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Stochastic evolutionary-based optimization for rapid diagnosis and energy-saving in pilot- and full-scale Carrousel oxidation ditches

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Real-time simulation and stochastic evolutionary-based optimization in pilot-scale and full-scale Carrousel oxidation ditches

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Abstract

Accurate modeling of Carrousel oxidation ditches (ODs) is of great importance in optimizing their operating conditions to reduce energy consumption, ensure qualified effluent, and achieve even deposits of sludge. This paper presents a hybrid model composed of a three-dimensional (3D) three-phase computational fluid dynamics (CFD) model, a multi-site artificial neural network (ANN) model with back propagation, and an accelerating genetic algorithm (AGA) model to achieve real-time simulation and synchronized system optimization in the Carrousel OD. The 3D three-phase CFD model provided comprehensive, precise simulation of OD systems by treating activated sludge as a pseudo-solid phase and considering water-sludge-gas interactions. By coupling the 3D three-phase CFD model with a multi-site ANN model, the resulting hybrid model provided computationally fast, accurate predictions of liquid flow field, sludge sedimentation, dissolved oxygen distribution, and water quality parameters in the OD. An evolution theory-based AGA model, which incorporated the ANN model to compute fitness values, was used to perform global optimization of the operating conditions in the OD, and so identify optimum conditions that reduced energy consumption, prevented uneven deposits of sludge, and satisfied effluent standards. The proposed hybrid model was successfully applied to pilot-scale and full-scale ODs. The results showed the potential of the hybrid model to realize rapid prediction of phase motions and interactions in the OD, and to achieve real-time OD process optimization.

Keywords: three-dimensional three-phase; artificial neural network; accelerating

genetic algorithm; rapid feedback; global optimization; oxidation ditch

Highlights:

- Proposed CFD, ANN and AGA hybrid model applied to pilot- and full-scale ODs.
- Hybrid model precisely simulated liquid-gas-solid motions and interactions.
- Computational speed of hybrid model 86,400 times faster than CFD counterpart.
- Optimized energy consumption, effluent quality, and even sludge deposition.
- Hybrid model reduced energy consumption by 31% in full-scale OD.

1. Introduction

As modified activated sludge treatment processes [1], oxidation ditches (ODs) are continuous loop reactors containing multi-channels in which surface aerators and rotating impellers provide circulation, mixing, and uneven distribution of dissolved oxygen (DO) to remove contaminants [2]. ODs are utilized worldwide because of their reliable removal efficiency, convenient management, and low sludge production [3]. However, there remain many challenges [4]; namely, a typical OD occupies a large area of land, the deposition of sludge is usually uneven thereby reducing the effective area of the OD, and the OD equipment often consumes a large amount of energy to ensure effluent quality. Therefore, reliable design and successful operation of ODs are necessary to meet prescribed effluent quality standards, achieve even deposition of sludge, and minimize operating costs.

Accurate understanding of the physical-chemical-biological processes in ODs is essential when determining equipment upgrades and optimized operating conditions to meet environmental and economic criteria. A growing number of mathematical models have been proposed to simulate multi-phase behavior and simultaneous nitrification and denitrification (SND) in OD systems. Notably, activated sludge models (ASMs) proposed by the International Water Association (IWA) [5] are widely used to predict effluent water quality and biomass production of wastewater treatment plants. Subsequently, many models have been built to reflect the hydraulic, chemical, and biological processes in ODs by coupling a computational fluid dynamics (CFD) model with an ASM [6-7]. More recently, a three-dimensional (3D) three-phase CFD

model has been developed at Peking University, which produced reasonable simulations of liquid flow velocity and concentrations of DO, COD and nutrients that matched experimental data [8]. This model represented activated sludge flocs as a pseudo-solid phase in order to characterize sludge transportation and gas/liquid-solid interactions within the OD. However, the numerical model was limited by its complexity (involving a large number of modules and input parameters) and high computational cost. In a recent study [8], more than 20 parameters were needed to model floc features and biological processes, and approximately 24 hours were required to simulate one operational mode. Hence, it was difficult to achieve real-time simulation and respond to sudden changes.

For fast prediction of the behavior of ODs, a multi-layer artificial neural network (ANN) with back propagation (BP) algorithm was introduced in combination with the CFD model because of their effectiveness at solving non-linear problems [9, 10] and handling large, complicated systems while requiring relatively few inputs [11,12]. A substantial body of literature is available on the use of ANN in modeling wastewater treatment processes. Researchers have applied ANN to estimate wastewater process parameters [13], to develop control schemes [14], and to predict the wastewater treatment performance of wastewater treatment plants (WWTPs) at laboratory and full scale (including conventional activated processes [15], anaerobic-anoxic-oxic systems [16], sequencing batch reactors [17] and submerged membrane bioreactors [18]). However, few studies have simulated wastewater treatment performance in ODs using ANN-based real-time prediction. This may be because sufficient, comprehensive data

are required to train the model, and these data cannot be obtained easily by common experimental measurements or by 1D/2D mathematical models considering only one or two phases.

Since WWTPs are complex non-linear systems [19], their control and optimization are difficult to achieve. In practice, implementation of these tasks relies heavily on operator experience and empirical guidelines [20], both of which tend to be insufficiently detailed and subject to considerable uncertainty. As a result, model-based control approaches have been proposed for different objectives such as nitrate control [21] and DO control [22]. However, few control methods have considered sludge settling. In an OD system, the uneven deposition of sludge reduces the effective area [23] and leads to malodorous septic sludge occurring in dead zones [24]. It is therefore necessary to evaluate sludge settling in order to achieve acceptable effluent standard at low operational cost.

In this paper, a hybrid model incorporating CFD, ANN and an accelerating genetic algorithm (AGA) was proposed to provide real-time feedback and to perform global optimization based on comprehensive simulation of the coupled physical-chemical-biological processes in the OD. Fig. 1 illustrates the model framework. First, a 3D three-phase CFD model, validated by experimental results, was employed as a data engine to provide adequate information by which to train the ANN model. Next, a multi-site ANN model with BP algorithm was used to extract the outputs of the CFD model and to achieve real-time simulation at arbitrary positions along the ditch. Finally, an AGA model based on stochastic evolutionary theory was

combined with the ANN model to determine the optimum operation mode that simultaneously met effluent quality, evenness of sludge deposition, and operating cost criteria. The paper describes the successful application of the CFD - ANN - AGA hybrid model to pilot-scale and full-scale Carrousel ODs. The hybrid model is demonstrated to be a useful tool by which to gain insight into the characteristics of ODs and to optimize their operational conditions.

2. Methodology

2.1 Experimental set up and operation of the pilot-scale oxidation ditch

A pilot-scale Carrousel OD was fabricated with plexiglass with a total working volume of 1.40 m^3. The pilot OD consisted of four straight channels (1.15 m long, 0.35 m wide and 0.50 m still water depth; Fig. 2), the ends of each were joined by semi-circular connecting channels, one of radius 0.35 m, the other of radius 0.70 m. Two surface impellers (Impeller 1 and Impeller 2) and four submerged stirrers (Stirrer 1, Stirrer 2, Stirrer 3 and Stirrer 4) were inserted in the semi-circular channels to drive the circulating flow in the reactor; the flow direction is indicated by arrows in Fig. 2. Table 1 lists the rotational speeds and angular directions of the impellers and stirrers used in the CFD model (calibration: Case II; validation: Case IV) and ANN model (training and validation: Case I, II and III; test: Case IV). A series of 1 m long gas distributors controlled by the rotameter were located at the bottom of the second and third channels to supply air in the ditch, and hence form aerobic zones. Synthetic wastewater was stored in a tank of 1.8 m^3 total volume. The wastewater was composed of 1 m^3 tap water, 250 g sugar, 107.2 g NH_4Cl, 61.3 g $Na_3PO_4 \bullet 12H_2O$, 10 g

$CaCl_2$, 3 g $FeSO_4 \bullet 7H_2O$, 500 g $NaHCO_3$, 12 g $MgSO_4$, and 50 mL trace element solution; this provided COD and NH_4^+-N concentrations of 250 mg/L and 50 mg/L, respectively. The synthetic wastewater was pumped into the OD at a flow rate of 0.1 m^3/h to guarantee a hydraulic retention time of 14 h; and 60 L of mixed liquor was discharged daily from the outlet of the ditch to maintain the sludge retention time of 25 d. A settling tank of volume 0.15 m^3 was used to separate the activated sludge which was recycled to the ditch at a 100% sludge recycle ratio. During experiments, the temperature was maintained at 20-24 °C, and the pH was approximately 7.8. Twice weekly, the liquid velocity was monitored at Sections 1-1, 2-2 and 3-3, and the mixed liquor suspended solid (MLSS) was measured 0.1 m above the bed at locations M1, M2, M3, M4, M5, and M6. DO concentrations were recorded twice daily, 0.25 m above the bed at locations W1, W2, W3, outlet, W4, and W5. Water samples were also collected twice daily 0.25 m above the bed at W1, W2, W3, outlet, W4, and W5, for water quality analysis in order to monitor the concentrations of ammonia nitrogen, nitrate, total nitrogen (TN), and COD.

2.2 Three-dimensional three-phase CFD model

The 3D multi-phase hydrodynamics model used to describe the movement of wastewater, activated sludge and gas in the OD is based on the following continuity and momentum conservation equations:

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

and

$$\frac{\partial}{\partial t}(\alpha_q \rho_q \vec{v}_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q \vec{v}_q) = -\alpha_q \nabla p + \nabla \cdot \tau_q + \alpha_q \rho_q g + \sum_{p=1} (R_{pq} + m_{pq} \vec{v}_{pq} - m_{qp} \vec{v}_{qp})$$

$$+(\vec{F}_q + \vec{F}_{lift,q} + \vec{F}_{vm,q})$$

(2)

where α_q is the volume fraction of the phase q, such that $\sum_{q=1}^{3} \alpha_q = 1$, ρ_q is the density of phase q, $\vec{v}_q$ is the velocity vector of phase q, S_q is the source term relating to the phase q, m_{pq} is the mass transfer from phase p to q, and the subscripts q=1, 2 and 3 denote wastewater, gas and active sludge, respectively. p is the pressure shared by all phases, $\vec{g}$ is the vector of gravitational acceleration, $\vec{R}_{pq}$ is the interaction force vector between phases, $\vec{v}_{pq}$ is the interphase velocity vector, $m_{pq}\vec{v}_{pq} - m_{qp}\vec{v}_{qp}$ denotes the momentum change due to mass transfer between the phase p and q, $\vec{F}_q$ is the external body force, $\vec{F}_{lift,q}$ is the lift force, $\vec{F}_{vm,q}$ is the virtual mass force and τ_q is the q phase stress-strain tensor.

The advection-dispersion species transport equation was used to describe the growth, decay, and transformation of activated biomass (e.g. heterotrophs and autotrophs) and contaminants (e.g., soluble COD, ammonia nitrogen and nitrate) in the OD,

$$\frac{\partial}{\partial t}(\alpha_q \rho_q Y_{q,i}) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q Y_{q,i}) = -\nabla \cdot (\alpha_q \vec{J}_{q,i}) + m_{q,i} + R_{q,i} \quad (3)$$

where $Y_{q,i}$ is the mass fraction of species i in the phase q, $m_{q,i}$ is the mass transfer of the species i from the other phases to phase q, $\vec{J}_{q,i}$ is the diffusion flux of species i in phase q, and $R_{q,i}$ is the source term representing the production rate of species i for biochemical reactions (which is obtained from the modified ASM1). The rate of

oxygen mass transfer from the gas to liquid phase is determined from:

$$\rho_3 = K_L a_L (\alpha S_{O(S)} - S_O) \quad (4)$$

in which $K_L a_L$ is the mass transfer coefficient, calculated as the sum of surface and bottom aeration. $S_{O(S)}$ is the saturated DO concentration in clean water, S_O is the oxygen concentration in the liquid phase, and α is a coefficient.

Using Gambit, an unstructured mesh containing 161,987 tetrahedra was created representing the OD geometry, and refined in the aerator and rotating zones. The equations were solved at steady state using the finite volume method software Fluent 6.3. Open boundary conditions were set at the inlet and outlet of the ditch. At the inlet, prescribed values were input for wastewater flow velocity, activated sludge concentration, and concentrations of soluble constituents. No-slip boundary conditions were applied at all fixed, solid walls. The rotating equipment was simulated by either a fan model or a moving wall model. The water surface was treated as a rigid-lip slip wall, in order to complete the degasification process. Pressure was set to be atmospheric at the effluent outlet.

2.3 Artificial neural network model

ANNs are parallel models inspired by the biological neural networks of the human brain [9] that contain a large number of interconnected processing neurons [10]. The calculation procedure can be separated into two stages: a forward phase during which information from input nodes is propagated forward to compute information at output nodes, and a backward stage during which connection weights are modified based on the differences between computed and observed information

signals at the output nodes.

To provide sufficient data to train and validate the ANN model, 364 sets of operating conditions, summarized in Appendix A, were calculated using the 3D three-phase model. Following the Code for Design of Outdoor Wastewater Engineering (GB50014-2006), the total coefficient of variation of the sewage treatment capacity of a general wastewater treatment plant is taken to be approximately 2.0; thus, the calculated inflow rates were 100, 150 and 200 L/h. Given that the concentration of TN in the typical domestic wastewater varies from 25 to 75 mg/L and the ratio of carbon to nitrogen (C/N) ranges from 3 to 7 [25], the simulated concentrations of TN were set to 25, 50 and 75 mg/L, and the C/N ratios were 3, 5 and 7. For a general OD, Hartley [26] observed that the average concentration of sludge in the OD was 3.0-4.5 g/L; herein, input values of average concentration of sludge in the OD were therefore set to 3.0, 3.5, 3.9 and 4.5 g/L. The aeration rates were 1.4, 1.8, 2.2, 2.6 and 3.0 m^3/h. Reference points were located at W1, W2, W3, outlet, W4 and W5 (Fig. 2) where W1 was the starting point of the aeration zone, W2 was at the center of the aeration zone, W3 was at the end of the aeration zone, W4 and W5 were close to the start and end of the curved channel. These locations were chosen because they reflect the local hydrodynamics structures and primary water quality parameters in the aerobic and anoxic zones. Information at the six reference locations was extracted from the 3D three-phase CFD model simulations in order to train and validate the ANN model.

The constructed ANN with BP algorithm consisted of one input layer, two

hidden layers, and one output layer, as shown in Fig. 1. Grid input data comprised: inflow discharge, TN, C/N ratio, average sludge concentration, aeration rate, speed of impellers and stirrers, and the locations of the reference points (in terms of stream-wise distance along the inlet to each of the reference points). Grid output data consisted of the liquid velocity and the concentrations of ammonia nitrogen, nitrate, TN, DO, COD and MLSS, accounting for all the primary hydrodynamics and water quality parameters in the OD. The Levenberg–Marquardt algorithm (LMA) was implemented to train the network, noting the ability of LMA to achieve high generalization accuracy and fast convergence [27]. The tangent sigmoid transfer function (tansig) was applied at both hidden and output layers to avoid possible undesirable, negative estimates possibly arising at the output layer. Of the 2,184 groups of data listed in Appendix A, 70% were treated as the training set to cultivate the learning ability of the multi-site ANN model, and 30% were treated as the validation set to find the optimum structure with the best predictive ability [28]. Measurements under experimental conditions (Table 2) were treated as the test set to verify the performance of the multi-site ANN model in terms of the mean square error (MSE).

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(x_{ci} - x_{mi})^2 \tag{5}$$

and normalized standard error (OF),

$$OF = \frac{\sqrt{\frac{1}{n(n-1)}\sum_{i=1}^{n}(x_{ci} - x_{mi})^2}}{\frac{1}{n}\sum_{i=1}^{n}x_{ci}} \tag{6}$$

where x_c and x_m represent calculated and measured values, respectively, and n is the total number of data values in each set.

To determine the effects of aeration rate and rotational speeds of the impellers and stirrers on the hydrodynamics and effluent water quality while optimizing the operating conditions in the OD, the constructed multi-site ANN model was extended to conduct real-time simulations of the liquid velocity and the concentrations of MLSS and DO at multiple sites along the ditch, and to predict the concentrations of ammonia nitrogen, nitrate nitrogen, TN, and COD at the outlet. The grid inputs of the inlet condition were fixed as follows: 100L/h of inflow rate, 3.9 g/L of MLSS, 50 mg/L of NH_4^+-N and 7 of C/N. The aeration rates ranged from 1.4 to 3.0 m^3/h. The standard deviation (*Std*) of sludge was used to describe quantitatively the evenness of activated sludge in the OD, and was given by:

$$Std=\sqrt{\frac{\sum_{i=1}^{n}(MLSS_i-\overline{MLSS})^2}{n-1}}$$

(7)

where $MLSS_i$ is the sludge concentration at point i , $\overline{MLSS}$ is the average sludge concentration, and n is the number of points. Obviously, a lower *Std* represents a more uniform distribution of sludge.

2.4 Optimization model using an accelerating genetic algorithm

The genetic algorithm (GA) is a global search method used to deal with complex optimization problems based on the mechanism of intra-group chromosome information exchange and survival of the fittest in the process of biological evolution

[29]. GA utilizes simple coding techniques and algorithmic mechanisms, and has no restrictions on the specific form of the objective function and the number of optimization variables [30]. Consequently, GA has been successfully applied in many fields [11, 12, 29, 30]. However, the standard genetic algorithm has the disadvantages of premature convergence and large computational complexity, lowering both its accuracy and computational speed [31]. To overcome these shortcomings, the accelerating genetic algorithm (AGA) was developed to accelerate convergence to the optimal solution and to save computation time [32, 33]. The AGA involves the following steps (Fig. 1): determination of the initial parameters (e.g., population size, the number of smart individuals, range of variables); the encoding of variables; initialization of the parent population; calculation of the objective function and fitness value; selection; crossover; mutation; evolution; and accelerating cycles [32, 33]. During implementation, the processes of selection, crossover and mutation were parallelized, and the smart individuals were used to modify adaptively the search range. As a result, the AGA is faster computationally and has more opportunities to reach the global optimal solution than GA [33].

3. Results and discussion

3.1 Simulation of pilot-scale oxidation ditch using 3D three-phase CFD model

By representing activated sludge as a pseudo-solid phase, the 3D three-phase CFD model replicated the liquid-gas-solid interactions and sludge sedimentation in OD, and good agreement was obtained between the simulated and measured liquid velocity and activated sludge concentration, with normalized standard errors of 9.6%

and 2.8% [8]. Likewise, the normalized standard errors between the simulated and measured ammonia nitrogen, nitrate, DO and COD concentrations were 1.5%, 3.3%, 9.9% and 1.5%, respectively, indicating that the 3D three-phase CFD model satisfactorily reproduced the key multi-phase motions and interactions in the OD.

3.2 Verification of the multi-site ANN model

Table 3 presents the optimum ANN structure, after training and validation, for simulations of liquid velocity, and concentrations of MLSS, ammonia nitrogen, nitrate, DO and COD at multiple sites in the OD. Using the test set to verify further the performance of the multi-site ANN model, satisfactory agreement was achieved between measured and predicted results (Fig. 3 and Table 3). For all parameters considered, the correlation coefficients $R^2 > 0.9$; moreover, for ammonia nitrogen, nitrate, TN, DO and COD, $R^2 > 0.99$. In all cases, MSE < 0.3 (between measured and the simulated results), and the normalized standard errors of the liquid velocity, MLSS, ammonia nitrogen, nitrate, TN, DO and COD concentrations were 1.36, 0.23, 0.33, 0.32, 0.33, 1.13 and 0.04%, respectively. Therefore, the multi-site ANN model fully replicated the power of the 3D three-phase CFD model to simulate precisely the liquid-gas-solid motions in the OD. In short, the multi-site ANN model proved highly capable of predicting the local hydrodynamics, transport and deposition of activated sludge, and water quality indexes at different locations in the OD.

3.3 Improved simulation time

All simulations were performed on a workstation equipped with two Intel Xeon 2.93 GHz processors and 24 GB RAM. For the 3D three-phase model, 24 hours of

CPU time were required to reach steady state in each case considered [8]. By comparison, the multi-site ANN model trained using the 3D three-phase model required only 1 s of CPU time to calculate the same operational mode case. The trained multi-site ANN model was 86,400 times faster to run than the 3D three-phase CFD model on its own, a 99.99% total time saving.

3.4 Effect of aeration rate and rotational speed

3.4.1 Liquid velocity and activated sludge

Fig. 4 shows the stream-wise profiles of liquid flow speed and concentration of activated sludge in the OD for three modes of operation (Table 1). As the rotational speed of the impellers and stirrers increased from 40 - 50 rpm (Case I) to 115 - 180 rpm (Case III), the averaged liquid velocity in the OD increased from 0.045 m/s to 0.070 m/s at an elevation 0.1 m above the channel bed. Peak liquid velocity occurred in the third channel (between W2 and W3); the flow velocities in the first and fourth channels were generally low (Fig. 4a). Profiles of activated sludge at 0.1 m from the bed (Fig. 4b) showed that sludge tended to settle out at the ends of the first and fourth channels where the velocity was relatively low. At an aeration rate of 1.4 m^3/h, the *Std* of sludge deposition with increasing rotational speed was 0.37 (Case I), 0.23 (Case II) and 0.15 (Case III), indicating that a more uniform distribution of sludge was obtained at faster rotational speed. As the aeration rate increased to 3.0 m^3/h, the location of sludge deposition remained fairly constant, but its distribution became much more uniform with *Std* values of 0.25 (Case I), 0.20 (Case II), and 0.10 (Case III) for the same rotation mode. Hence, both increased rotational speed and increased aeration

rate accelerated the liquid velocity and enhanced the even deposition of activated sludge.

3.4.2 Water quality

At higher aeration rates and rotational speeds of the impellers and stirrers, the average concentration of DO increased significantly (Fig. 5a and 5b), especially in the third channel. On the one hand, as the aeration rate and rotational speed increased, the effluent concentrations of ammonia nitrogen (Fig. 6a) and COD (Fig. 6d) decreased asymptotically to almost zero and 17.5 mg/L respectively, owing to enhanced nitrification in the aerobic zones at the higher DO levels, thereby increasing the removal efficiency of inlet ammonia nitrogen and COD. On the other hand, increased aeration rate and rotational speed caused the effluent concentration of nitrate to rise steeply (Fig. 6b) due to progressive accumulation through active nitrification and decreased consumption by inhibited denitrification at high values of averaged DO concentration. Consequently, the effluent TN concentration, given by the sum of ammonia nitrogen and nitrate, initially declined, reached a minimum, and then increased as the aeration rate and rotational speed increased (Fig. 6c). Too low or too high an aeration rate led either to the DO concentration in aerobic zones falling below 0.5 mg/L or to the DO concentration in anoxic zones exceeding 0.5 mg/L (Figs. 5a and 5b), which would affect the SND and the removal efficiency of nitrogen. When the aeration rate was low (1.4 m^3/h), the concentration of TN was particularly sensitive to the rotational speed of stirrers and impellers, a factor which played a key role in increasing the DO concentration in the aerobic zone through surface aeration

(Fig. 5a), thereby completing SND and thus reducing the effluent concentration of TN. However, when the aeration rate was high (3.0 m^3/h), increased rotational speed caused the low DO area to shrink considerably, inhibiting the nitrification process, and hence increasing the effluent concentration of TN. It should be noted that the lowest concentration of TN did not occur at the highest aeration rate or rotational speed; in practice, it would be necessary to commence from intermediate aeration rates and rotational speeds and then control them jointly to ensure the highest effluent efficiency is achieved.

3.5 Optimization of pilot-scale oxidation ditch

According to the Discharge Standards of Pollutants for Municipal Wastewater Treatment Plant (GB 18918-2002), the effluent concentrations of COD, ammonia nitrogen, and TN must be lower than 50 mg/L, 5 mg/L and 15 mg/L, respectively, for treated effluent to reach the first-class A level. The critical velocity to ensure an even deposition of sludge was determined as 0.06 m/s (Fig. S1). Within the application ranges of the aerator, surface impeller, and submerged stirrer, the constraints are expressed as:

$$COD_{out} < 50 \text{ mg/L} \tag{8}$$

$$NH_4^+ - N_{out} < 5 \text{ mg/L} \tag{9}$$

$$TN_{out} < 15 \text{ mg/L} \tag{10}$$

$$\bar{v} > 0.06 \text{ m/s} \tag{11}$$

$$1.4 \text{ m}^3/\text{h} \le Air \le 3 \text{ m}^3/\text{h} \tag{12}$$

$$40 \text{ rpm} \le Impeller(i) \le 180 \text{ rpm} \tag{13}$$

$$40\ \text{rpm} \le Stirrer(j) \le 120\ \text{rpm} \tag{14}$$

where COD_{out}, NH_4^+ - N_{out}, and TN_{out} are the effluent concentrations of COD, ammonia nitrogen and TN, respectively; Air represents the aeration rate; $Impeller(i)$ is the rotational speed of the i-th surface impeller; and $Stirrer(j)$ is the rotational speed of the j-th submerged stirrer. The objective function could be expressed:

$$E_{\min} = \min E \tag{15}$$

where E represents energy consumption. The energy consumption of each component used in the OD was measured by a power meter socket (LINI-T UT230C); Fig. S2 presents curves of energy consumption against aeration rate, rotational speed of surface impeller, and rotation speed of submerged stirrer

Before using AGA to optimize the operating conditions in the OD, all key parameters, including the population size, number of smart individuals and generation number, must be determined. Different population sizes were used to build the AGA model, as shown in Fig. S3a. During the first 20 generations, the energy consumption decreased largely overall, with relatively small fluctuation. Energy consumption remained stable after 50 generations, and so the generation number was set to 50. Fig. S3a also shows that a small population size could not produce all the important information and readily lead to a local optimum. However, a large population size resulted in increased computation and low efficiency. Hence, the population size was prescribed to be 500. In Fig. S3b, the population size was kept fixed at 500, while different numbers of smart individuals were calculated. A larger number of smart individuals resulted in a low convergence rate because the intervals of the variables

changed slowly. However, fewer smart individuals would lead to local optima because of information loss. Thus, the number of smart individuals was set to 30.

Table 4 lists the optimization results obtained by AGA. The lowest energy consumption is 216.90 W, meeting the first-class A level of effluent quality standards in China, while achieving an even deposition of sludge.

4. Application to a full-scale OD

4.1 Full-scale OD at Ping Dingshan WWTP, China

The full-scale bioreactor at the Ping Dingshan WWTP, Henan Province, China, comprised a four-channel circular ditch with a total working volume of 26,000 m^3, and wastewater flow rate up to 50,000 m^3/d. Each straight channel was 130 m long, 10 m wide, and had mean water depth of 4 m (Fig. 7). The larger semi-circular connecting channel at the right-hand end of the straight channel had a center-line radius of 20.4 m. Each of the smaller semi-circular channels had a center-line radius of 10.15 m. The OD contained a total of 13 sets of surface aerators and 9 sets of submerged impellers (Fig. 7), not all of which were necessarily operated at any one time. Each set of aerators consisted of 45 discs; and each disc was 10 m long (about 0.5 m of which was submerged) and 1.4 m in diameter with rotational speed of 53 rpm. Each surface aerator provided an oxygenation mass addition rate of 65 kgO_2/h and required a power input of 37 kW. And each single submerged impeller had two 2.0 m diameter blades, and required a power input of 4.19 kW. The submerged impellers were installed 2.2 m below the liquid free surface, and when running, the wastewater mixture could be accelerated through the impellers. Under existing

operating conditions, a total of 9 surface aerators and 3 submerged impellers operated simultaneously (Fig. 7). Table S1 summarizes the characteristics of the influent and effluent water quality indexes under existing operating conditions. The designed averaged concentration of sludge was 4.0 g/L, and the sludge retention time was 15 d. The hydraulic retention time was 12.48 h, of which the wastewater spent 2.50 h in aerobic zones occupying 20,800 m^3 working volume and 9.98 h in anoxic zones of 5200 m^3 working volume. Throughout operation of the OD, the wastewater temperature was 18.2-25.5 °C, and the pH was approximately 7.4.

Horizontal flow velocity components in the straight and semicircle portions were measured using an XZ-3 probe (an intelligent current meter; manufactured by Nanjing Automation Institute of Water Resources and Hydrology, Ministry of Water Resources of China). On-line DO measurements were acquired using an Endress + Hauser meter (made in Germany). Measurements were sampled at three stream-wise locations and at four different depths: 0.5 m below the surface (Surface Layer), 1 m below the surface (Top Layer), 2 m below the surface (Middle Layer), and 3 m below the surface (Bottom Layer) (Fig. S4).

4.2 Development of hybrid CFD, ANN and AGA model

In the 3D three-phase CFD model used to simulate the full-scale OD, prescribed influent flow velocity, activated sludge concentration, and concentrations of soluble constituents were applied at the inlet boundary and atmospheric pressure at the outlet boundary. A rigid-lid approximation was applied at the water surface, and a no-slip boundary condition was assigned to all fixed walls. Rotating devices were simulated

by the fan model and the moving wall model. The wall roughness height was set as 0.02 m, and the roughness constant was 1 [34]. All other parameters used in this simulation were chosen to be the same as those in the pilot-scale OD simulation [8].

Fig. S5 presents a comparison of predicted and measured liquid velocity at Sections 1-1, 2-2 and 3-3 under existing operating conditions; reasonable agreement is evident, as indicated by the normalized standard error of 5.3%. Fig. S6 presents color contours of magnitude of horizontal velocity components; the visualization shows the presence of an uneven flow pattern under existing operating conditions in the oxidation ditch; in particular, the horizontal flow speed near an internal wall is usually lower than that near the corresponding external wall. Fig. S7 shows that the predicted DO concentration profiles are in reasonable agreement with their measured counterparts at transects in the aerobic zone (Section 2-2) and anoxic zone (Section 3-3), with a normalized standard error of 2.6%. Table S2 lists the corresponding measured and calculated effluent concentrations of COD, ammonia nitrogen, and TN, with normalized standard errors of 9.2 %, 15.0 % and 8.6 %, respectively. These validation results established that the CFD model accurately reflected the characteristics of liquid velocity, DO profiles and effluent quality in the full- scale OD.

The calibrated 3D three-phase CFD model was then used to simulate a total of 260 groups of operational modes (Appendix B), and the results transferred as node inputs to the ANN model. The input data were randomly divided into training, validation, and test sets. Fourfold cross validation was used to limit the bias caused by

random selection of training set. Node outputs comprised estimates of concentrations of ammonia nitrogen, nitrate, TN, and COD, and the liquid velocity in the OD. The training algorithm was LMA, and tansig was used as the transfer function in both the hidden and output layers. Table 5 presents the optimum ANN structure used for simulating average liquid velocity and effluent water quality indexes; the high values of correlation coefficient demonstrate the close match between the CFD and ANN predictions. Importantly, the CPU time reduced from 32 h using CFD to 1.2 s using ANN for the same operation mode.

The aim is to achieve low operating costs, a relatively even distribution of activated sludge, and first-class A level effluent water quality. To achieve this, the correlation between average liquid velocity and *Std* of MLSS was determined at reference locations along the OD, each an elevation 0.5 m above the bed of the ditch, for all operation modes considered (Fig. S8); it was thus found that the critical velocity required to achieve an even distribution of sludge was 0.15 m/s. Based on Yang et al.'s study [34], 6 surface aerators were needed to meet the oxygen demand requirements in the Ping Dingshan OD. The overall constraints could be expressed as:

$$COD_{out} < 50 \text{ mg/L} \tag{16}$$

$$NH_4^+ - N_{out} < 5mg/L \tag{17}$$

$$TN_{out} < 15 \text{ mg/L} \tag{18}$$

$$\bar{v} > 0.15 \text{ m/s} \tag{19}$$

$$N_{aerator} \geq 6 \tag{20}$$

where $\bar{v}$ represents the average liquid velocity, and $N_{aerator}$ is the number of surface

aerators. The objective function is:

$$E_{\min} = \min E \tag{21}$$

The population size of the AGA was set to 300, the number of smart individuals was 20, and the generation number was 100. Table 6 lists the five best sets of results. Here, the effluent TN concentration has reduced from 19.7 mg/L (existing condition) to less than 14 mg/L (Table 6), meeting the effluent quality standards of first-class A level. Compared with 345.57 kWh energy consumption under existing conditions, the improved conditions saved 106.81 kWh (31%) of the energy, resulting in a cost saving of about 65,000 € per annum, assuming a tariff of 0.07 €/kWh [35].

5. Conclusion

Oxidation ditches involve complicated interacting physical-chemical-biological processes, and so require optimized operating conditions in order to meet water quality standards, sludge deposition requirements, and economic constraints. Rapid feedback control and real-time optimization are therefore urgently required for many WWTPs. This paper has described a hybrid model combining a 3D three-phase CFD model, a multi-site ANN model and an AGA model that achieves real-time prediction and optimization in both pilot-scale and full-scale ODs. Although the 3D three-phase CFD module correctly simulated the key liquid-sludge-gas motions and interactions in the OD system, the model was too expensive computationally to be applied routinely to cases involving rapid feedback. This drawback greatly limits the application of CFD in practice, especially to OD systems that undergo sudden changes. In contrast, the ANN model was capable of very rapid adjustment to new processes, but required

large quantities of comprehensive data for training and validation. Neither experimental measurements under different operating conditions nor corresponding predictions from 1D/2D mathematical models involving one or two phases can provide all the data required by the ANN model. To enhance the modelling capability, a considerable improvement was achieved by combining the complementary best features of the 3D three-phase CFD model and multi-site ANN module. The CFD model solved the data shortage problem and ensured accurate simulation data for the multi-site ANN model. The ANN model provided rapid feedback on liquid velocity, MLSS concentration and water quality parameters for each scenario at arbitrary sites along the oxidation ditch. This information enabled the AGA model to calculate fitness values and hence realize global optimization of the operating conditions based on the concept of stochastic evolution. When applied to the pilot-scale OD, the hybrid model led to a speed up in computational speed that was 86,400 times faster than CFD simulations would have cost. It was demonstrated that a 31% saving in total energy could possibly be made under an optimum operating condition compared to the existing operating condition in a full-scale OD. The hybrid model presented herein is potentially very useful in providing further insights into the behavior of ODs, and in helping achieve real-time process optimization control in practice.

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