Simulation of a full-scale activated sludge reactor: an approach to airflow rate optimization

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Abstract. Wastewater systems are high-energy consuming processes that discharge considerable amounts of pollutants into aquatic ecosystems, thus requiring appropriate optimization. Therefore, a full-scale activated sludge process was studied in this work through mathematical modeling of heterotrophic and nitrifying microorganisms. The airflow rate was introduced as the controlling parameter to accomplish the degradation of pollutants. Moreover, a sensitivity analysis was performed to determine the most sensible parameters that should be evaluated through further experiments, aiming to improve the model. The obtained results indicated that readily biological oxygen demand degradation and the oxidation of ammonia to nitrite could be achieved with an airflow rate of 35 m² air d⁻¹. The sensitivity analysis showed that heterotrophic kinetic parameters and oxygen mass transfer coefficient through diffusers are the most sensitive to the system. These results also proved that the air-diffusing systems can work at 0.3% of their maximum capacity to accomplish degradation. Future studies should consider other oxygen-consuming variables.

1. Introduction
Wastewater treatments are processes that help to improve the disposal of water back to ecosystems with qualities that avoid eutrophication; and by accomplishing this, waterbodies and local species can be preserved [1]. Two main wastewaters can be produced: those from domestic uses and those from industrial activities. The former ones are characterized by high organic content, while the latter can greatly vary depending on the industrial activity. Those wastewaters that contain readily biodegradable matter (bCOD) can be treated through activated sludge processes, in which the biomass sedimented in a secondary clarifier is returned to the main bioreactor. This process can carry out aerobic activities such as bCOD removal and nitrification; this latter is divided by ammonium-oxidizing (AOB) and nitrite-oxidizing (NOB) microorganisms.

On the other hand, mathematical modeling of biological systems is a well-known tool to optimize and describe the performance of microbial activities. The application of these tools has been widely used to scale up and increase operational efficiency [2,3].

Accordingly, in this work, mathematical modeling was proposed to study a full-scale activated sludge reactor; the biological removal of bCOD, nitrification, and oxygen mass transfer through diffusion were the main processes studied. Additionally, a sensitivity analysis was performed to identify the most sensitive parameters to the output variables aiming to calibrate and validate the modeling in further research.
2. Materials and methods

2.1. System configuration

The reactor under study is part of a wastewater treatment plant that receives effluents from a set of different factories in the Mamonal industrial sector in Cartagena de Indias, Colombia (more detailed information is lacking due to confidential agreements). Figure 1 shows the plant configuration that is formed by a coarse screen for large solids removal, a system of water transport through pumping, a chamber for grit removal, an activated sludge reactor with sludge recirculation, a secondary clarifier, and a sludge drier pond. The system boundary for the mathematical model herein proposed is marked off with the dashed lines; there, $X_R$ was defined through a mass balance in the secondary clarifier based on the settleability (Table 1). In that other, the main parameters that were supplied by the factory and used for the mathematical model are represented in Table 1. The inflow rate, inlet soluble COD $\{S_0\}$, and operational parameters were those measured for average and pick hours.

![Figure 1. Diagram of the wastewater treatment plant. The dashed line marks off the system boundaries for the mathematical model and simulation.](image)

2.2. Mathematical model

The mathematical model considered 7 processes in which 6 were biological, characterized by growth and decay of the microorganisms, and 1 was physicochemical, characterized by oxygen transfer to the liquid phase; these processes are defined as follows.

1. Growth of heterotrophic microorganisms.
2. Growth of ammonium oxidizers.
3. Growth of nitrite oxidizers.
4. Oxygen transfer to the liquid phase.
5. Decay of heterotrophic microorganisms.
6. Decay of ammonium oxidizers.
7. Decay of nitrite oxidizers.

The mathematical model is shown in Table 2 in a Peterson matrix representation [4] in which the above-mentioned processes are numbered in the first column and defined mathematically in the last column. The components studied were: bCOD, dissolved oxygen ($O_2$), nitrogen in form of total ammonium ($N_{AM} = N_{NH_3} + NH_4^+$), total nitrite ($N_{NO_2} = N_{NO_2^-} + N_{HNO_2}$), nitrate ($N_{NO_3}$), heterotrophic microorganisms ($X_H$), ammonium-oxidizing microorganisms ($X_{AM}$), and nitrite-oxidizing microorganisms ($X_N$).
The stoichiometric yields are shown in each component column and were determined based on Equation (1) to Equation (3) and literature reports; for the S consumption, Equation (1) was used, and stoichiometric yields were defined based on a COD balance as it was suggested by Wichern, *et al.* [4]. For ammonium and nitrite consumption, Equation (2) and Equation (3) were used [5] to define stoichiometric yields of ammonium and nitrite regarding oxygen. Differential equations were defined by mass balances for all the components in the reactor.

The three biological processes were studied through double Monod equations, $r_1$ to $r_4$ in Table 2, as this kinetic is the most-accepted criteria to describe microbial growth [1]; in this case, oxygen is the shared substrate for all the aerobic microorganisms while bCOD, ammonium, and nitrite are the other substrates for heterotrophic, AOB and NOB, respectively. The kinetic parameters were taken from the literature and are shown in Table 3.

$$S \text{ (Substrate)} + O_2 \rightarrow X_B \text{ (Biomass)} + H_2O + CO_2,$$

$$NH_4^+ + 1.5O_2 \rightarrow NO_2^- + 2H^+ + H_2O,$$

$$NO_2^- + 0.5O_2 \rightarrow NO_3^-. \tag{3}$$

**Table 1.** The main influence parameters of the wastewater, the plant design parameters, and the operational conditions correspond to average routine measurements (more detailed information was not available).

| Main influent parameters | Units | Average value | Pick value |
|--------------------------|-------|---------------|------------|
| Inflow rate (Q)          | m$^3$ d$^{-1}$ | 151           | 353        |
| [COD], S                 | g O$_2$ m$^{-3}$ | 555           | 746        |
| NAM                      | g NAM m$^{-3}$    | 45            | 61         |
| Temperature              | ºC    | 25            | -          |

| Operational conditions | Value |
|------------------------|-------|
| COD/BOD$_5$            | 3.20  |
| VSS/TSS                | 0.70  |
| [COD], S               | 20.00 |
| [TSS], X$_e$           | 20.00 |
| Q$_e$/Q                | 0.75  |
| Settleability          | 99.00 |
| pH                     | 7.50  |

| Design parameters       | Value |
|-------------------------|-------|
| Reactor volume (V)      | 266.0 |
| Depth                   | 3.6   |
| Cross-sectional area    | 74.0  |
| Airflow rate (Q$_a$)    | 0 - 11750 |

Yields coefficients (Y parameters from Table 2) are stoichiometric ratios between microorganisms and compounds and were taken from the literature [1,6,7]. Respecting the kinetic of AOB and NOB, the substrates are the undissociated form of ammonium and nitrite, respectively; and as these component distributions are pH and temperature dependent, NH$_3$ and HNO$_3$ were determined from acid/basic equilibrium [8,9].

In terms of mass transfer, oxygen is a key substrate for the three microbial processes studied, and a competitive growth will take place; then, a proper oxygen mass transfer estimation is important. Therefore, the oxygen mass transfer coefficients were determined from the theoretical equations proposed by Schierholz, *et al.* [10], for air sparged through fine bubbling ($K_{L}a_0$) and the mass transfer
through the liquid-air surface ($K_{L_A}$); to this aim, an empirical parameter ($\alpha$) was needed and taken from the literature [10], as well as oxygen diffusivity in water [11], and water kinematic viscosity [1].

### Table 2. Peterson Matrix of the mathematical model. Processes considered: growth and decay of heterotrophic, ammonium, and nitrite oxidizers, respectively; and oxygen transfer.

| Components | Rate |
|------------|------|
| $1$          | $r_1 = \mu_{\text{max}/1} \frac{S}{K_s+S} \cdot \frac{O_2}{K_{O_2/1} + O_2} \cdot X_{H}$ |
| $2$          | $r_2 = \mu_{\text{max}/2} \frac{N_{\text{NH}_3} + N_{\text{NH}_4}}{K_{\text{NH}_3} + K_{\text{NH}_4}} \cdot \frac{O_2}{K_{O_2/2} + O_2} \cdot X_{\text{AM}}$ |
| $3$          | $r_3 = \mu_{\text{max}/3} \frac{N_{\text{NO}_2} + N_{\text{NO}_3}}{K_{\text{NO}_2} + K_{\text{NO}_3}} \cdot \frac{O_2}{K_{O_2/3} + O_2} \cdot X_N$ |
| $4$          | $r_4 = k_{i_1} \cdot \mu_{\text{AM}} \cdot (O_{2_{\text{sat}}} - O_2)$+$k_{i_2} \cdot \mu_{\text{AM}} \cdot (O_{2_{\text{sat}}} - O_2)$ |
| $5$          | $r_5 = b_{x_1} \cdot X_H$ |
| $6$          | $r_6 = b_{x_2} \cdot X_{\text{AM}}$ |
| $7$          | $r_7 = b_{x_3} \cdot X_N$ |

*a* $N_{\text{AM}} = N_{\text{NH}_3} + N_{\text{NH}_4}$;  
*b* $N_{\text{NO}_2} = N_{\text{NO}_2} + N_{\text{NO}_3}$;  
*c* Saturation at 25ºC and not considering salinity is 8.24 mg O$_2$ L$^{-1}$ [1].

### 2.3. Sensitivity analysis

A sensitivity analysis was performed to determine the most influential parameters over each component defined in Table 2. In that order, Equation (4), which represents the sensitivity function ($F_s$), was used for this purpose as it has been done in other works [2,12,13]; where $y_n$ represents any component, $t$ the simulation time, $\theta$ any of the kinetic parameters or mass transfer coefficients used in the rate expressions (Table 2), and $\delta$ is the increasing fraction of parameter. In this work, a unique sensitivity of all the above-mentioned parameters over each of the 8 components was evaluated using an increase fraction $\delta$ of 10% and a simulation time of 20 days.

$$F_s(t_{m,n}) = \left(y_n(t_{m} + \delta \cdot \theta_{m}) - y_n(t_{m} - \delta \cdot \theta_{m})\right) \cdot \left[2 \delta \cdot y_n(t_{m} \cdot \theta_{m})\right]^{-1}. \quad (4)$$

### 3. Results

#### 3.1. Running the mathematical model

Different model running was performed. Initially, the system was studied under the average conditions shown in Table 1, and dissolved oxygen as an optimization criterion; from there, it was obtained that after 6 days the system achieved the stationary stage (SS), the airflow rate was optimal at 23 m$^3$ air d$^{-1}$, which is only 0.2% of the maximum aeration capacity (Table 1), bCOD removal and ammonium conversion to nitrite were kept both over 98.8% w/w. The $X_H$ and $X_{\text{AM}}$ concentrations in the SS were 78 g VSS m$^{-3}$ and 6 g VSS m$^{-3}$, respectively, while oxygen was 1.7 g O$_2$ m$^{-3}$, NOB was washed out as the solid retention time (SRT) is 4 days and due to the oxygen concentration and the half-saturation constant ($K_{O_2/X3}$ Table 3), NOB grows at the half of the maximum growth rate ($\mu_{\text{max}/3}$, Table 3), which means that a solid retention time superior to 4.2 days is needed to allow its growth.
Table 3. Kinetic parameters that were taken from the literature.

| Kinetic parameters for each type of microorganism | Units          | X_1             | X_2             | X_3             |
|-------------------------------------------------|---------------|-----------------|-----------------|-----------------|
| Maximum specific growth rate \( \mu_{\text{max}} \) | d^{-1}        | 6.00 [1]        | 1.45 [14]       | 0.48 [14]       |
| Decay rate \( b \) | d^{-1}        | 0.12 [1]        | 0.20 [6]        | 0.17 [6]        |
| S half-saturation coefficient \( K_s \) | g bCOD \( (m^3)^{-1} \) | 20.00 [1]       |                 |                 |
| \( N_{\text{AM}} \) half-saturation coefficient \( K_{\text{AM}} \) | g \( N_{\text{AM}} \) \( (m^3)^{-1} \) | 0.30 [9]        |                 |                 |
| \( N_{\text{NO2}} \) half-saturation coefficient \( K_{\text{NO2}} \) | g \( N_{\text{NO2}} \) \( (m^3)^{-1} \) | 2.2 \times 10^{-4} [9] | | |
| \( O_2 \) half-saturation coefficient oxygen \( K_{O2} \) | g \( O_2 \) \( (m^3)^{-1} \) | 0.16 [13]      | 0.74 [15]       | 1.75 [15]       |

*a Units of nitrogen are in N-NH_3, which is the substrate form used by ammonium oxidizers [9].

*b Units of nitrogen are in N-HNO_3, which is the substrate form used by nitrite oxidizers [9].

Based on the above-mentioned optimal conditions, the simulation was studied considering the influent variations that are defined by the peak hour parameters (Table 1); thereby, 18 hours and 6 hours a day the system received average and pick loads, respectively.

The simulation using the optimal airflow rate determined before is shown in Figures 2(a) and Figure 2(c); the results show that bCOD was below 20 g m^{-3}, which is the threshold value demanded by the environmental regulation. For ammonium, the conversion is halved due to the oxygen concentration (below 1 g \( O_2 \) m^{-3}) in the pseudo-SS, and the AOB growth rate is affected at these conditions (see \( K_{O2}^{-x2} \), Table 3). Moreover, this half ammonium conversion could be attractive if a further anammox system is intended to fully treat nitrogen compounds [5]. As the inlet fluctuates, there is a pseudo-SS and it can be observed by all the component fluctuation after 10 days. Regarding oxygen, it is suggested to keep the concentration between 1.5 g \( O_2 \) m^{-3} and 2 g \( O_2 \) m^{-3} in aerobic systems [1], which was not achieved in this case (Figure 2(a)); therefore, a new optimization of the airflow rate was performed considering the influent fluctuations (see Figure 2(b) and Figure 2(d)). The optimal airflow rate was 35 m^3 air d^{-1}, and oxygen in the pseudo-SS fluctuates from 3.2 g \( O_2 \) m^{-3} to 0.7 g \( O_2 \) m^{-3}, which due to the short period of low oxygen concentration it can be acceptable. Regarding components, biomass concentration kept similar in both cases, while bCOD and nitrite were below both 10 g m^{-3}.

Figure 2. Modeling simulation under optimal airflow rate; (a) and (c) show results of simulation the first simulation; (b) and (d) show the results of the second simulation.
The 2 cases, airflow rate at 23 m$^3$ d$^{-1}$ and 35 m$^3$ d$^{-1}$, represent less than 0.3% of the maximum capacity of the aeration system. Even though, the aeration shall be optimized to avoid solid sedimentation in the reactor, as there is not mechanical stirring and liquid homogenization is enhanced only by the air diffusing system. Also, other oxygen uptake processes shall be considered to fully describe the system.

3.2. Sensitivity analysis
The sensitivity analysis was done from Equation (4), and results were computed as $\sum_{i}^{n} \sum_{j}^{n} F(m,n)$, where m represents parameter influence over each of the components, and n represents the outcomes of the components in time. It was obtained that the decay rate for heterotrophic microorganisms ($b_i$) was largely more influential parameter than the rest; the sensitivity (expressed as a relative percentage to $b_i$) of the other most influential parameters were: 3.4% for the oxygen half-saturation constant for $X_H$, microorganisms ($K_{O2,s}$), 3.4% for the maximum growth rate for $X_H$ ($\mu_{max,s}$), and 1.3% for the oxygen mass transfer coefficient from air bubbling ($K_I,a_b$). All this means that further experimental estimation of these parameters should be considered to improve the mathematical model description of the system.

4. Conclusions
This work was focused on the simulation and optimization of an activated sludge reactor. It was obtained that working with less than 0.3% of the maximum aeration capacity, the conversions of contaminants were achieved. A sensitivity analysis shows that kinetic parameters of heterotrophic microorganisms and oxygen mass transfer coefficient were the most influential for the model, meaning that their experimental estimation is necessary to increase the model accuracy. Moreover, in further research, it is important to study other oxygen-consuming processes. Finally, the model herein developed described a significant improvement of the system energy consumption and removal efficiency.

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