Simulation on flow field and gas hold-up of a pilot-scale oxidation ditch by using liquid-gas CFD model
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ABSTRACT
A liquid–gas two-phase computational fluid dynamics (CFD) model was developed to simulate flow field and gas hold-up in a pilot-scale oxidation ditch (OD). The volume of fluid (VOF) model and the mass flow inlet boundary condition for gas injection were introduced in this model. The simulated values of the flow velocities and the gas hold-up were verified by experimental measurements in the pilot-scale OD. The results showed that the gas hold-up at test-site 3, immediately downstream of the surface aerator, was the highest among all three test-sites. Most of the gas existed in the upper portion of the ditch and was close to the inner side of the channel. Based on the liquid–gas two-phase CFD model, three operating conditions with different setting height ratios of the submerged impellers were simulated. The simulated results suggested that the setting heights of the submerged impellers have significant impacts on the flow velocity distribution. Lowering the setting height could increase the flow velocity in the pilot-scale OD. An optimal setting height ratio of 0.273 was proposed, which would be beneficial for minimizing sludge sedimentation, especially near the inner side of the curve bend.

Key words | computational fluid dynamics, gas hold-up, hydrodynamic, mathematical modelling, oxidation ditch, two-phase flow

NOMENCLATURE
\[ \vec{F} \] body force, N
\[ \vec{g} \] gravity vector, m/s²
\[ H \] vertical distance between two measuring points, m
\[ \Delta h \] liquid level difference of the U-type pressure gauge, m
\[ m_{qp} \] mass transfer from phase q to phase p
\[ m_{pq} \] mass transfer from phase p to phase q
\[ p \] pressure, Pascal
\[ \Delta p \] differential pressure, Pascal
\[ S_{q,t} \] mass source of the q\textsuperscript{th} phase, kg/(m\textsuperscript{3}·s)
\[ t \] time, s
\[ \vec{v} \] velocity, m/s
\[ \vec{v}_q \] velocity of the q\textsuperscript{th} phase, m/s

GREEK LETTERS
\[ \alpha_q \] volume fraction of the q\textsuperscript{th} phase
\[ \varepsilon_g \] gas hold-up
\[ \mu \] viscosity, kg/(m·s)
\[ \rho \] density, kg/m\textsuperscript{3}
\[ \rho_q \] density of the q\textsuperscript{th} phase, kg/m\textsuperscript{3}
\[ \rho_L \] density of liquid, kg/m\textsuperscript{3}
\[ \rho_G \] density of gas, kg/m\textsuperscript{3}
ABBREVIATIONS

CFD  Computational fluid dynamics  
COD  Chemical oxygen demand  
DO   Dissolved oxygen  
OD   Oxidation ditch  
WWTP Wastewater treatment plant

INTRODUCTION

With rapid economic development and accelerated urbanization, the number of wastewater treatment plants (WWTPs) has been dramatically increasing in China, e.g. it increased from 1,040 in 2006 to 6,031 in 2014, according to the reports of Ministry of Environmental Protection of China (2006–2014). Since oxidation ditch (OD) has advantages of low operation maintenance requirements and costs, less susceptibility to shock loading or hydraulic surge and less sludge production (Stamou 1994; US EPA 2000), it becomes the most commonly used wastewater treatment process in China (Xie et al. 2014). Hydrodynamic characteristics are critical to the operation of ODs, and have been widely investigated recently (Pougatch et al. 2007; Fayolle et al. 2010). However, the measurement of hydrodynamic characteristics is expensive and inconvenient to be conducted using experimental analysis (Stamou 1995). On the other hand, computational fluid dynamics (CFD) is a powerful tool for the simulation of fluid flow and heat transfer (Achouri et al. 2014; Karpinska & Bridgeman 2017). It has been widely utilized in environmental engineering research and applications, including those on ODs (Brannock et al. 2010; Lakghomi et al. 2012; Karpinska & Bridgeman 2016, 2017). Fluid flow, as well as interactions among liquid, gas and solid phases, are the primary areas in OD simulation using the CFD model (Stamou 2008; Liu et al. 2014; Wei et al. 2015; Sánchez et al. 2018). Fayolle et al. (2007) used an Euler-Euler two-fluid model to predict flow and oxygen transfer characteristics in four different aeration tanks equipped with fine bubble diffusers. The model reproduced experimental results well in terms of axial liquid velocities and local gas hold-up. Lei & Ni (2014) used a three-dimensional (3D) three-phase fluid model, coupled with species transport and biological process models, to simulate flow field, dissolved oxygen (DO), sludge sedimentation, and variations of COD and nitrogen in a pilot-scale OD with gas distributors at the bottom of channels. The validation results were in agreement with the laboratory data. All the above-mentioned ODs or aeration tanks have aerating apparatus such as gas distributors or air diffusers at the bottom, not on the surface. Littleton et al. (2007) used a CFD model to simulate the velocity and oxygen-distribution gradients in a full-scale Orbal OD, and the simulated results were found to be comparable with the measured data. Although the surface aerator was used in their study, only oxygen source and sink parameters were introduced in the model due to complexity of the two-phase model. Liu et al. (2014) and Wei et al. (2015) used a volume of fluid (VOF) two-phase model to describe flow in a full-scale OD with aeration impellers. The optimal impeller radius and the submergence depth of aeration impellers were studied by using the simulated results of the flow field. However, the simulated results were not validated by experimental data and the simulated results of gas hold-up were not discussed in the paper. Wei et al. (2016) used a two-phase model, based on the large eddy simulation with the Smagorinsky model, to simulate hydraulic characteristics and average volume fractions of water in a pilot-scale OD with surface aerators. Comparisons between the simulated velocities and the experimental ones showed good agreement, but the average volume fractions of water were not validated by experimental data. In our previous studies, the flow field and the sludge concentration of an OD with surface aerators and submerged impellers were simulated well by using a liquid–solid two-phase model, and an optimal operation state was proposed to prevent sludge deposition (Xie et al. 2014). However, the gas distribution which was mainly influenced by surface aerators has not been studied. The surface aerators not only participate in the process of aeration but also in the driving of the flow. Meanwhile, the aeration process and the flow field interact with each other. So aeration process with surface aerators is more complicated than aerators with air diffusers. The simulation of flow field and gas hold-up for ODs with surface aerators by CFD model has seldom been studied and validated. In addition, not only the aqueous phase affects the flow, other phases (gas phase and solid phase) influence the flow field as well (Lei & Ni 2014). The interaction between the liquid phase and the gas phase for ODs with surface aerators has seldom been discussed.

The objectives of this paper were to study the flow field and the gas hold-up of a pilot-scale OD with a surface aerator and submerged impellers by using a two-phase liquid–gas CFD model. The VOF model and the mass flow inlet boundary condition for gas injection were introduced in this model.
to simulate the gas hold-up. The optimal setting height of the submerged impeller and its relationship with the gas hold-up were investigated. This study provides a practical platform for the simulation of DO and gas hold-up by using the liquid–gas two-phase model with oxygen transfer terms to assist both of the design and operation optimization of ODs.

**METHODS**

**Description of the pilot-scale OD**

The studied OD is a Carrousel 2000 OD with a total working volume of 0.750 m³. This pilot-scale bioreactor is a four-channel circular ditch, with a water depth of 0.550 m. The photo of the experimental set-up is shown in Figure 1(a), and the schematic diagram of the OD is shown in Figure 1(b). The pilot-scale OD was fabricated from Plexiglas. The straight portion of each channel is 1.000 m in length and 0.200 m in width. The radius of the outer semi-circle is 0.410 m and that of the inner semi-circle is 0.200 m. The thickness of the internal wall is 0.010 m. In order to study the characteristics of surface aerators in detail, only one set of surface aerator and five sets of submerged impellers are installed in this bioreactor. The drive axle of the horizontally running surface aerator is parallel to the water surface as shown in Figure S1 (available with the online version of this paper). The surface aerator is positioned across the fourth channel of the tank, as shown in Figure 1(b). The two submerged impellers of QT1 and QT2 are in the anoxic zone, while QT3, QT4 and QT5 are in the aerobic zone, as shown in Figure 1(b). The rotational speed of the surface aerator and the submerged impellers are 3.14 and 6.28 rad/s, respectively. Three test-sites (1 to 3) are selected for flow velocity and gas hold-up characterization (Figure 1(b)). Test-site 1 is far away from the surface aerator and the other two test-sites are upstream and downstream of the surface aerator, respectively. The flow velocities and the gas hold-up of these three test-sites would be representatives of the OD.

**Mathematical modelling**

A 3D liquid–gas phase CFD model was employed to predict the flow field and gas hold-up. The CFD model was developed by using the 13.0 version of a commercial CFD code FLUENT (ANSYS, Inc., Pennsylvania, USA). The mass and momentum conservation equations were solved by the software using the Navier-Stokes equations (Littleton et al. 2007). Furthermore, the simulation of ODs or aeration tanks with gas distributors or air diffusers at the bottom, like the bubble column reactors, has been extensively investigated with the Euler-Euler approach (Fayolle et al. 2007). The Euler-Euler model could be applied to simulate bubbly flows, but it is time-consuming. The VOF model, which could simulate two or more fluids and track the volume fraction of each fluid throughout the domain, has been used for surface aeration simulation (Liu et al. 2014; Wei et al. 2015). Thus, it was adopted for the investigation on interaction between the liquid phase and the gas phase in this study. Moreover, the governing equations are the momentum equation and the volume fraction equation for the multiphase flow (Anderson 1995; Warsi 1998). The momentum equation for the VOF model could be expressed as follows:

\[
\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot [\mu (\nabla \vec{v} + \nabla \vec{v}^T)] + \rho \vec{g} + \vec{F} \tag{1}
\]

where \(t, \rho, \vec{v}, \mu, \vec{g}, \) and \(\vec{F}\) are time, density, velocity, pressure, viscosity, gravity vector, and body force, respectively.
The tracking of the interface between the two phases was accomplished by the solution of the continuity equation. For the $q^{th}$ phase, the equation of volume fraction has the following form:

$$\frac{1}{\rho_q} \frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q) = S_{nq} + \sum_{p=1}^{2} (m_{pq} - m_{qp})$$

(2)

where $m_{qp}$ is the mass transfer from phase $q$ to phase $p$; and $m_{pq}$ is the mass transfer from phase $p$ to phase $q$. $\rho_q$, $\alpha_q$, $\vec{v}_q$, and $S_{nq}$ are density, volume fraction, velocity, and mass source of the $q^{th}$ phase, respectively.

The primary-phase volume fraction was computed based on the following constraint:

$$\sum_{q=1}^{2} \alpha_q = 1$$

(3)

**Geometry and grid generation**

The 3D model of the pilot-scale OD with surface aerator and submerged impellers was built with the pre-processor Gambit (Figure S2, available online). The total computed volume of the OD is 0.730 m$^3$. The 3D grid meshes were also created by using the Gambit. All meshes were unstructured and composed of tetrahedrons. The grids near the surface aerator and submerged impellers were refined because of the complex structure. Furthermore, different grid sizes were tested: the different numbers of tetrahedral cells were 2,003,409; 3,255,222; or 3,509,905. The simulated velocities of different grids were compared with each other at Test-site 3, which is 0.300 m in height. The grid independency was verified (Supplementary material Figure S3, available online). Finally, the grid with 3,255,222 cells was chosen as the best compromise between precision and computational effort.

**Boundary conditions**

The boundary conditions are related to the surface aerator, the submerged impellers, and the gas injection. Water and air were used for the simulation of liquid and gas, respectively. Because the liquid phase inlet and outlet had insignificant effects on the flow field of an OD (Stamou 1993), the effects of inlet and outlet were not considered in the model based on the assumption of stable fluid. For an OD, surface aerators and submerged impellers are the most significant devices as they are the main sources of power input. Moreover, structures of the surface aerators and the submerged impellers are too complex to decrease computational costs with a personal computer. Consequently, a moving wall model was adopted for the water surface simulation (Yang et al. 2010; 2011). In this study, there are one set of surface aerators in the ditch, and nine rotation discs along the drive axle for the surface aerator, as shown in Figure S4 (available online). The part-cylindrical moving zone is 0.100 m in width and 0.100 m in radius. The complete moving zone was formed by the sidewalls, the outer wall, and the surface. Each rotation disc served as a moving wall, which was the main source of the drag force. The fluid in each moving zone got the velocity and momentum from the moving walls firstly, and then the velocity and momentum were passed to the rest of the fluid in the OD. The slip wall boundary condition was assigned at the location of the surface aerator, and the rigid-lid assumption was introduced. The moving wall motion was used for the rotation disc, and the rotational speed was set as 31.4 rad/s. The roughness height and the roughness constant of the moving wall were set as 0.02 m and 1, respectively. In addition, a fan model was adopted for simulation of the submerged impellers (Yang et al. 2011). It was assumed that a submerged impeller was an infinitely thin circle, and the pressure difference across the impeller was estimated by the area of the disc, density of the fluid and the average flow velocity in the ditch. A circle with a diameter of 0.200 m was used for each impeller. A VOF two-phase model was used in ANSYS FLUENT (13.0). The gas injection depended on the gas inlet in the region of the surface aerator. The mass-flow-inlet boundary condition was introduced for the gas inlet, depending on the rate of aeration. The gas outlet was set on the top surface except the area occupied by the surface aerator. Therefore, the pressure-outlet was selected for this outlet boundary condition under the downward gravity, and it was set as the atmospheric pressure as well (Lakghomi et al. 2012; 2014).

**Different run models at different setting heights of the submerged impellers**

The setting height of a submerged impeller, measured from the bottom of the ditch, has impacts on the flow field, especially on the average flow velocity near the bottom of OD. Therefore, run models with different setting heights of the submerged impellers were constructed to optimize the flow field as well as develop relationships between the setting height and the gas hold-up. The setting height of a submerged impeller herein referred to the distance between...
the horizontal rotating axis of the submerged impeller and the bottom. The ratio of the setting height of a submerged impeller to the entire water depth of the ditch was defined as the setting height ratio of the submerged impeller in this study. Three setting height ratios of 2.273, 0.364, and 0.545 were used in this study, as presented in Table 1. The lowest setting height of the submerged impellers was 0.150 m due to the limited space between the submerged impellers and the bottom of the ditch.

EXPERIMENTAL MEASUREMENTS IN THE PILOT-SCALE OXIDATION DITCH

Measurements of the flow velocity

The working water depth in the OD is 0.550 m. The locations of the surface aerator and five submerged impellers (QT1, QT2, QT3, QT4 and QT5) are shown in Figure 1(b). The radii of the surface aerator and the submerged impellers are 0.100 and 0.050 m, respectively. The submergence depth of the surface aerator with helical discs is 0.080 m under the water surface, and the aerator’s rotational speed is 3.14 rad/s. The setting height of the horizontal rotating axis of the submerged impellers with an S-shaped blade is 0.300 m above the bottom of this pilot-scale OD. The actual liquid velocity profiles were measured at three different locations (test-sites 1, 2, and 3) as shown in Figure 1(b) by using an acoustic Doppler velocimeter (Flow Tracker; measurement range: 0.001–4.5 m/s; SonTek/YSI Inc., San Diego, CA, USA) with a 3-D probe. The measurements were taken at 12 locations in a vertical section of each test-site. There are four points in each layer of three water depths (Top, Middle, and Down). The details of the sampling locations are shown in Figure 2.

Measurements of the gas hold-up

The differential pressure method was used to measure the gas hold-up (Kara et al. 1982; Tang & Heindel 2005b). A U-type pressure gauge was used to measure the differential pressure between two locations at different heights to calculate the difference of their average gas hold-up. According to the Bernoulli equation,

$$\varepsilon_G = \frac{\Delta p}{\rho_L g H}$$

where $\varepsilon_G$, $\rho_L$, $\Delta p$, $g$, and $H$ are the gas hold-up, density of liquid, differential pressure, gravity, and the vertical distance between the two measuring points, respectively.

Because a U-type pressure gauge was used for the measurement of differential pressures, where $\Delta p = (\rho_L - \rho_G)g\Delta h$ is the differential pressure between the two measuring points. Equation (4) could be transformed into:

$$\varepsilon_G = \frac{(\rho_L - \rho_G)g}{\rho_L g} \frac{\Delta h}{H}$$

where $\rho_G$ and $\Delta h$ are the density of gas and the liquid level difference of the U-type pressure gauge, respectively. Owing to $\rho_L \gg \rho_G$, Equation (5) could be transformed into Equation (6):

$$\varepsilon_G = \frac{\Delta h}{H}$$
Consequently, the average gas hold-up could be calculated by measuring the liquid level difference of the U-type pressure gauge \((\Delta h)\) and the vertical distance between the two measuring points \((H)\). Three sections (test-sites 1 to 3) were selected for the measurements of the gas hold-up.

**RESULTS AND DISCUSSION**

**Comparison of the simulated and the measured flow velocities**

Comparisons of the simulated and the measured flow velocities are shown in Figure 3. Because the operational conditions of the submerged impellers in the actual pilot-scale OD are similar to those in Run model H3 (Table 1), the simulated velocities for H3 were compared with the measured data. The velocity profiles in the liquid-gas model are in a good agreement with the measured data, especially in the x-direction, which is the main flow direction in the channel of the OD. Moreover, the velocities in the x-direction are the highest among all three directions. Consequently, the velocities in the x-direction were chosen for further analysis. It can be seen from Figure 3(a) that the velocities at test-site 1 stay relatively constant when the distance from the internal wall increases. However, the velocities in the x-direction at test-site 2 near the external wall are higher than those near the internal wall, as shown in Figure 3(b). This may because the velocities at test-site 2 are influenced by the surface aerator and the curve bend. Due to the inertia and the centrifugal forces, the fluid is dragged towards the external wall. As shown in Figure 3(c), velocities near the internal wall at the big circular channel are relatively low at all of the Top, Middle and Down layers. Consequently, it may enhance sludge sedimentation and reduce the effective treated volume. To prevent the sludge sedimentation, some optimization patterns would be needed. The optimization of flow field is discussed later.

![Figure 3](https://iwaponline.com/wst/article-pdf/78/9/1956/513835/wst078091956.pdf)
The contours of the velocity profiles at the Top layer (height of 0.450 m above the bottom), the Middle layer (height of 0.250 m above the bottom) and the Down layer (height of 0.100 m above the bottom) of the OD calculated by the two-phase model are shown in Figure 4. The vectors of velocity distribution of horizontal section of the OD are shown in Figure S5 (available with the online version of this paper). In the Top layer near the water surface, the velocities in the zone of the surface aerator at the fourth channel are significantly higher than those in other areas, as shown in Figure 4(a) and Figure S5(a). However, in the Down layer near the bottom of OD, the velocities at the third and fourth channels are much lower than those at the first and second channels, as shown in Figure 4(c) and Figure S5(c). Therefore, the optimization of the flow field is necessary to increase the average velocities at the third and fourth channels near the bottom of OD so as to minimize sludge settling in these zones.

Generally, the velocity distribution characterization in the whole tank is summarized as the following.

- In the Top layer near the water surface, the velocities in the zone of the surface aerator at the fourth channel are significantly higher than those in other areas, as shown in Figure 4(a) and Figure S5(a).
- The velocities at the curve bend are higher than those of the straight channel since the fluid was dragged towards the external wall at the curve bend because of the centrifugal forces and inertia force.
- The simulated flow velocity profiles are in good agreement with the experimental measurement as shown in Figure 3. The velocity distribution have the same law compared with our previous studies (Yang et al. 2010; 2011; Xie et al. 2014).

Comparison of the simulated results and the measured data in gas hold-up

Comparisons between the simulated average gas hold-up values by using the liquid-gas two-phase model and the measured data are shown in Figure 5. The measured values of the average gas hold-up at test-sites 1 and 2 are zero, while the simulated values at these two sections are relatively small. The simulated value at average gas hold-up at test-site 3 is maximum, owing to its short distance to the surface aerator. Moreover, the measured value (0.020) and the simulated average value (0.0204) of the gas hold-up are very similar to that at test-site 3.

The gas hold-up contour profiles of the three vertical sections (test-sites 1, 2, and 3) simulated by the two-phase model are shown in Figure 6(c). It is noted that the gas hold-up at the test-site 3 is the largest one among all three sections. Most of the gas is present in the upper portion of the ditch and close to the inner side of the channel. This might be induced by the liquid movement of the channel and the working zone of the surface aerator.

Optimization of the setting height of the submerged impellers

Three setting height ratios of submerged impellers were used for the optimization of the flow field and for the exploration...
of the relationships between the setting height of the submerged impeller and the gas hold-up. Average flow velocities at the Top, Middle, and Down layers under three run models are shown in Figure 7. The average flow velocity of run model H1 is faster than those of the other two run models at each layer. This might be induced by the decrease of internal flow resistance under run model H1 since the setting height (0.150 m) of the submerged impellers is the closest to the bottom of the OD. The gas hold-up under all three conditions at all three locations are identical, as shown in Figure 6. As a result, the setting height of the submerged impeller has insignificant, if any, impact on the gas hold-up distribution in the OD.

Figure 8 shows the flow velocity contour profiles of a horizontal section at the Down layer of the OD under three run models with the submerged impellers at the different setting heights. As can be seen, the flow velocity of the run model H1 is faster than those of the other two run models at the third and the fourth channels in Figure 8, as the same situation in the anoxic zone (Figure 1(b)). Comparisons of simulated velocities on a transversal line at the Down layer at the height of 0.100 m above the bottom in test-site 3 under three run models are shown in Figure 8(d). The run models with setting height ratios smaller than that of run model H1 were not tested in this study, because the space between the submerged impellers and the bottom of ditch is too small to set up submerged impellers. It is obvious that the flow velocities under run model H1 are higher than those two run models, especially near the inner side of the curve bend of OD channels. Higher velocities could be beneficial for minimizing sludge sedimentation. All the flow field results suggest that run model H1 with a setting height ratio of 0.273 for submerged impellers is the optimal one among all three run models.

In this study, the optimal setting height ratio has been investigated to minimize sludge sedimentation by using a
flow field and the gas hold-up distribution in a pilot-scale OD. The conclusions from this study are as follows:

(1) The simulated flow velocity profiles using the liquid–gas model are in good agreement with the experimental measurement. Approaches for modelling the gas hold-up distribution in ODs with surface aerators were presented by the VOF model.

(2) The simulated average gas hold-up values agree reasonably well with the measured data. Most of the gas is presented in the upper portion of the ditch and close to the inner side of the channel.

(3) The simulated results suggest that the setting heights of the submerged impellers have significant impacts on the flow velocity distribution in the OD, and lower setting heights could significantly increase the flow velocities in the third and the fourth channels in the pilot-scale OD. An optimal setting height ratio of 0.273 would be beneficial for minimizing sludge sedimentation, especially near the inner side of the curve bend.

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