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Abstract

The one-equation SGS LES model has shown promise in revealing flow details as compared to the dynamic model, with the additional benefit of providing information on the modelled SGS turbulent kinetic energy (Niceno et al., 2008). This information on SGS turbulent kinetic energy (SGS-TKE) offers the possibility to more accurately model the physical phenomena at the sub-grid level, especially the modelling of the SGS turbulent dispersion force (SGS-TDF). The use of SGS-TDF force has the potential to account for the dispersion of particles by sub-grid scale eddies in an LES framework, and through its use, one expects to overcome the conceptual drawback faced by Eulerian-Eulerian LES models. But, no work has ever been carried out to study this aspect. Niceno et al. (2008) could not study the impact of SGS-TDF effect as their grid size was comparable to the dispersed bubble diameter.

A proper extension of research ahead would be to quantify the effect of sub-grid scale turbulent dispersion force for different particle systems, where the particle sizes would be smaller than filter-size. This work attempts to apply the concept developed by Lopez de Bertodano et al. (1994) to approximate the turbulent diffusion of the particles by the sub-grid scale liquid eddies. This numerical experimentation has been done for a gas-liquid bubble column system (Tabib et al., 2008) and a liquid-liquid solvent extraction pump-mixer system (Tabib et al., 2009; Tabib et al., 2010). In liquid-liquid extraction system, the organic droplet size is around 0.5 mm, and in bubble columns, the bubble size is around 3-5 mm. The simulations were run with mesh size coarser than droplet size in pump-mixer, and for bubble column, two simulations were run with mesh size finer and coarser than bubble diameter. The magnitude of SGS-TDF values in all the cases were compared with magnitude of other interfacial forces (like drag force, lift force, resolved turbulent dispersion force, force due to momentum advection and pressure). The results show that the relative magnitude of SGS-TDF as compared to other forces were higher for the pump-mixer than for the coarser and finer mesh bubble column simulations. This was because in the pump-mixer, the ratio of "dispersed
phase particle diameter to the grid-size” was smaller than that for the bubble column runs. Also, the inclusion of SGS-TDF affected the radial hold-up, even though the magnitudes of these SGS-TDF forces appeared to be small. These results confirm that: (a) the inclusion of SGS-TDF will have more pronounced effect for those Eulerian-Eulerian LES simulation where grid-size happens to be more than the particle size, and (b) that the SGS-TDF in combination with 1-Equation-SGS-TKE LES model serves as a tool to overcome a conceptual drawback of Eulerian-Eulerian LES model.

*Keywords*: CFD; Bubble column; pump-mixer; liquid-liquid; turbulent dispersion force; LES; multiphase; eulerian-eulerian.
1. Introduction

Multi-phase systems in chemical and process industries are governed by exchange of momentum, heat, mass and chemical reactions between the phases. The understanding of these processes can be enhanced by incorporating relevant physics in a fluid dynamics framework. A tool like multiphase computational fluid dynamics (CFD) has the potential to simulate such phenomena, and it is continuously being developed/tested to incorporate multiphase physics. The key to develop an accurate multiphase CFD model lies in effective representation of the turbulence phenomena and the local interfacial exchanges between the phases. Hence, within the multiphase CFD, there has been growing research in areas pertaining to capturing turbulence phenomena, which involves: (a) study of physics like turbulence modulation by dispersed phase, (b) development/application of turbulence models (like, variants of Large Eddy simulation (LES) models for capturing turbulence), and (c) towards accurately modelling the interfacial forces between phases that represent the momentum exchange, in particular, the much discussed “turbulent dispersion force”. Any development in these research areas is effective in improving the accuracy of two commonly used multiphase CFD approaches: ie the Euler–Lagrange approach and the Euler–Euler approach. The present work attempts to cover some ground in related areas, mainly pertaining to the use of Eulerian-Eulerian Large Eddy Simulation and sub-grid scale turbulent dispersion force (SGS-TDF). The Eulerian-Eulerian approach remain a popular choice to study systems with high density/high volume fraction dispersed phase , as it is computationally prohibitive to conduct the Eulerian-Lagrangian simulations of dispersed phase particles for the high volume fraction systems. Also, it is expected that the inclusion of sub-grid-scale turbulence dispersion model will help to address the drawbacks of Eulerian-Eulerian LES approach as described below. To get a good perspective on the context of this
manuscript, a brief description of status of Eulerian-Eulerian LES and interfacial forces is given below, which is followed by the objective of the current work.

The Eulerian-Eulerian Large Eddy Simulation (LES) turbulence model has shown significant promise in unearthing flow details in multiphase systems like, in gas-liquid multiphase systems (Deen et al., 2001; Dhotre et al., 2008; Tabib et al., 2008; Zhang et al., 2008; Niceno et al., 2008); in liquid-solid particle systems involving stirred vessel (Derksen., 2006), in fluidized bed (Chiesa et al., 2005) and particle laden flow (Riber et al., 2009). Though, there is one drawback while applying the Eulerian-Eulerian LES, that is in-order to maintain the consistency of the assumption of interpenetrating continua, the largest interface details should be smaller than the grid size, which means that the cell size must be larger than the particle size. That implies that the grid might not be fine enough to capture all turbulence details, hence making the basic assumption of LES invalid. In other words, lots of details moves to sub-grid scale (SGS) level, and this needs to be captured accurately. Researchers have tested various variants of LES models like, Constant Smagorinsky model, Dynamic Smagorinsky model and One-equation SGS turbulent kinetic energy LES (1-Eq-SGS-TKE) model. The smagorinsky and Dynamic model do not make the information on sub-grid-scale level available explicitly. Niceno et al. (2008) were the first to apply the 1-Eq-SGS-TKE LES model to Eulerian-Eulerian multiphase gas-liquid flow. Their results reveal that the one-equation SGS model gives superior results to the well-established dynamic model, with the additional benefit of giving information on the modelled SGS energy. They suggested that the sub-grid scale (SGS) information can be used to access the sub-grid scale interfacial forces, in particular the sub-grid scale turbulent dispersion force. In their work, the effect of sub-grid scale turbulent dispersion force could not be determined as the particle size was almost equivalent to the mesh-grid size. As mentioned earlier, the above work has been one of those very rare research instances, where importance of incorporating sub-grid scale contributions
was suggested. A proper extension of research ahead would be to quantify the effect of sub-grid scale turbulent dispersion in LES framework. We study a bit about the development of turbulent dispersion force in the next section.

Development of interfacial forces: The multiphase formalism involves use of phasic ‘function of presence’ approach in Navier-Stokes equation to formally account for co-sharing of a control volume by different phases. The use of this ‘function of presence’ leads to a term denoting interfacial momentum force \(( T_i \nabla X_i )\), which is the dot product of total stress term \(( T_i )\) and gradient of ‘function of presence’ term \(( \nabla X_i )\), and, represents force induced by local flow perturbations at the interface by influence of second phase. Here, the total stress is comprised of total bulk pressure and total shear stress contribution (comprising of shear stress at interface and “total stress minus the interfacial stress” term). The subsequent averaging (ensemble averaging for RANS turbulence or spatial filtering for LES model) of Navier-Stokes equation and the interfacial momentum term, leads to additional terms that can be attributed to form drag, skin drag, and other parts that can be modeled as non-drag forces (lift force, virtual mass force and turbulent dispersion force). These models needs to be expressed in terms of resolved quantities of the flow (mean or filtered variables), and, they should also be able to take into account the effect of unresolved motion (fluctuating or sub-grid scale) on the continuous phase and particle dispersion. In case of multiphase LES, so far the trend has been to neglect the unresolved sub-grid scale contributions as they remain unidentifiable both theoretically and experimentally. Generally, the modelling of these interfacial forces is complex because they depend upon the local liquid mean velocity, its gradient, the local turbulence parameter, and also strongly dependent on the dispersed phase particle size. But, the most debated amongst these forces is the formulation of turbulent dispersion force. This is because the derivations of the dispersed phase mass and momentum equations do not lead to a natural model for dispersion. The turbulent dispersion force
signifies the turbulent diffusion of the dispersed phase by the random motion of continuous phase eddies. The ‘classical’ model for including the dispersion effect is to include a flux of dispersed material in a continuity equation which is proportional to the gradient of number density (or volume fraction). The limitation of this model is that it gives a flux of the dispersed phase, even when the velocity of the dispersed phase is zero. In formalism employing the favre averaging, the dispersion term in continuity equation vanishes, and the dispersion effect makes its appearance as a force in the momentum equations. Different authors have come up with different expressions to model this turbulent dispersion force, like (a) Lahey et al., (1993); Carrica et al., (1999); Drew; (2001) considered the force to be proportional to the gradient of the void fraction in the momentum equations of the dispersed phase; (b) Lopez de Bertodano (1991); Lahey et al.,(1993); and Alajbegovic et al.,(1999) assumed that the dispersion force is proportional to the product of the turbulent kinetic energy of the liquid phase and the volume fraction gradient of the dispersed phase; (c) Drew (2001) and Lopez de Bertodano (1998) have proposed that the dispersion force is proportional to the Reynolds stress tensor of the dispersed and continuous phase, respectively, and a scalar coefficient, which is a function of the Stokes number (i.e., the ratio of the response times of the bubbles or particles and liquid eddies); (d) Dhotre et al. (2007) proposed random dispersion model (RDM) in-place of empirical TDF and obtained good agreements with their LIXN facility, without the need of introducing any adjustable coefficients, while, (e) Burns et al. (2004) double averaged the local instant equations to obtain a Favre averaged drag model which accounted for TDF as well. Their model generalizes well with most current models of turbulence dispersion, and was seen to possess a wide degree of universality. In the model validations carried out by Lopez de Bertodano (1991, 1998), Lahey et al. (1993) and Alajbegovic et al. (1999), there were some sources of uncertainties arising due to liquid-phase k-ε turbulence model. It is expected that the LES turbulence model which resolves the
larger scale would be able to resolve the turbulent dispersion better, but the effect of sub-grid scale eddies in causing turbulent dispersion has to be modeled. Hence, there is a need to apply and gain insights from application of Eulerian-Eulerian multiphase LES with SGS Turbulent dispersion. For our case, it was deemed suitable to use Bertodano model, as we could adapt it for SGS level using SGS-TKE.

Hence, the objective of our present study is to analyze the importance and effect of sub-grid scale turbulent dispersion force on different particle systems, where the particle sizes would be smaller than filter-size. A numerical exercise in quantifying the sub-grid scale turbulent dispersion force (SGS-TDF) and its effect for different particle systems would help to understand how the dispersion of sub-grid particles is being quantified, and how much effect it has on the flow profile. The work attempts to adapt the concept developed by Lopez de Bertodano et al. (1994) to approximate the turbulent diffusion of the particles by the sub-grid scale liquid eddies. This work attempts to do so for a gas-liquid bubble column system (Tabib et al., 2008) and a liquid-liquid solvent extraction pump-mixer system (Tabib et al., 2009; Tabib et al., 2010). In liquid-liquid extraction system, the organic droplet size is around 0.5 mm, and in bubble column, the bubble size is around 3-5 mm. To study the effect of sub-grid turbulent dispersion, the bubble column was simulated with two different mesh sizes, a grid size coarser and a grid size finer than the bubble size. The pump-mixer was simulated with mesh size coarser than the droplet diameter. The effect of SGS-TDF was studied on averaged axial velocity and hold-up profile obtained from LDA and PIV experimental measurements.

2. Model Description

The two-fluid model based on the Euler-Euler approach employing LES turbulence model is described below. Here, each fluid (or phase) is treated as a continuum in any size of domain under consideration. The phases share this domain and interpenetrate as they move
within it. This Eulerian modelling framework uses the phasic function of presence (to account for space occupation by a given phase) instead of volume averaging step, and this allows us to directly derive a set of mass and momentum transport equations for each phase by applying filtering (LES framework) or ensemble averaging (for RANS). These transport equations without mass transfer can be written as:

Continuity equation

$$\frac{\partial}{\partial t}(\rho, \alpha_r) + \nabla \cdot (\rho, \alpha_r \mathbf{u}_r) = 0$$

(1)

Momentum transfer equations

$$\frac{\partial}{\partial t}(\rho, \alpha_r \mathbf{u}_r) + \nabla \cdot (\rho, \alpha_r \mathbf{u}_r \mathbf{u}_r) = -\nabla \cdot (\alpha_r \mathbf{t}_{ij,r}) - \alpha_r \nabla P + \alpha_r \rho_r g + M_{F,r}$$

(2)

In this work, the phases are continuous phase (r=a) and dispersed phase (r=b). The terms on the right hand side of eqn (2) are respectively representing the stress, the pressure gradient, gravity and the filtered momentum exchange between the phases, due to interface forces. The pressure is shared by both the phases. The stress term of phase r is described as follows:

$$\mathbf{t}_{rr} = -\mu_{eff,r} \left( \mathbf{v}_r + (\mathbf{v}_r)^f - \frac{2}{3} \nabla (\mathbf{v}_r) \right)$$

(3)

where, $\mu_{eff,r}$ is the effective viscosity and the Strain rate S is $\left( \mathbf{v}_r + (\mathbf{v}_r)^f \right)$. The effective viscosity of the continuous phase is composed of two contributions: the molecular viscosity and the turbulent viscosity.

$$\mu_{eff,a} = \mu_{l,a} + \mu_{t,a}$$

(4)

The continuous phase turbulent eddy viscosity $(\mu_{t,a})$ is formulated based upon the Large eddy...
simulation (LES) turbulence model, as described below.

Large Eddy Simulation Turbulence Model

Equations for LES are derived by applying a filtering operation to the Navier-Stokes equations. The filtered equations are used to compute the dynamics of the large-scale structures, while the effect of the small scale turbulence is modeled using a Sub Grid Scale model. Thus, the entire flow field is decomposed into a large-scale or resolved component and a small-scale or subgrid-scale component. In case of LES, the velocities (u) in continuity equations and momentum equations (eqn.1-2) represent the resolved velocities or grid scale velocities. The eqn. 5 defines this resolved velocity, called so, as they are resolved by the numerical simulation.

\[ u = u_i - u_s \]  

(5)

where, \( u_i \) is the true instantaneous velocity of fluid, and \( u_s \) is the sub-grid scale (SGS) velocity, which is not resolved by the numerical simulation. These SGS parts of velocity components, gives rise to additional stress terms and additional interface forces. The SGS stress terms of a given phase is related to the resolved scale strain tensor \( S \). In case of LES models, like smagorinsky (Smagorinsky, 1963) and dynamic (Germano et al. 1991; Lilly er al. 1992) model, only the deviatoric part of the SGS stress is modelled, while its trace is implicitly added to the pressure. This means with such LES models the information on the amount of SGS kinetic energy (\( k_{sgs} \)) is lost in algebraic models, and hence unavailable to use for computing SGS dispersion force or SGS droplet induced turbulence. The use of 1-Eq-SGS-TKE LES model (Davidson et al. 1997) overcomes this drawback, and computes the turbulent eddy viscosity in a manner as described below:

\[ \mu_{T,a} = \rho_a C_k \Delta k_{sgs,a}^{1/2} \]  

(6)
where, \( k_{sgs} \) is obtained by solving for transport equation for SGS kinetic energy for continuous phase (\( r=a \)):

\[
\frac{\partial}{\partial t}(\rho \alpha k_{sgs}) + \nabla \cdot (\rho \alpha \mathbf{u} k_{sgs}) = -\nabla \cdot \left( \alpha \frac{\mu_{sgs}}{\sigma} \nabla k_{sgs} \right) + \alpha \left( G - C_s \frac{k_{sgs}^{3/2}}{\Delta} \right) + S_{T_k}
\]  

(7)

Where, \( G \) is the production term, defined as:

\[
G = \mu_{T,a} \overline{S_{ij}}
\]  

(8)

and \( S_{T_k} \) is the source term for production as described in section on bubble induced turbulence.

The model constants are \( C_\varepsilon=1.05 \) and \( C_k=0.07 \). The 1-Eqn-SGS-TKE LES model was incorporated in ANSYS CFX-12 platform using user-subroutines and user-functions.

While, the effective dispersed phase viscosity is computed based on the effective continuous phase viscosity as follows:

\[
\mu_{eff,b} = \left( \frac{\rho_a}{\rho_b} \right) \mu_{eff,a}
\]  

(9)

Such a model (eqn. 9) is simple to implement and gives approximate turbulence estimate for computation of dispersed phase. This approach has been widely used in numerous works (Deen et al. 2000). The justification for using such a simple approximate dispersed phase turbulence model lies in the fact that dispersed phase turbulence has less effect on continuous phase, and the scope of work is to capture the turbulence in the continuous phase.

Interfacial forces
The total interfacial force acting between the two phases may arise from several independent physical effects:

\[ M_{I,a} = -M_{I,b} = M_{D,a} + M_{L,a} + M_{VM,a} + M_{TD,a} \]  

(10)

The forces indicated above represent the interphase drag force, lift force, virtual mass force and turbulent dispersion force respectively. The origin of the drag force is due to the resistance experienced by a body moving in the liquid. Viscous stress creates skin drag and pressure distribution around the moving body creates form drag. The later mechanism is due to inertia and becomes significant as the particle Reynolds number becomes larger. The lift force arises from the net effect of pressure and stress acting on the surface of a dispersed phase. The sign of this force depends on the orientation of slip velocity with respect to the gravity vector. The turbulent dispersion force signifies the turbulent diffusion of the dispersed phase by the eddies in the continuous phase. For simulating liquid-liquid flow, the contributions of lift force and virtual mass force can be neglected as they are negligible, while for the gas-liquid system, all the forces except the virtual mass force has been considered. The virtual mass force is proportional to relative acceleration between phases and is negligible once pseudo-steady state is reached. Based on observation made by Hunt et al. (1987), Thakre and Joshi (1999), Deen et al. (2001) and Sokolichin et al. (2004) and our own observation for this system (Tabib et al, 2008), the added mass force is known to have had no effect on the simulation. Hence, it was neglected. In case of Large eddy simulation, there would be additional forces at the SGS level. An attempt is made here to take account of sub-grid-scale turbulent dispersion force by using sub-grid-scale-turbulent kinetic energy in Bertodano Model. The interphase momentum transfer due to drag force is given by:

\[ M_{D,a} = -F_{drag,a} = -\frac{3}{4} \alpha_p \rho \frac{C_D}{d_b} |U_o - U_a| (U_o - U_a) \]  

(11)
where, $C_D$ is the drag coefficient taking into account the character of the flow around the particle, and $d_b$ is the particle diameter. In case of droplets and bubble, the drag coefficient was determined through the empirical correlations of Ishii and Zuber (1979), which allow for an increase in drag (and reduced rise velocity) due to multiple particle (droplet) interactions, as a function of the dispersed phase volume fraction. For the viscous regime, the drag coefficient was determined according to:

$$C_{D,a} = \frac{24}{Re} \left( 1 + 0.1 Re^{0.75} \right)$$  \hspace{1cm} (12)

where the Reynolds number, $Re$, is modified to allow for the dispersed phase volume fraction and is given by:

$$Re = \frac{\rho_a |U_a - U_o| d}{\mu_a} \left( 1 - \alpha_o \right)$$  \hspace{1cm} (13)

For the distorted regime,

$$C_{D,a} = \frac{2}{3} d \sqrt{\frac{(\rho_a - \rho_o) g}{\sigma}} (1 - \alpha_o)^{-0.5}.$$  \hspace{1cm} (14)

The drag coefficient was chosen according to:

$$C_D = \max \left( C_{D,a}, C_{D,o} \right)$$  \hspace{1cm} (15)

The lift force in terms of the slip velocity and the curl of the continuous phase velocity can be described as:

$$M_{L,a} = C_L \epsilon_a \rho_L (u_b - u_a) \times \nabla \times u_a$$  \hspace{1cm} (16)
where, $C_L$ is the lift coefficient. The sign of this force depends on the orientation of slip velocity with respect to the gravity vector. The lift force will have significant effect on radial profile of dispersed phase hold-up. The choice of lift coefficient was done on the basis of corresponding bubble size as suggested by Kulkarni (2003) and Tomiyama (2004). The value reported by Kulkarni (2003) follows the same trend as reported by Tomiyama (2004), but the absolute value is less in the bubble size range of 6–8 mm. For the sieve sparge bubble column, the average bubble diameter is 3 mm, and the lift coefficient value is taken negative ($C_L = -0.05$). The sensitivity analysis of lift force had been conducted in a previous article by Tabib et al (2008). The study had showed that the positive value of lift coefficient makes the bubbles move outwards towards the column wall, which leads to a flatter hold-up profile and lower centreline velocity. The negative values of lift coefficient acts to move the bubble in the centre and results in higher dispersed-phase hold up at the centre. The lift force sensitivity analysis results can be seen in Tabib et al (2008). In this work, we concentrate on sub-grid scale turbulent dispersion effects in a LES framework.

The turbulent dispersion force, derived by Lopez de Bertodano [51], is based on the analogy with molecular movement. It approximates a turbulent diffusion of the dispersed phase by the liquid eddies. In this case since larger eddies are resolved, and effect of smaller eddies need to be modeled, so we consider the sub-grid-scale turbulent kinetic energy in the formulation.

$$M_{TD,a} = -C_{TD} k_{sgs,a} \rho_a \nabla \epsilon_a$$  \hspace{1cm} (17)

where, $k_{sgs}$ is the SGS turbulent kinetic energy per unit of mass. $C_{TD}$ is the turbulent dispersion coefficient. In this work, a value of 0.1 is considered for $C_{TD}$ while computing SGS-TDF and this SGS-TDF magnitude is compared with all the interfacial forces (including the resolved turbulent dispersion force). The LES in principal takes care of the gas dispersion
by large-scale eddies as these are resolved. Hence, unlike other forces, the resolved turbulent dispersion force has not been included in the model, but only computed to compare with the sub-grid scale-turbulent dispersion force. It was observed that the SGS-TDF magnitude far less than that obtained using $C_{TD} = 0.1$ is required to obtain the experimental hold-up profiles. This also shows that even a small magnitude of SGS-TDF force is enough to affect the flow profile. Hence, the research work towards finding a suitable $C_{TD}$ values to be used in SGS-TDF is also a direction that needs to be pursued.

Bubble induced turbulence

In regions of higher volume fraction, the turbulence within the wake can be higher than the shear-induced turbulence. The fluctuations induced by bubble wake can be incorporated in the model as bubble-induced turbulence (BIT). The attempts at incorporating the bubble-induced turbulence in a LES framework has been done before (Niceno et al. (2008); Deen et al. (2001)). There are two approaches that have been used to account this: One involves incorporating the effect as enhanced eddy viscosity by including a term call bubble induced viscosity (Sato and Sekoguchi, 1975), and second approach is by adding extra production terms into the SGS-turbulent kinetic energy equation (following the procedure described by Pfleger and Becker (2001) or Simonin and Viollet, 1988). The results obtained by various researchers suggest that the models employing the second approach of extra production term has been more effective. In this work, the influence of Pfleger model on the SGS-TDF has been analyzed and results are discussed in section 4.1. The Pfleger model (eqn 18) computes the bubble induced turbulence as the energy input of the bubble wakes resulting from the forces acting between a gas bubble and the surrounding liquid and the local slip velocity.

$$ST_k = C_k \left| M_{\alpha,\beta} \right| \left| u_G - u_L \right|$$  \hspace{1cm} (18)
3. Experimental details, simulation and geometry details:

3.1 Experimental dataset

Bubble column: The experimental details and dataset for validating the bubble column simulation was obtained using laser Doppler velocimetry (LDV) by Bhole et al., (2006) and Kulkarni et al., (2007). This dataset was used previously by Tabib et al., (2008) for validation of LES and RANS CFD code. The same dataset has been used in this work too. In this case, the effects of variation of SGS turbulent dispersion force on hold-up and axial velocity has been studied quantitatively in comparison with the LDA experimental data.

Pump-Mixer: particle image velocimetry studies have been carried out at CSIRO for a single phase operation of the pump-mixer unit. The prediction of axial average velocity profile from this single phase study has been used to compare predictive performance of different models (RANS, LES-Smagorinsky, LES-Dynamic) by Tabib et. al. (2009, 2010). The LES study has been extended to multiphase after validation in single phase system. For multiphase operation of pump-mixer involving aqueous water and organic kerosene phase, it was not possible to obtain velocity measurements using laser based techniques (PIV, LDA). This was because of the high degree of opacity introduced by high organic volume fraction (around 50%). Hence, the CFD results for multiphase has been validated using the torque measured while experiments. The torque experienced on impeller surface as computed from CFD data (0.682 Nm) is close to the experimental value (0.705 Nm) in multiphase system. In this case, the effects of variation of SGS turbulent Dispersion force on hold-up and axial velocity has been studied qualitatively.

3.2 Accuracy and Resolution of LES Model
The accuracy and resolution of a LES simulation is determined by criteria like spatial resolution (grid size), the resolved kinetic energy, and the temporal resolution. The following three criteria have been discussed below:

Spatial resolution criteria: Fig 1 shows the hexahedral grid arrangement used for simulating the pump-mixer, and Figure 2 shows it for the bubble column. For bubble column, two mesh sizes are used to study the effect of SGS-TDF, one coarser than particle size and other finer than the particle size. Generally for accurate LES results, the grid should be sufficiently fine, so that only smaller, isotropic eddies are modelled. In other words, the modelled SGS stress should account for a negligible fraction of the total stress. Baggett et al. (1997) suggested that SGS stress becomes isotropic when filter width is a fraction of turbulent dissipation length scale (preferably, 0.1). This ratio is computed as \( \frac{(\nu \bar{\gamma}^2)}{k \varepsilon} \), where, the turbulent length scale can be computed from \( k \) and \( \varepsilon \) values of the \( k-\varepsilon \) model. Figure 3 shows the contour plot of ratio of “filter width to turbulent dissipation length scale”, and gives an indication of suitability of grid. For pump-mixer (Fig. 3A), the volumetric average of ratio \( \frac{(\nu \bar{\gamma}^2)}{k \varepsilon} \) is around 0.6, and the contour plot shows a horizontal plane at impeller region. For bubble column, Fig 3B shows that for the coarser mesh, in the central region the ratio is around 0.1, and for finer mesh (Fig 3C), the ratio is less than 0.1 in most of the regions as expected. But, for maintaining consistency with the interpenetrating continuum assumption of multiphase Eulerian-eulerian approach, the largest interphase details of dispersed phase should be smaller than the grid-size. Thus, the grid chosen for pump-mixer and coarse mesh bubble column meets these criteria and is adequate. The incorporation of SGS turbulent dispersion force to account for particle dispersion by sub-grid eddies is expected to take care of the information lost by coarse mesh. The finer mesh (Fig 3C), though it violates the eulerian-eulerian consistency, has been used to study the effect of
SGS turbulent dispersion in situations where sub-grid scale eddies may not be dominant. Mesh details are covered in section 3.3.

Resolved kinetic energy criteria: The other issue in LES is resolved kinetic energy. Pope (2000) suggested that the ratio of resolved turbulent kinetic energy to the total turbulent kinetic energy \( \left( \frac{k_r}{k_{total}} \right) \) be used as a measure to analyze the adequacy of the fluid flow being resolved by LES. For a well-resolved flow, the ratio is greater than 80%. Figure 4 helps to judge the present LES simulation on the basis of the resolved energy criteria. For pump-mixer (Fig 4A), the ratio is above 70% when averaged over the tank, and in regions with higher turbulence near impeller and in bulk, the ratio is greater than 80%. For bubble column with coarser mesh (Fig 4B), the volume averaged ratio is around 60%, while for bubble column with the finer mesh, the LES resolves more flow, with the volume averaged ratio being around 75%. Hence, the results from the pump-mixer and coarse mesh bubble column LES run can be considered to be moderately resolved and acceptable for analysis with inclusion of SGS-TDF.

Temporal resolution: The time-step should be selected in such a manner that the LES is able to capture the physics associated with flow structures displaying dominant frequencies, and numerically, the code should be converging.

Thus, care has been taken to resolve the flow adequately, though it is not as finely resolved as per Pope’s criteria (2000). There are two reasons, we went with a coarser mesh: (1) A coarser mesh should help to highlight the importance of sub-grid scale turbulent dispersion force while satisfying interpenetrating continuum assumption. In other words, we seek to check whether for a coarser mesh LES run, the sub-grid scale coupling forces should be accounted, which hasn’t been done yet. (2) The computational time required for going with a finer resolution LES is prohibitive, and also it would not have enabled us to carry out SGS turbulent dispersion force studies.
3.3 Simulation details

Gas-Liquid Bubble Column:

The bubble column unit comprises of a cylindrical column with 0.15m diameter and 1m height. The gas inlet through the spargers was incorporated by creating mass source points at the specified position to mimic the exact sparger. Based on the superficial gas velocity (0.02 m/sec), the mass flow rate was specified for each source point. Along the walls, no-slip boundary conditions were adopted. At the outlet of the column, the atmospheric pressure was specified as boundary condition. Two different mesh sizes have been used to study the effect of SGS turbulent dispersion. The coarser mesh (Fig 2B) size considered was about 5 mm at the centre (roughly the size equivalent to bubbles) and has 36000 nodes. This mesh can be considered a bit coarser with respect to the bubble size, than the one used by Niceno et al. (2008), as our objective is to study the effect of sub-grid scale turbulent dispersion force. The other with finer mesh (Fig 2C) has about 0.4 million nodes. The LES run has been initialized from a perturbed RANS simulation (Tabib et al. 2008). The simulations were performed for a time-span of around 100 sec, with a time-step size of 0.01 s for coarser mesh and 0.001 s for finer mesh. The simulation with coarser grid takes around 4 days computational time on a single processor, while the one with finer grid takes around 6 weeks computational time on 4 processors.

Liquid-Liquid Pump-Mixer

The pump mixer unit comprises of a square mixer box (of dimensions 450mmx450mmx450mm) equipped with a Lightnin R320 impeller (of diameter 230 mm and positioned about 5 mm above the false bottom). The mixer has been modelled with an impeller speed of 200 rpm (tip speed of 2.4 m/s) using the sliding mesh approach for impeller motion. There is a separate inlet section for the organic and aqueous phases located in the
bottom section below, where they flow in at a rate of 15 l/min each. The outlet from the mixer box is in the form of an overflow via a weir to a rectangular settler (of dimensions 1410mmx450mm). The LES run has been initialized with a perturbed RANS transient solution run to achieve steady flow (around 20 impeller rotations). The mesh consisted of 587000 cells (hexahedral elements) with relatively fine mesh near the impeller to better resolve the velocity fields. In pump mixers, the turbulent structures are generated by large and rotating geometrical features and flow curvature. Hence, the near wall spacing criteria is relaxed with use of appropriate wall functions. The simulations were performed for a time-span of around 10 sec, which corresponds to around 33 revolutions of the impeller. The time-step is around $5 \times 10^{-3}$ s. The selected time-step ensures proper convergence and capture of transient flow structures. The monitoring of local transient averages indicated the attainment of this pseudo steady state. In experiments, the flow field reaches a quasi-steady state after few impeller rotations. Computationally, the number of impeller rotations required to achieve this quasi-steady state depends upon the grid density and initial values of a transient simulation. In this case, the LES runs are initialized from the perturbed RANS solution. This resulted in the flow field achieving a pseudo-steady state in around 20 impeller rotations; hence 10 s simulation time was sufficient to compute averages. The 10 s simulation run takes about 4 weeks of computational time on 4 processors. The average droplet diameter was taken as 0.6 mm, based on the results from experimental photographic techniques (Tabib et al. 2009).

4. Results

The main objective of this paper is to quantify the sub-grid scale turbulent dispersion force, and study whether its inclusion benefits the Eulerian-Eulerian LES simulation. Hence, the results are presented in two sub-sections: Section 4.1 deals with quantification of sub-grid turbulent dispersion force with respect to other forces (like drag, lift, turbulent dispersion
etc.). The effect of mesh size on sub-grid turbulent dispersion force has been shown. Section 4.2 deals with effect of turbulent dispersion force on radial hold-up and velocity profiles. This is done by comparing the results of simulation run with and without incorporating the turbulent dispersion force. Generally, the phase-averaged variables are preferred for comparison of results in an un-stationary random periodic flows (as in pump-mixer) since it helps us to study the effect of relative position of impeller blade on the flow field at a given location. Thus, phase-averaging is extremely useful to compare flow-fields arising out of two different impellers as the mean-flow and fluctuating flow can be obtained as function of impeller angle. However, here we have used the time-averaged profiles for validation and comparison for two reasons: first, our objective was to study the effect of sub-grid-scale turbulent dispersion force on the average volume fraction dispersion and on the average flow field in general, regardless of the effect of blade position, and secondly, we had validated the single phase model with the time-averaged experimental single phase dataset, before extending the model to multi-phase. The time-averaged profiles are popular and convenient to use for validation/comparison.

4.1 Quantification of SGS turbulent dispersion force with respect to other forces

The use of 1-Equation-SGS-TKE LES with SGS-TDF model has enabled us to compute the values of sub-grid scale turbulent dispersion force. It is not possible to experimentally measure/validate the dispersion caused by sub-grid eddies. The smagnitude of sub-grid turbulent dispersion force (instantaneous as well as time-averaged) is shown in Figure 5 for bubble column and Figure 6 (A-C) for pump-mixer. For pump-mixer, the instantaneous values are plotted at 10 s, and for coarse mesh bubble column, they are plotted at 100 s. The averaged SGS-TDF value helps us to give the true picture for comparing. The instantaneous contours (in Figure 5 and 6) give a good idea on how instantaneous SGS-TDF is computed and how it varies with the two parameters: the instantaneous dispersed phase
volume-fraction gradient and the instantaneous SGS-TKE. In case of pump-mixers, the region near the impeller is a region of high SGS-TDF on account of higher sub-grid scale energies here (Fig 6A-C). In case of bubble-column, the SGS-TKE term being weak has less pronounced effect on SGS-TDF as compared to ‘gradient of dispersed phase volume fraction’ (Fig 6A-C). The relative influence of averaged SGS-TDF within a particular flow system can be gauged by comparing its magnitude and its directional dominance with respect to other averaged forces (drag force, lift force, force due to advection of momentum and pressure, resolved turbulent dispersion force), as shown in Fig 6-10. Figure 6 (D-F) compares the time-averaged forces for the pump-mixer. Figure 7 compares the time-averaged forces in bubble column (drag, lift, TDF, SGS-TDF etc.) for simulation involving coarser mesh and has two contours showing relative influence of bubble induced turbulence as evaluated using Simonin and Pfleger model, while Figure 8 compares the time-averaged forces for the finer mesh bubble column run. These runs with finer and coarser mesh describe the variation in relative importance of SGS-turbulent dispersion force with mesh size. All these results give us many insights. Like, the time-averaged profiles show that the relative strength of SGS-TDF magnitude with respect to other forces in the coarse bubble-column run (Figure 5D, 7E) is higher than that in finer mesh bubble column (Figure 8E), but it is much lower than the relative strength of SGS-TDF values in the pump-mixer (Figure 6D). This indicates that SGS-TDF force will have more influence in pump-mixer. To quantify further, Fig 7E (and Fig 5D) shows that the magnitude of SGS-TDF in coarse bubble column (~1e-8, in most regions) is three orders of magnitude lower than the drag force magnitude (~1e-4) in the same system (Fig 7A). On the other hand, the magnitude of SGS-TDF values in pump-mixer (~1e-6 , as seen in Fig 6D) is an order of magnitude higher than that in coarse bubble column, and is comparative in magnitude to the drag force in that system (~1e-6, as seen in Fig 6E). Hence, the effect of SGS turbulent dispersion force is more pronounced in the pump-mixer. The
reason being that the ratio of mesh size with respect to dispersed phase organic droplet size (around 0.5 mm) in pump-mixer is higher than in bubble column (where mesh size is equivalent to the bubble size~5mm). Hence, the sub-grid eddies in pump-mixer would have more effect as captured by the computational model and this suggests that SGS-turbulent dispersion forces should be accounted in LES for coarse meshes.

The influence of sub-grid scale bubble induced turbulence (SGS-BIT) on SGS-TKE and subsequently on SGS-TDF has been incorporated using the Pfleger model. The contour plot of ratio of “production of SGS-KE from SGS bubble induced term” to “production of turbulence from shear-strain rate” for coarse mesh bubble column simulation has been shown using the Pfleger model (Fig 7G). The volumetric average for the ratio is 0.2 for Pfleger model. The contour plot reveals that the SGS-BIT may need to be considered for such analysis, though it may not play as dominant role as compared to the shear induced turbulence.

The comparison between coarser and fine mesh effect on SGS-TDF in bubble column also helps to give an insight into the suggestions made by Niceno et al. (2008). The lower values of SGS-TDF for finer mesh bubble column (Fig 8E) as compared to coarser mesh (Fig 7E) suggests no major role of sub-grid eddies in the simulations where particle size is larger than mesh size (ie. in finer mesh simulation).

Figure 9 show that the SGS-TDF has a dominant component in the transverse direction (radial direction) than in the flow direction (axial direction) for both the bubble column and pump-mixer. While, drag forces and momentum advection force is dominant in the axial direction (or in the flow direction, components not shown here). The magnitude of SGS-TDF force appears small as compared to the force exerted by mass flow (which is dominant only in flow direction and is shown in Figure 5D and Figure 6D), but, the SGS-TDF force do
influence the radial profiles of hold-up and axial velocity (as will be seen in results described in section 4.2). In next section, we cover the effect of SGS-TDF on the averaged hold-up and the averaged axial velocity.

4.2 Effect of TDF on Velocity profiles and on Gas-Hold up profile

Bubble Column: Fig. 10 shows the LES model validation for radial profile of averaged averaged hold-up for the sieve plate bubble column with respect to LDA experiments. The profile obtained by One-Equation-SGS-TDF LES model (with SGS-TDF in coarse mesh, without SGS-TDF in coarse mesh, without SGS-TDF in finer mesh) has been compared vis-a-vis the experimental LDA dataset at two axial locations corresponding to height to diameter ratio of 2 and 3 (corresponding to z=0.35 m and z=0.45 m respectively). The model in general shows that axial flow is distinctly upward in the central region, while a downward counter flow is observed in the near wall region. The point of flow reversal is clearly seen at a radial location of around r/R = 0.6-0.8 m. The variation in mesh size (wrt dispersed phase particle size) has been used to to determine the effect of sub-grid turbulent dispersion force. The inclusion of SGS-TDF in the coarser mesh has seen to have immense influence on the results (Figure 10). The average gas hold-up profile increases and the profile becomes much flatter as compared to the run without SGS-TDF in coarse mesh. This effect is caused even though the magnitude of SGS-TDF is low as compared to other forces. The result of coarse mesh with TDF can be improved further to approach the experimental hold-up profile and the results of finer mesh without TDF by using a much lower SGS-Turbulent dispersion coefficient and hence a lower magnitude of SGS-TDF force. This highlights the need for inclusion of SGS-TDF for LES runs with coarser mesh. Hence, the need is to model the SGS-TDF and SGS-turbulent dispersion force appropriately. The SGS-TDF force can counter balance the lift force (when the lift coefficient is negative) and its use is physically justified.
Pump-Mixer: Figure 11 shows the effect of including SGS turbulent dispersion force (SGS-TDF) on average dispersed phase volume fraction in regions near the impeller and away from impeller. The simulations show that around the impeller there is more radial dispersion of dispersed phase with the inclusion of SGS-TDF (Fig 11B) as compared to without SGS-TDF (Fig 11A). This can be attributed to the higher magnitude of SGS-TDF force in radial transverse direction. Fig 11 (C) and (D) show the effect at a location 0.15 m axially above the impeller without and with TDF resp., while Fig 11 (E) and (F) shows the effect at a location 0.3 m above the impeller respectively. As we move away from the impeller, the radial dispersion becomes less pronounced. This could be because of higher sub-grid scale turbulence energy near the impeller, which signifies that the sub-grid scale eddies have more influence near the impellers. Away from impeller, Fig 11 (C) and (D) shows some radial dispersion of dispersed phase happening with inclusion on SGS-TDF, but it is not as pronounced as near the impeller. Near the upper wall of pump-mixer (Fig 11 (E) and (F)) not much radial dispersion is seen. Though in all the regions, an increase in dispersed phase hold-up is seen which can be attributed to the inclusion of SGS-TDF. The SGS-TDF enhances the residence time of dispersed phase by making it move radially, and this is reflected in higher hold-up profiles in the mixer unit. Similarly, Fig. 12 shows the effect of including SGS Turbulent dispersion force on average axial velocity of continuous phase in a multiphase system. Fig 12 compares the predicted CFD values to the experimental values of time averaged axial velocity along the y direction at location $x= -0.168$, $z = 0.323$ for the pump-mixer operating in single phase. The experimental data shown in Fig 12 was obtained for single phase system using PIV. The results from single phase LES was validated against this dataset. With the inclusion of SGS-TDF force in multiphase run, it is seen that the central peak velocity dampens a bit. The multiphase model has been validated with torque measurements as mentioned earlier. It is not possible to measure the local flow velocities and
local hold-ups in the pump-mixer, owing to high opacity arising from dispersed kerosene phase. Hence for this case, we rely on numerical experimentation and checking qualitative trend.

Thus, this small numerical exercise has helped us to better understand the status of SGS-Turbulent dispersion force. The future direction lies in developing of SGS-TDF models, and studying them with different particle systems, like solid-gas systems having diameter in 50-100 micron range, where it may not be possible to use the grid-size equivalent to particle diameter.

5. Conclusions

This work has helped to quantify the sub-grid scale turbulent dispersion force (SGS-TDF), and has shown how its inclusion in modelling could be beneficial to overcome the drawbacks associated with typical Eulerian-Eulerian LES simulations. An attempt has been made to use the information on the SGS kinetic energy obtained from the one-equation-SGS-Turbulent kinetic energy LES model to model the sub-grid-scale turbulent dispersion phenomena. In the current study, the effect of SGS-TDF was studied for two different particle systems: the gas-liquid bubble column was simulated with two different mesh sizes, a grid size coarser and a grid size finer than the bubble size (= 5 mm), and the liquid-liquid pump-mixer was simulated with a grid size coarser than the droplet diameter (0.5 mm). In comparison with bubble column (both coarser and finer), the SGS-TKE values and the relative influence of SGS-TDF as compared to other forces were stronger for the pump-mixer. This was because in pump-mixer, the ratio of “dispersed phase particle diameter to grid-size” was smaller than for the bubble column. Also, the inclusion of SGS-TDF affected the radial hold-up profiles and this happens despite of the fact that the magnitudes of SGS-TDF forces appeared to be small enough to cause a influence. The result of coarse mesh with TDF can be improved further to approach the experimental hold-up profile and the results of
finer mesh without TDF by using a much lower SGS-Turbulent dispersion coefficient and hence a lower magnitude of SGS-TDF force. This highlights the need for inclusion of SGS-TDF for LES runs with coarser mesh. Hence, the need is to model the SGS-TDF and SGS-turbulent dispersion force appropriately. These results suggest that the inclusion of SGS-TDF will have more pronounced effect for those Eulerian-Eulerian LES simulation where grid-size happens to be more than the particle size. As expected, the SGS-TDF in combination with 1-Equation-SGS-TKE LES model also serves as a tool to overcome a drawback of Eulerian-Eulerian LES model. The future direction lies in developing of SGS-TDF models, and studying them with different particle systems, like solid-gas systems.

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Nomenclature

\[ C_D \] drag force coefficient, dimensionless

\[ C_L \] lift force coefficient, dimensionless

\[ C_{TD} \] turbulent dispersion coefficient, dimensionless

\[ C_{VM} \] added mass force coefficient, dimensionless

\[ C_s \] smagorinsky Constant, dimensionless

\[ C_\mu \] constant in \( k-\varepsilon \) model, dimensionless

\[ d_b \] bubble diameter, m

\[ g \] gravitational constant, m/s^2
\( G \) generation term, kg/ms\(^2\)

\( k \) turbulent kinetic energy per unit mass, m\(^2\)/s\(^2\)

\( k_{sgs} \) sub-grid-scale turbulent kinetic energy per unit mass, m\(^2\)/s\(^2\)

\( M_i \) total interfacial force acting between two phases, N/m\(^3\)

\( M_d \) drag force, N/m\(^3\)

\( M_L \) lift force, N/m\(^3\)

\( M_{VM} \) added mass force acting, N/m\(^3\)

\( M_{TD} \) turbulent dispersion force, N/m\(^3\)

\( P \) pressure, N/m\(^2\)

\( R \) radial distance, m

\( R_c \) column radius, m

\( Re_B \) Reynolds Number (= \( d_b V_S/\nu \)), dimensionless

\( S \) strain rate, 1/s.

\( T \) time, s

\( u \) velocity vector, m/s

\( u' \) fluctuating velocity, m/s

\( u_i \) average axial liquid velocity, m/s

\( u_{inst} \) instantaneous velocity, m/s.

\( u_{sgs} \) sub-grid scale velocity, m/s.
\( V_s \)  axial slip velocity between gas and liquid, \( m^2/s \)

\( v_c \)  centerline axial liquid velocity, \( m/s \)

\( z \)  axial distance along the column, \( m \)

**Greek symbols**

\( \varepsilon \)  fractional phase hold-up, dimensionless

\( \bar{\varepsilon} \)  average fractional phase hold-up, dimensionless

\( \epsilon \)  turbulent energy dissipation rate per unit mass, \( m^2/s^3 \)

\( \mu \)  molecular viscosity, \( Pa \, s \)

\( \mu_{\text{eff}} \)  effective viscosity, \( Pa \, s \)

\( \mu_t \)  turbulent viscosity, \( Pa \, s \)

\( \rho \)  density, \( kg/m^3 \)

\( \sigma_k \)  Prandtl number for turbulent kinetic energy, dimensionless

\( \sigma_\varepsilon \)  Prandtl number for turbulent energy dissipation rate, dimensionless

\( \tau_k \)  shear stress of phase \( k \), \( Pa \)

**Subscripts**

\( r \)  = phase; \( a \) : continuose phase, \( b \) = dispersed phase

**References**


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