



## LES of bubble column bubbly flows accounting SGS turbulent dispersion and added mass stress effects

Journal:	<i>Chemical Engineering &amp; Technology</i>
Manuscript ID	ceat.202300142.R1
Wiley - Manuscript type:	Research Article
Date Submitted by the Author:	n/a
Complete List of Authors:	Long, Shanshan; University of Nottingham Ningbo China, Mechanical, Materials and Manufacturing Engineering Yang, Xiaogang; Univ Nottingham Ningbo China, Mechanical, Materials and Manufacturing Engineering Yang, Jie; University of Hull, School of Natural Sciences Sommerfeld, Martin; Otto von Guericke Universität Magdeburg, Fakultät für Verfahrens- und Systemtechnik Xue, Chenyang; University of Nottingham Ningbo China
Keywords:	Added Mass Stress, Bubble Column, LES Simulation, Mass transfer, Turbulent Dispersion

SCHOLARONE™  
Manuscripts

1  
2  
3 Shanshan Long<sup>1</sup>

4 Xiaogang Yang<sup>1,\*</sup>

5  
6 Jie Yang<sup>2</sup>

7  
8 Martin Sommerfeld<sup>3</sup>

9  
10 Chenyang Xue<sup>1</sup>

### 11 12 13 **LES of bubble column bubbly flow considering SGS turbulent diffusion effect and bubble oscillation**

14  
15 The present study will demonstrate through Euler/Euler LES modelling that turbulent dispersion of  
16 bubbles can effectively indicate the impact of turbulent eddies on bubble dynamics, i.e. the bubble  
17 oscillation behavior. This finding builds on previous work using Euler/Lagrange LES modelling approach  
18 and leads to a significant improvement in predicting bubble lateral dispersion. Spatially filtered terms  
19 were proposed for the SGS turbulent dispersion and added mass stress force models, with a modification  
20 made to the SGS eddy viscosity to reflect bubble turbulent dispersion and oscillations. The proposed  
21 model substantially improves the prediction of bubble volume fraction distribution, bubble and liquid  
22 phase velocity profiles, turbulent kinetic energy spectrum, and mass transfer.  
23  
24

25 **Keywords: Added Mass Stress, Bubble Column, LES Simulation, Mass Transfer, Turbulent Dispersion**

26  
27 <sup>1</sup>Department of Mechanical, Materials and Manufacturing Engineering, The University of Nottingham  
28 Ningbo China, University Park, Ningbo 315100, PR China

29 <sup>2</sup>School of Natural Sciences, University of Hull, Hull HU6 7RX, UK

30 <sup>3</sup>Faculty of Process and Systems Engineering, Otto-von-Guericke-Universität Magdeburg, Zeppelinstraße  
31 1, 06130 Halle, Magdeburg, Germany  
32

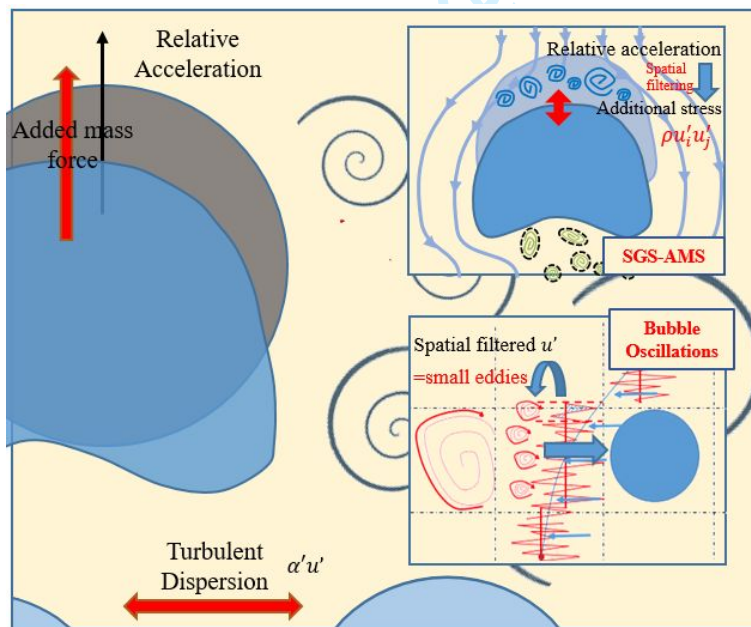
33  
34 1 \*Corresponding author: Professor Xiaogang Yang Email: Xiaogang.Yang@nottingham.edu.cn  
35  
36  
37

### 38 4 **1. Introduction**

39  
40  
41 6 When applying two-fluid model Euler/Euler large eddy simulation, the filtering process involves the use  
42 of phasic ‘function of presence’ approach to the momentum equation by accounting for co-sharing of a  
43 control volume by different phases. As a result, this leads to the terms denoting interfacial momentum  
44 forces, contributed by the dot product of total stress term and gradient of ‘function of presence’ term,  
45 and indicates the forces induced by the local flow perturbations at the interface of the second phase  
46 (bubbles). The subsequent averaging (ensemble averaging for RANS turbulence or spatial filtering for LES  
47 model) to the momentum equation and the interfacial momentum terms leads to the additional terms  
48 that can be attributed to the drag and other parts that can be modelled as non-drag forces such as lift  
49 force, added mass force and turbulent dispersion force (SGS-TDF) together with the added mass stress  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60

1  
2  
3 15 force (SGS-AMS). In case of conducting two-phase LES, these interfacial momentum exchange terms need  
4  
5 16 to be modelled in terms of the resolved quantities of the flow or filtered variables while taking into  
6  
7 17 account the effect of unresolved fluctuating on sub-grid scale. It should be mentioned that most of the  
8  
9 18 previously reported work on two-phase or three-phase LES has overlooked or neglected the unresolved  
10  
11 19 sub-grid scale contributions. Several previous studies have also indicated the important role played by the  
12  
13 20 turbulence terms of the interfacial momentum transfer on the bubble dynamics, in particular related to  
14  
15 21 the added mass stress force which has proved to be effective in improving the phase distribution  
16  
17 22 prediction, e.g. bubbly mixing layer [1], air-lift [2], and vertical liquid-liquid pipe flows [3].  
18

19  
20 24 Due to the bubble's dynamic response to the surrounding carrier phase, the bubble mass centre changes  
21  
22 25 with its entrainment, which leads to bubble oscillations and tumbling motion [4]. To consider the bubble  
23  
24 26 dynamic motion using Euler/Euler LES modelling approach, one may interpret that the interactions  
25  
26 27 between bubble and the surrounding turbulent eddies give rise to the bubble deformation in case of no  
27  
28 28 bubble coalescence or break-up taking place as shown in Figure 1. Thus, the interphase forces acting on  
29  
30 29 the dispersed phase are strongly affected by interactions between the bubbles and the turbulent shear  
31  
32 30 caused by nearby turbulent eddies, and these interfacial momentum transfer must be properly  
31  
32 31 implemented in the sub-grid scale LES [5-9].  
33



34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60

Figure 1

By taking both phase velocity fluctuations and bubble volume fraction fluctuations into account, the spatial filtering of the drag force and added mass force terms will give rise to the extra terms proportional to the area density and slip velocity correlation i.e., turbulent dispersion, and the correlation of bubble volume fraction and gradient of SGS stress. Based on the SGS eddy diffusivity hypothesis, the SGS-TDF and SGS-AMS will be used to mimic the turbulent dispersion effect in the framework of Euler/Euler two-fluid model approach, revealing the bubble dynamics in the bubble column in the present study. The modified SGS eddy viscosity  $\nu_T$  accounting for the bubble dynamic response to the turbulent eddies induced shear will be implemented in modelling the SGS-TDF and SGS-AMS terms [10].

## 2. Mathematical modelling and numerical methods

### 2.1 Governing equations

The two-fluid model based LES modelling has been adopted in the present study. By applying the phase-weighted filtering to mass and momentum conservation equations, the governing equations can be written as

$$\frac{\partial}{\partial t}(\rho_k \alpha_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\alpha_k \rho_k \mathbf{u}_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \mathbf{u}_k) = -\nabla \cdot (\alpha_k \boldsymbol{\tau}_k) - \alpha_k \nabla p + \alpha_k \rho_k \mathbf{g} + \mathbf{M}_{F,k} \quad (2)$$

where  $\mathbf{u}_k$  is the filtered velocity vector for phase  $k$  in grid-scale, given as  $\tilde{\mathbf{u}}_k = \mathbf{u}_k + \mathbf{u}'_k$  while  $\tilde{\mathbf{u}}_k$  is the instantaneous velocity and  $\mathbf{u}'_k$  stands for the sub-grid scale (SGS) fluctuation, which needs to be modelled. The terms on the right-hand side of Equation (2) respectively represent the stress, the pressure gradient, gravity and the filtered interphase momentum exchange, which arises from the actions of the interphase forces. The stress term is given by

$$\boldsymbol{\tau}_k = -\mu_{eff} \left( \nabla \mathbf{u}_k + (\nabla \mathbf{u}_k)^T - \frac{2}{3} I (\nabla \cdot \mathbf{u}_k) \right) \quad (3)$$

where  $\mu_{eff}$  is the effective viscosity of the liquid phase, which may be assumed to be composed of the contributions from the molecular viscosity, the turbulent eddy viscosity and the bubble induced turbulence, i.e.

$$\mu_{eff} = \mu_{L,L} + \mu_{T,L} + \mu_{BI,L} \quad (4)$$

The extra viscosity due to the bubble-induced turbulence is now usually modelled based on Sato's model, given by

$$\mu_{BI,L} = \rho_L C_{\mu,BI} \alpha_G d_B |\mathbf{u}_G - \mathbf{u}_L|. \quad (5)$$

However, as will be discussed later in this section, this viscosity due to the bubble-induced turbulence may also be contributed by the relative bubble dynamic response to those turbulent eddies that have equivalent or slightly larger length scale and entrapped the bubbles [11, 12]. The filtered momentum exchange term can be classified as different contributions from the interphase forces, defined by

$$\mathbf{M}_{F,L} = -\mathbf{M}_{F,G} = \mathbf{M}_{D,L} + \mathbf{M}_{L,L} + \mathbf{M}_{AM,L} + \mathbf{M}_{TD,L} + \mathbf{M}_{AMS,L} \quad (6)$$

where the terms on the right-hand side of Equation (6) are interphase forces acting on the bubbles that are caused by the filtered drag, lift and added mass plus turbulence dispersion and so-called added mass stress. The formulations of the filtered drag, lift and added mass forces employed in the Euler/Euler LES modelling are summarised in Table 1.

**Table 1**

Forces	Expressions
Drag	$\mathbf{M}_{D,L} = \frac{3}{4} \alpha_G \rho_L \frac{C_D}{d_B}  \mathbf{u}_G - \mathbf{u}_L  (\mathbf{u}_G - \mathbf{u}_L),$ $C_D = \frac{2}{3} E_0', E_0' = \frac{g \Delta \rho d_B^2}{\sigma}$
Lift	$\mathbf{M}_{L,L} = \rho_L C_L (\mathbf{u}_B - \mathbf{u}_L) \times (\nabla \times \mathbf{u}_L),$ $C_L = \begin{cases} \min[0.288 \tanh(0.121 Re_B), f(E_0')] & E_0' \leq 4 \\ f(E_0') & 4 < E_0' < 10 \\ -0.29 & E_0' > 10 \end{cases}$ $E_0' = \frac{g(\rho_l - \rho_g) d_h^2}{\sigma}, d_h = d(1 + 0.163 E_0'^{0.757})^{1/3}$
Added mass	$\mathbf{M}_{AM,L} = \alpha_G \rho_L C_{AM} \left( \frac{D\mathbf{u}_G}{Dt} - \frac{D\mathbf{u}_L}{Dt} \right)$

81

1  
2  
3 82 The turbulent dispersion term  $\mathbf{M}_{TD,L}$  can be obtained by phase-weighted filtering the instantaneous  
4  
5 83 interphase drag force term, expressed by Equation (7) after taking a certain derivations and  
6  
7 84 simplifications, given by

$$85 \quad \mathbf{M}_{TD,L} = \frac{3}{4} \rho_G \frac{C_D}{d_G} |\mathbf{u}_G - \mathbf{u}_L| \left( \frac{\overline{\alpha'_G u'_G}}{\alpha_G} - \frac{\overline{\alpha'_L u'_L}}{\alpha_L} \right) = \frac{3}{4} \rho_G \frac{C_D}{d_G} |\mathbf{u}_G - \mathbf{u}_L| \frac{\nu_{SGS}}{\sigma_{SGS}} \left( \frac{\nabla \alpha_G}{\alpha_G} - \frac{\nabla \alpha_L}{\alpha_L} \right). \quad (7)$$

86 The bubble oscillation in the bubble column bubbly flow can be thought of as a result of the interactions  
87 between bubbles and the surrounding turbulent eddies in the frame of Eulerian-Eulerian modelling,  
88 leading to the deformation of the bubble shapes if bubbles are not subjected to coalescence and break-  
89 up. The liquid-phase turbulence eddy viscosity can be modified as the sum of the filtered turbulent shear  
90 and SGS eddy viscosities to reflect the modification due to bubble dynamic response to the turbulent  
91 eddies, i.e.

$$92 \quad \mu_{T,L} = \rho_L (C_s \Delta)^2 |S| \left( 1 + C_b \alpha_G \frac{\lambda}{d_B} \left( \frac{1}{1 + St_{SGS}} \right)^{\frac{3}{2}} \right) \quad (8)$$

93 where  $\lambda$  represents the different turbulent length scales in the range between the integral and  
94 Kolmogorov scales ( $L > \lambda > \eta$ ),  $C_s$  is a model constant,  $S$  is the characteristic filtered rate of strain tensor and

95  $St_{SGS}$  is the local Stokes number expressed as  $St_{SGS} = \frac{\tau_{\text{bubble}}}{\tau_{L,SGS}}$ . The bubble response time scale can be

96 estimated using  $\tau_{\text{bubble}} = \frac{4(\rho_G + 0.5\rho_L)d_B^2}{3\mu_L C_D Re_B}$  while the characteristic time of turbulent eddies in sub-grid scale

97 can be estimated by  $\tau_{L,SGS} = \frac{\Delta}{\mathbf{u}'_{L,SGS}}$ . Since  $\alpha_L + \alpha_G = 1$  in two-phase flow system and  $\nabla \alpha_L + \nabla \alpha_G = 0$ , this

98 would yield Equation (9):

$$99 \quad \mathbf{M}_{TD,L} = C_{TD} \frac{3}{4} \rho_G \frac{C_D}{d_G} |\mathbf{u}_G - \mathbf{u}_L| \frac{(C_s \Delta)^2 |S| \left( 1 + C_b \alpha_G \frac{\Delta}{d_B} \left( \frac{1}{1 + St_{SGS}} \right)^{\frac{3}{2}} \right)}{\sigma_A} \left( \frac{1}{\alpha_L} + \frac{1}{\alpha_G} \right) \nabla \alpha_L \quad (9)$$

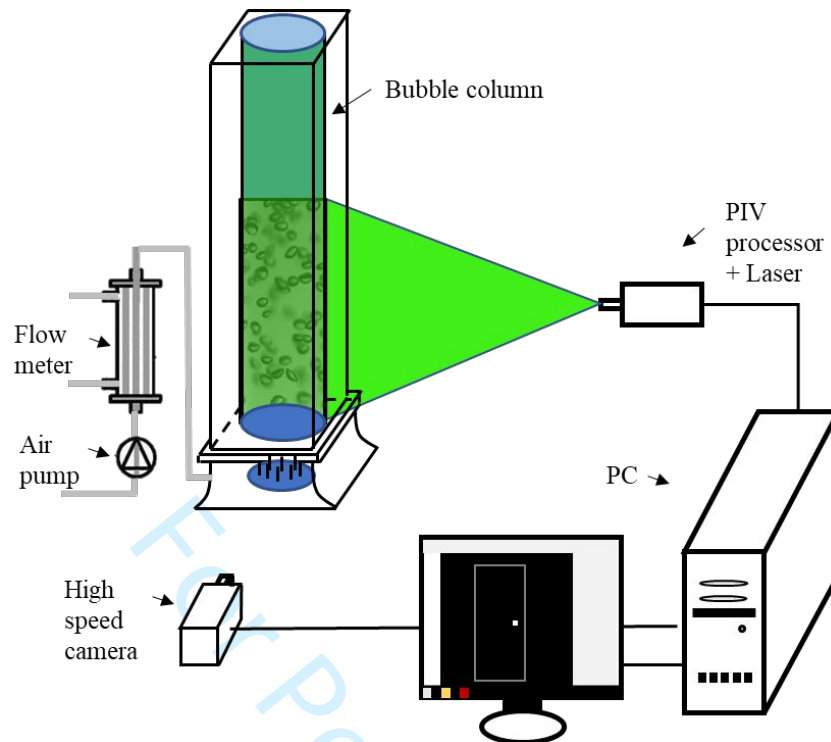
100 For simplicity, Equation (9) is referred to as the modified sub-grid turbulent dispersion force model (SGS-  
101 TDF) hereafter. As shown in Figure 1, the filtering of the instantaneous added mass force will also result  
102 in the mean and turbulent contributions in SGS scale when taking the filtering to the instantaneous added  
103 mass force, which can be expressed as:

$$104$$

$$105 \quad \overline{\chi_G \tilde{\mathbf{M}}_{AM,L}} = \overline{\chi_G \rho_L C_{AM} \left( \frac{D\mathbf{u}_L}{Dt} - \frac{D\mathbf{u}_G}{Dt} \right)} = \alpha_G \rho_L C_{AM} \left( \frac{\partial \bar{\mathbf{u}}_L}{\partial t} + \bar{\mathbf{u}}_L \cdot \nabla \bar{\mathbf{u}}_L - \frac{\partial \bar{\mathbf{u}}_G}{\partial t} + \bar{\mathbf{u}}_G \cdot \nabla \bar{\mathbf{u}}_G \right) + \rho_L C_{AM}$$

$$106 \quad \left( \nabla \cdot \overline{\alpha_G \mathbf{u}'_{L,i} \mathbf{u}'_{L,j}} - \nabla \cdot \overline{\alpha_G \mathbf{u}'_{G,i} \mathbf{u}'_{G,j}} \right) + \alpha_G \rho_L C_{AM} \left( \frac{\partial \bar{\mathbf{u}}_L}{\partial t} + \bar{\mathbf{u}}_L \cdot \nabla \bar{\mathbf{u}}_L + \bar{\mathbf{u}}_L \cdot \nabla \bar{\mathbf{u}}_L \right) \quad (10)$$





131  
132 **Figure 2**

133 In the simulation, the number weighted bubble size distribution (BSD) among the entire bulk phase  
 134 obtained in the experiment was adopted to account for the actual bubble size change. Considering bubble  
 135 volume fraction for the present study  $\alpha_G < 0.04$ , the bubble number density transport may be more  
 136 appropriately used to describe the bubble size distribution if bubbles move with small collision, negligible  
 137 breakup and coalescence rates, given by

$$138 \quad \frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{u}_G n) = 0. \quad (11)$$

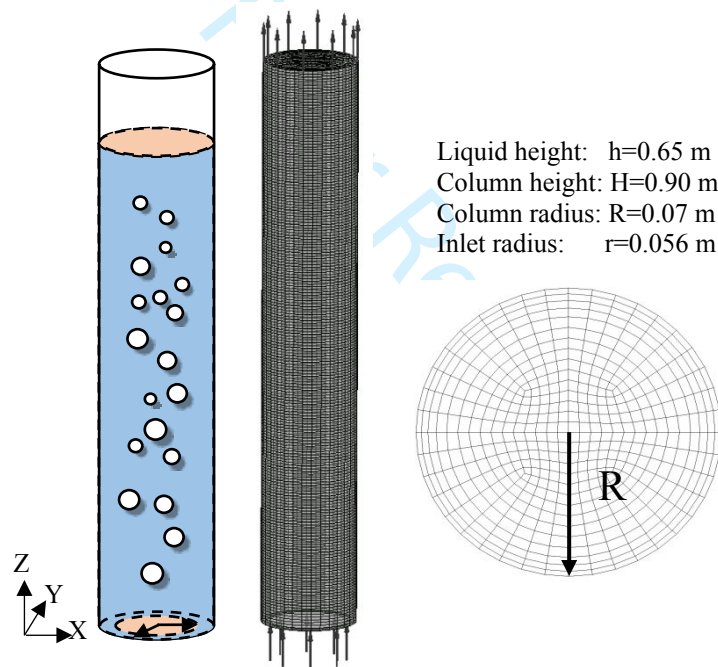
139 The Sauter mean diameter can then be obtained by

$$140 \quad d_{G,32} = \left( \frac{6\alpha_G}{\pi n} \right)^{1/3}. \quad (12)$$

141 As the local bubble equivalent diameter is in the same order as the SGS grid scales, therefore, the bubble  
 142 size can be characterised with the 0-th moment of the bubble size distribution i.e., only taking the local  
 143 mean bubble diameter, i.e. specification of one equivalent bubble diameter rather than a range of bubble  
 144 sizes. This MUSIG approach requires much less computational effort and offers a surprisingly good  
 145 agreement with available experimental data [13]. For Euler/Euler LES modelling, the boundary conditions  
 146 were specified as described below. At inlet, a mass flow rate was specified, corresponding to the  
 147 experimental conditions used by Sommerfeld *et al.* [4] and the author's experiment. At the top surface of



1  
2  
3 148 the reactor, a pressure-constant boundary is specified. No-slip condition was applied to the inner wall of  
4  
5 149 the bubble column. A central-differencing discretisation scheme was used for convective and diffusive  
6  
7 150 terms in the momentum equations, while a second-order backward Euler scheme is employed for the  
8  
9 151 transient term. The mesh set-up for the bubble column for the current LES modelling as shown in Figure  
10  
11 152 3 was satisfied the condition that the cell size of  $\Delta z^+=100$  in the main flow direction and  $\Delta r^+=5$  in the radial  
12  
13 153 direction with a growth rate of 1.2 and total 95,400 cells. With caution and from the perspective of the  
14  
15 154 computational cost,  $\bar{d}_B/\Delta = 0.6375$  in the core-region was used in the LES modelling. This grid resolution  
16  
17 155 adopted is considered to be reasonably close to Milelli's limit [14]. In the LES simulation, the time step  $\delta$   
18  
19 156  $t_E$  was chosen in terms of CFL criterion,  $\min(\frac{|u_L|\delta t_E}{\Delta}, \frac{|u_G - u_L|\delta t_E}{\Delta}) < 1.0$ , varying from 0.0005 s to 0.001s for  
20  
21 157 capturing the transient behaviour of turbulent eddy evolution in the bubble column. The simulations were  
22  
23 158 run to last for 100 seconds while the instantaneous velocities at given positions were monitored and  
24  
25 159 recorded during the calculation process.



160  
161  
162 **Figure 3**

### 163 **3. Results and discussion**

#### 164 **3.1 Effects of accounting for the turbulent dispersion and added mass stress in LES on bubble transport**

165 To highlight the importance of the turbulent dispersion and added mass stress in affecting the bubble transport in Eulerian-Eulerian LES modelling, the results obtained by using our modified SGS-TDF and SGS-

AMS models are also compared with those using Euler/Lagrange LES simulation [7] and experimental data as shown in Figure 4. The time-averaged bubble axial velocity profiles predicted by using the modified and standard turbulent dispersion force models at height  $z=0.325\text{m}$  are illustrated. Our Euler/Euler LES simulation has employed the forces that include the time averaged drag, lift, buoyancy, added mass forces together with the modified SGS-TDF and SGS-AMS (Cases 2: D+L+AM+SGS-TDF and Case 3: D+L+AM+SGS-TDF+SGS-AMS). It can be seen that the Euler/Euler LES by implementing either the modified SGS-TDF force or SGS-AMS models (Cases 2 and 3) performs better than the simple use of the momentum exchange terms, drag, lift and added mass forces (Cases 1), for prediction of the bubble velocity profiles.

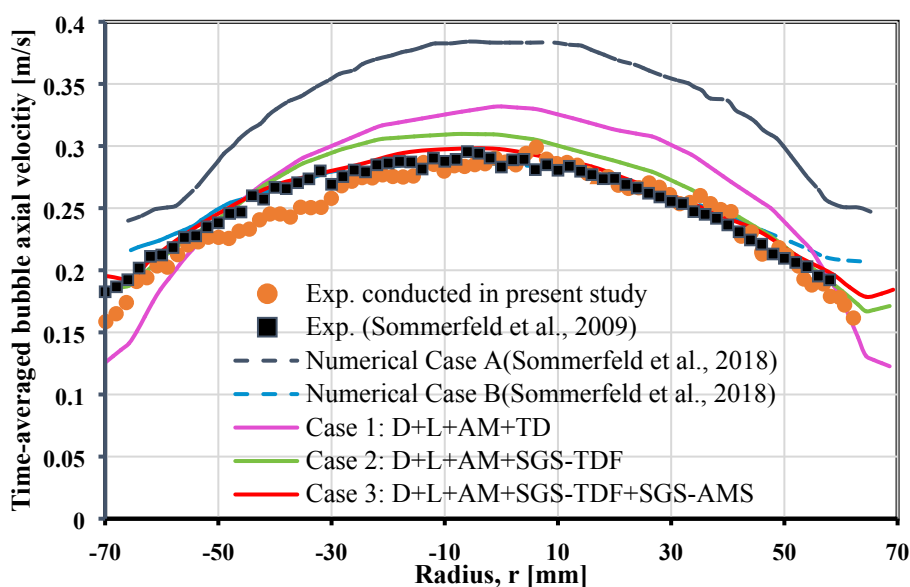


Figure 4

The bubble axial velocity profile predicted by neglecting the SGS-TDF and SGS-AMS contributions shows an apparent difference from the experimental result with over-prediction of the bubble axial velocity in the central core region but under-prediction of its value nearing the bubble column wall. This clearly demonstrates that the inclusion of the modified SGS-TDF and SGS-AMS in the LES simulation has a remarkable influence on the bubble radial dispersion. It can be observed from Figure 4 that the predicted profiles by using the modified SGS-TDF model and the modified SGS-TDF and SGS-AMS are consistent with their predicted velocity profiles, especially in the case that the SGS-AMS model is implemented into the modelling. The fact that the results obtained by considering the fluctuating  $\overline{\alpha'_k \mathbf{u}'_k}$  and  $\nabla \cdot (\overline{\alpha_k \mathbf{u}'_{k,i} \mathbf{u}'_{k,j}})$  with dynamic response to surrounding eddies are improved and are better consistent with the experimental results highlights the need for inclusion of the SGS-TDF and SGS-AMS for properly modelling bubble

186 dispersion especially bubble radial migration in the bubble column bubbly flow. Figure 5 shows the time-  
 187 averaged radial bubble volume fraction distribution obtained by using the standard SGS-TDF (Case 1), the  
 188 modified SGS-TDF (Case 2) and the modified SGS-TDF plus SGS-AMS models (Case 3), compared with the  
 189 Euler/Lagrange LES simulation results reported by Muniz and Sommerfeld [20]. This may be attributed to  
 190 the inclusion of the modified SGS-TDF and SGS-AMS models that can effectively modulate the bubble  
 191 lateral dispersion in the LES simulation.

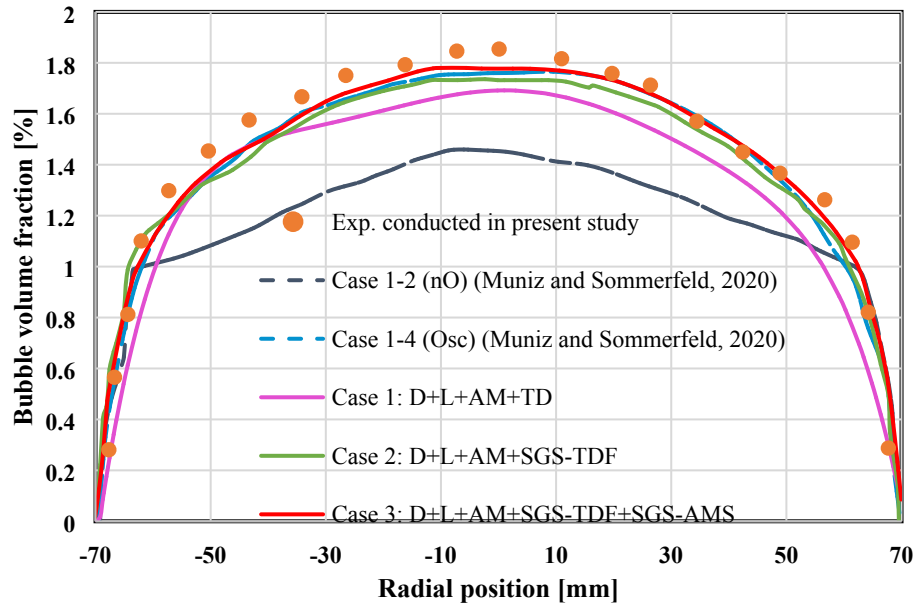


Figure 5

### 3.2 Quantification of SGS-turbulent dispersion force and added mass stress contributions and effect on bubble dynamics

To characterise the effect of the contributions from SGS-TDF and SGS-AMS on turbulent dispersion, the ratios of cross-sectional averaged SGS-TDF and added mass stress force to the overall sum of drag, lift and added mass forces at different cross-sections along the height of the bubble column have been obtained. Figure 6(a) shows the quantification of the ratio of the cross-sectional averaged SGS-TDF to the sum of drag, lift and added mass forces along the bubble column height. By comparing the magnitude of the contribution from drag, lift and added mass forces, along the height, the ratio can reach around 12% but gradually decreases with the height. The decrease in the ratio of the SGS-turbulent dispersion force to the overall contribution from drag, lift and added mass forces along the column height reveals that the bubble lateral dispersion is highly affected by the turbulent dispersion force, implying that a stronger SGS-TDF may promote the bubble group oscillations [4]. In terms of the ratio of total added mass stress force to

206 the sum of the averaged drag, lift and added mass forces, the magnitude of the ratio can also reach 9% in  
 207 the lower part of the bubble column but follows the same trend as the ratio of SGS-TDF to the sum of  
 208 drag, lift and added mass forces as shown in Figure 6(b). Figure 7 shows the distribution of SGS-AMS and  
 209 SGS-TDF terms obtained from the LES at different height in the bubble column together with the bubble  
 210 volume fraction gradient and shear strain rate distribution from  $H=0.1-0.6\text{m}$  at  $t=100\text{s}$ . Thus, the present  
 211 study has highlighted the importance of the contributions of SGS-TDF and SGS-AMS in the LES modelling  
 212 of bubble column bubbly flow.

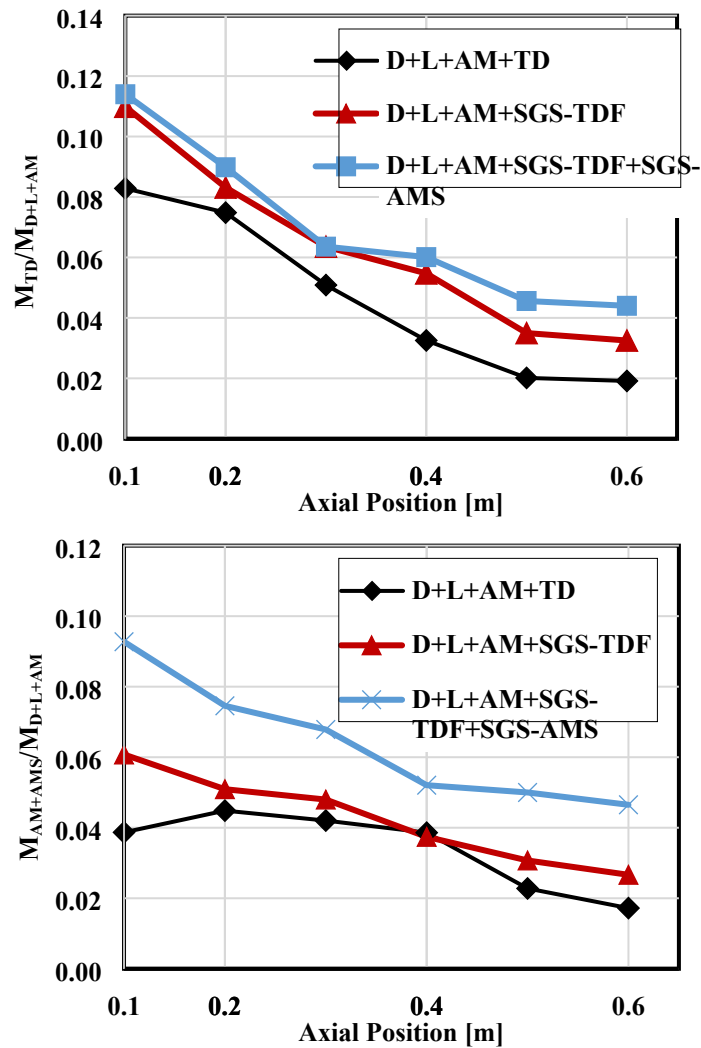


Figure 6

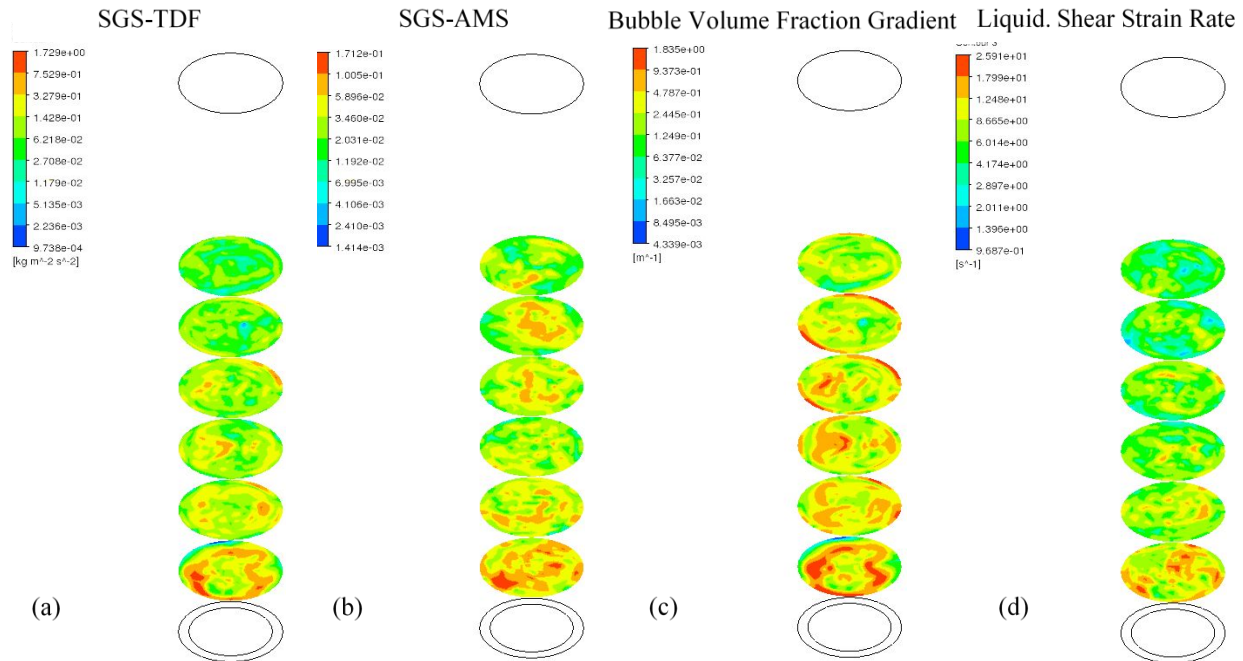


Figure 7

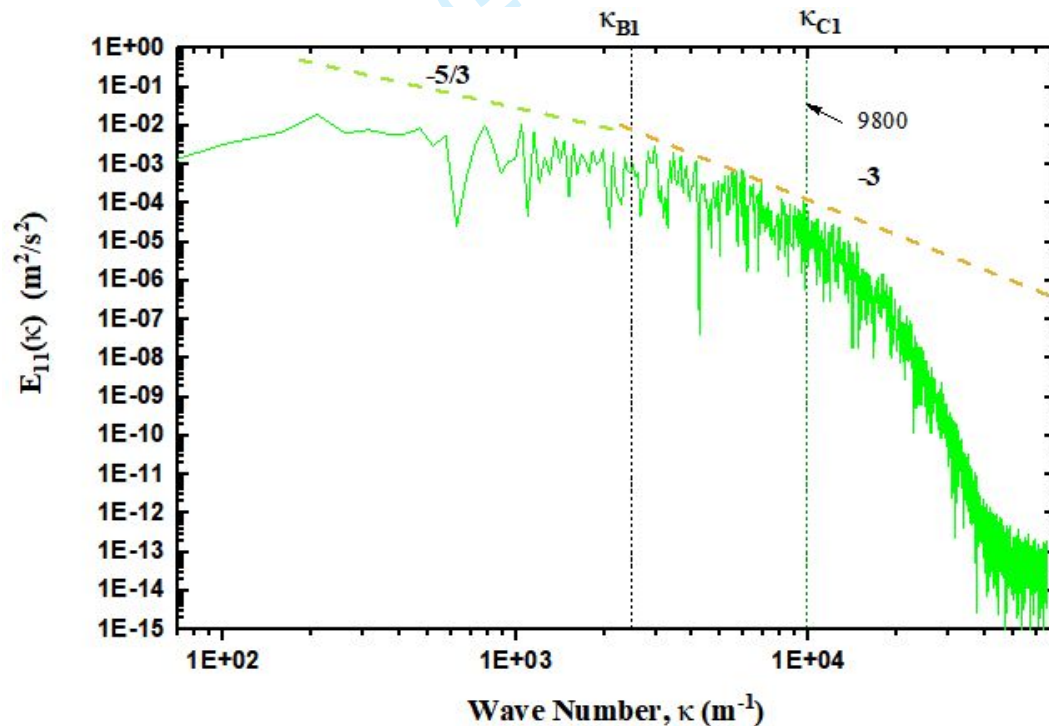
### 3.3 Effects of inclusion of turbulent dispersion and added mass stress on turbulent kinetic energy spectra and interfacial mass transfer

In order to assess the impact of inclusion of SGS-TDF and SGS-AMS models on the calculation of the turbulent kinetic energy of the liquid phase, the one-dimensional LES-filtered turbulent kinetic energy power spectral densities (PSD)  $E_{11}(\kappa)$  obtained for Cases 1, 2 and 3 are presented in Figure 8. The liquid axial turbulent velocity is monitored at the centre of the cross section at  $z = 0.325$  m. The turbulent energy spectrum is obtained by taking the Fast Fourier Transform (FFT) of the time correlation of axial turbulent velocity fluctuations based on the Welch method. As can be seen from Figure 8, the PSD predicted by using the modified SGS-TDF and SGS-AMS models can be still approximated and described by using Pope's model spectrum [16] but considering the bubble volume fraction influence and the relation between one-dimensional and three-dimensional spectrum, defined by

$$E_{11}(\kappa_{11}) = \int_{\kappa_{11}}^{\infty} \frac{E(\kappa)}{\kappa} \left(1 - \frac{\kappa_1^2}{\kappa^2}\right) d\kappa$$

$$= \int_{\kappa_{11}}^{\infty} \frac{C(1 - \alpha_G) \varepsilon^{2/3} \kappa^{-5/3} \left[ \frac{\kappa L}{\sqrt{(\kappa L)^2 + C_L}} \right]^{5/3 + p_0} \exp[-\beta\{[(\kappa\eta)^4 + C_\eta^4]^{1/4} - C_\eta\}]}{\kappa} \left(1 - \frac{\kappa_1^2}{\kappa^2}\right) d\kappa$$
(13)

The parameters  $\beta$  and  $p_0$  are found to be equal to 5.2 and 2.0, respectively. The use of the modified SGS-TDF and SGS-AMS models gives a -5/3 scaling in smaller wave number zone while presents a -3 scaling law measured based on the wave number  $\kappa_1$  larger than the typical wave number characterized by the equivalent bubble size, i.e.  $\kappa_B = \frac{2\pi}{d_B} \approx 2464 \text{ m}^{-1}$ . It can be seen from Figure 9(c) that the transition for different scaling laws in  $E_{11}(\kappa)$  takes place in the wave number at about  $\kappa_1 \approx 2500 \text{ m}^{-1}$ , where the left of the transition location shows the -5/3 slope while the right side of the transition gives rise to the -3 scaling, clearly indicating the feature of feeding of bubble induced turbulence to the turbulent kinetic energy. This -3 scaling were also demonstrated by the experimental work as well as DNS [17-19].



(a)



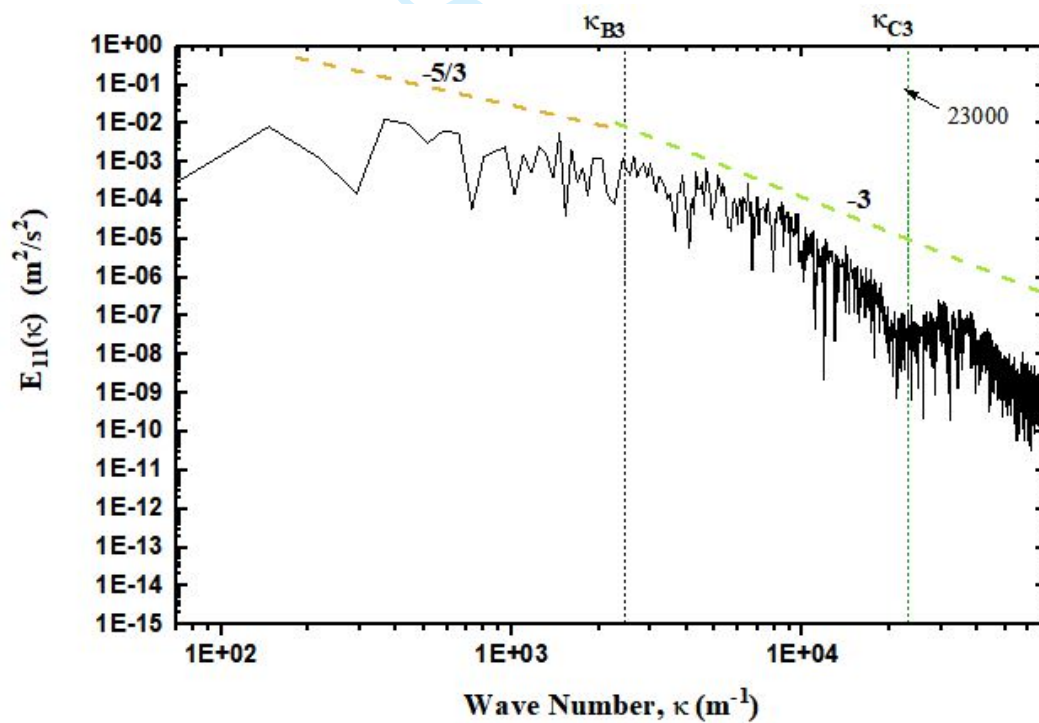
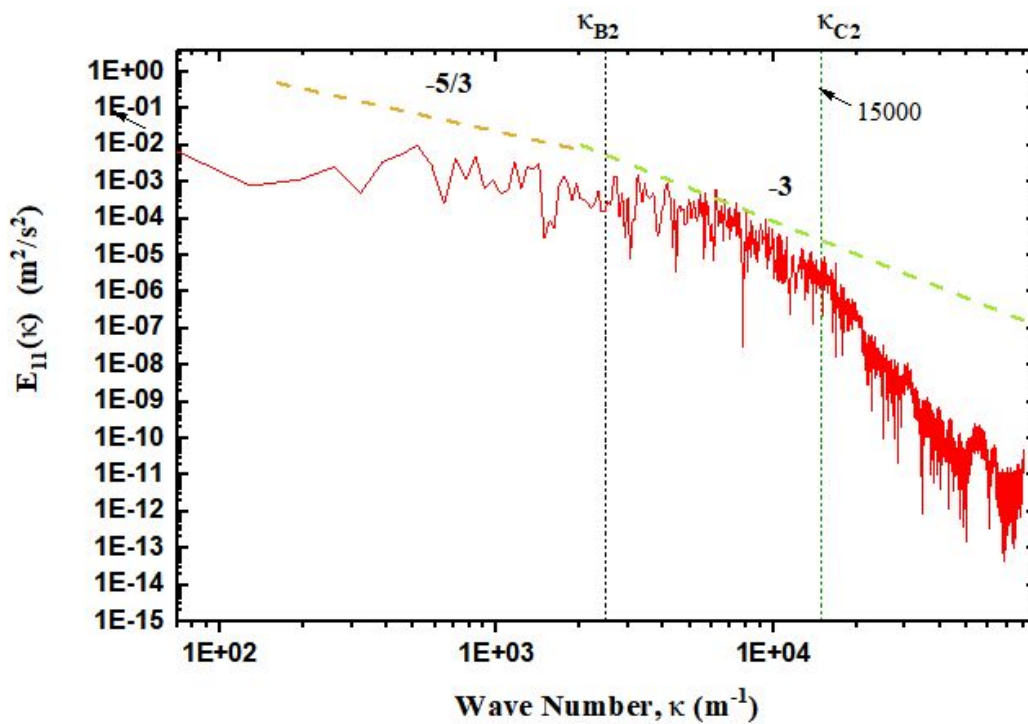


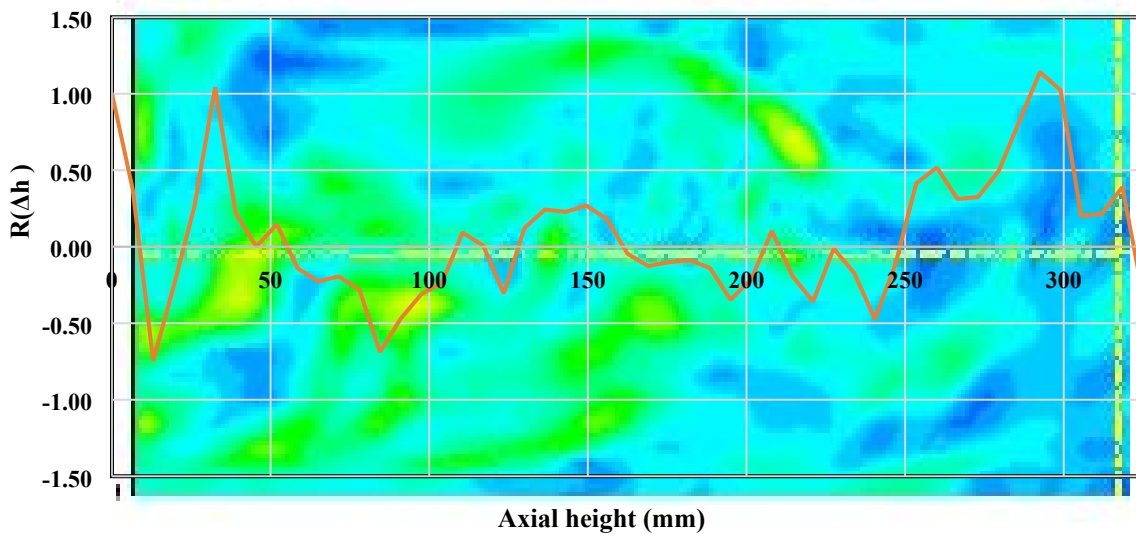
Figure 8

### 244 3.4 Spatial correlation between local bubble volume fraction and shear strain rate

245 In order to assess the effect of accounting the SGS-AMS on the evolution of bubble transport in the bubble  
 246 column, the correlation between the local bubble volume fraction fluctuation and the added mass stress  
 247 was assessed. The spatial correlation between the local bubble volume fraction and shear strain rate  
 248 fluctuation to characterise the interaction of bubbles with SGS turbulent eddies along the axial height of  
 249 the bubble column is proposed, defined by

$$250 R_{\alpha_G \bar{s}_{ij}}(\Delta h) = \frac{\overline{\alpha'_G(h_0) |\bar{s}'_{ij}(h_0 + \Delta h)|}}{\sqrt{\alpha_G'^2(h_0)} \sqrt{|\bar{s}_{ij}^2(h_0)|}} \quad (14)$$

251 Figure 9 presents the  $R_{\alpha_G \bar{s}_{ij}}(\Delta h)$  variations along the centreline at different axial height from  $\Delta h = 0$  to  $\Delta h$   
 252  $= 0.325\text{m}$  of the bubble column. It can be seen from the figure that along the centreline, higher value of  
 253 bubble volume fraction is always accompanied by larger variations in the correlation coefficient  $R_{\alpha_G \bar{s}_{ij}}(\Delta h)$   
 254 along the height. The change of the turbulence induced shear strain rate strongly affect the entrainment  
 255 of the bubbles, causing the local bubble volume fraction fluctuations as can be seen from Figure 10.

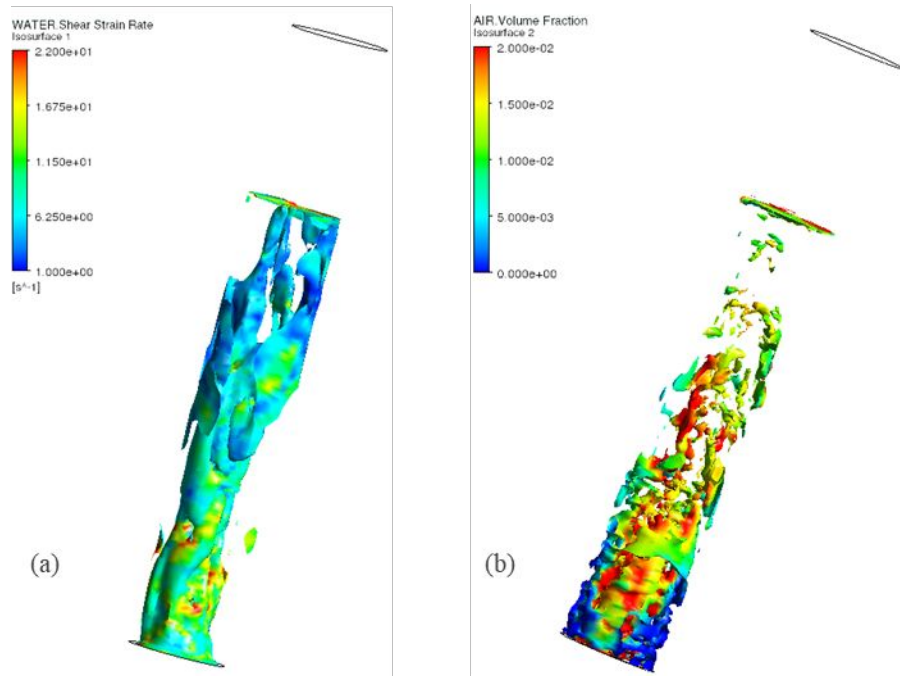


256

257

Figure 9



**Figure 10**

#### 4. Conclusions

It was affirmed that bubble dynamics in the bubble column can be captured by using the adequate SGS-TDF and SGS-AMS models in Eulerian-Eulerian LES modelling, when mimicking the bubble transport in the bubble column. This can imply that the modified SGS-TDF and SGS-AMS models may play an equivalent role in indicating the bubble fluctuating motion predicted by using Euler/Lagrange LES modelling approach but with the stochastic dispersion model [4]. Though the case presented in the present study has been confined to a circular cylindrical bubble column, it has been revealed that the proposed modelling can be also applied to other cases such as square bubble column. The cross-sectional averaged absolute ratios of SGS-TDF force to the time averaged drag force and SGS-AMS force to the time averaged added mass force along the height of the bubble column are found to be around 5%-10% with the higher percentage taking place in the lower part of the column, indicating the needs to include the contributions from the SGS-TDF and SGS-AMS forces for radial re-distributing bubble volume fraction profiles. The SGS-TDF has more influences in the radial direction while the SGS-AMS has more influences in the main flow direction. The turbulent kinetic energy spectrum obtained at the given locations by jointly applying the modified SGS-TDF and SGS-AMS models has shown the existence of a -5/3 scaling law followed by an approximate -3 scaling law in the slope of the spectrum. In addition, a correlation of the local extra eddy viscosity and

277 turbulent shear stresses gradients in both phases has been proposed.

278

279 **Acknowledgements**

280 This work was financially supported by the National Natural Science Foundation of China (Grant Nos.

281 21761132026, 91534118).

282

283 **Symbols used**

A	[m <sup>-1</sup> ]	Area density
C <sub>D</sub>	[-]	Drag coefficient
C <sub>TD</sub>	[-]	Turbulent dispersion coefficient
C <sub>L</sub>	[-]	Lift coefficient
C <sub>AM</sub>	[-]	Added mass coefficient
d	[m]	Bubble diameter
E <sub>0</sub>	[-]	Eötvös number
f	[Hz]	Frequency
<b>M<sub>D</sub></b>	[N/m <sup>3</sup> ]	Drag force
<b>M<sub>L</sub></b>	[N/m <sup>3</sup> ]	Lift force
<b>M<sub>AM</sub></b>	[N/m <sup>3</sup> ]	Added mass force
<b>M<sub>AMS</sub></b>	[N/m <sup>3</sup> ]	Added mass stress force
<b>M<sub>TD</sub></b>	[N/m <sup>3</sup> ]	Turbulent dispersion force
<b>g</b>	[m/s <sup>2</sup> ]	Gravity acceleration
Q	[s <sup>-2</sup> ]	Invariant Q-criterion
Re	[-]	Reynolds number
S	[s <sup>-1</sup> ]	Characteristic filtered rate of strain
Sh	[-]	Sherwood number
Sc	[-]	Schmidt number
<b>u</b>	[m/s]	Velocity vector
t	[s]	Time
ω	[s <sup>-1</sup> ]	Water vorticity

**Greek letters**

α	[-]	Phase volume fraction, gas holdup
---	-----	-----------------------------------

1				
2				
3	284	$\sigma_{TD}$	[-]	Turbulent Schmidt number of gas phase
4				
5	285	$\gamma$	[-]	Volume increment ratio
6				
7	286	$\nu_t$	[m <sup>2</sup> /s]	Turbulent kinematic viscosity
8	287	$\varepsilon$	[m <sup>2</sup> /s <sup>3</sup> ]	Turbulence dissipation rate
9				
10	288	$\lambda$	[m]	Characteristic length scale of eddy
11				
12	289	$\tau$	[Pa]	Shear stress
13	290	$\mu$	[Pa · s]	Liquid dynamic viscosity
14				
15	291	$\mu_{\text{eff}}$	[Pa · s]	Effective viscosity of the liquid phase
16				
17	292	$\Delta$	[m]	LES delta
18	293	$\kappa$	[m <sup>-1</sup> ]	Wave number
19				
20	294	$\gamma$	[-]	Volume increment ratio

### Subscripts

21	295			
22				
23	296	$B$		Bubble
24				
25	297	$G$		Gas phase
26				
27	298	$L$		Liquid phase
28				
29	299	max		Maximum
30	300	SGS		Sub-grid scale
31				
32	301	$i$		$i$ -th component
33				
34	302	$j$		$j$ -th component

303

304

### References

- 305
- 306 [1] H. Ayed, J. Chahed, V. Roig, *AIChE Journal*, **2007**, 53 (11), 2742–2753. DOI: 10.1115/icone18-29517.
- 307 [2] M.A. Atiya, A.M. Rahman, A. Abd Al-Jabbar, *Al-Khwarizmi Engineering Journal*, **2011**, 7 (4): 61–75.
- 308 [3] M. Rezig, G. Bellakhal, J. Chahed, *AIChE Journal*, **2017**, 63(9), 4214–4223. DOI: 10.1002/aic.15736.
- 309 [4] M. Sommerfeld, M. Muniz, T. Reichardt, *Journal of Chemical Engineering of Japan*, **2018**, 51(4), 301–
- 310 317.
- 311 [5] N.G. Deen, T. Solberg, B.H. Hjertager, *Chemical Engineering Science*, **2001**, 56(21–22), 6341–6349.
- 312 [6] M. Sommerfeld, D. Broder, *Industrial & Engineering Chemistry Research*, **2009**, 48(1), 330–340.
- 313 [7] V.V. Buwa, V.V. Ranade, *Chemical Engineering Science*, **2002**, 57(22–23), 4715–4736.
- 314 [8] R. Rzehak, M. Krauß, P. Kováts, K. Zähringer, *International Journal of Multiphase Flow*, **2017**, 89, 299–
- 315 312. DOI: 10.1016/j.ijmultiphaseflow.2016.09.024

- 1  
2  
3 316 [9] A. Kulkarni, K. Ekambara, J. Joshi, *Chemical Engineering Science*, **2007**, 62(4), 1049–1072.  
4  
5 317 [10] S. Long, J. Yang, X. Huang, G. Li, W. Shi, M. Sommerfeld, X. Yang, *International Journal of Heat and*  
6  
7 318 *Mass Transfer*, **2020**, 161, 120240. DOI: 10.1016/j.ijheatmasstransfer.2020.120240  
8  
9 319 [11] D.A. Drew, S.L. Passman, *Theory of multicomponent fluids*, Springer Science & Business Media, **2006**.  
10 320 [12] M. Bhole, J. Joshi, D. Ramkrishna, *Chemical Engineering Science*, **2008**, 63(8), 2267–2282. DOI:  
11 321 10.1016/j.ces.2008.01.013  
12  
13 322 [13] Z. Huang, D.D. McClure, G.W. Barton, D.F. Fletcher, J.M. Kavanagh, *Chemical Engineering Science*,  
14  
15 323 **2018**, 186, 88–101. DOI: 10.1016/j.ces.2018.04.025  
16  
17 324 [14] M. Milelli, *A numerical analysis of confined turbulent bubble plumes*, Ph.D. Thesis, ETH Zurich, **2002**.  
18 325 [15] M. Muniz, M. Sommerfeld, *International Journal of Multiphase Flow*, **2020**, 128, 103256. DOI:  
19 326 10.1016/j.ijmultiphaseflow.2020.103256  
20  
21 327 [16] S.B. Pope, *Turbulent flows*, IOP Publishing, **2001**.  
22  
23 328 [17] V.N. Prakash, J.M. Mercado, L. van Wijngaarden, E. Mancilla, Y. Tagawa, D. Lohse, C. Sun, *Journal of*  
24  
25 329 *Fluid Mechanics*, **2016**, 791, 174–190. DOI: 10.1017/jfm.2016.49  
26  
27 330 [18] J.M. Mercado, D.C. Gomez, D. Van Gils, C. Sun, D. Lohse, *Journal of Fluid Mechanics*, **2010**, 650, 287–  
28 331 306. DOI: 10.1017/s0022112009993570  
29  
30 332 [19] G. Riboux, D. Legendre, F. Risso, *Journal of Fluid Mechanics*, **2013**, 719, 362–387. DOI:  
31 333 10.1017/jfm.2013.12.  
32  
33 334  
34  
35 335  
36  
37 336  
38  
39 337  
40 338  
41  
42 339  
43  
44 340  
45 341  
46  
47 342  
48  
49 343  
50 344  
51  
52 345  
53  
54 346  
55 347  
56  
57  
58  
59  
60

348 **Figure 1.** Schematic of contribution from SGS-TDF and SGS-AMS in bubbly flow.

349 **Figure 2.** Schematic of a bubble column with imaging system and data acquisition.

350 **Figure 3.** Schematic of mesh set-up in the bubble column for LES modelling.

351 **Figure 4.** Comparison of time-averaged bubble axial velocity distribution at  $z=325\text{mm}$  by using three  
352 models with experimental and numerical data obtained from Sommerfeld et al. (Dot: experimental  
353 data[4]; Dash: E-L simulation data [4].

354 **Figure 5.** Comparison of time-averaged normalized bubble volume fraction distribution at  $z=325\text{mm}$  by  
355 using three models with experimental and numerical data obtained from Sommerfeld et al. [15]

356 **Figure 6.** Quantification of (a) SGS turbulent dispersion force (TDF) contribution: and (b) total added mass  
357 force (AM) contribution: cross-sectional averaged AM over the sum of drag, lift and added mass force  
358 ratio along the bubble column height  $H=0.1-0.6\text{m}$ .

359 **Figure 7.** Distribution of (a) SGS-TDF; (b) SGS-AMS; (c) bubble volume fraction gradient; (d) liquid phase  
360 shear strain rate at different height from  $H=0.1-0.6\text{m}$  at  $t=100\text{s}$  in Case 3.

361 **Figure 8.** Predicted turbulent kinetic energy spectrum of liquid axial velocity at middle point at  $z=325\text{mm}$   
362 by using (a) case 1: D+L+AM+TD; (b) case 2: D+L+AM+SGS-TDF; (c) case 2: D+L+AM+SGS-TDF+SGS-AMS.

363 **Figure 9.** Spatial correlation coefficient  $R_{(\alpha_G \bar{S}_{ij})}(\Delta h)$  along the height of the bubble column from  $z=0$   
364 to  $z=325\text{mm}$ . The background was superimposed with the contours of instantaneous liquid phase shear  
365 strain rate at  $X=0$ , YZ-Plane.

366 **Figure 10.** Iso-surfaces of (a) bubble volume fraction  $\alpha_B = 0.016$  colored by local water shear strain rate  
367 and (b) water shear strain rate  $S_{ij,L} = 10 \text{ s}^{-1}$ , colored by local bubble volume fraction at  $t=100\text{s}$ .

369 **Table 1.** Interphase force closure.

## 371 CEAT Graphic Abstract

