinsky SGS model alone is known to over-estimate the sub-grid-scale dissipation, and it therefore requires some modifications, such as the dynamic approach of Germano et al. [1991] or proper near-wall treatment.

II.3 The filtered equations

The filtered two-fluid transport equations for dispersed multi-phase flows, and its single-fluid variant for interfacial flows are described in Lakehal [2004]. In the Boundary-fitting context where the phases are treated separately, the filtered mass and momentum equations are equivalent to those governing the large scales of motions for single-phase, incompressible flow of a Newtonian fluid, i.e.

\[ \nabla \cdot \mathbf{u} = 0 \]  

\[ \frac{\partial \tilde{\mathbf{u}}}{\partial t} + \mathbf{u} \cdot \nabla \tilde{\mathbf{u}} = -\frac{1}{\text{Re}_e} \nabla \cdot \mathbf{\tau} \]  

where \( \mathbf{u} \) is the resolved velocity vector, made non-dimensional by the reference velocity \( u_* \), and \( p \) is the dynamic pressure normalized by \( \rho u_*^2 \). All the barred quantities are filtered through the convolution product:

\[ \tilde{f}(x) = G \ast f(x) = \int f(x - x'; \delta) G(x - x'; \delta) dx' \]  

where \( G \) represents an appropriate spatial filter obeying the normalization condition. The above set of equations is solved in each domain using proper material properties, and the separate flow solutions are coupled through the jump conditions, once the filtered interface topology equation is solved (\( \partial_t \tilde{f} + \mathbf{u} \cdot \nabla f = 0 \)). The effect of the small scales appears...
through the SGS stress term, $\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j$, that must be modeled. If the non-resolved velocity $\bar{u}_i = \bar{u}_i - \bar{u}_j$ is defined, the SGS stresses can be decomposed into three parts:

$$\tau_{ij} = L_{ij} + C_{ij} + R_{ij} \quad (7)$$

where $L_{ij}$ is the Leonard term, $R_{ij}$ is the cross-scale term, and $C_{ij} = \bar{u}_i \bar{u}_j$ is the true SGS Reynolds stress, the deviatoric part of which is the only quantity to be modeled. This can be achieved by an eddy viscosity model or by other approaches such as the multi-scale approach of Hughes et al. [2001].

II.4 SGS and near interface modeling

The SGS Reynolds stress is modeled here by means of the Smagorinsky [1963] kernel:

$$\tau_{ij} = -2 \nu \tilde{S}_{ij} + \delta_{ij} \tau_{ij}/3 \quad (8)$$

where

$$\nu = \ell^3 \tilde{S}_{ij} = (C_s \Delta)^2 (2 \tilde{S}_{ij} \tau_{ij})^{1/2} \quad (9)$$

denotes the eddy viscosity and $\tilde{S}_{ij}$ the resolved strain rate. The length scale $\ell = (C_s \Delta)$ is based on the cell size $\Delta = (\Delta_x \Delta_y \Delta_z)$. The value of the model constant has been traditionally determined from isotropic decay of turbulence, and takes values between 0.15 and 0.22. In the presence of shear, however, be it near the wall or in the vicinity of evolving surfaces, the value of the model constant has to be reduced by use of a damping function to accommodate the near-wall/interface limiting behavior in low-Re number flow regions. This is usually achieved by the incorporation of the Van Driest damping function in front of the length scale. Similar “corrections” need obviously to be introduced in case the model is employed for interfacial flows, where the lighter phase perceives the surface like a rigid wall.

The DNS data of this flow have shown that as the interface deforms in response to the imposed shear, the RMS velocity normal to the interface is finite as compared to wall flows, and thus the turbulent kinetic energy (TKE) $k = 1/2 (u^2 + v^2 + w^2)$. It is therefore more judicious to infer a damping function by reference to the two-equation model involving $k$, rather than the one-equation model. With this the model could be made somewhat sensitive to the turbulent kinetic energy behaviour at the interface. Within the two-equation framework the damping function can be expressed as follows:

$$f_{C_{ij}} = \left( \frac{\nu \ell}{k} \right)^2 \quad (10)$$

where $P$ and $\epsilon$ stand for the production and dissipation of the turbulent kinetic energy, respectively (cf. Eq. 13). The model constant $C_s$ should be equal to 0.09 in order to accommodate the equilibrium conditions ($P = \epsilon$). Figure (2) below shows the DNS results of the shear structure and the production to dissipation term corresponding to the two configurations, R1 and R2, which designate the flat interface case (almost) and the wavy case, respectively. Figure (3) shows the DNS results of the RMS velocities and the derived damping function. The best fit to the DNS data, which is also reported in the right panel of the figure, reads

$$f_{C_{ij}} = 1 - \exp(-0.00013 \psi^3 - 0.00038 (\psi^3)^2 - 1.08 \psi^{-0.53} (\psi^3)) \quad (11)$$

This has been incorporated into the SGS model in the following form:

$$\ell^2 = (f_{\mu} C_s \Delta)^2 \quad (12)$$

and has been used for the simulations presented in this paper. Note that the determination of the interface distance function poses serious problems in interface-tracking codes (e.g. more in VOF then in Level Sets), where it requires special and tedious Reconstructed Distance Function (RDF) algorithms [Lakehal & Liovic, 2005]. This explains the reasons why we have deliberately chosen for SGS modelling validation the pseudo-spectral, Boundary-fitting code, where the interface distance function is determined as in any other channel flow DNS solver.

III ■ SIMULATION RESULTS

The comparison between LES and DNS results shows appreciable deviations, similar to those obtained by Hughes et al. [2001] for single phase channel flow at the same

![Figure 2: DNS results of the production-to-dissipation ratio and the structure parameter $-\tilde{u} \tilde{w}/k$.](image-url)
Reynolds number. Details of the comparison are discussed in the context of figure (4), where the mean streamwise velocity and shear stress profiles are compared as a function of the non-dimensional distance to the interface. As was to be expected, the simple SGS model fails in reproducing the boundary layer characteristics. The velocity profile is grossly under-predicted as well as the shear stress distribution. Combining the SGS model with the near-interface damping function (11) leads to much better and meaningful results, though a slight deviation is observed near the interface. The trend of the shear stress is correctly predicted by the model with the damping function, albeit slightly under-estimated.

The RMS velocity fluctuations in three directions are plotted versus the non-dimensional distance to the interface in figure (5). In this graph the comparison includes the results of the under-resolved DNS, or LES without SGS model. It is clearly shown that without a sub-grid-scale approximation the results deviate considerably from the DNS, in particular the peak of turbulence intensity. While the fluctuations are underestimated in the streamwise directions, they are grossly overestimated in the spanwise and vertical directions. The simple SGS model without near-interface treatment is clearly dissipative, and this can be judged from the shift of the peak in turbulence intensity, which corroborates with the shift in the shear stress observed in figure (4). Introducing the near-interface treatment via (11) enhances considerably the quality of the results, although the streamwise fluctuations are somewhat under-estimated.

A further analysis of the results focuses on the energy transfer mechanisms obtained by analyzing the contribution of each term in the turbulent kinetic energy balance. For incompressible turbulent flow the transport equation for the turbulent kinetic energy, \( k \), can be derived from the Navier–Stokes equation, and is given by

\[
\frac{Dk}{Dt} = -\mu \frac{\partial U_i}{\partial x_j} - \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \mu \frac{\partial U_i}{\partial x_j} \right) - \frac{1}{2} \frac{\partial}{\partial x_j} \left( \mu_i \mu_j \right) + \frac{1}{2} \frac{\partial^2}{\partial x_j \partial x_j} \left( \frac{U_i U_j}{U_m n_m} \right) - \frac{\partial}{\partial x_j} \left( \frac{\partial U_i}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \frac{\partial U_i}{\partial x_j} \right) + \text{Turb. Transp.}
\]

Figure 3: DNS results of RMS velocity fluctuations and \( f_\mu \) distributions.

Figure 4: Comparison of mean velocity and shear stress profiles in wall coordinates: (—), DNS; (— —), LES with SGS and (11); (-), LES with SGS alone.
Écoulements diphasiques

Figure 5: RMS fluctuations: Lines and symbols are used to identify DNS and LES, respectively. (●), LES with simple SGS model; (◊), LES with SGS and (11); and (+), Under-resolved DNS.

where \( \frac{D}{Dt} \) is the substantial derivative. Figure 6(left) compares only the most important terms on the right-hand-side of equation (13), i.e. production, dissipation and pressure diffusion, for DNS and LES simulations, with and without near-interface correction (11). Significant differences can be observed close to the interface. In all the LES simulations, the dissipation rate close to the interface was found to balance entirely the viscous diffusion (result not shown), exactly as in the DNS of this flow and of similar wall flows. The quantities presented are scaled with \( u_* \). The production and dissipation terms are underestimated by the Smagorinsky model alone, and feature near-interface asymptotic behaviors well below the DNS. The correction brought by the damping function substantially improves the energy budget, especially in the viscosity-affected region, \( z^+ < 20 \). The considerable under-predicted levels of production and dissipation are in line with the earlier results of mean velocity and shear stress distributions.

The last comparison between DNS and LES data concerns the pressure-strain correlations, which serves to redistribute energy among the Reynolds stresses, and promote isotropy of turbulence. The trace of the Reynolds stress tensor \( R_{ij} \) is used to define the pressure-strain correlation

\[
P_{Si} = \frac{1}{\rho} \frac{\partial u_i}{\partial x_j}, \quad i = 1, 2, 3
\]

A positive value of \( P_{Si} \) implies a transfer of energy into component \( i \) from the other components, and vice versa. Figure 6(right) shows the profiles of the pressure–strain correlation. In all cases, the streamwise component, \( P_{S1} \), transfers energy into the spanwise \( (P_{S2}) \) and the normal \( (P_{S3}) \) components. The redistribution between the terms, which has previously shown that near–interface turbulence is more isotropic than near–wall turbulence dependents in this case dramatically on the SGS model in the viscous layer. More than all the other terms, the comparison of the results for this quantity clearly shows the benefits of resorting to a near-interface damping to limit the dissipative behavior of the Smagorinsky model.

IV /// CONCLUSIONS

The LES approach is potentially promising for tackling interfacial turbulent multi-fluid flows. The filtered single-fluid formulation provides further accuracy by directly predicting interface topologies as they evolve in time and space, and turbulence motions down to the interface. This study aims at paving the way for future use of LES for this class of flow, where the lighter phase sees the heavier phase as an impermeable wall. The simple Smagorinsky model has been tested in combination with a DNS-based near-interface damping function to simulate the flow over a deformable interface. Only the data on the gas side have been explored. The results have been compared to existing DNS data. The present LES seems to face the same problem as the simulation of wall-bounded flows: the simple eddy-viscosity models give physi-
cally unrealistic results. The present investigation shows that the model has to be modified to explicitly account for turbulence decay near the interface. Since this could not be done through a dynamic modeling approach, a new damping function based on the DNS of the stratified gas-liquid flow over a sheared interface has been derived. Only with this correction could the model provide relevant, less-dissipative turbulent statistics. For later use of the model within the interface-tracking context (VOF in particular), the determination of the interface distance function will require tedious Reconstructed Distance Function (RDF) algorithms, such as that of Lakehal & Liovic [2005]. The situation is somehow less problematic within the Level set approach, where the interface distance function is a result of the simulation.

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