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DRAG MODELLING IN CFD SIMULATION TO GAIN INSIGHT OF PACKED COLUMNS

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A three dimensional CFD model was developed to analyze the flow behavior of countercurrent gas-liquid flow on an inclined plate. The influence of countercurrent gas flow was analysed by varying gas flow rates for each liquid flow rates. The simulation results are compared and discussed with experimental results. Experiments are performed in the same geometry and the measurements are done using the optical techniques. The average velocity profile and the film thickness are considered in this work. From the comparison of velocity profiles, it can be found that increasing the gas flow rate for a constant liquid flow rate, decreases the velocity along the flow direction which is mainly due to the influence of the drag force from the countercurrent gas flow. This trend is also shown for two different liquid Reynolds number and two different testing systems.

1. INTRODUCTION

In the area of separation, distillation and absorption are the most widely used processes in chemical industries. Due to the advantages like high separation efficiency and low pressure drop, packed columns are of more interest than tray columns during recent years and gaining more and more importance in various applications. The efficiency of the packed columns strongly depends on the flow behaviour of liquid inside the packing. It is very important to understand the same for designing the internals and also to optimise the process. Experimental investigation of the flow inside the packing is very complex and the accuracy is also limited. With the recent computational developments, CFD (Computational Fluid Dynamics) is used to investigate the flow behaviour which will reduce the experimental effort for analyzing the influence of various parameters.

Many works have been performed using CFD for studying the hydrodynamical behaviour of gas and liquid flows in the structured packing. J.M. van Baten et. al (2002) studied the gas and liquid phase mass transfer in KATAPAK-S structures using CFD simulations. The gas phase mass transfer was in good agreement with the theoretical correlation of Subawalla et. al (1997), where as the liquid phase mass transfer was one order of magnitude less than the correlation. Gu et. al (2004) studied the hydrodynamics of falling film flow on inclined and wavy plates corresponding to the surface texture of structured packing using 2D CFD simulation. It was reported that the liquid flow patterns are dependent on the microstructures of the plate when there is no gas flow. Yuan et. al (2005) proposed a novel internal in packed columns and performed both 2D CFD simulation and experimental analysis of two phase cross/countercurrent flow with the novel internal in the packed column. The installation of this internal increase the radial gas velocity and decreases the axial velocity which in turn reduces the pressure drop. Ataki (2006) also performed the 3D CFD study to analyse the wetting behaviour in structured packing elements without countercurrent flow and also validated with experimental studies. Raynal et. al (2007) proposed multi-scale approach for analyzing the gas-liquid flows in structured packing. As a first step, 2D studies were performed in micro scale and the results are further extended for 3D studies in meso scale. In this work, 3D CFD study concerning the hydrodynamics of the countercurrent flow behaviour of gas and liquid inside the packing internals will be carried out.

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It is very tedious to study the flow behavior inside the complex packing structure directly. As a base case a simplified geometry is required to understand the flow behaviour in principal. To simplify the problem initially, smooth inclined plate will be used to study the flow behaviour using 3D CFD model. Further the work will be extended to more complex packing structure which resembles the packing used in industrial applications.

In previous work, Hoffmann et. al, (2006) investigated the influence of different parameters like contact angle (CA), inclination angle and surface tension for multiphase flows, but without considering the effect of countercurrent flow using three dimensional CFD and validated with experimental studies. Xu et. al. (2008) analysed the flow on an inclined plate considering the mass transfer into account using 3D CFD model.

The main target of this work is the development of a 3D CFD model to study the hydrodynamic performance of gas-liquid countercurrent flow which occurs in a packing segment in distillation or absorption. So the smooth inclined plate is chosen to analyse the same. The influences of the parameters like surface tension, contact angle was included. The influence of drag force between the gas and liquid phase is taken into account for the countercurrent gas flow. The comparison between experimental and simulation profiles are shown and discussed. Experiments are performed using new micro Particle Image Velocimetry (µPIV) method (Paschke et. al, 2007) which enables the measurement on non-transparent materials. To show the influence of countercurrent gas flow, average velocity profiles are calculated and compared with the case without countercurrent flow. From the simulation, it can be seen that the drag force is inevitable while considering the countercurrent flow. The long term target of the project is to develop a model for multiphase operations which also take mass and heat transfer into account.

2. DETAILS OF NUMERICAL STUDY

To analyse the fluid flow behaviour, a three dimensional smooth inclined plate is considered. The dimensions of the plate are 0.12m*0.01m*0.05m is shown in Fig.1 which resembles the experimental set up.

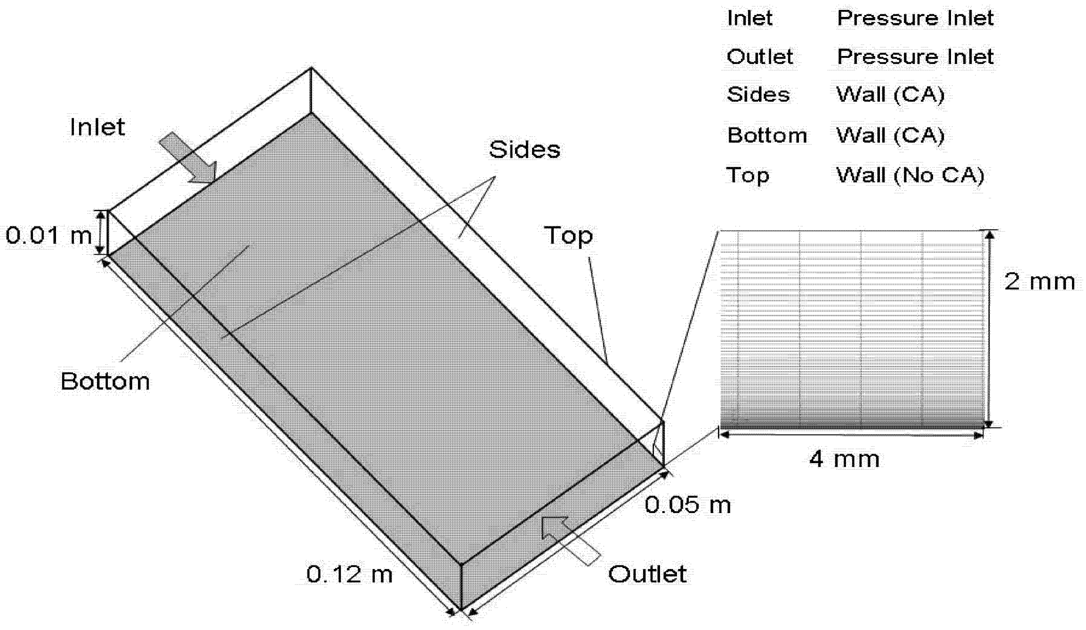

Fig. 1 Geometry, Boundary conditions and mesh details

The boundary conditions on the sides of the plate are assigned as walls to resemble the experimental set up held by steel supports on the left and on the right side. The whole geometry is meshed using Gambit 2.3, a meshing tool from Ansys Inc. The geometry consists of two different meshing zones. The mesh is very fine in the liquid region and the region around the gas-liquid interface. The coarser mesh is used in the region more than half the height of the plate which consists only of gas phase. The very fine mesh enables to capture the gas-liquid interface. The geometry consists of $0.516*10^6$ cells and an inclination angle (α) of the plate is 60°.

Water-Air and Water/Glycerol-Air are used as a testing system. The physical properties of the liquid and gas used in the simulations are given in Table 1(Dow, product database).

Table 1 Physical properties of the used system.

	Water	Air	Water-Glycerol*
Density ρ (kg/m^3)	997	1.185	1099.3
Kinematic viscosity ν (m^2/s)	$8.926*10^{-7}$	$1.545*10^{-5}$	$2.929*10^{-6}$
Surface Tension γ (N/m)	0.0728	-	0.069
Static contact angle with air-steel θ	70 – 80°		70°

* mass fraction of glycerol = 40%

The simulations are carried out with the commercial tool Fluent 6.3, ANSYS Inc. The Volume of Fluid (VOF) model (Hirt et. al, 1981) with geometric reconstruction scheme was used which is one of the limiting cases of Euler-Euler homogenous model (Fluent 6.3, 2007). The model considers that the gas and liquid phase are not interpenetrating. The influence of surface tension source term is taken into account by Continuum Surface Model (CSF) proposed by Brackbill et. al (1992).

For the liquid inlet condition, parabolic velocity profile is defined based on the theory of Nusselt solution. In the liquid region, i.e., below the Nusselt film thickness, the velocity is defined as follows considering the inclination angle (α),

$$u(y) = \frac{1}{2} \cdot \frac{g \cdot \delta^2 \cdot \sin\alpha}{\nu} \cdot \left[\frac{2 \cdot y}{\delta} - \left(\frac{y}{\delta} \right)^2 \right] \tag{1}$$

where δ, being Nusselt film thickness is defined as

$$\delta = \left(\frac{3 \cdot \nu^2 \cdot}{g \cdot \sin\alpha} \right)^{1/3} \cdot \mathrm{Re}_l^{(1/3)} \tag{2}$$

in which liquid Reynolds number, Re_l is defined as

$$\mathrm{Re}_l = \frac{u_{ave} \cdot \delta}{\nu} \tag{3}$$

As the aim of this work is to analyse the hydrodynamic behaviour of the gas-liquid countercurrent flow, the influence of mass and heat transfer has been neglected. The impact of the drag force is taken into account using frictional pressure drop model developed by Woerlee et.al (2001) which is shown in eqn. (4)

$$\frac{\partial P}{\partial X} = -a_e \cdot f_i \cdot \rho_g \cdot \left(\overline{u_{eff}} - u_x\right) \cdot \left|\overline{u_{eff}} - u_x\right| \quad (4)$$

In eq. 4 a_e is the effective interfacial area per unit volume and f_i is the interfacial friction factor. Stephan et. al (1992) developed a correlation to describe the interfacial friction in countercurrent flow based on their experimental results in a rectangular channel which can be described as in eqn. (5)

$$f_i = 0.079 \cdot \mathrm{Re}_g^{-0.25} \cdot (1 + 115 \cdot \delta^{*N}) \quad (5)$$

Where Re_g is the gas phase Reynolds number which can defined as $Re_g = (u_{eff} * \rho_g * D_h)/\mu_g$ and $N = 3.95 * (1.8 + 3.0/Bo)$, δ^* is the dimensionless ratio of film thickness and Bo is the Bond number. Equation (5) is also an extension of famous Blasius equation for single phase flow.

These models have been implemented in Fluent using User Defined Function (UDF). Since the two phases share a common velocity field, the algebraic sign of the drag force source term is opposite to the interfacial velocity so as to ensure it as resistance. The PISO algorithm with neighbor correction is used as Pressure-Velocity Coupling method (Fluent 6.3, 2007). The simulations are carried out unsteady conditions until the residuals; mass flow rate reaches a pseudo-steady state.

The simulations are performed by decreasing liquid load. For each liquid load, countercurrent gas load was increased. Nicolaiewsky (1999) illustrated that only experiments with decreasing liquid loads were more reproducible than increasing liquid loads and avoided the scattered results. So the same strategy is also adapted in the simulations.

3. EXPERIMENTAL SET UP

For the experimental analysis of the countercurrent flow behavior a measuring cell is built and the new micro Particle Image Velocimetry (μ-PIV) method is used. The sketch of the experimental set up is shown in Fig. 2 and the detailed description can be found in Paschke et. al (2007, 2008).

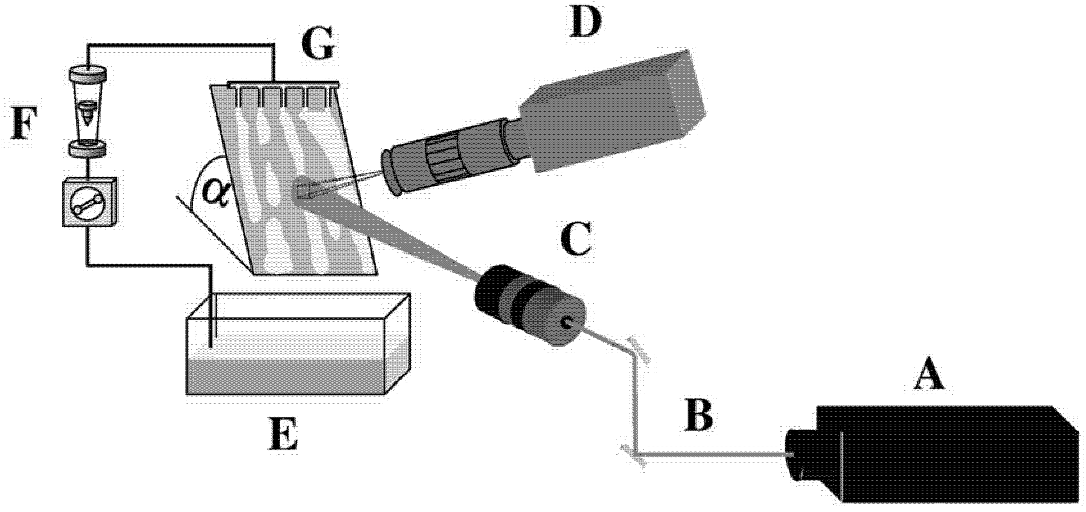

Fig. 2 A: Laser (ND:YAG) B: Mirror (Light Arm) C: Laser Light Optic D: CCD Camera with band-pass Filter and microscopic lens E: Collecting Water Tanks F: Peristaltic Pump with Rotameter G: Feed Tubes a: Angel of Inclination Paschke et. al (2007, 2008)

This method is characterized by the fact that the measurements are carried out through the gas-liquid interface, so that the measurements on non transparent smooth and structured solid surface materials are enabled. The setup enables the countercurrent flow analysis in a wide working range and for different material systems. With the aid of an overflow weir the liquid is fed on the top of the stainless steel plate and flows down the measurement cell as a closed free liquid film flow. The width and height of the plate is same as mentioned above, but the length is 300mm. The gas inlet is close to the liquid outlet at the end of the plate. To minimize the wall effects and take the entrance area into account the measurement position is in the middle of the plate and 11cm behind the inlet weir. The time–weighted average velocity profile can be calculated after processing the images from optical measurements.

4. RESULTS AND DISCUSSION

The influence of the countercurrent flow has been shown for two different testing systems. For each case, the profile without and with countercurrent flow is presented. For analyzing the influence of countercurrent gas flow, the study has also been performed for different gas phase velocities. The F-factor used to express countercurrent gas velocity in distillation and absorption can be defined as

$$F = u_{eff} \cdot \rho_g^{0.5} \tag{6}$$

The flow in the simulation and experiment is laminar, as the liquid phase Reynolds numbers are always lower than 300 and the velocities of the gas phase i.e., F-factor is also in the range of 1.5 and 2.5 which resembles the range used in industrial operating conditions.

The position-weighted average profiles are calculated in simulation by analyzing the local profiles on different positions along the length and width of the plate. The measuring position is around center of the plate along the width and around 110mm along the length, which is the same as the experimental measuring position.

In Fig. 3, the averaged velocity profile against film thickness in the bottom of the plate is shown for the case with Re_l=224 for pure water-air system. The profiles from both simulation and experiment are compared for the cases without and with countercurrent flow.

The agreement between experiment and simulation is adequate and both exhibit the similar parabolic profile. In simulation, the influence of the countercurrent gas flow can be noticed only around the interface of the phases, but not at the bottom of the plate. Velocity at the gas-liquid interface reduces due to the influence of countercurrent gas velocity and in turn increases the film thickness. In comparison with the profiles from simulation, experimental profiles are slower at the bottom of the plate and become faster around the interface. Also the experimental film thickness is slightly higher than the simulation. Experimental measurements have error in the y direction is same like the depth of focus which is almost equal to +/- 0.04mm. This error depends on the properties of the testing system such as refractive index.

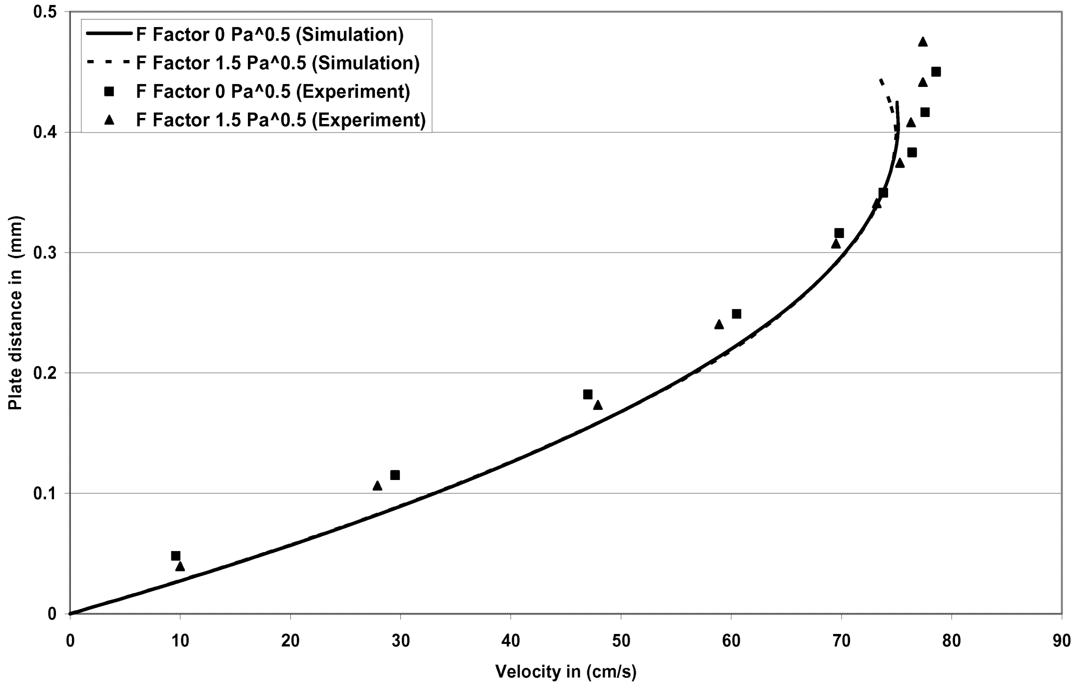

Fig. 3 Comparison of velocity profile from experiment and simulation for pure water system with $Re_l = 224$*, with and without countercurrent gas loads at temperature 25 deg C*

To understand further the influence of countercurrent velocity of gas, a simulation study is required for the cases with increase in friction factor between the gas and liquid phase. But for this testing system, increasing the gas load is not possible due to restriction in experimental set up and decreasing the liquid Reynolds number leads to film break up. So, another testing system enabling the above requirement is chosen and measurements are carried out. This can be achieved by increasing the countercurrent gas load or decreasing the liquid Reynolds number. Therefore, additional experiments and simulations are performed on Water/Glycerol mixture with Reynolds number of liquid 64 & 32 and for two different F-factors.

The average velocity profile against the film thickness for the Water/Glycerol mixture with $Re_l = 64$ and $Re_l = 32$ is shown in Fig. 4 and Fig. 5 respectively. The case without and with countercurrent flow of two different countercurrent F-factor of 1.5 and 2.5 $Pa^{0.5}$ is compared. As seen in the previous case, the velocity profiles from experiment and simulation exhibits the similar parabolic behaviour for the case without countercurrent flow, whereas the experimental velocity profile for the case with countercurrent flow varies.

The velocity profile from the experiment which starts like parabolic profile in the bottom of the plate changes and looks more linear near the gas liquid interface. This can be mainly due to two reasons. Firstly, the deceleration due to the countercurrent gas phase. Secondly, due to formation of waves, this was observed in the experiments. To confirm the formation of waves using simulation, simulations should be performed for considerably longer time. In simulation, the velocity profile for the case with countercurrent flow is always parabolic. For the case with countercurrent F-factor of 1.5, the deceleration in velocity occurs only around the interface but further increase of F-factor to 2.5, leads to change in velocity profile from the bottom of the plate i.e., around 0.3mm and also around the interface. But in experiment, deviation in the bottom of the plate can be seen for both the increase in F-factor. The similar trend can be seen for both the liquid Reynolds number.

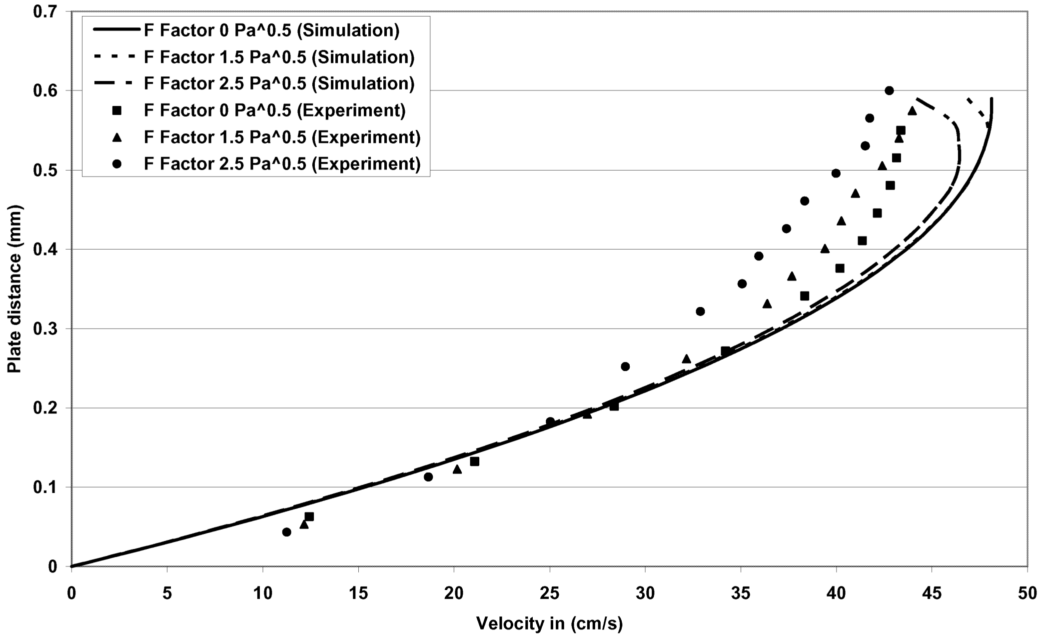

Fig. 4 Comparison of velocity profile from experiment and simulation for water/Glycerol -Air system with Re_l = *64, with and without countercurrent gas loads*

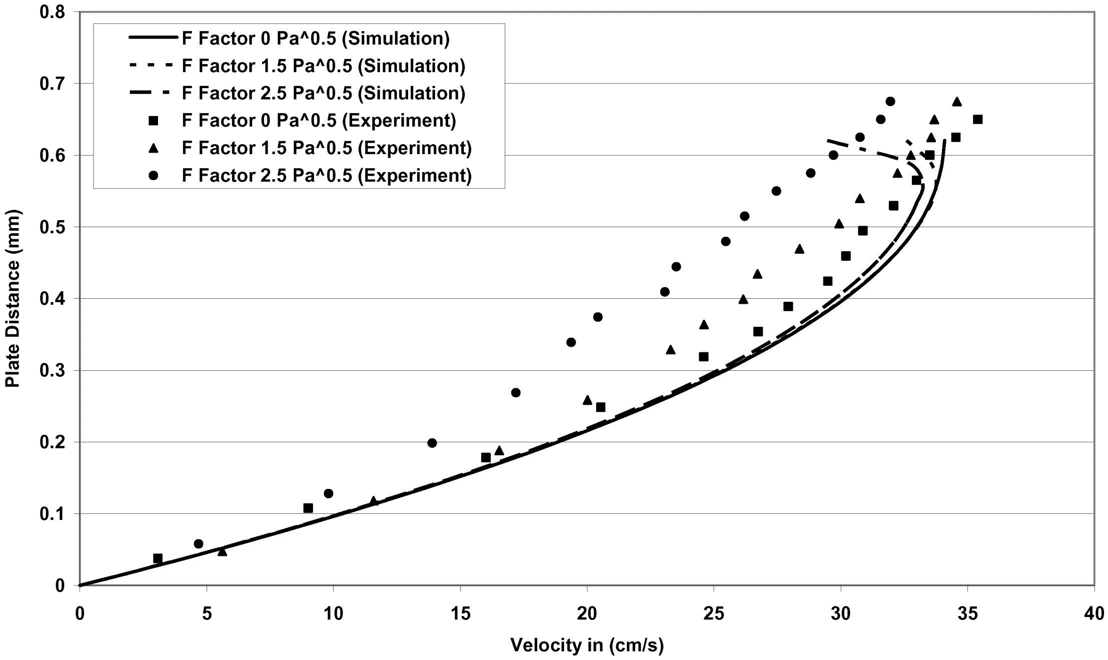

Fig. 5 Comparison of velocity profile from experiment and simulation for water/Glycerol -Air system with Re_l = *32, with and without countercurrent gas loads*

The deviation between the profile from experiment and simulation is higher and this can be due to various reasons. As described before, in simulation velocity profile is position-weighted average profile whereas in the experiments it is time-weighted average profile. The other factors like small changes in liquid flow rate, inclination angle, physical properties of the testing system like viscosity, density may leads to deviation. In the experiments, in the pure wave regions where the fluctuation of velocity is higher, the error is also higher and this error increases with increase in wave formation which can be seen as straight line region in Fig. 4 & Fig. 5. Also the influence like the wall effects, alignment of inlet weirs plays a role. The deviation between the profile for the case with countercurrent and without is also lesser in simulation compared to experiment. This can be because friction factor defined using the pressure drop model is not enough to predict the same and some correction factor need to be introduced.

In Fig. 6, the behaviour of mean film thickness along the length of the plate for increase in F-factors has been shown for two different liquid Reynolds number. The slight increase of mean film thickness with increase in F-factor is clearly seen for both the Reynolds number. This also shows that the increase in F-factor for lesser in Reynolds number increases the liquid hold up because the liquid flow rate is not sufficient enough to withstand the countercurrent gas flow rate.

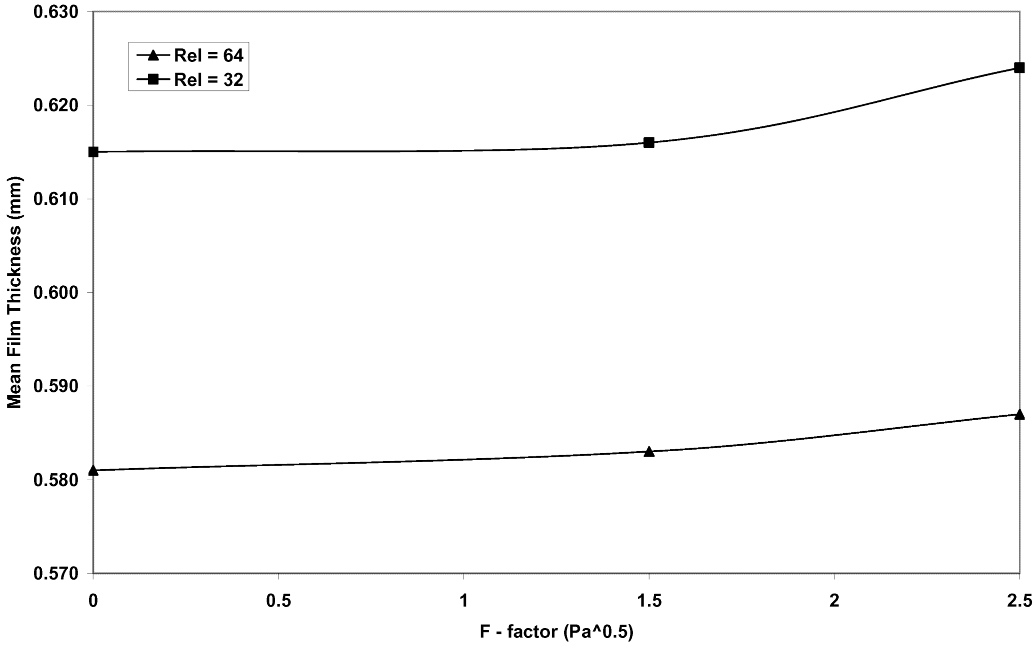

Fig. 6 Average Film thickness against F-factor for two different Reynolds number of Water/Glycerol-System

Overall, the VOF model can be utilized for studying the influence of countercurrent flow. Further studies should be carried out for real structured packing and also taking mass transfer into account.

5. CONCLUSION

A Three dimensional CFD study was carried out to investigate the influence of countercurrent gas flow on a liquid film flow using VOF model. The influence of surface tension, contact angle, drag between the phases was taken into account in the simulations. Experimental measurements were carried out using the newly developed µPIV method which enables the measurements in non-transparent solid surfaces. The experimental measurements and simulations are performed for two different testing systems, water-air and water/glycerol-air. For each liquid load, simulations and experiments were done for increasing gas load to study the influence of countercurrent flow.

From the comparison of experiment and simulation, it can be seen that the increase of countercurrent gas load, decreases the liquid velocity and increases the film thickness. The similar trend can be seen for two liquid Reynolds numbers. In simulation, the change in velocity profile is observed only near the interface not at the bottom of the plate when there is slight increase of countercurrent gas velocity. While further increasing the gas velocity, the profile also changes at the bottom of the plate. This shows the influence of drag force due to the countercurrent gas velocity. Furthermore, the influence of the different parameters like deviation in physical properties of the liquid, small deviation in inclination angle should be studied.

After finalizing the accurate model, further studies should be carried out for packing structures resembling industrial structured packing also considering mass transfer into account.

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Dow, The Dow Chemical Company, product database resources in their website www.dow.com

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NOMENCLATURE

a_e	effective interfacial area per unit volume	(m^2/ m^3)
Bo	Bond Number	(--)
d_h	Hydraulic Diameter	(m)
f_i	Interfacial friction factor	(-)
F	F-factor	($Pa^{0.5}$)
N	Dimensionless constant	(-)
P	Pressure	(bar, Pa)
Re	Reynolds number	(-)
δ^*	dimensionless ratio of film thickness	(-)
u_{eff}	Effective gas velocity	(m/s)
μ	Dynamic Viscosity	(kg/m s)
ν	Kinematic viscosity	(m^2/s)
ρ	Density	(kg/m^3)
δ	Film thickness	(m)
g	Gravity	(m/s^2)
Subscripts		
g	Gas phase	
l	Liquid phase	