

Effect of gas distributor on mass transfer performance of mechanically stirred reactors

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Abstract: To address the prominent issues associated with traditional mechanically stirred reactors, such as the tendency of forming localized flow dead zones at the bottom of the vessel, poor bubble dispersion, and uneven gas phase distribution, this study employs numerical simulation methods to analyze the characteristics of the gas-liquid two-phase flow field within the reactor. The study focuses on investigating the influence of the structural parameters of the gas distributor on gas phase distribution, fluid flow conditions, and gas-liquid mass transfer performance. The results indicate that the orifice diameter of the gas distributor has a significant impact on the distribution of the gas phase. While maintaining low shear stress level and avoiding damage to the growth of microorganisms or microbial communities in the ore leachate, reducing the orifice diameter can effectively improve bubble breakup and dispersion, enhance the uniformity of bubble distribution within the vessel, alleviate the problem of bubble stagnation in dead zones, and thereby increase gas hold-up and the volumetric oxygen mass transfer coefficient. The research findings reveal the mechanisms by which key structural parameters of gas distributor influence flow field characteristics and mass transfer performance, providing important theoretical references for the structural optimization of multi-phase reactors in fields such as mineral processing and biometallurgy.

Keywords: gas distributor, orifice diameter, gas hold-up, volumetric oxygen mass transfer coefficient

1. Introduction

Due to the excellent operational flexibility, adaptability, and high mixing efficiency, mechanically stirred reactors have been widely used in the mining industry for projects such as biometallurgy, the processing of hard-to-treat gold ores, and tank-based bioleaching of sulfide ores (Ahmed et al., 2026). In gas-liquid-solid multi-phase reaction systems, such as mineral bioleaching, the mass transfer rate of dissolved oxygen is a key bottleneck limiting the growth and metabolism of leaching microorganisms as well as the rate of metal sulfide oxidation, while the degree of gas dispersion in the slurry is a critical prerequisite for determining the rate of dissolved oxygen (Rawlings et al., 2003; Chen, 2020). Typically, the effectiveness of gas dispersion is largely influenced by the structure of the gas distributor (Gelves et al., 2014).

Understanding and optimizing the complex hydrodynamics in multi-phase stirred tanks has been a major focus of international research, particularly concerning bubble dispersion mechanisms and mass transfer modeling. Recent advancements in experimental measurements, such as invasive imaging (Wang et al., 2023) and high-resolution mesh sensors (Perez et al., 2025), have provided crucial insights into local gas hold-up and initial mass transfer behavior. Concurrently, computational fluid dynamics (CFD) has significantly broadened the analytical toolkit. Beyond the traditional Euler-Euler frameworks, researchers have increasingly adopted coupled approaches like CFD-PBM (Mao et al., 2026; Yu et al., 2025) and CFD-MUSIG (Krysa and Soos., 2022), as well as the Euler-Lagrange approach coupled with the Volume of Fluid (VOF) method (Marx et al., 2024) and the CLSVOF method (Lai et al., 2026) to capture microscopic bubble breakage and coalescence. These advanced techniques have been instrumental in revealing how microbubble dispersion characteristics can be internally optimized to

enhance gas-liquid mixing (Li et al., 2022). Building upon these hydrodynamic insights, international research has heavily focused on the critical role of gas distributor design across diverse industrial applications. The geometric configuration of spargers fundamentally dictates phase dispersion and eliminates localized dead zones, whether in dynamic membrane-agitated reactors (Gan et al., 2024), slurry bubble columns (Li et al., 2024a), or wastewater treatment systems (Zheng et al., 2022). Extensive studies have evaluated various distributor parameters, including spatial arrangement (Maluta et al., 2023), opening orientation (Kumari et al., 2024), and the use of microporous structures (Liu et al., 2019). Specifically, the orifice diameter and hole configuration have been shown to directly govern gas retention and phase surface area (Chen et al., 2022; Jonach et al., 2025). Furthermore, studies evaluating gas-liquid mass transfer in complex environments confirm that the volumetric mass transfer coefficient (k_{La}) is highly sensitive to the interaction between the distributor and the agitation system. Studies on unbaffled multi-impeller reactors under supercritical conditions (Nolasco et al., 2025), large-scale aerated stirred bioreactors (Jamshidian et al., 2025), and complex two-layer blade assemblies (Liu et al., 2024) demonstrate the necessity of co-optimizing these components.

Despite this extensive international progress in structural optimization and advanced modelling, a key challenge in biological systems remains unresolved. Currently, traditional stirred reactors still face prominent issues when handling mining applications or high-density multiphase flow systems, such as uneven gas phase distribution, the tendency for localized dead zones at the vessel bottom, and solid particle deposition. Furthermore, the mechanisms by which gas distributors influence the flow field and mass transfer within the reactor remain unclear. Therefore, this paper employs numerical simulation methods to analyse the characteristics of the gas-liquid two-phase flow field inside the reactor, focusing on investigating the effects of the orifice diameter on gas phase distribution, flow patterns, and mass transfer performance. The research findings can provide important theoretical references for the structural optimization of multi-phase reactors in fields such as mineral processing and biometallurgy.

2. Research models and numerical simulation methods

2.1. Geometric model and reactor configuration

This study focused on a 500-liter gas-liquid two-phase reactor model. The interior of the reactor featured a four-layer composite impeller arrangement: the middle-upper and upper layers were four-folded-blade impellers, the middle-lower layer was six-straight-blade turbine impellers, and the lower layer was six semicircular turbine impellers, all of which were designed to enhance fluid mixing and gas-liquid contact. Based on this, a 3D physical model of the reaction was created using SOLIDWORKS software and exported, as shown in Fig.1. The 3D model of the gas distributor was shown in Fig.2, and the specific structural parameters were listed in Table 1. To isolate the effect of orifice diameter on gas dispersion while maintaining an approximately constant total inlet area, the total opening area was kept approximately constant for all four distributor configurations, and the number of openings was correspondingly adjusted according to the orifice diameter. The number of openings and total opening area for each configuration were summarized in Table 1.

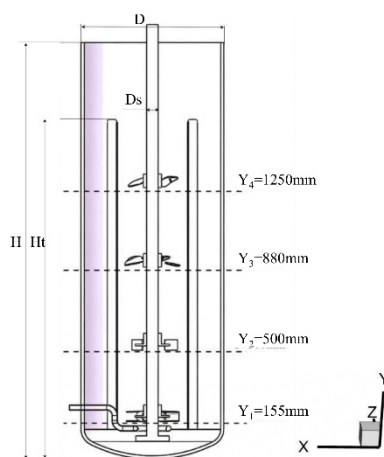


Fig. 1. Physical model of the reaction vessel

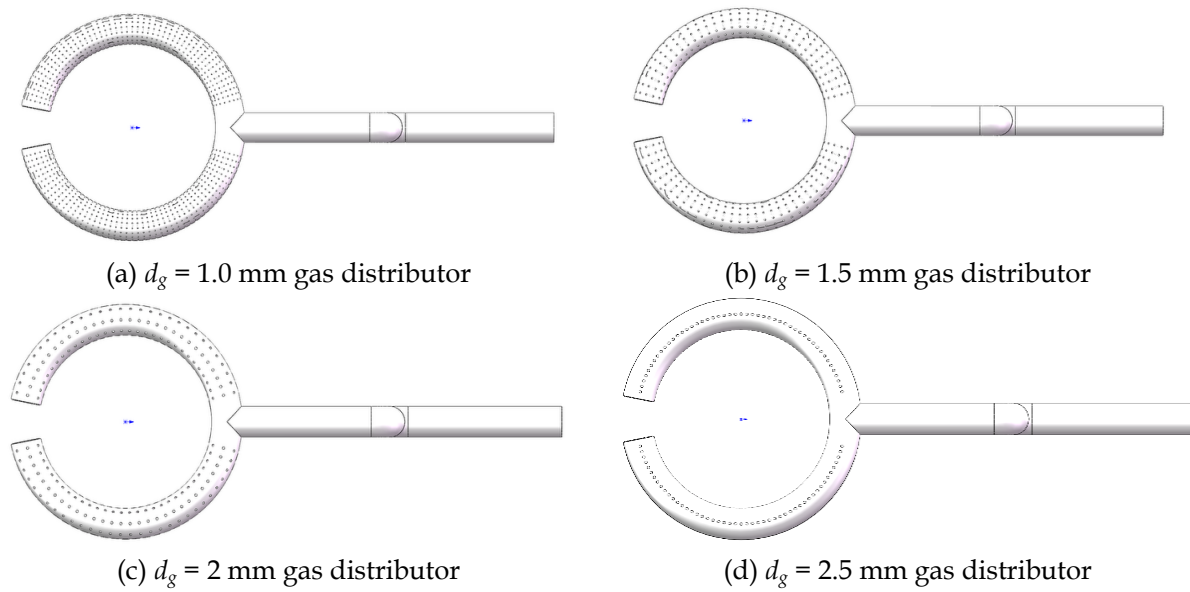


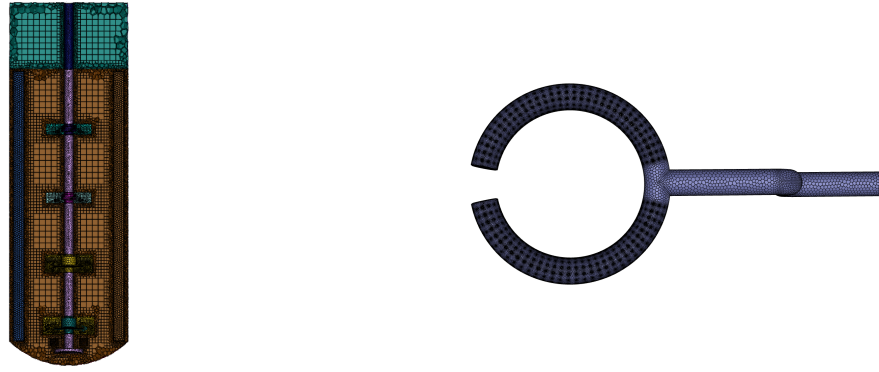
Fig. 2. Gas distributor

Table 1. Reactor model parameters

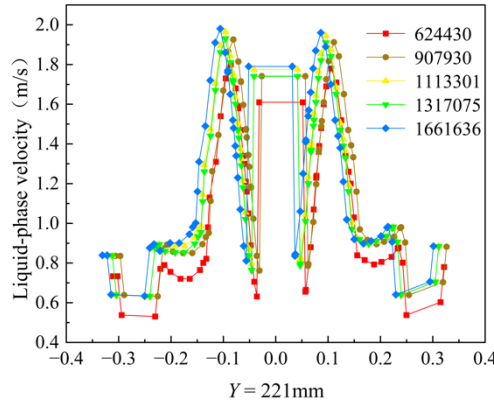
Name	Value	Name	Value
Reaction tank diameter D/mm	646	Reaction tank height H/mm	1975
Stirring shaft diameter D_s/mm	54	Liquid level H_l/mm	1609
Baffle length /mm	1470	Baffle width /mm	60
Number of baffles	4	Wall thickness /mm	5
Four-fold blade diameter /mm	224	six-straight-blade turbine impellers diameter /mm	242
Gas distributor orifice diameter d_g/mm		six semicircular turbine impellers diameter /mm	242
Number of openings / N			1, 1.5, 2, 2.5
Total opening area A_0/mm^2			1862, 828, 466, 298
Distance from the blade to the bottom of the tank /mm			1462, 1463, 1464, 1463
			198, 535, 901, 1275

2.2. Grid partitioning and independence verification

Fluent-meshing software was used to perform an unstructured mesh generation on the reactor model. Compared to tetrahedral mesh, hexahedral mesh offered higher computational accuracy with fewer mesh elements (Jamshidian et al., 2023). Therefore, hexahedral mesh was used to model the reactor, as shown in Fig.3(a). Taking a 2- mm gas distributor as the subject of study, with the rotational speed set to 400 r/min and the medium defined as water, the liquid-phase velocity distribution at the cross-section of the reactor at $Y = 221$ mm was used as the evaluation metric to examine different numbers of mesh elements. The simulation results under different mesh counts were shown in Fig.3(b). When the mesh count exceeded 900 k, the liquid-phase velocity at the $Y = 221$ mm cross-section of the reactor became essentially consistent. Therefore, a mesh count of approximately 900 k was selected for the reactor. Using this method, the number of grid cells in the reactor was determined to be 2,166,006, 1,211,334, 907,930, and 901,642, respectively, for gas distributors with orifice diameters ranging from 1.0 mm to 2.5 mm.



(a) Grid partitioning



(b) Independence verification

Fig. 3. Grid partitioning and independence verification

2.3. Numerical model

2.3.1. Continuity equation

The continuity equation, also known as the mass conservation equation, is based on the continuous medium model of fluids (Moraga et al., 2016). This model assumes that the fluid velocity and density are continuously differentiable in both the time and space dimensions and that the change in mass of a fluid element is conserved relative to the increment in mass flow rate. The differential form of the equation is as follows:

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

In the equation, ρ is the fluid density, kg m^{-3} , t is time, s , $\mathbf{u}$ is velocity, m s^{-1} , and ∇ is the Hami differential operator.

2.3.2. Equation of momentum conservation

The net force exerted by a fluid on an element is equal to the rate of change of the element's momentum with respect to time. Combining this with the law of momentum conservation, we can derive the equations of momentum conservation in each coordinate direction:

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu_t \frac{\partial u_i}{\partial x_j} \right) + (\rho - \rho_a) g_j \quad (2)$$

where u_i and u_j are the velocity components in the i and j directions, respectively, P is the static pressure, Pa , μ_t is the turbulent viscosity, Pa s , g represents the acceleration due to gravity, m s^{-2} , and the subscripts i and j follow Einstein's summation convention in three-dimensional space.

2.3.3. Multiphase flow models

The Euler-Euler method uses the Eulerian framework to treat gas-liquid two-phase flow as a continuous

medium. It features low computational cost and good scalability, and is therefore widely used in numerical simulation studies of gas-liquid two-phase flow (Giorgio et al., 2023; Gupta and Roy., 2013). Based on the Euler-Euler framework, combined with the particle balance model (PBM) or the interfacial concentration model, it is possible to further describe the collective behavior of bubbles and mass transfer processes. In particular, the PBM establishes particle balance equations by considering dynamic mechanisms such as bubble coalescence, fragmentation, and deformation, thereby enabling the prediction of bubble size distribution, number density, and their dynamic evolution. For bubble flow systems, the PBM equations are expressed as follows:

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

$$B_B = \int_v^\infty g(\varepsilon, v) n(\varepsilon, t) d\varepsilon \quad (4)$$

$$D_B = n(v, t) \int_0^v g(v, \varepsilon) d\varepsilon \quad (5)$$

$$B_C = \frac{1}{2} \int_0^v Q(v - \varepsilon, \varepsilon) n(v, t) d\varepsilon \quad (6)$$

$$D_C = n(v, t) \int_0^\infty Q(v, \varepsilon) n(\varepsilon, t) d\varepsilon \quad (7)$$

In the equation, $n(v, t)$ is the probability density function of bubble size, $u_{gt}(v, t)$ is the average velocity of a bubble with volume v , B_B , D_B , B_C and D_C represent the rates of bubble formation and extinction following coalescence and fragmentation, respectively, $n(\varepsilon, t)$ is the number density of bubbles with volume ε , $g(\varepsilon, v)$ is the bubble fragmentation rate function, and $Q(v, \varepsilon)$ is the bubble coalescence rate function.

2.3.4. Turbulence models

The RNG k - ε model significantly improves the accuracy of rapid strain flow by adding an additional term to the turbulent kinetic energy equation. In particular, it provides a more precise description of the turbulent energy distribution in high-Reynolds-number flows (Yakhot et al., 1992). The formula is as follows:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left(\alpha_k \mu_{eff} \frac{\partial k}{\partial x_j} \right) + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (8)$$

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \frac{\partial(\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left(\alpha_\varepsilon \mu_{eff} \frac{\partial \varepsilon}{\partial x_j} \right) + G_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} - R + S_\varepsilon \quad (9)$$

where k is the turbulent kinetic energy per unit mass, $\text{m}^2 \text{s}^{-2}$, ε is the turbulent energy dissipation rate per unit mass, $\text{m}^2 \cdot \text{s}^{-3}$, μ_{eff} is the effective viscosity, $\text{Pa} \cdot \text{s}$. G_k is the turbulent kinetic energy generated by the mean velocity gradient, $\text{kg} \text{m}^{-1} \text{s}^{-3}$, G_b is the turbulent kinetic energy generated by buoyancy, $\text{kg} \text{m}^{-1} \text{s}^{-3}$, Y_M is the dissipation term resulting from compressible pulsational expansion, $\text{kg} \text{m}^{-1} \text{s}^{-3}$, R is the additional source term in the RNG model, $\text{kg} \text{m}^{-1} \text{s}^{-3}$, S_k and S_ε are user-defined source terms, $\text{kg} \text{m}^{-1} \text{s}^{-3}$.

2.3.5. Mass transfer models

During the reaction process, attention is typically focused on the oxygen mass transfer coefficient between the gas and liquid phases, which can be expressed as the volumetric oxygen mass transfer coefficient $k_L a$ (Chisti and Jauregui-Haza, 2002). This coefficient can be broken down into two components: k_L and a . The value of a can be calculated using the following equation:

$$a = \frac{6\alpha_g}{d} \quad (10)$$

In this equation, α_g represents the gas hold-up, and d represents the average bubble diameter.

Various theoretical models have been proposed for calculating the mass transfer coefficient k_L . Among these, the diffusion theory and the surface renewal theory are the two most widely used classical theories in the study of mass transfer in two-phase flow (Ma et al., 2024). Based on the diffusion theory,

the mass transfer coefficient can be described as:

$$k_L = \frac{2}{\sqrt{\pi}} \sqrt{D_L} \left(\frac{\varepsilon}{\nu_l} \right)^{1/4} \quad (11)$$

where D_L is the molecular diffusion coefficient of oxygen in the liquid phase, taken as $2.42 \times 10^{-9} \text{ m}^2\text{s}^{-1}$ according to the reference (Tsimpanogiannis et al., 2021), ε is the turbulent dissipation rate, and ν_l is the kinematic viscosity of the liquid phase.

2.3.6. Shear stress equation

Shear stress is primarily generated by fluid turbulence induced by the relative motion between the agitator blades and the wall. For Newtonian fluids, the following formula is typically used to simulate and calculate the shear stress within a stirred reactor (Wu and Patterson, 1989):

$$\tau = \sqrt{\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2} \quad (12)$$

where τ_{xy} , τ_{yz} , τ_{zx} represent the three components of the shear stress, whose basic form is:

$$\begin{aligned} \tau_{xy} &= -\mu_e \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \\ \tau_{yz} &= -\mu_e \left(\frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z} \right) \\ \tau_{zx} &= -\mu_e \left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right) \end{aligned} \quad (13)$$

Here, μ_e represents the effective viscosity, defined as the sum of the molecular viscosity and the turbulent viscosity, u_x , u_y , and u_z are the velocity components in the x , y , and z directions, respectively.

2.4. Material and boundary condition settings

ANSYS Fluent 2024 was used to solve the meshed grid. The rotating region of the stirred reactor was modeled using the multiple reference frame (MRF) method, and the Eulerian-PBM model was employed to simulate the gas-liquid two-phase flow field inside the reactor. The rotational speed was set to 400 r/min. The RNG k - ε two-equation model was selected, and the turbulent viscosity was calculated by solving the transport equations for k and ε . The parameters for the gas and liquid phases were shown in Table 2. The outlet was set as a pressure outlet with a pressure of 0.05 MPa, the aeration rate of the entire reactor is 0.67 vvm, the inner diameter of the aeration pipe is 22 mm, and the velocity at the pipe inlet is defined as 14.6 m s^{-1} through calculation. The convergence residual for the numerical calculation was set to 10^{-3} , and the time step was set to $1 \times 10^{-4} \text{ s}$. The population balance model was set to “discrete” and six groups of bubble diameter distributions were constructed. The Bin-3 group size was used as the initial bubble size at the inlet. The average diameters of the bubbles in each size group are shown in Table 3. The Luo coalescence model was selected for bubble coalescence and bubble fragmentation (Luo and Svendsen, 1996; Li et al., 2024b).

Table 2. Gas-liquid two-phase parameters

Name	Viscosity/Pa • s	Density/kg • m ⁻³
Gas phase	1.7894×10^{-5}	1.225
Liquid phase	5×10^{-3}	1050

Table 3. Average bubble diameter

Orifice diameter d_g (mm)	Bin-0	Bin-1	Bin-2	Bin-3	Bin-4	Bin-5
1.0mm	1.697	1.200	0.848	0.600	0.424	0.300
1.5mm	2.016	1.459	1.055	0.764	0.553	0.400
2.0mm	2.519	1.823	1.319	0.954	0.690	0.500
2.5mm	3.024	2.188	1.583	1.146	0.829	0.600

3. Numerical simulation results and analysis

3.1. CFD model validation

To evaluate the reliability of the established CFD model for predicting the gas-liquid mass transfer characteristics of the stirred reactor, experimental measurements were carried out in cooperation with a medical equipment company in Chengdu. The dynamic dissolved oxygen method was adopted to determine the volumetric mass transfer coefficient (k_La) of a 500 L stirred reactor. The k_La data obtained under typical operating conditions were taken as the validation benchmark, and can be compared with numerical simulation results to quantitatively verify the prediction accuracy of the CFD model.

During the experiment, purified air was continuously supplied under specified operating conditions until the dissolved oxygen (DO) signal reached a stable value. The stabilized DO concentration was defined as the 100% saturation concentration. Subsequently, the air supply was interrupted and replaced by high-purity nitrogen to remove dissolved oxygen from the liquid phase. The deoxygenation process was terminated when the DO concentration decreased below 1% and the fluctuation rate was less than $0.3\% \text{ min}^{-1}$. Afterward, purified air was reintroduced, and the DO recovery process was recorded at 1 s intervals until the DO concentration exceeded 97% of the initial saturation value.

The oxygen transfer process can be described by:

$$dC_L / dt = k_La(C_{O_2}^* - C_L) \quad (14)$$

where C_L represents the dissolved oxygen concentration in the liquid phase, $C_{O_2}^*$ is the equilibrium dissolved oxygen concentration, and k_La is the volumetric oxygen mass transfer coefficient.

After integration, Eq. (14) can be expressed as:

$$\ln(C_{O_2}^* - C_L) / (C_{O_2}^* - C_0) = -k_Lat \quad (15)$$

where C_0 denotes the initial dissolved oxygen concentration. Therefore, the k_La value is obtained from the absolute slope of the linear fitting curve between $\ln(C_{O_2}^* - C_L) / (C_{O_2}^* - C_0)$ and time.

As illustrated in Fig. 4, data comparison has been conducted at 10 distinct vertical positions located at a radial distance of 220 mm from the central axis of the reactor. With a maximum relative error of only 9.6%, the deviations at all measurement positions are maintained at a low level, falling well within the acceptable tolerance range for both numerical simulations and instrumental measurements. These results support the capability of the CFD model to predict k_La in the present stirred reactor.

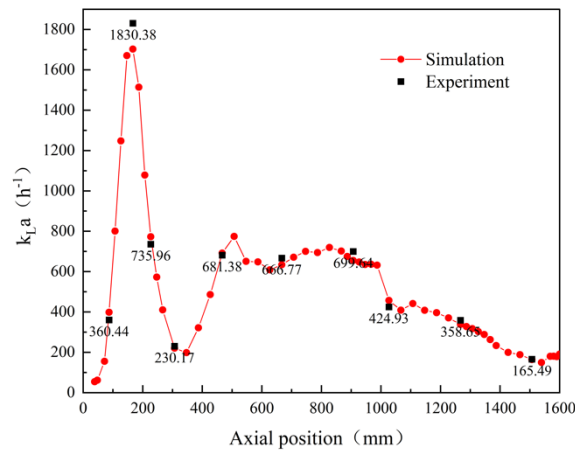


Fig. 4. Experimental verification

3.2. Liquid-phase velocity

The distribution of liquid-phase velocity vectors provides a visual representation of the flow intensity and flow structures inside the reactor. Fig. 5 provides the velocity vector distribution at the $Z = 0$ mm cross-section. As can be seen from the figure, the region near the impeller blades has the highest liquid velocity, with values consistently exceeding 6.0 m s^{-1} . At the bottom of the reactor, as the orifice diameter of the gas distributor decreases from 2.5 mm to 1.0 mm, the high-velocity region gradually

expands. This is because jets from smaller-diameter orifices have greater penetrating power, then the high-velocity jets directly impact the area around the impeller, enhancing fluid flow in that region. Furthermore, when the orifice diameter is small, the backflow at the bottom-most blade becomes more pronounced, and the high-velocity region downstream of the blades extends further. Therefore, a small-orifice diameter can significantly increase the turbulence intensity in the area around the agitator blades and alleviate the problem of dead zones at the bottom.

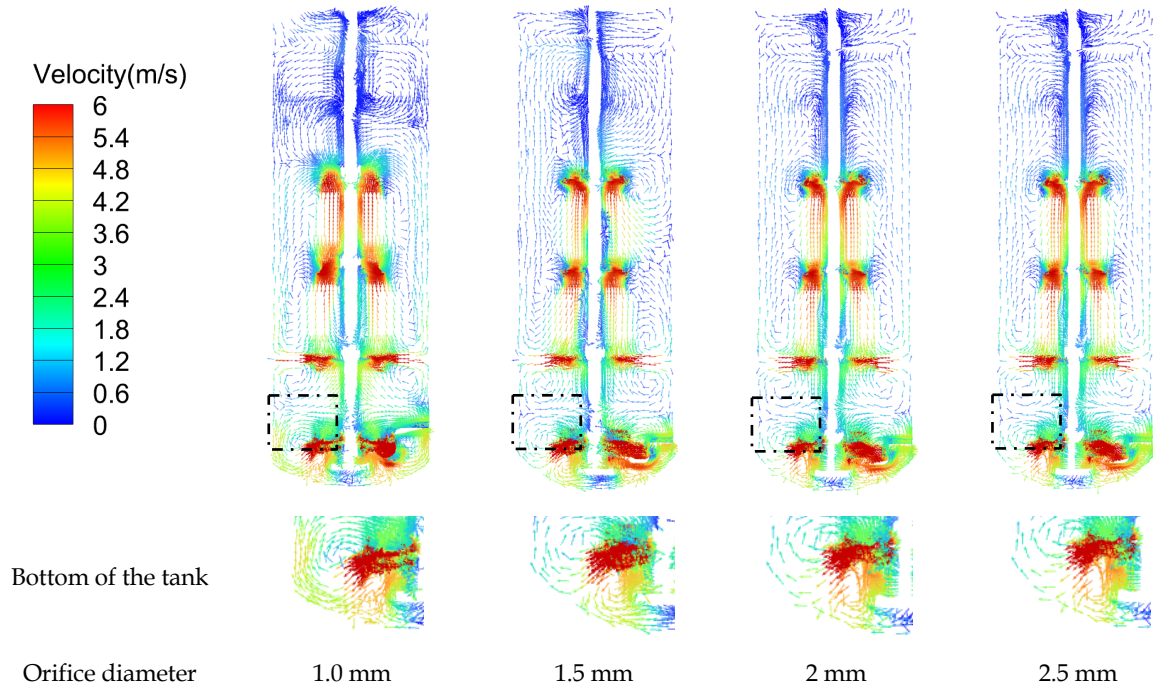


Fig. 5. Velocity vector distribution at cross-section $Z = 0$ mm

3.3. Shear stress

Typically, the shear stress exhibits a highly non-uniform spatial distribution within the reactor. Due to the influence of the agitation structure, localized high-shear-stress zones form near the edges of the impeller blades and in the wall-adjacent regions of the baffles. Fig. 6 presents the distribution of shear stress at different cross-sections. As can be seen from the figure, the shear stress is distributed nonuniformly within the reaction vessel. The tip of the bottom-most impeller blade has the highest linear velocity and the highest shear stress level. At the wall and baffle surfaces, local high-shear regions form due to friction between the fluid and the wall. As the axial height increases, the shear stress gradually decreases. Under constant aeration conditions, the orifice diameter of the distributor has a certain effect on the shear stress within the tank, that is reducing the orifice diameter increases the level of shear stress within the tank.

Fig. 7 shows the shear stress distribution at cross-section $Y = 195$ mm. As can be seen from the figure, the shear stress near the impeller reaches approximately 1.1 Pa. At the reactor wall, due to friction between the baffle and the fluid, it shows a secondary peak. In contrast, the shear stress level in the flow field is generally below 0.5 Pa. A comparison of different distributor orifice diameters reveals that the trends of shear stress distribution within the reactor are generally consistent. However, the maximum shear stress at the 1.0 mm orifice diameter is 6.77% higher than that at the 2.5 mm orifice diameter. Lee et al. (2023) reported a critical shear stress of approximately 1.8 Pa for *E. coli* bio aggregates under pore-throat flow conditions. Therefore, the maximum shear stress of approximately 1.1 Pa obtained in the present study is lower than the critical value reported. It should be noted that microbial shear tolerance may vary with microbial strain, growth state, surface properties, and environmental conditions. Accordingly, the slight increase in shear stress associated with reducing the distributor orifice diameter remains within the range considered in this study, while its biological implications require verification for the specific microorganisms and operating conditions of interest.

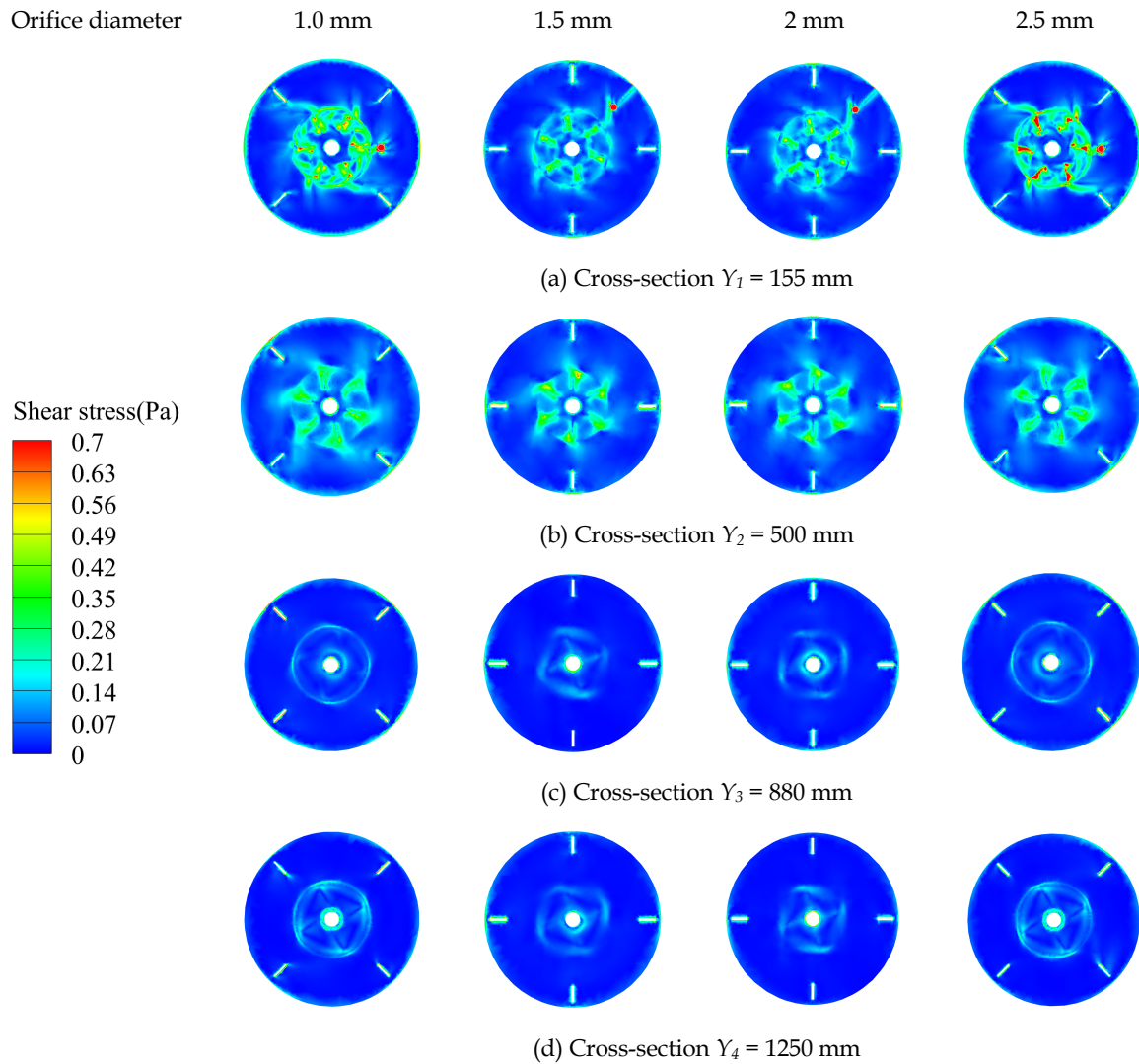


Fig. 6. Diagram of shear stress distribution at different cross-sections

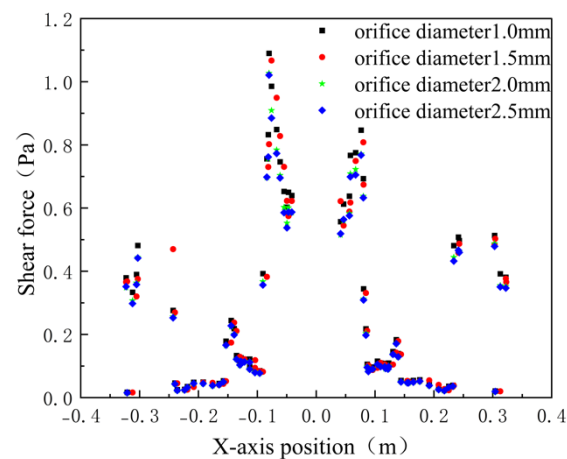


Fig. 7. Shear stress distribution at cross-section $Y = 195$ mm

3.4. Gas hold-up

Gas hold-up is a key indicator of bubble dispersion efficiency and gas-liquid mass transfer potential. Fig. 8 gives the gas hold-up distribution at cross-section $Z = 0$ mm. Based on the characteristics of the flow field distribution, as the orifice diameter decreases, the local gas hold-up in the tank bottom and

wall regions increases significantly, and gas dispersion in the central shaft region becomes pronounced. At the same time, gas diffusion from the vicinity of the impeller to other areas of the tank is enhanced, improving the spatial uniformity of the gas-liquid distribution. This principle confirms that gas distributors with small orifice diameters can generate a large number of dispersed bubbles. By slowing the rise of the bubbles and prolonging the gas residence time, they ultimately increase the gas hold-up and improve the uniformity of gas phase distribution.

Fig. 9 shows the distribution of gas hold-up at different cross-sections. As can be seen from the figure,

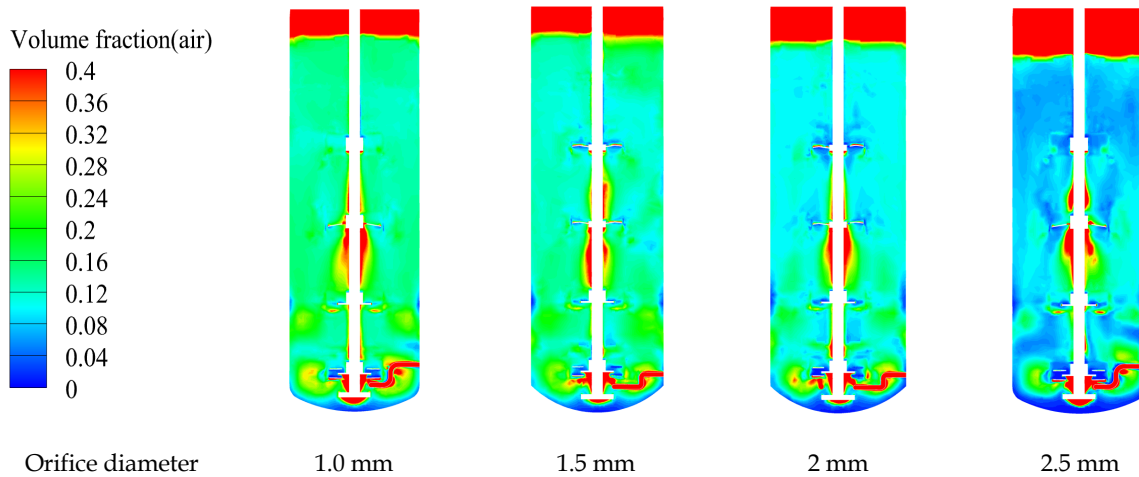


Fig. 8. Gas hold-up distribution at cross-section $Z = 0$ mm

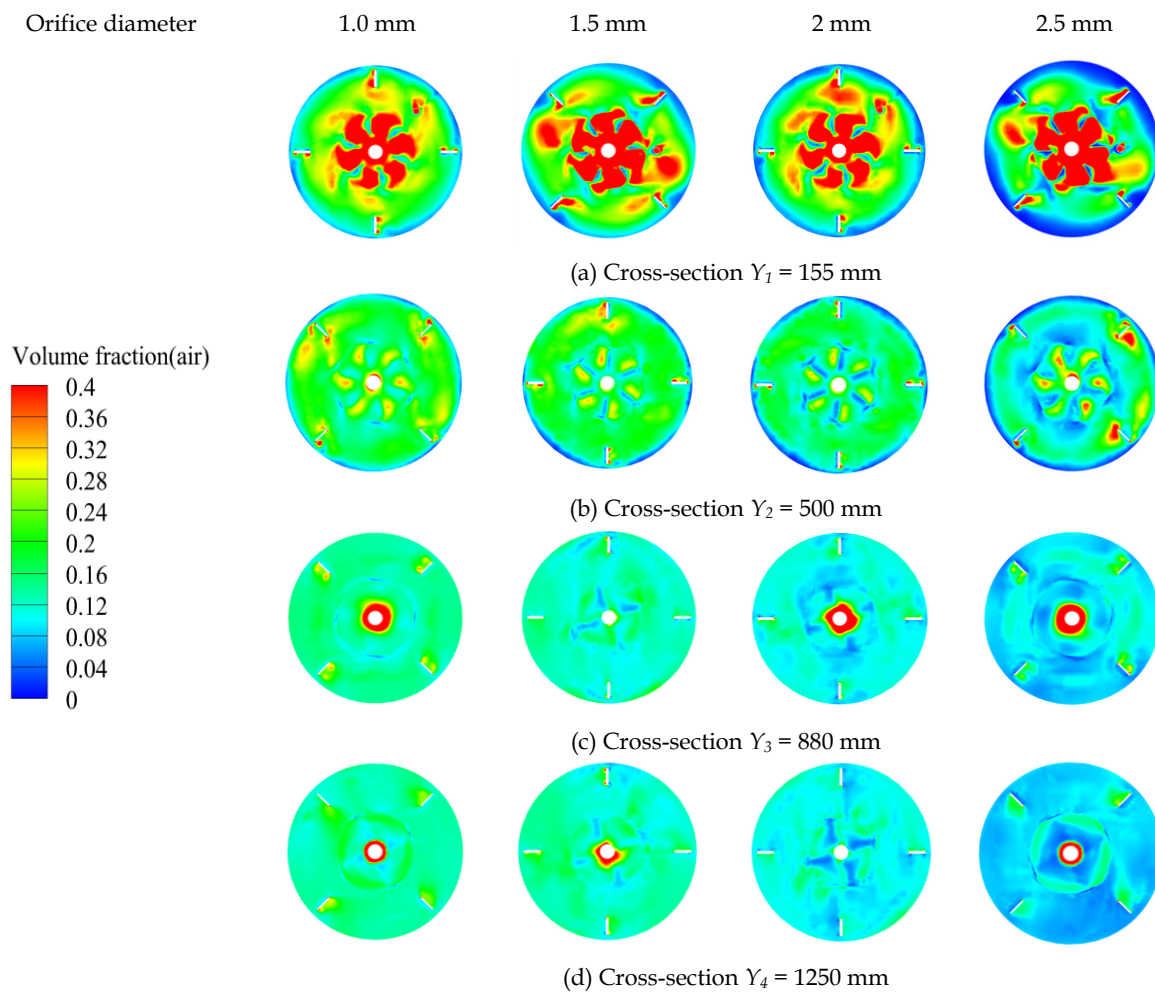


Fig. 9. Distribution of gas hold-up at different cross-sections

for a given orifice size, a large number of bubbles below the Y_1 cross-section have not yet overflowed, forming localized accumulations between the impeller blades and the distributor, which results in an abnormally high gas hold-up. At the Y_3 and Y_4 cross-sections, the gas hold-up is relatively low, and there is significant unevenness on either side of the baffle. The reason is that the baffle effectively suppresses the formation of large-scale vortices and impedes the upward movement of bubbles, resulting in an uneven distribution of bubbles on either side of the baffle. At cross-sections at the same height, as the orifice size decreases, the local gas hold-up shows a significant upward trend. This indicates that reducing the orifice diameter can effectively increase the local gas hold-up and improve the uniformity of bubble distribution, which helps enhance mass transfer efficiency.

Fig. 10 illustrates the effect of orifice diameter on the average gas hold-up in the reactor. As the aeration time increases, the average gas hold-up in the reactor tends to increase for all orifice diameters. Furthermore, after 60 seconds, gas inflow and outflow reach a dynamic equilibrium, and the average gas hold-up curves in the reactor all tend to stabilize. When the orifice diameters of the gas distributor are 1.0 mm, 1.5 mm, 2 mm, and 2.5 mm, respectively, the average gas hold-up in the reactor reaches 14.9%, 12.5%, 10.8%, and 9.9%, respectively. This indicates that, under the same airflow rate, a distributor with a smaller orifice diameter can generate a greater number of fine bubbles, which not only increases the specific surface area of gas-liquid contact but also prolongs the residence time of the bubbles in the tank, thereby improving the gas hold-up in the tank.

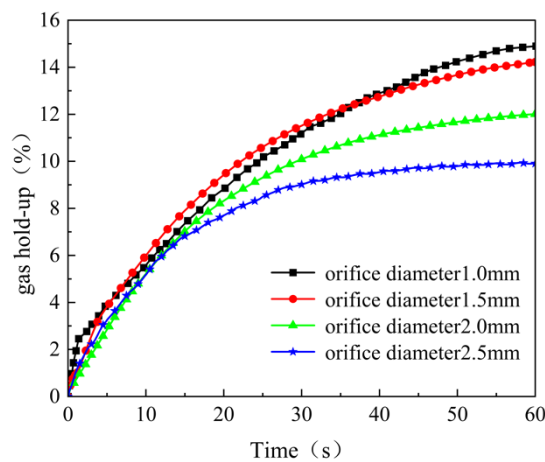


Fig. 10. Effect of orifice diameter on the average gas hold-up

3.5. Bubble size

As can be seen from Eqs. (10) and (11), the interfacial area decreases with increasing bubble diameter, while a smaller bubble diameter generally favors a larger gas-liquid interfacial area and thus improves k_{La} . The smaller bubble diameter and the more uniform distribution, the larger the gas-liquid contact surface area, which is more conducive to the mass transfer process.

Fig. 11 presents the distribution of bubble sizes under different distributor orifice conditions. As shown in the figure, as the orifice diameter increases from 1.0 mm to 2.5 mm, the average bubble diameter inside the tank increases from 1.1 mm to 2.45 mm. The proportion of small-diameter bubbles decreases significantly, and the bubble size distribution shifts from concentrated to dispersed, with the size distribution range expanding from 1.4 mm to 2.5 mm. When the orifice diameter is 1.0 mm, the proportion of small-diameter bubbles in the tank is highest, and their spatial distribution is uniform.

3.6. k_{La}

During the operation of a stirred reactor, the mass transfer performance is typically characterized by the volumetric oxygen mass transfer coefficient k_{La} , which is closely related to parameters such as bubble size and gas hold-up (Bouaifi et al., 2001).

Fig. 12 shows a contour of the volumetric oxygen mass transfer coefficient k_{La} at various cross-sections within the reactor for different gas distributor orifices. As shown in the figure, the k_{La} distribution patterns in the reactor are generally consistent at different gas distributor orifice sizes. For

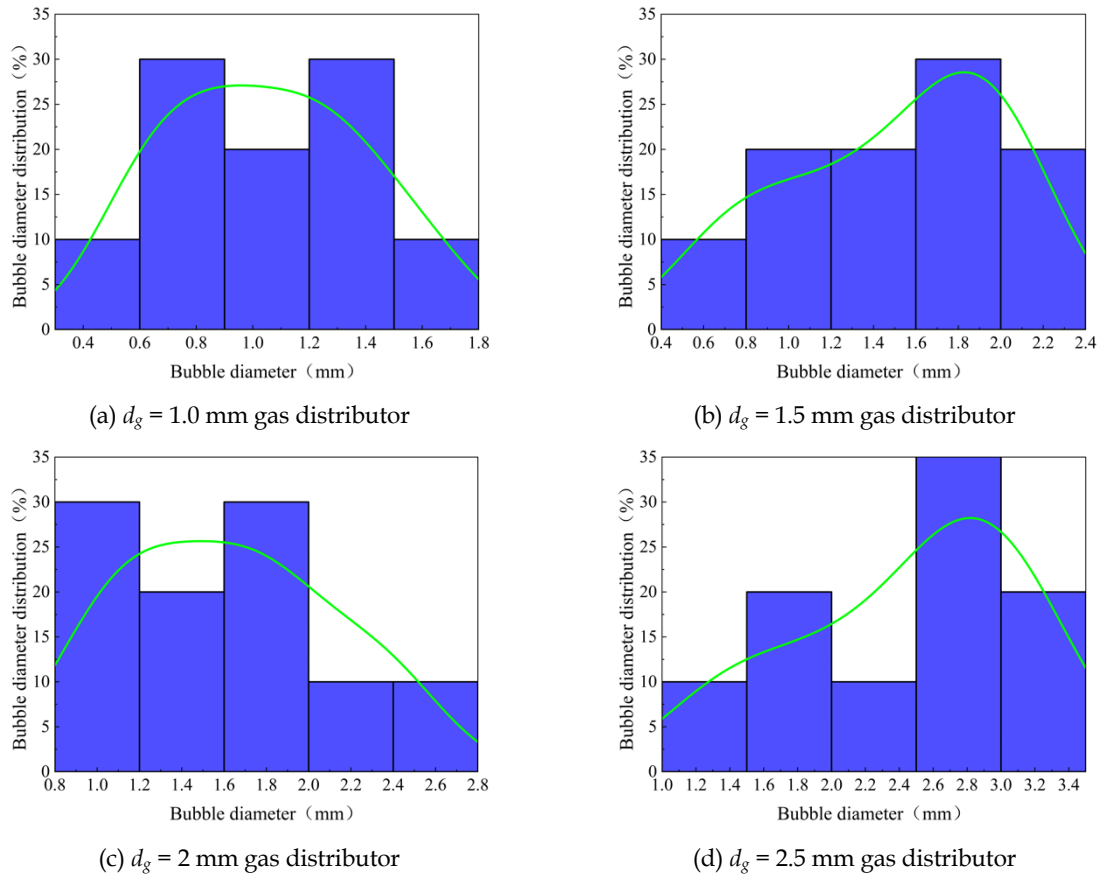
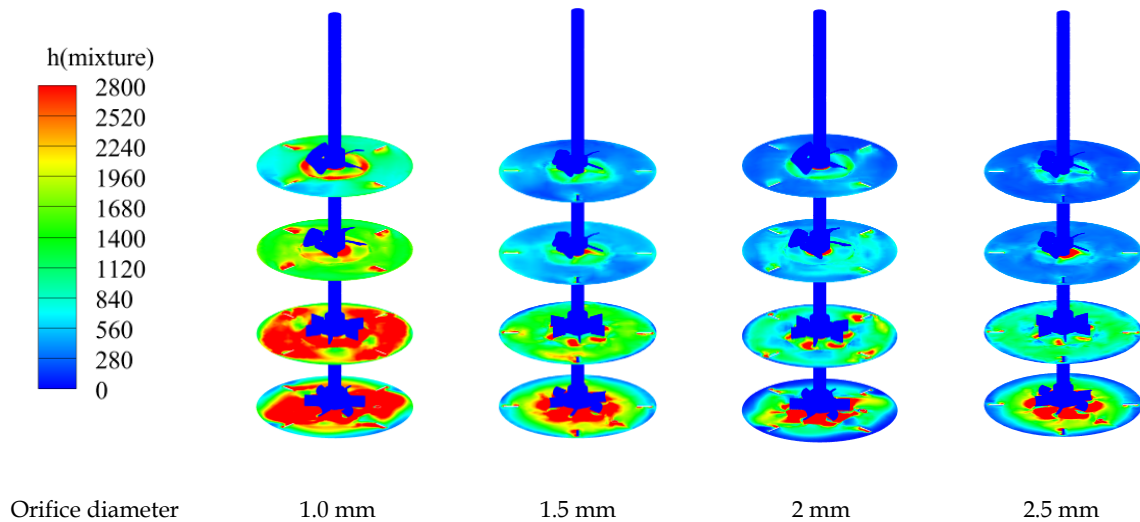


Fig. 11. Bubble size distribution chart

Fig. 12. k_{La} distribution at different cross-sections

the same orifice diameter, k_{La} increases significantly in the region of the stirrer blades at different cross-sectional heights. This is because the energy dissipation rate near the blades is slightly higher, and large bubbles are broken down into smaller bubbles under strong shear stress, which significantly increases the contact surface area between the gas and liquid phases and, consequently, enhances mass transfer.

Under the same orifice diameter condition, the lower-layer and lower-middle-layer blades possess stronger radial pumping capacity, enabling them to transport broken bubbles radially toward the tank wall area, which helps expand the high mass transfer zone. In contrast, the four-fold blades in the upper and middle-upper layers feature a downward-pressing blade structure that suppresses upward gas

movement. After being broken up, bubbles around the blades tend to diffuse downward, resulting in a significant reduction in the local k_{La} value for that cross-section.

When the orifice diameters of the gas distributor are 2.5 mm, 2 mm, 1.5 mm, and 1.0 mm, respectively, the average k_{La} values inside the tank are 537.10 h⁻¹, 641.52 h⁻¹, 781.13 h⁻¹, and 1618.17 h⁻¹, respectively. As the orifice diameter decreases, the k_{La} increases by 201.28%. On the one hand, as the orifice diameter decreases and the number of openings increases, the resulting bubbles are smaller, leading to a higher average gas hold-up in the tank and a significant increase in the gas-liquid mass transfer contact area. On the other hand, with smaller orifice diameters, the liquid circulation velocity inside the reactor is higher, the turbulence intensity of the liquid phase is significantly enhanced, the thickness of the gas-liquid mass transfer boundary layer is reduced, and mass transfer resistance is lowered. The combined effect of these factors results in reactors equipped with small-orifice gas distributors exhibiting superior mass transfer performance.

4. Conclusions

The study employs numerical simulation methods to investigate gas-liquid two-phase flow in a mechanically agitated reactor, and explore the influence of gas distributor structural parameters on the flow patterns, gas phase distribution, and mass transfer performance. The main conclusions are as follows:

- (1) Reducing the orifice diameter enhances jet penetration, increases the range of high velocities at the bottom of the reactor, and improves the phenomenon of dead zone. The shear stress of the fluid inside the reactor increases slightly within a controllable range.
- (2) An analysis of the effects of orifice diameter on gas hold-up and bubble size distribution shows that as orifice diameter decreases, the bubble distribution becomes more uniform, and the average gas hold-up in the tank increases by 50.5%. Smaller orifice diameters help reduce bubble size and increase the proportion of smaller bubbles, with the average bubble size decreasing from 2.45 mm to 1.1 mm.
- (3) The distribution of the volumetric oxygen mass transfer coefficient (k_{La}) verifies that within the tank of a small orifice diameter gas distributor, the k_{La} has been significantly improved by 201.28%. At the same time, the distribution of k_{La} within the tank became more uniform, which helps enhance the overall gas-liquid mass transfer efficiency.

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