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The Numerical Simulation on Internal Gas-liquid Two Phase Flow Field of Three Layers of Air Stirred Reactor

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Abstract: The gas-liquid two phase flow field, overall gas holdup, local gas holdup and bubble size distribution of the three layers ventilation stirred reactor ware numerically simulated by using the computational fluid dynamics (CFD) and multiple reference frame (MRF) methods. And the Euler-Euler double fluid model, the K-e turbulence model with cyclone correction coefficient and the population balance model (PBM) that considering the influence of bubbles breakage and coalescence on bubble size ware used in the numerical simulation. The experimental bench was built and the gas-liquid mixing reaction ware tested under the same working conditions with the numerical simulation. The following conclusions could be got from the comparison between the numerical simulation results and experimental values: the numerical simulation results of the flow field in the stirred reactor are in good agreement with the experimental values; the overall gas holdup distribute uniform, but there are some local areas with high gas holdup and the error was about 13.44%; the bubble coalescence and breakage of area around impeller is faster than others and it is good to the mixing reaction.
Keywords: the stirred reactor, CFD, MRF, the Eulerian multiphase model, PBM

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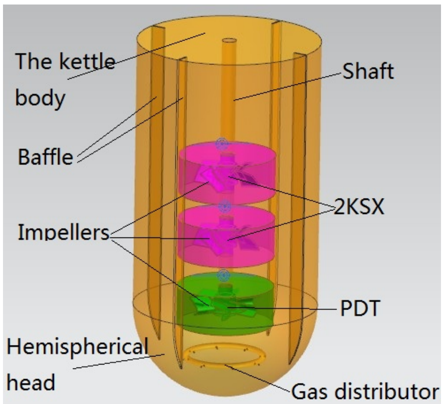
1. INTRODUCTION

The mechanical stirred reactors of multiphase are widely used in Bio-Chemical process industry production field, such as the petrochemical, pharmaceutical, metallurgy and wastewater treatment, which have the advantages of strong practicability and flexible operation. In recent decades, with the development of the industrial, the multiple impellers are adopted in stirred reactor[1]. The changes of the flow field in stirred reactor is very complex, though some experimental works have been done[2-5] in two-phase stirred reactor of multilayer, but the most can be see from the literature is macroscopic research, and the local characteristics is less, and the demands of the design and amplification in stirred reactor without the local research are difficult to be met, Such as the coefficient of mass transfer[6-10], the local gas holdup[11-13], turbulence length[14-17] and the changes of bubble size[18-20]. But the numerical simulation method can be used to study the flow field of gas liquid two-phase in stirred reactor with the rapid development of computational fluid dynamics (CFD).

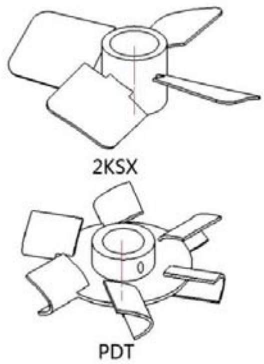
Usually, two methods of Euler-Lagrange and Euler-Euler are used to solve the two-phase problem of numerical simulation[21-24]. The Euler-Lagrange is used to track every dispersed phase that casts large amount of calculation and higher consumption, and it is difficult to achieve the simulation of high gas holdup. While, the Euler-Euler is used in a different way, which is used a method to treat gas liquid two-phase as interpenetrative quasi continuous phase that can effectively save the resources and time in computing. The gas liquid two phase flow field in the stirred reactor was simulated by Gosman[25] etc. with the method of the Euler-Euler two-fluid model. The impeller of monolayer 6-RT in reactor was simulated by using Euler-Euler two-fluid model and multiple reference frame (MRF) and good results from the velocity of fluid, the distribution of gas-liquid and the prediction of bubble size could be got by Lane[26] etc. The Euler-Euler two-fluid mode and the snapshot ware combined to simulate the gas-liquid flow field in stirred reactor of six blade turbine impeller by Ranada[27], and in which accurately predictions of the cavitation of the back of blade by gas condensating and the good agreements between numerical simulation results and experimental values in stirring speed and gas holdup could be got. Numerical simulation of flow field is done by Khopkar[28] in the stirred reactor which has three layers of downstroke PT impeller by the means of Euler-Euler double fluid model, and the distribution of flow field with different speed and different ventilation has been accurately forecasted, in which the method of snapshot in blade area is adopted. Accurately predictions about the distribution of bubble size in stirred reactor with Rushton impeller by using the population model (PBM) ware made and the numerical simulation results are confirmed in good agreement with the experiment values by Montanete[29-30] etc. , in which the Euler-Euler double fluid model is seen to be the key to solve the problem of bubble size.

In this paper, it is based on experimental test. The Euler-Euler double fluid model and population balance model (PBM) are combined to numerically simulate the flow field in stirred reactor of three layers ventilation, in which is based on the theory of multiple reference frame. And the characteristics of flow field was analyzed, the simulation calculations of the overall and local gas holdup ware accurately carried on and accurate forecasts about the change rule of bubble size in the stirred reactor ware made. A relatively complete numerical simulation model is established in this paper, and some theoretical basis are provided for this class of stirred reactor with multilayer and gas-liquid.

2. THE STIRRED REACTOR



(a)



(b)

Fig.1 3D model figure of reaction kettle

In this paper, the object of the numerical simulation is three layers of gas liquid ventilation stirred reactor. The size of 3D model is based on the experiment, and the ratio is 1:1. As shown in figure 1(a), the stirred tank is composed of the cylinder and hemispherical head, and the diameter of cylinder T=380mm, the total height of stirred reactor H=2T; there are four baffles on the inner wall of stirred reactor, and the width W_B=0.10T; three layers of impellers are set up at the distance of 0.5T, 0.9T, 1.2T from the bottom, and above two layers is 2KSX, the lower layer is PDT, the contour diameter of impeller is 0.3T just as the figure 1(b) shows; in the distance of 0.2T away from the bottom is equipped a gas distributor with 16 hole diameter is d=0.008T, and the diameter of gas distributor is D=0.42T.

3. THE GAS-LIQUID TWO-PHASE THEORY MODEL

3.1 Euler-Euler double fluid model

The dispersed phase such as bubble and liquid are regarded as equivalently continuous medium in the Euler-Euler double model, and assuming the bubble and fluid can mutual penetration and can exist as quasi fluid independently. The control conservation equations those are similar to continuous fluid are used in the two phase of gas and liquid under the Euler coordinate, and it is as known as double fluid model. The amount of calculation of Euler-Euler are much less than the Euler-Lagrange, and it is usually been most commonly used. The numerical simulation of the stirred reactor is based on the Euler-Euler in this paper.

The form of basic control equation:

Continuity equation:

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q\right)+\nabla \cdot\left(\alpha_q \rho_q \vec{v}_q\right)=0 \tag{1}$$

In the formula, ρ_q, α_q, υ_q represent density, the phase holdup and the average speed. For the gas-liquid system, namely liquid (L) and gas (g).

Momentum equation:

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q \vec{v}_q\right) + \nabla \cdot \left(\alpha_q \rho_q \vec{v}_q \vec{v}_q\right) = \\ -\alpha_q \nabla P + \nabla\left(\alpha_q \mu_{eff,q}\left(\nabla \vec{v}_q + \left(\nabla \vec{v}_q\right)^T\right)\right) \\ + \alpha q \rho q \vec{g} \pm \vec{F}_{\lg} \tag{2}$$

In the formula, ***P*** is for the pressure between gas and liquid, $\mu_{eff,q}$ is for effective viscosity, F_{lg} is for the interphase momentum transfer term.

The continuity equation and momentum equation are seen as the N-S equations of the gas-liquid two phase flow in the stirred reactor. The parameters are necessary to been closed to solve the partial differential equation, the effective viscosity of liquid can be solved by the turbulence model and the interphase momentum transfer can be closed through the various expressions of interphase force.

3.2 PBM model

PBM model is applied in the gas liquid two phase system in the stirred reactor, the effect of bubble coalescence and breakage on the influence of bubble size distribution, and the behavior of bubble changes can be systematically studied and known deeply from the level of mechanism. It is the key that whether bubble coalescence and breakage can be used as a more real expression of bubbles and the interaction between bubble and fluid by PBM model.

The PBM model is used in the gas-liquid two phase system, and the expression can change to be what is like below when bubble coalescence and breakage are only considered.

$$\frac{\partial}{\partial t} n(v,t) + \frac{\partial}{\partial t}\left(u_{gt}(v,t) n(v,t)\right) = B_B - D_B + B_C - D_C \tag{3}$$

In the formula, $n(v,t)$ is for the probability density function of bubbles number; B_B, D_B, B_C, D_C are respectively for the bubble creation and dissolution rate after coalescence and breakage; $g(\varepsilon; v)$ is for the bubble breakage rate function; $Q(v, \varepsilon)$ is the bubble coalescence rate function.

$$B_B = \int_v^\infty g(\varepsilon; v) n(\varepsilon, t) d\varepsilon \tag{4}$$

$$DB = n(v,t) \int_0^v g(v, \varepsilon) d\varepsilon \tag{5}$$

$$BC = \frac{1}{2}\int_0^{\nu} Q(\nu-\varepsilon;\varepsilon)n(\nu-\varepsilon,t)n(\nu,t)d\varepsilon \tag{6}$$

$$DC = n(\nu,t)\int_0^{\infty} Q(\nu;\varepsilon)n(\varepsilon,t)d\varepsilon \tag{7}$$

4. THE SIMULATION OF GAS-LIQUID TWO PHASE IN THE STIRRED REACTOR

4.1 Modeling and meshing the region of gas-liquid two phase

The main content of article is to study the gas-liquid two phase field in the stirred reactor, so the computational domain is composited of two parts, and the height $H=H_0+H_1$. H0 is for the initial liquid height, and H1 is for the initial gas height above the liquid, taking $H_1=0.42T$. Because the numerical simulation is based on the experimental test, so taking the two phase medium consistent with the experiment, water is for the liquid and argon is for the gas.

The three layers of ventilation stirred reactor is the research object, it contains three layers of impeller, gas distributor, other parts and the structure is complicated. The stirred reactor model should be parted by the software GAMBIT pretreatment before meshing. In order to ensure the accuracy and amounts of the calculation, the hexahedron and unstructured tetrahedral ware both applied to mesh. The impellers, gas distributor and some irregular regions ware meshed with unstructured tetrahedral, and the good quality and fast convergent hexahedron ware adopted to mesh the rest of the regions. In addition, in order to make the features of important areas to be described accurately, the impellers and gas distributor regions are refined, finally we get the grid cell number is 912585, and the stirred reactor grid is shown in figure 2.

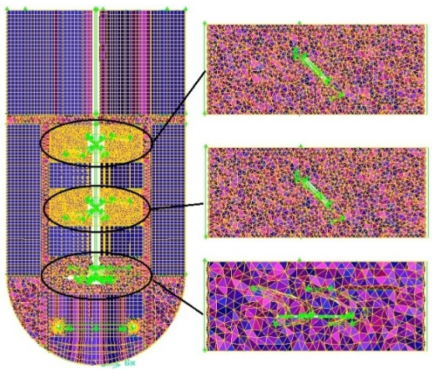


Fig.2 Sectional view of mesh

4.2 Theoretical models and boundary conditions

In this paper, the numerically simulation of the flow field was based on the theory of multiple reference frame, and Eulerian two-flow model and population balance model ware used in the stirred reactor. The k-epsilon model with belt vortex correction coefficient is used in turbulence model, SIMPLEC algorithm is adopted in continuity equation and The Second Order Wind Format (Second Order Upwind) was also used in momentum equation and the momentum, turbulent kinetic energy and turbulence dissipation rate discrete format.

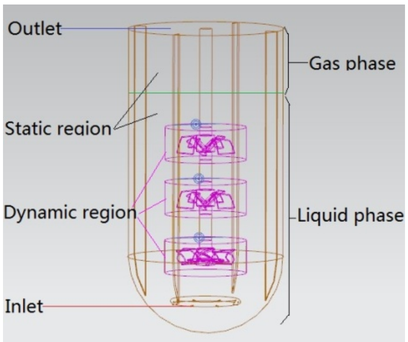


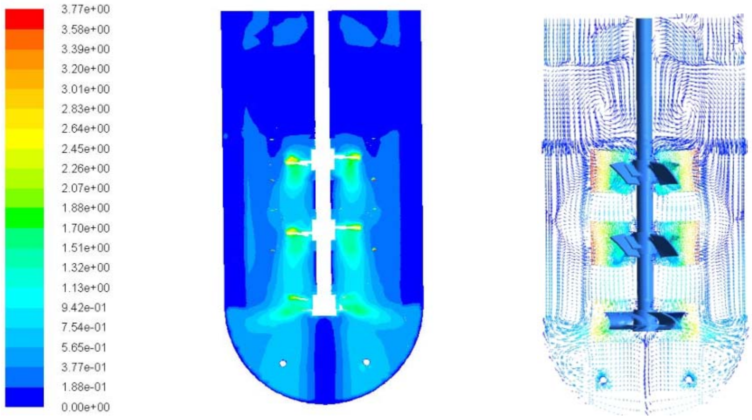
Fig.3 The computation domain model of stirred reactor

The computational domain model of the numerical simulation in stirred reactor is shown in figure 3. The three layers of impellers ware set to be the dynamic region, the rest ware static region and the wall between the dynamic and static region are coupled by INTERFACE. The dynamic region was set as reference frame by the method of multiple reference frame (MRF), the impellers and shaft wall ware handled by Rotating formula and the rest of the wall in the stirred reactor ware set to no slip wall that ware dealt with standard wall function. The inlet round face of gas distributor was set to be the velocity inlet and the surface on the top of the stirred reactor was set to be the pressure outlet. The stirred reactor was ventilation, so the bubbles in the stirred reactor are no longer in a state of balance. And the population balance model (PBM) was used to couple the bubble coalescence and breakage, and the variation range of the bubble size is 1mm to 10mm.

4.3 The simulation analysis of flow field in the stirred reactor

In this article, the numerical simulations are based on experiments, many working conditions, such as under the same inlet velocity with 210r/min, 300r/min, 360r/min different rotations and under the same rotation with the different inlet velocity of 20L/min, 30 L/min, 40 L/min, 50 L/min, 60 L/min, 70 L/min, 80 L/min ware simulated. Because of the large amount of simulation data, so the typical image that can represent the entire flow field ware just shown.

4.3.1 The distribution of velocity field in the stirred react



(a) contour (b) vector

Fig.4 Contours and vector of velocity (Condition: 360r/min, 50 L/min)

As shown in figure 4 is the numerical simulation vector of velocity of the gas- liquid two phase flow field in the stirred reactor, and the inlet velocity 50L/min, the rotation 360r/min was taken as the example. A round the impeller areas is the regions with the higher speed, away from the impeller is lower. From the velocity distribution it can be seen clearly, the axial flow was mainly produced by above and middle impellers and the radial flow was mainly produced by below impeller. When the radial flow reach to the inner wall of the stirred reactor and then two tributaries ware collided, the upward parts are affected by the upper two impellers to join in the axial movement and when the downward flow arrive to the bottom of the stirred reactor lead to a collision and then continue to return to the radial flow. So it can be seen from the figure 4, the whole flow field can be divided into three circulation area in the stirred reactor. A circle flow field by the influence of the upper two layers of impellers of axial flow at the upper middle region of the stirred reactor was formed; due to the radial force of the lower impeller and the role of the inner wall of the stirred reactor, a obvious cycle flow field at the bottom of the reactor was formed; in addition, there is a relatively week circle flow field between the middle and the lower impeller.

In addition, it can be got from the results of the numerical simulation under three kinds of speed 210r/min, 300r/min and 360r/min that the higher the speed, the more obvious the cycle flow field, and also the forming time more little, and the results are in good agreement with the experimental phenomena.

4.3.2 The gas-liquid two phase distribution in the stirred reactor

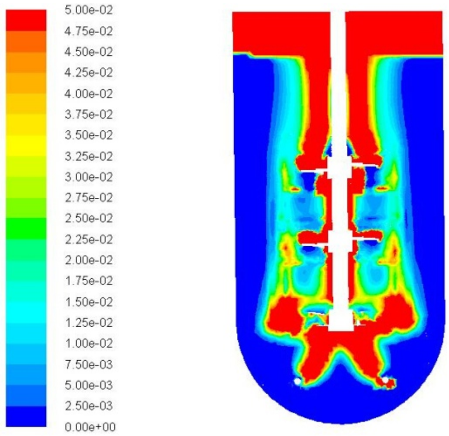
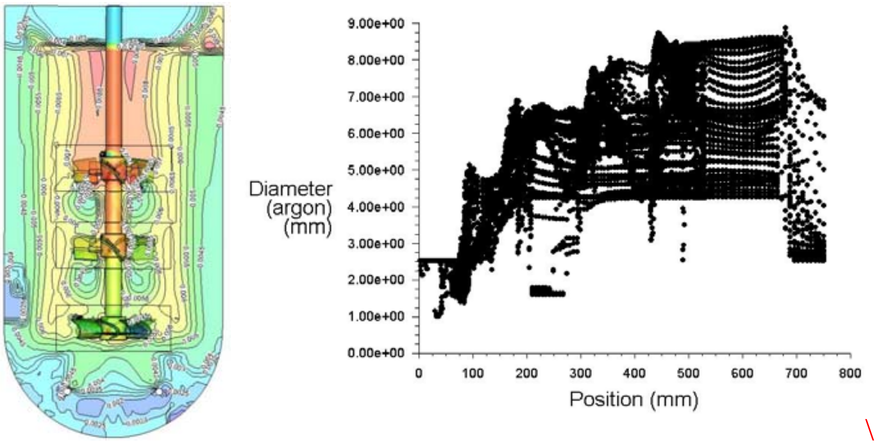


Fig.5 Gas-liquid distribution (Condition: 360r/min, 50 L/min)

The distribution of gas-liquid two phase after the flow field is stable is shown in figure 5. It can be seen from the figure, the change of the gas holdup causes the liquid level to rise in the stirred reactor. The high local gas holdup mainly focuses on the entrance of gas distributor, the impeller and the gas liquid interface, it is higher near the region of impellers than near the wall of reactor, and the gas holdup shows a trend of decreasing as far away from the shaft.

4.4 Particle size distribution

By studying the bubble size distribution, it can be learned to control and optimize the stirred reactor and the reaction conditions from the micro level. As shown in figure 6, it is the numerical simulation results of bubble size distribution under the working condition of 360r/min and 50L/min. From the figure 6(a), the mainly survival particle size range is 5.3mm to 7.1mm under this conditions and it is about to account for 50% of the total live particle size in the stirred reactor. In the radial direction, the bubble size increases from the impeller to T/4, and this is due to the shearing force the makes the closer near blade, the more difficult large size bubbles survived; the bubble size decreases from T/4 to the wall, because it is affected less far away from the cycle flow field and bubbles will collide when they reach to the wall of reactor. In the axial direction, the bubble size overall distribution trend is increasing gradually from the bottom of the stirred reactor to the top, there are two main reasons, A is due to the internal fluid pressure, as the bubbles rise and because of the physical function the bubble size increases gradually; B is because of the turbulence in the stirred reactor, as the bubbles rise, the influence weakens and the bubble size increases.



(a) contour (b) scatter distribution

Fig.6 The bubble size distributions

The figure 6(b) is the scatter distribution of bubble size in the shaft section. It is can be seen from the figure that bubble size at the bottom is smaller and it nearly has no change when the position rises, and the bubble size keeps between 1mm-2.5mm, when it is near the gas distributor the bubble size increases. Because of the shearing force, the range of the bubble particle size is larger. Between far from the blade area and gas-liquid interface the live particle size is stable, and it keeps from 4mm to 8mm.

5. ANALYZING THE RESULTS BETWEEN EXPERIMENTS AND NUMERICAL SIMULATIONS

5.1 The experimental device

The experiments are carried on in the fluid mixing laboratory in Wei-Hai Chemical Machinery Co., LTD. As shown in figure 7 is the multi-function experimental platform, and it is mainly composed of drive motor, lifting equipment, water tank, cylinder, experimental heads, impellers, the control devices and output devices, etc. In the experiment process, the position and speed of the impellers can be controlled by the control devices.

The gas-liquid two phase mixing system was applied in this article, adding water into the reactor until the water level height is 1.55T before the experiments. The stirring speed is controlled by the control box and the inlet speed of the gas is controlled by the flowrator in the process of mixing. The experimental data ware Collected by the observation, camera, recording the change of liquid level height in the process of experiments.

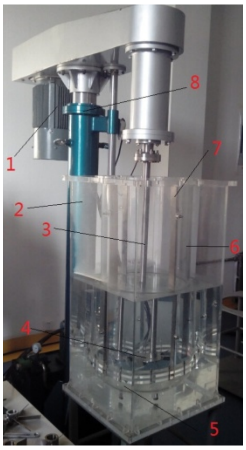


Fig.7 The experimental device of stirred reactor
1-Motor; 2-Tank; 3-Shaft; 4-Impeller; 5-Hemispherical head; 6-Vessel; 7-Baffle; 8-The lifting device

5.2 The gas holdup

5.2.1 The overall gas holdup

As shown in the figure 8 is the experimental values of overall gas holdup under working conditions of different stirring speed and different gas inlet velocity. It ca be seen from the figure that the overall gas holdup rise as the gas inlet velocity increases when the stirring speed is determined, and the lower the inlet velocity is, the less the overall gas holdup increases. It can be told from figure 8, when the inlet velocity is more than 70L/min the overall gas holdup is to stable under the stirring speed of 210r/min and 300r/min, and the gas holdup is no longer rising as the inlet velocity increasing; but when the stirring speed is 360r/min, the overall gas holdup is still following the law of rising with the inlet velocity. From above it can come to the conclusion that the relationships between the overall gas holdup and stirring speed and inlet velocity: the overall gas holdup increases with the stirring speed; the overall gas holdup increases with the inlet velocity under the condition of high speed; when the stirring speed is low, and it also follows the law above under the condition of low inlet velocity, but under the high inlet velocity the overall gas holdup is stable and no longer changing.

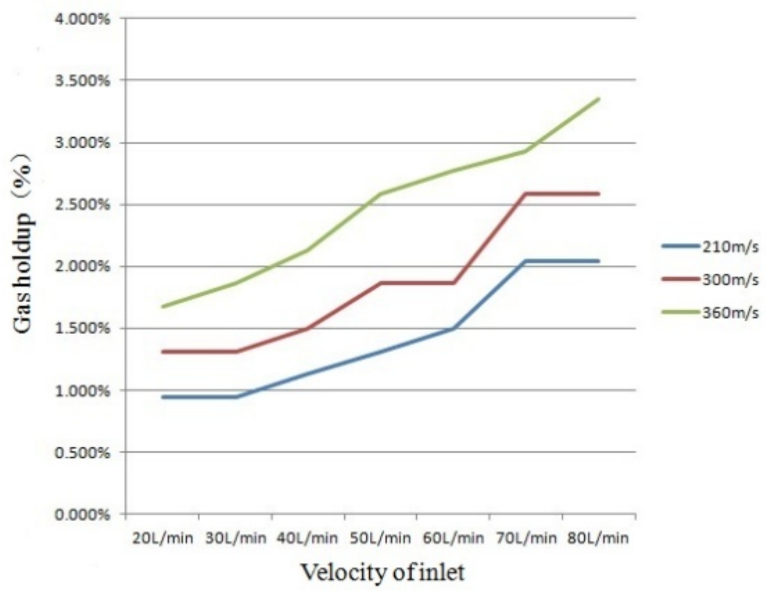


Fig.8 Comparison of overall gas holdup experimental results under different conditions

Under the condition of 360r/min, as shown in figure 9 is the comparison of overall gas holdup between numerical simulation results and experimental values. It can be seen from the figure, the overall gas holdup of the stirred reactor rises with the inlet velocity increases both in experiments and numerical simulations. The numerical simulation results are in good agreement with the experimental values, and the average relative error is 13.34%.

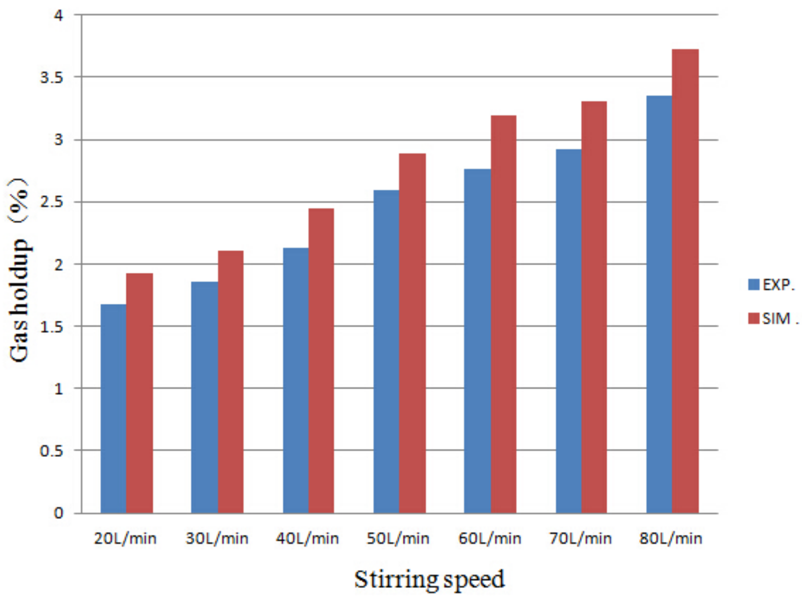
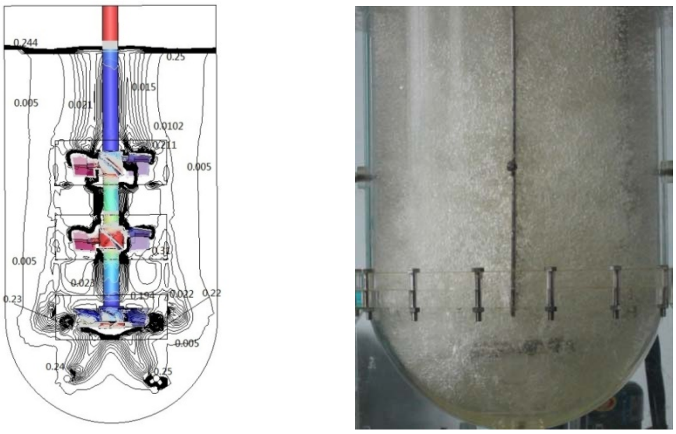


Fig.9 Comparison of overall gas holdup between the simulation and experimental results

5.2.2 The local gas holdup

The local gas holdup can describe the distribution of the gas more specific in the stirred reactor. Taking the condition of stirring speed of 360r/min and inlet velocity of 50L/min for example, the numerical simulation results of local gas holdup is shown in figure 10(a). And the figure 10(b) is the experimental picture, it can be seen clearly from the comparison between simulations and experiments, the distribution of the gas holdup is well-distributed in general under the working conditions, but at the same time there are areas with high local gas holdup, and those areas named gas enrichment area. The gas enrichment areas are mainly concentrated in the exit of gas distributor, near the area of upper and lower impellers and the gas liquid interface area.



(a) simulation (b) experiment

Fig.10 Local gas holdup distributions

It can be seen from the figure 10, the gas holdup is well-distributed in the stirred reactor and the numerical simulation result is 2.9%, there is a peak appearing in the gas enrichment area, in which the average gas holdup is much higher than the average, and the highest gas holdup is about 25%. From the figure 10, it showed that the gas gets into the stirred reactor by the distributor and there is a high-speed gas flow area near the exit of distributor, and this is the reason that the local gas holdup of this area is higher; because of the existence of the circle flow field between the upper and lower impeller and forming a backflow zone, so it is enriching bubbles and the local gas holdup is far higher than other areas; it is due to the disturbance of the impellers and the effect of the baffles that the gas liquid interface is fluctuating great, and making some of the gas above the liquid to spread into the liquid, so the gas holdup near the gas liquid interface in higher, but mostly the areas is less in this case, and the changes is not obvious.

6. CONCLUSION

The following conclusions can be obtained from the numerical simulations and experiments on the three layers of ventilation stirred reactor.

(1) The numerical simulation results are in good agreement with the experimental values, it showed that using the Eulerian multiphase model, multiple reference frame (MRF) and population balance model (PBM) to simulating this kind of stirred reactor is feasible.

(2) In this article, the overall gas holdup is well-distributed, but there are also higher local gas holdup in the stirred reactor that is studied. And the average relative error is 13.34% between numerical simulations and experiments, both are in good agreement with each other, which can be told from the reference [30].

(3) To this stirred reactor, under the lower stirring speed, the gas holdup will increase with the inlet velocity, but when the inlet velocity increases to a certain value the gas holdup is no longer getting change; under the higher stirring speed, it will follow the law that the gas holdup increases with the inlet velocity.

(4) The faster the bubble coalescence and breakage, the much better to the stirring reactions. It can be seen from the numerical simulations that the changing range of the bubble diameter is larger around the impeller area and it is stable far away from the mixing area, and it shows that the bubble coalescence and breakage is faster than other areas in the stirred reactor.

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