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Numerical investigation on the effects of Drag force models on fluid dynamic behavior of CO_2 –IL system

Anees Ahmed[*], Khadija Qureshi, Masroor Abro

Department of Chemical Engineering, Mehran University of Engineering & Technology, Jamshoro

[*]*Corresponding Author E-mail: aneesahmed.solangi@gmail.com*

ABSTRACT

Our country ranks fifth in the list of countries most vulnerable to climate change according to the global climate Risk index 2021 published by the environmental think tank GERMANWATCH and Carbon dioxide CO_2 is major contributor to Global Warming. Ionic Liquids are potential green solvent for the carbon dioxide capturing. Therefore, multi bubble CO_2 capturing system model is simulated and sensitivity of different drag and non-drag force (virtual mass, lift force) models is investigated by measuring key fluid dynamic parameters, i.e., gas holdup, local bubble size, mean interfacial area in CO_2-[bmim][BF_4] bubble column system. Simulations were performed under the low velocity condition, and it was observed that, the Drag and non-drag forces models play key role on local and global fluid dynamics of bubble column. It was further expected that, results could be relatively more sensitive to such models under the high velocity conditions.

Keywords:

CO_2 absorption
Fluid dynamics
Bubble Column
Momentum closures

1. Introduction:

Global Warming is one of the major contributors to the Global climate change. Global warming is increasing day by day due to release of enormous amount of greenhouse gases in atmosphere. Carbon dioxide (CO_2) is one of major greenhouse gas emissions, which undergoes a continuous rise all over the world and contributes more than 60% in global warming. Therefore, CO_2 capture has become a major concern to limit increasing global warming ultimately to avoid sever consequences on environment and ecosystem. Typically used industrial CO_2 capture units are Packed Bed column [1], Tray column [2], Membrane Separators [3] and Bubble Column [4]. The bubble column is preferred over other multiphase equipment due to its simplicity, no moving parts, low operation cost, high heat and mass transfer coefficient, good mixing characteristics, and ability to accommodate wide range of residence time. At this time, ionic liquids (ILs) are regarded as green solvents due to their key features such as wide liquidus range, negligible vapor pressure and high thermal and chemical stability [5]. Moreover, ILs offer physical absorption of CO_2 reducing the overall cost and energy requirement of CO_2 desorption and their regeneration [6]. CFD simulation of gas-liquid-solid or gas-liquid bubble columns has attracted great attention in the past years. The precise prediction of the hydrodynamic parameters in bubble columns is a challenging task due to their complex transport phenomenon. Inside the bubble column, an interaction exists between the dispersed gas and the liquid that is affected by the momentum enclosures (e.g. drag force, Virtual Mass Force lift force, etc.,) and turbulence in respective column. Therefore, simulation for the bubble columns is dependent on the correct modeling of momentum enclosures (Drag Force, Lift Force, virtual mass force) and turbulence models. The drag force calculates the gas phase velocity and residence time of the bubbles, hence; it has a great effect on the flow patterns in the bubble columns. Several drag models are proposed by researcher such as Ishii & Zuber Drag model, Schiller Naumann Drag model, Grace et al Drag Model, and Dong et al Drag model. The lift force which is the perpendicular component of the hydrodynamic force relative to the flow direction defines the flow pattern in the bubble columns. A bubble traveling through a fluid in shearing motion experience lift force perpendicular to the direction of motion. Several lift models are proposed by researcher such as Auton et al Lift model, Tomiyama et al Lift Model, Legendre & Magnaudet. The virtual mass force is the work performed by the bubbles from the acceleration of the liquid surrounding the bubbles. The usage of proper mass coefficient in particular conditions can assist in obtaining clearer vision of the flow pattern in the bubble columns which matches the experimental data [7] especially at the sparger region. In general, numerical studies used constant virtual mass coefficient 0.5 is often used for spherical bubbles. The effect of these models cannot be neglected however role of these models for CO_2-IL hydrodynamic behavior is found scant in literature carried out up to now. Therefore, the role of momentum enclosures models for study of viscous liquids like Ionic Liquids is incorporated in this research. A proper selection of these model could lead maximum accuracy of CFD modeling in terms of reproducing the experimental results with higher agreement.

2. Methodology:

2.1. Model Equations:

In this study, gas-liquid hydrodynamics are modeled in E-E framework, which allows a separate mathematical treatment for each phase that is considered as an interpenetrating continuum and the movement for each phase in Eulerian reference frame. k–ε turbulence model is used for the conservation equations of continuity and momentum for continuous Phase.

$$\frac{\partial}{\partial t}\left(\alpha_p\rho_p\right) + \nabla\left(\alpha_p\rho_p v_p\right) = 0 \tag{01}$$

The equation of continuity for dispersed phase in Eulerian multiphase model is given below:

$$\frac{\partial}{\partial t}\left(\alpha_p\rho_p\right) + \nabla\left(x_p\rho_p v_p\right) = S_i \tag{02}$$

The Equation for momentum conservation:

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\alpha_p\rho_p v_p\right) + \nabla\left(\alpha_p\rho_p\, v_p v_p\right)\\ &= -\alpha_p\nabla p + \nabla\left[\alpha_p\mu_p^{eff}\left(\nabla v_p + \nabla v_p^T\right) + \alpha_p\left(\lambda_p - \frac{3}{2}\mu_p^{eff}\right)\nabla v_p\bar{\bar{I}}\right] + \alpha_p\rho_p\vec{g} + F_q\end{aligned} \tag{03}$$

Here

F_q accounts for momentum exchange terms such as drag equation , Lift equation, Virtual mass equations etc

The drag force is calculated with equation

$$F_D = \frac{3}{4}C_D\,\frac{\alpha_q\rho_p}{d}\left|v_q - v_p\right|\left(v_q - v_p\right) \tag{04}$$

For this study different correlations proposed for C_D are as follows:

Ishii & Zuber Drag Model

$$\mathrm{C_d} = \frac{2}{3}\mathrm{Eo}^{\frac{1}{2}} \tag{05}$$

Schiller Naumann Drag model

$$\begin{aligned}C_d &= \frac{24}{Re} \qquad Re \le 100\\ C_d &= 0.44 \qquad Re \ge 1000\end{aligned} \tag{06}$$

Grace et al Drag Model

$$C_d = \frac{4}{3}\frac{\rho_l - \rho_g}{\rho_l}\frac{g d_{32}}{V_T^2} \tag{07}$$

Dong et al Drag coefficient

$$\mathrm{C_D} = \begin{Bmatrix} 27.73\mathrm{Re}^{-0.849}\mathrm{Mo}^{0.020},\ 0.5 \le \mathrm{Re} \le 5 \\ 20.08\mathrm{Re}^{-0.636}\mathrm{Mo}^{0.046}, 5 \le \mathrm{Re} \le 50 \end{Bmatrix} \tag{08}$$

Lift Force Equation

$$\mathrm{F_L} = \mathrm{C_L}\frac{\rho \mathrm{V}^2 \mathrm{A}}{2} \tag{09}$$

For this study different correlations proposed for C_{lD} are as follows:

Auton et al Lift Model

$$\mathrm{C_L} = 0.5 \tag{10}$$

Tomiyama et al Lift Model

$$\mathrm{C_L} = \frac{1 + \frac{16}{\mathrm{Re}}}{1 + \frac{29}{\mathrm{Re}}} \tag{11}$$

Legendre and Magnaudet Lift Model

$$\mathrm{C_L} = (0.288 \tanh(\mathrm{Re}), \mathrm{f(Eo)} \tag{12}$$

Here

$$(\mathrm{Eo}) = 0.00105\mathrm{Eo}^3 - 0.0159\mathrm{Eo}^2 - 0.204\mathrm{E0} + 0.474$$

2.2. Physical domain and Material properties:

The dimension for flat bubble column is taken as 0.2 m in width, 0.45 m in height (height of quiescent liquid) and 0.05m in depth was used. The rectangular inlet of dimension (2.4 cm x 1.2 cm) is used as shown in Fig. 01,

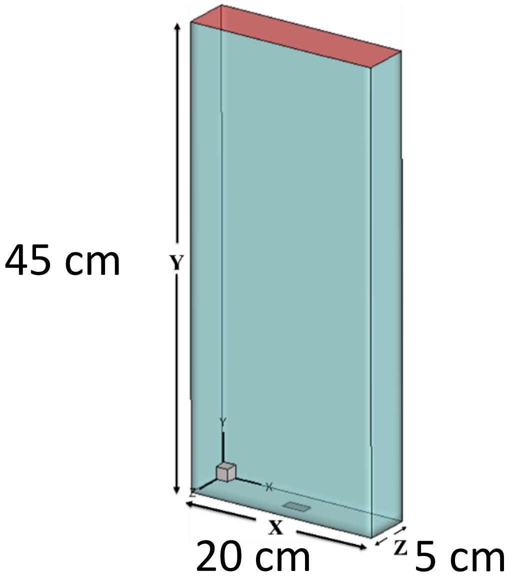


Fig. 01: Dimensional representation of the Bubble Column

The gas liquid system comprising of pure CO_2 as dispersed phase, and an ionic liquid (IL) $[BMIM][BF_4]$ as continuous phase was taken into consideration. The initial bubble size taken at inlet boundary condition was calculated using correlation proposed especially for ILs by Zhang, et al. [8], the correlation is given as

$$d_{inlet}\left[\frac{d_{orifice}\,\sigma}{\rho_l \mathrm{g}}\right]^{-1/3} = aFr^{b}Mo^{c} \tag{13}$$

Where $d_{orifice}$ is diameter of orifice, The values of a, b and c were 2.67, 0.029 and 0.016 respectively The viscosity (μ), density (ρ) and surface tension (σ) of ionic liquid at different conditions are taken from the literature [9], as enlisted in Table -1.

Table 01: Properties of Ionic Liquid

Temperature [K]	μ [Pa.s]	ρ [Kg/m3]	σ [N/m]
303	0.08827	1198.3	0.04448

2.3. Numerical setting and boundary conditions

In the present work, Finite Volume Method (FVM) based commercial CFD tool ANSYS Fluent 19.0 has been used to carry out all the simulations. The CO_2 is sparged with uniform initial bubble size via velocity inlet at bottom of bubble column with inlet velocity of 0.0006 m/s. The outlet domain is set as pressure outlet boundary at atmospheric pressure and no-slip condition is considered at walls for both phases. The PBM model is coupled with E-E framework to capture the phenomena of bubble breakage and coalescence phenomenon. Population balance was modeled using QMOM. For CO_2 dissolution in IL, a scalar transport equation is solved.

A transient condition was implemented in numerical setup and turbulence was modeled using standard k–ε model keeping the default model constants. Standard k–ε model has been proved to be satisfactory in several modeling strategies [10,11]. A time step size of 0.005 was selected to satisfy the criterion of CFL number and for each time step, 30 iterations were adequate to give solution convergence.

3. Results and Discussions:

Sensitivity analyses of Drag models *i.e.*, Ishii Zuber, Schiller Naumann, and Grace is carried out by comparing Local values as well as global values of CO_2 gas holdup, CO_2 Mean interfacial area and CO_2 mean bubble diameter with those measured by using experimentally validated Dong et al. model. Furthermore, the effect of incorporating Non-Drag Models (Virtual Mass and Lift Model) with drag model on CO_2 mean gas Holdup, Mean Bubble Diameter and Mean interfacial area is also studied in this work.

3.1 Validation of the CFD model:

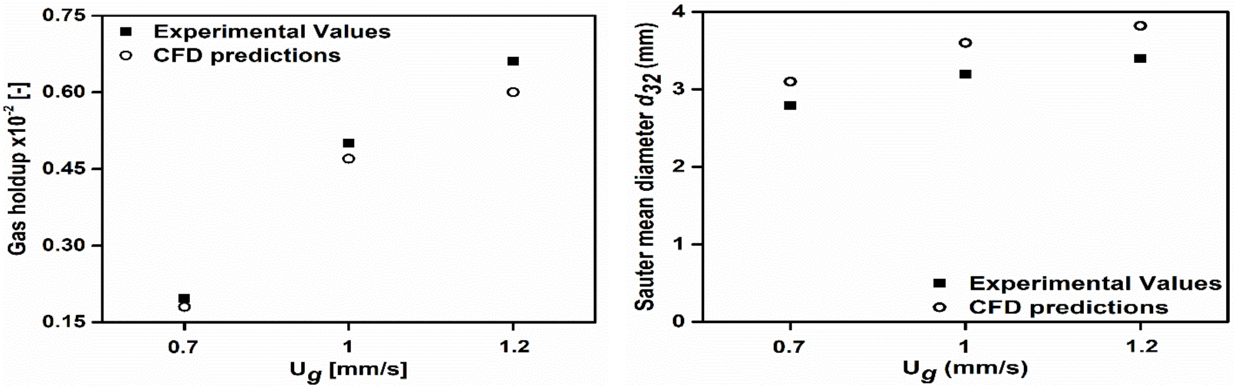


Fig. 02: Validation of the Dong Drag Model for CO_2-IL system model with experimental measurements.

Dong Drag model for CO_2 -IL System was validated by comparing the global values with the published experimental measurements [6], a satisfactory matching with the experimental data (Fig. 02). The study is further extended using flat bubble column from the pas literature.

3.2.1 Simulation Results:

Effect of Drag force models

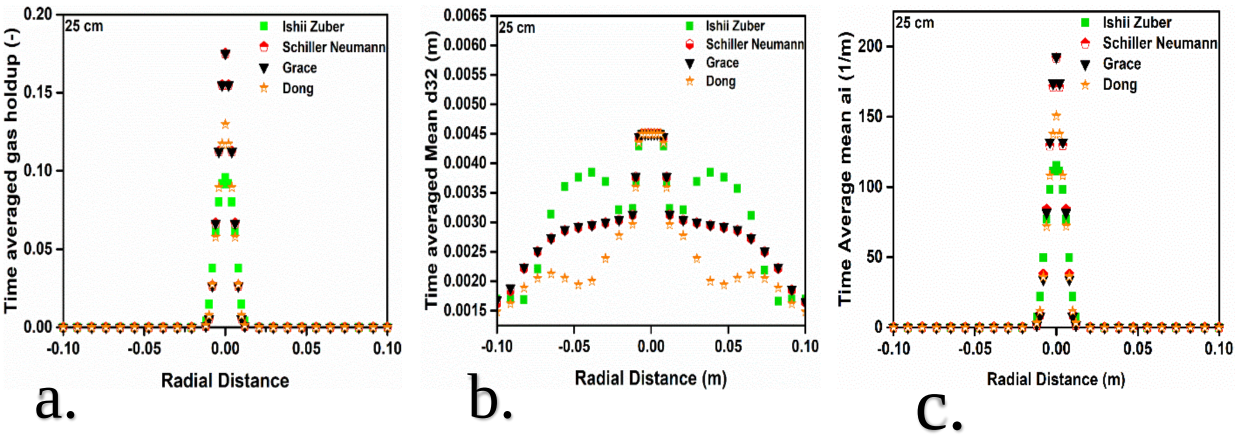


Fig. 03: Effect of different drag models on local values of a. gas holdup, b. bubble diameter, c. interfacial area

As depicted in Figs. 03a, 03b and 03c, the gas holdup as well as interfacial area obtained at different drag models reveals that the gas hold up and interfacial area is maximum at the center of the column and near the wall gas hold up as well as interfacial area decreases. Schiller Naumann and grace drag model overestimated the gas holdup and interfacial area as compared with dong drag model at superficial gas velocity of 0.0006 m/s. In contrast, the Ishii Zuber Drag slightly underestimated the gas hold and interfacial at same 0.0006 m/s superficial gas velocity at the sparger and axial position of 25cm of bubble column. The local profile of CO_2 mean bubble diameter d_{32} obtained at these drag models reveals that Ishii Zuber, Schiller Naumann and Grace Drag model accurately predict the CO_2 mean bubble diameter at the center of bubble column as compared with Dong drag model but overpredicted the bubble coalescence rate for region in between the center & walls of the bubble column.

As when drag force increase, gas phase velocity decrease, and gas hold up increases. The comparison between the different drag models states that the value of Mean global CO_2 gas holdup obtains by using Schiller Naumann and Grace Drag model is greater than Dong drag model due to reason that schiller Naumann drag model is most proper model for small spherical bubble but not for the big bubbles of any shape, such as spherical, elliptical or Cap. Therefore Schiller Naumann drag model underestimated the drag force at CO_2 superficial inlet velocity of 0.0006 m/s due to which the gas hold value increases.

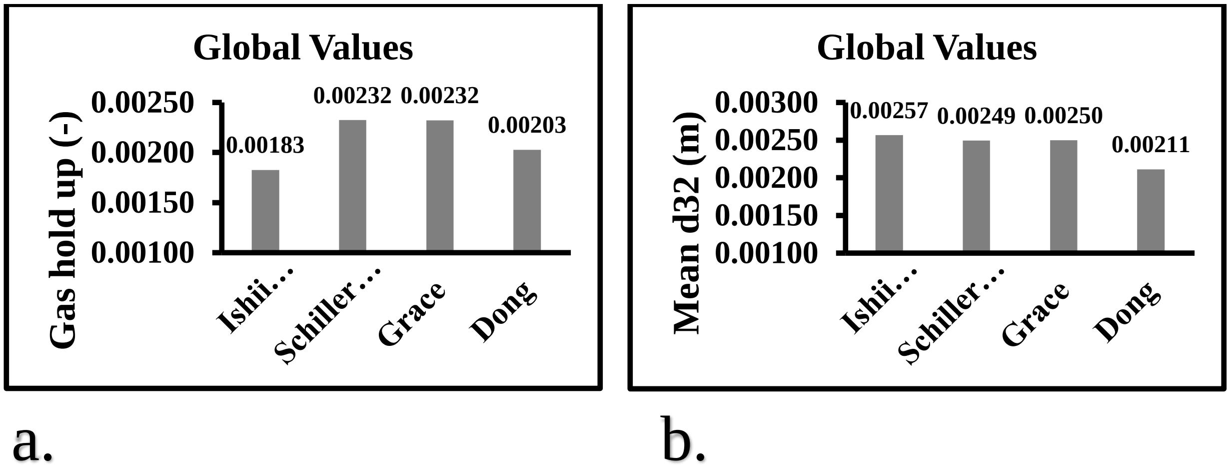


Fig. 04: Effect of different drag models on local values of a. gas holdup, b. bubble diameter.

It can also be observed from the study that Grace drag model also over-predicted global gas hold up values as same as Schiller Naumann drag model while the gas holdup value of the Ishii Zuber is not much higher than Dong Drag model. In comparison of global values of CO_2 mean bubble diameter with different drag models; Schiller Naumann, Grace as well as Ishii Zuber Drag Model overestimated the bubble diameter because these models over predicted the bubble coalescence phenomenon in region in between the column center & walls as mentioned in the Local profile of CO_2 Mean Bubble (refer to Fig. 04)

Effect of non- drag force models

The non-drag forces were incorporated in models according to the table 02.

Table 02: Cases Combinations of Drag and non-drag model

Sr#	**Closure**	**Drag**	**Virtual Mass**	**Lift**		
				Auton	**Tomiyama**	**Legendre & Magnaudet**
01	C1	✓	✗	✗	✗	✗
02	C2	✓	✓	✗	✗	✗
03	C3	✓	✗	✓	N/A	N/A
04	C4	✓	✗	N/A	✓	N/A
05	C5	✓	✗	N/A	N/A	✓

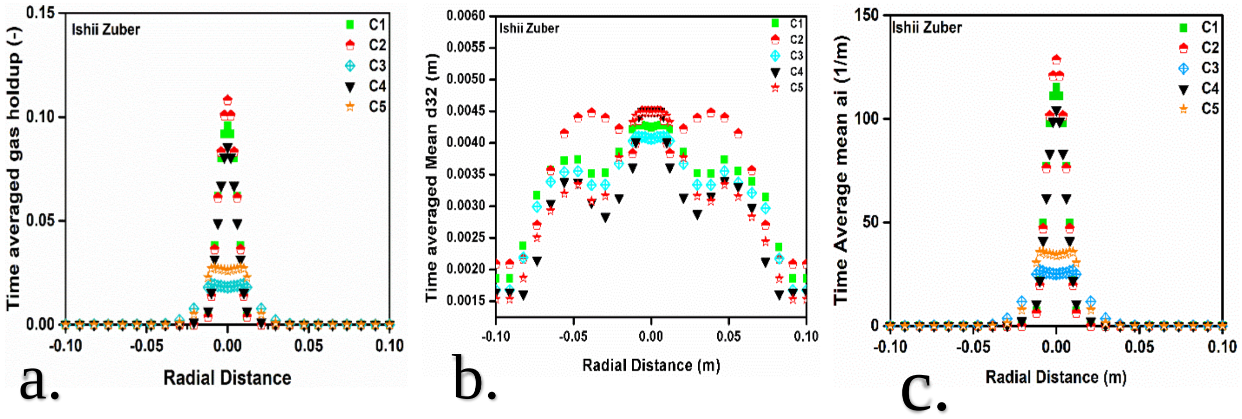


Fig. 05: Measurement of Local values a. gas holdup, b. bubble diameter c. interfacial area against different closures using Ishii Zuber Drag model.

Result of local gas holdup, bubble diameter and interfacial area for different combinations of drag and non-drag force models are plotted in Fig. 05. In previous section, it was observed that local gas hold up profile and interfacial area profile using Ishii Zuber drag model were slightly underestimated compared with the results of experimentally validated Dong drag model. However, this discrepancy was reasonably reduced by incorporating the virtual mass force with a constant value of 0.5 for virtual mass coefficient as suggested by Auton et al.. Furthermore, in the study of Ishii Zuber gas hold and interfacial area profile, it can also be concluded that incorporating Lift models; Auton, Tomiyama and Legendre & Magnaudet along with the Ishii Zuber Drag model increases the error value in comparison with the experimental validated Dong model in simulation of CO_2-IL system. The Comparison between the cases states that the local value of gas holdup is not same for all cases. By using Virtual mass model along with the Ishii Zuber drag model the gas holdup value increase in the center of bubble column. While in combination of drag with the lift model, Tomiyama lift model shows highest trend of gas hold up in the center of bubble column. From the local profile of CO_2 mean bubble diameter it can be reveal that all the combination of drag and non-drag model accurately predicts the CO_2 mean bubble diameter at the center of the bubble column but in the area in between the center and walls of the column, addition of the virtual mass cause the positive deviation, while addition of Auton, Tomiyama and Legendre & Magnaudet cause the negative deviation.

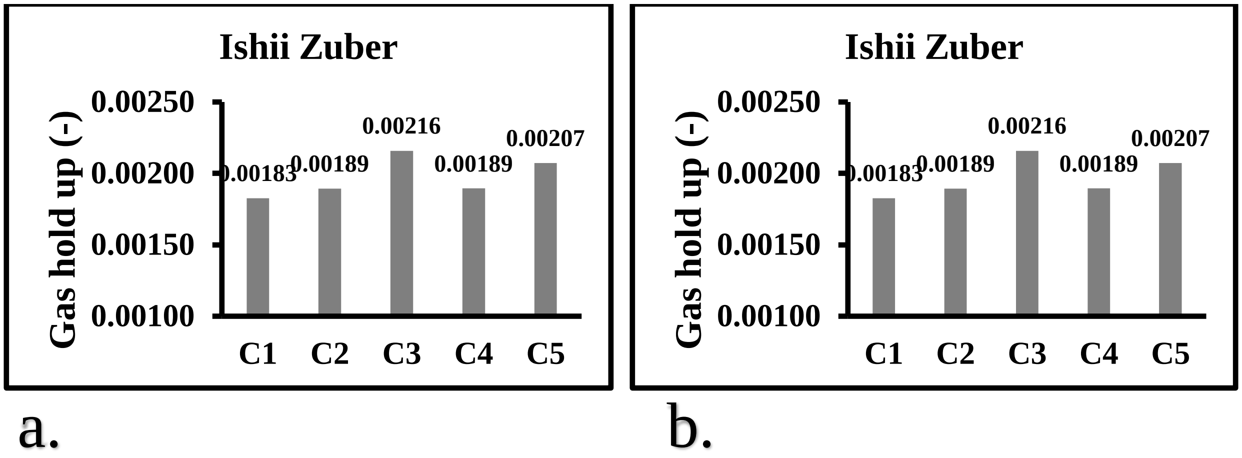


Fig. 06: Measurement of global values a. gas holdup, b. bubble diameter against different closures using Ishii Zuber Drag model.

The Global values of gas holdup and mean d_{32} is compared by incorporating the virtual mass and Lift models such as Auton, Tomiyama and Legendre & Magnaudet in Fig 06 (a), Fig 06 (b). This study leads to conclusion the error of the under estimation on Local as well as Global value of gas Holdup of the Ishii Zuber Drag model can be corrected by incorporating the constant virtual mass of 0.5 while incorporating Lift models; Auton, Tomiyama and Legendre & Magnaudet along with the Ishii Zuber Drag model increases the error value in comparison with the experimental validated Dong model in simulation of CO_2-IL system. From the study of the global values of the CO_2 mean bubble diameter incorporating virtual mass with drag has no effect of CO_2 mean bubble diameter.

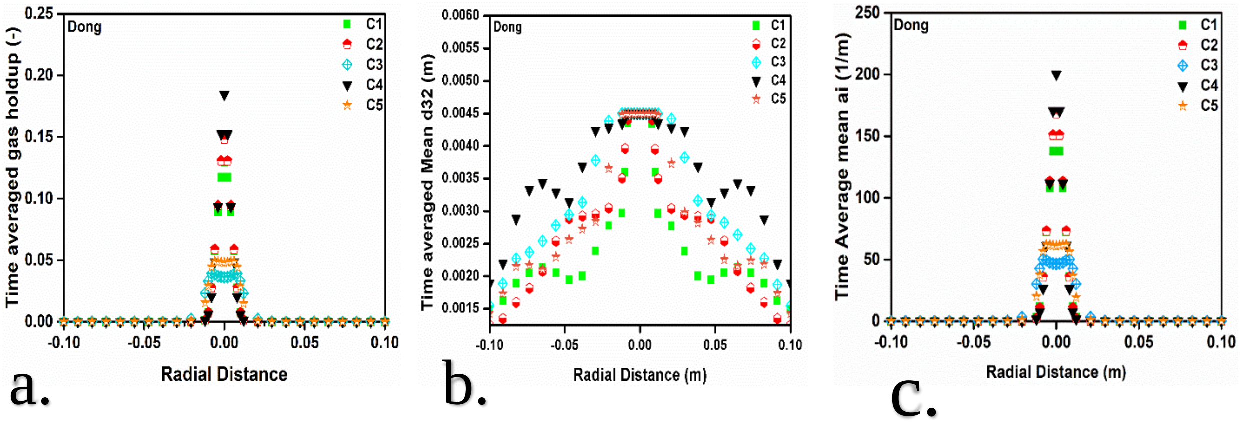
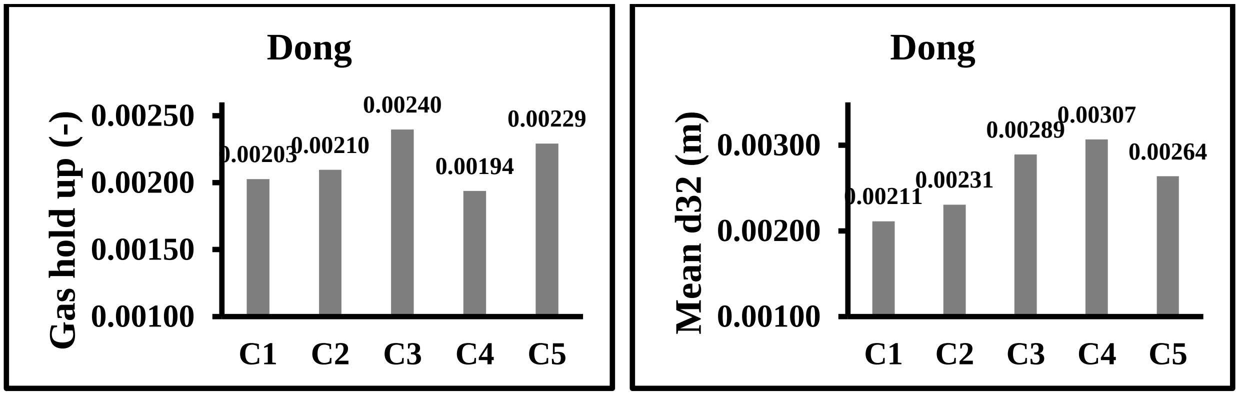


Fig. 07: Measurement of Local values a. gas holdup, b. bubble diameter c. interfacial area against different closures using Dong Drag model.

The local values of gas holdup, bubble diameter and interfacial area are compared using dong drag model in combination with virtual mass and lift models: Auton, Tomiyama and Legendre & Magnaudet as shown in fig 07 (a), fig 07 (b) and Fig 07 (c). The Local profile of the CO_2 gas hold and CO_2 Mean bubble diameter reveals that the dong drag model is enough to represent CO_2 -IL system as compared to experimental data. When Virtual mass or Tomiyama lift model is incorporated with the drag model positive deviation occur in the gas hold up and interfacial area values while incorporating the Auton lift model or Legendre & Magnaudet model makes the negative deviation in gas holdup and interfacial area results as compared to experimental reported data. The local profile of CO_2 mean bubble diameter reveals that combination of incorporating the non-drag models (virtual mass, Auton lift model, Tomiyama Lift model and Legendre & Magnaudet predicts same bubble diameter in the center of bubble column as compared with experimental data While in region in between the center and wall of bubble column positively deviate the results from the experimental data.



a. b.

Fig. 08: Measurement of Global values a. gas holdup, b. bubble diameter against different closures using Dong Drag model

The global values of gas holdup and Mean d_{32} using dong drag models is compared with values obtained using dong drag model in combination with virtual mass and lift model such as Auton, Tomiyama and Legendre & Magnaudet is shown in Fig 08 (a) and Fig 08 (b). The global profile of the gas holds up reveals that the incorporating the virtual mass leads to a very little positive deviation. Incorporating the Tomiyama lift model cause negative deviation while Auton and Legendre & Magnaudet leads to a high positive deviation. The global profile of the CO_2 mean bubble diameter reveals that incorporating the virtual mass with the dong drag model has not significant impact on result while incorporating lift model leads to deviation from the experimental data.

4. Conclusions

In this study Sensitivity of different drag models *i.e.,* Ishii Zuber Drag model, Schiller Naumann and Dong Drag Model are examined as well as the impact of using Virtual mass and Lift force with the drag models were investigated. The Main Conclusion drawn from this study are:

Validation of Model was obtained from the published experimental data with the Dong Drag model. The results showed the remarkable matching with the published results. On overall basis, the local results were marginally changed with variation in drag model. This could be attributed to existence of bubbly regime (low Reynold number condition) in bubble column. As expected, the interfacial area of CO_2 bubble is directly proportional to CO_2 gas holdup. The gas holdup, mean interfacial area and mean Bubble size were found maximum in the center of Bubble Column. In Comparison of Local values at different drag models Ishii Zuber, Schiller Naumann, Grace, and Dong at 25 cm column height, the Schiller Neumann and Grace models show positive deviation of gas hold up and interfacial in comparison with Dong Model while in contrast Ishii Zuber Drag model show the negative deviation in gas hold up and interfacial local profile. The local profiles as well as global values of selected parameters suggested that the dong drag model is enough for the representation CO_2-IL system at the low superficial gas velocity.

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