Numerical simulation of the gas–liquid two-phase flow in aeration tank based on different multiphase models

Jinnan Guo, Liang Dong, * and Jiawei Liu
Research Centre of Fluid Machinery Engineering and Technology, Jiangsu University, Zhenjiang, China
*Corresponding author e-mail: dongliang@ujs.edu.cn

Abstract. In this paper, the Eulerian model and Mixture model are used to study the free surface, internal flow and mass transfer in the aeration tank. The two multiphase models affect the liquid velocity, internal flow and oxygen mass transfer coefficient (kLa) of the tank. Eulerian model than the Mixture model significantly higher simulates the liquid velocity near the impeller, and the range of the main longitudinal circulation vortex is smaller than Mixture model. The error between the simulated kLa of Eulerian model and the experimental value is smaller than Mixture model. The results show that the Eulerian model is more suitable for the simulation of the gas–liquid two-phase flow in the aeration tank.

1. Introduction
China is a country with a severe shortage of water resources, and the problem of water pollution is increasingly prominent. Sewage treatment is an integral part of the construction of ecological civilization. The inverted umbrella aerator is an essential part of sewage treatment, which can effectively solve the problem of water pollution in life and industry.

Many researchers have devoted themselves to the study of gas-liquid two-phase flow using different multiphase models. Guo J. et al. [1] simulated the gas-liquid two-phase flow and mass transfer coefficient in the aeration tank through the Eulerian model. The results showed that the numerical simulation could well predict the flow in the aeration tank. Liu [2] studied the fluctuation of the free surface through the volume of fluid (VOF) model. Bandyopadhyay et al. [3] used the Eulerian model to simulate the gas-liquid two-phase flow at the elbow of the pipeline and achieved satisfactory results. Wang [4] simulated the gas-liquid two-phase flow field of four different inlets at the bottom of the bubble column using the Eulerian model coupled with the population balance model (PBM). Guo L. [5] used the VOF model to obtain the velocity and vorticity distribution of the free surface in a ditch, which confirmed that the VOF model could better simulate the velocity of the shallow liquid. Liang X. et al. [6] used the Eulerian model coupled with the population balance model (PBM) to simulate the bubble movement in a cylindrical bubble column. The simulated results of the time-averaged local gas holdups and normalized axial liquid velocities accorded well with the experiment. Based on the Navier-Stokes equation and the Mixture model, Chen et al. [7] simulated the flow of a ventilated cavity around a three-dimensional axisymmetric body and verified the validity of the model. Fu et al. [8] compared the Eulerian and Mixture model coupled with the standard k-ε turbulence model to simulate the flow in a contact zone of dissolved air flotation.
To accurately reveal the real flow situation in the inverted umbrella aerator, this paper compared different multiphase models to study the free surface, gas-liquid two-phase flow law and mass transfer coefficient, which provides the research basis for the gas-liquid two-phase flow in the aeration tank.

2. Model and Numerical calculation method

2.1. Model and grid
The models used in the simulation are the inverted umbrella aerator (rotating domain) and the cylindrical aeration tank with a diameter of 300mm (static domain). Figure 1 shows the object and size of the inverted umbrella aerator. In the simulation, the highest point of the blade is equal to the free surface, the liquid depth in the aeration tank is 200 mm, and the rotational speed of the inverted-umbrella aerator is 250 rpm. Computational domain and grid are shown in Figure 2.

![Figure 1. Object and size of inverted umbrella aerator](image1)

![Figure 2. Computational domain and grid](image2)

The gas holdup of a specific cross section in the aeration tank is taken as the grid independence test index. Six different numbers of grids are selected (the grid number of static domain is $5.79 \times 10^5$, $7.26 \times 10^5$, $8.68 \times 10^5$, $1.113 \times 10^6$, $1.412 \times 10^6$ 1.856$ \times 10^6$, and the grid number of corresponding rotating domain is $1.36 \times 10^5$, $1.81 \times 10^5$, $2.26 \times 10^5$, $2.72 \times 10^5$, $3.16 \times 10^5$, $3.62 \times 10^5$). The result of the grid independence test is shown in Figure 3. The result shows that when the grid number of static domain is...
greater than 1.1×10^6, the value of gas holdup is unchanged. Therefore, the final static domain grid number is 8.68×10^5, and the rotating domain grid number is 2.26×10^5.

Figure 3. Result of the grid independence test

2.2. Boundary condition and solution method
Fluent 15.0 is used for unsteady calculation, and the time step is set to 0.001s, the calculation time is 9s. The liquid phase is set as the primary phase, and the gas phase is set as the secondary phase. The top outlet is set as a pressure outlet [9], and the impeller is set as a rotating wall.

The solution method of pressure-velocity coupling is SIMPLE. The least-square method is used to deal with the gradient of the spatial discretization scheme. First-order upwind is used for momentum, volume fraction, turbulent kinetic energy and turbulent dissipation. The transient formulation adopts the first-order implicit.

2.3. Multiphase model
1. Eulerian model
   (1) Volume fraction equation:
   \[ V_q = \sum_v \alpha_q \, dV \]  
   Where, \( \sum_{q=1}^{n} \alpha_q = 1 \)
   (2) Mass-conservation equation:
   \[ \frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q) = \sum_{p=1}^{n} \left( \dot{m}_{pq} - \dot{m}_{qp} \right) + S_q \]  
   Where, \( \vec{v}_q \) is current velocity of q-phase; \( \dot{m}_{pq} \) is mass transfer from p-phase to q-phase; \( \dot{m}_{qp} \) is mass transfer from q-phase to p-phase; \( S_q = 0 \).
   (3) Momentum conservation equation:
   \[ \frac{\partial}{\partial t} (\alpha_q \rho_q \vec{v}_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q \vec{v}_q) = -\alpha_q \nabla p + \nabla \cdot \vec{f}_q + \alpha_q \rho_q \bar{\vec{g}} + \sum_{p=1}^{n} \left( \vec{R}_{pq} (\vec{v}_p - \vec{v}_q) + \dot{m}_{pq} \vec{v}_p - \dot{m}_{qp} \vec{v}_q \right) \right] + \left( \vec{f}_{\text{lift},q} + \vec{f}_{\text{slip},q} + \vec{f}_{\text{vm},q} + \vec{f}_{\text{td},q} \right) \right] \]  
   Where, \( \bar{\vec{g}} \) is stress-strain tensor of q-phase, \( \vec{f}_{\text{lift},q} \) is external volume force, \( \vec{f}_{\text{slip},q} \) is wall slip force, \( \vec{f}_{\text{vm},q} \) is virtual mass force, \( \vec{f}_{\text{td},q} \) is turbulent diffusion force, \( \vec{R}_{pq} \) is interphase force; \( \vec{v}_{pq} \) is interphase velocity

2. Mixture model
   (1) Continuity equation:
   \[ \frac{\partial}{\partial t} (\rho_m) + \nabla \cdot (\rho_m \vec{v}_m) = 0 \]  

(1)
Where: $\hat{v}_m$ is the average mass speed.

$$\hat{v}_m = \frac{\sum_{k=1}^{n} a_k \rho_k \hat{v}_k}{\rho_m}$$  \hspace{1cm} (5)

Where: $\rho_m$ is the mixed density: $\rho_m = \sum_{k=1}^{n} a_k \rho_k$; $a_k$ is the volume fraction of phase k.

(2) Momentum equation:

$$\frac{\partial}{\partial t} (\rho_m \hat{v}_m) + \nabla \cdot (\rho_m \hat{v}_m \hat{v}_m) = -\nabla p + \nabla \cdot [\mu_m (\nabla \hat{v}_m + \nabla \hat{v}_m^T)] + \rho_m \hat{g} + \vec{F} + \nabla \cdot \left( \sum_{k=1}^{n} a_k \rho_k \hat{v}_{dr,k} \hat{v}_{dr,k} \right)$$  \hspace{1cm} (6)

Where: $\vec{F}$ is the volume force, $\mu_m$ is the density of mixed phase; $\hat{v}_{dr,k}$ is the drift velocity of the secondary phase k

3. Results and discussion of gas-liquid two-phase flow

3.1. Analysis of free surface

Figure 4 shows the top view of the free surface near the inverted umbrella aerator simulated by different multiphase models.

![Velocity](image)

Figure 4. Top view of the free surface

It can be seen from the figure that the fluctuation of liquid level changes with the calculation time. After 7s, the liquid level tends to be stable. Different multiphase models do not affect the flow pattern of the liquid surface. The liquid in the tank is still affected by centrifugal force and ejects along the working face of the blade through the upper plate, forming a hydraulic jump. Different multiphase models mainly affect the liquid velocity in the aeration tank. The liquid velocity near the impeller of the Eulerian model is higher than the Mixture model. The larger the initial velocity is, the wider the hydraulic jump area is. The mass transfer efficiency and the concentration of dissolved oxygen are improved. The study of free surface can reveal some gas-liquid two-phase flow laws, but the internal flow and mass transfer process need further study.
3.2. Analysis of internal flow
After the flow is stable \((t=9s)\), streamlines and air volume fraction of the cross-section in the aeration tank is shown in Figure 5.

![Streamlines and Air Volume Fraction](image)

Figure 5. Gas-liquid two-phase flow in the aeration tank

It can be seen from the figure that the flow on the left and right sides is the same during the rotation of the impeller, and vortex occurs because of centrifugal force. Under the rotating action of the inverted umbrella aerator, the liquid in the tank diffuses to the wall until it reaches the wall and the liquid moves in two parts. Part of the liquid moves along the free surface to the impeller under wall resistance, which forms convection with the liquid diffused to the wall, and forms a clear circulation vortex at free surface (Vortex A). At the same time, circulation vortex also appears in the liquid area outside the impeller (Vortex B) under the influence of Vortex A. The main reason is that the liquid has begun to circulate longitudinally and renew the liquid level before it reaches the wall due to the impact of reverse moving liquid and the lifting capacity of inverted umbrella aerator. The other part of the liquid flows along the wall to the bottom of the tank. Then it flows up to the free surface through the impeller to complete the renewal of the liquid with the lifting capacity of the inverted umbrella aerator. In this process, circumfluence vortices (Vortex C) appears in the middle section.

In addition, a gas-liquid two-phase interfacial area is generated under the rotating action of the inverted umbrella aerator, which is the central area of oxygen mass transfer. The larger the gas-liquid interfacial area is, the higher the oxygen mass transfer efficiency is. It can be seen from the figure that different multiphase models will affect the internal flow. In the Eulerian model, the range of the main longitudinal vortex (Vortex C) is smaller than Mixture model, which results in a lower mixing efficiency of oxygen than Mixture model.

3.3. Analysis of mass transfer coefficient
The oxygen mass transfer coefficient \(k_{La}\) is the characteristic of oxygen mass transfer of the inverted umbrella aerator under certain conditions. It is the mass of oxygen transferred from gas phase to liquid phase in unit volume in unit time. The mass transfer of oxygen plays a decisive role in the biochemical reaction in the aeration tank, and it is necessary to separate \(k_{La}\) into two parameters: liquid-phase mass transfer coefficient \(k_L\) and interfacial area \(a\). The microscopic phenomena of gas-liquid two-phase flow in the aeration tank driven by the inverted umbrella aerator are explained from the two aspects \((k_L\) and \(a\)) respectively.

Mass transfer coefficient in different multiphase models are simulated, and the specific data is shown in Table 1. As can be seen from the table, compared with the Mixture model, the error of the oxygen
mass transfer coefficient of the Eulerian model is smaller. The main reason is that the vortex of the Eulerian model caused by centrifugal force is closer to the experiment [10], which makes the interfacial area smaller than the Mixture model.

| Table 1. Comparison of mass transfer coefficient in different multiphase models |
|---------------------------------|-----------------|-----------------|-----------------|-----------------|
| t=9s   | Interfacial area/m$^2$ | Liquid-phase mass transfer coefficient/m$\cdot$s$^{-1}$ | Oxygen mass transfer coefficient/s$^{-1}$ | $k_{la_exp}$/s$^{-1}$ |
| Eulerian model          | 8.2             | 0.00028         | 2.29×10$^{-3}$ | 2.1×10$^{-3}$ |
| Mixture model            | 10.5            | 0.00027         | 2.83×10$^{-3}$ |

In conclusion, the Eulerian model can more accurately describe the flow and mass transfer in the aeration tank.

4. Conclusion
In this paper, Fluent 15.0 is employed to simulate the internal flow of the aeration tank, and the free surface, flow field and mass transfer coefficient of the aeration tank under different multiphase models (Eulerian model and Mixture model) are compared. The conclusion is that the Eulerian model can more accurately describe the flow and mass transfer in the aeration tank.

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