Application of Mechanical Relations in Mathematical Modeling to Oxygenate Synthetic Wastewater through a Circular Rotary Aerator

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Abstract. This paper expounds the issue about the evolution of the dissolved oxygen concentration in synthetic wastewater with a circular rotary by setting a mathematical model. The mathematical model is based on the Lewis and Whitman relations to transfer oxygen to water, and includes the mechanistic models proposed by Lee, to determine the global oxygen transfer coefficient and the oxygen saturation concentration in water, as a function of the fifth power temperature. For this purpose, historical data from aeration experiments with two types of discs and two levels of COD concentration were compared. The equation allows to include the effect of the variation of the temperature and atmospheric pressure. Finally, through the data obtained, it’s concluded that the estimation error is not affected by the type of disc, the COD concentration of the synthetic wastewater or by the interaction of both, and is less than + - 0.086 mg / L dissolved oxygen.

1. Introduction

The biological treatment of wastewater is understood as the elimination of pollutants through the biological activity of microorganisms present in biological reactors. In this way, biodegradable organic substances, colloidal particles and dissolved pollutants, among others, will be removed, turning them into gases and biomass (new cells), separable by sedimentation. For this, it requires concentrations of dissolved oxygen, which occurs through the aeration process, which consists of putting the water in intimate contact with the air, in order to ensure an appropriate supply of oxygen for the consumption of the microorganisms responsible for the treatment [1]. Aeration is one of the most energy-intensive processes and accounts for about 50 to 90 percent of the electricity needed by a wastewater treatment plant. [2].

Samples of real wastewater for aeration experiments present difficulties in their preservation, which, if not given due attention, will change their physical and chemical characteristics. For this reason, synthetic sewage is used, since it makes it easier to handle the concentrations and substances that will constitute water as pollutants. In this research, partially submerged discs are used as aerator elements at the laboratory level to transfer oxygen to samples of synthetic sewage. The discs are fixed on an axis that rotates at 50 RPM. During the circular motion, a layer of liquid wets the undefiled surface of each disc, and physical contact is established between the liquid and the air, causing the transfer of atmospheric oxygen. This liquid layer, with oxygen gained, is mixed with the entire mass of liquid in the container, thus increasing the concentration of dissolved oxygen over time. Through the surface of the same liquid...
contained in the container, oxygen is also transferred, but in small quantities, so it is considered negligible. The rate of transfer of atmospheric oxygen to wastewater is affected by several factors involved in the process of transfer from the gas phase to the liquid phase, including: the temperature of the liquid, the temperature and pressure of atmospheric air, the concentration and type of dissolved and suspended pollutants in the water, the type of aeration system or mechanism, the characteristics of the vessel and its elements for homogenisation of the liquid. The increase in temperature leads to a lower level of oxygen saturation in the water, and this in turn causes a low driving force for the transfer of oxygen [3]. There are mathematical models that allow describing the phenomenon of mass transfer of oxygen from the air to contaminant-free water. The oldest model is the one proposed by Lewis and Whitman [4], who propose the process of transferring gases to liquids, through two films located at the gas-liquid interface. This model relates the oxygen transfer rate to the dissolved oxygen concentration in the liquid. There are also other mechanistic models to determine mass transfer coefficients and oxygen solubility in liquids [5]. In addition, it was possible to find relationships that allow estimating the concentration of oxygen saturation in liquids (Henry's law) [6], and the deviations with atmospheric pressure, temperature and the presence of contaminants in the water. The objective of the research is to formulate a mathematical model that considers the factors that affect the process of oxygen transfer, from atmospheric air to wastewater, to be available within scientific knowledge; in the field of wastewater, a tool that allows dynamically predicting the evolutionary process of dissolved oxygen concentration.

2. Materials and methods

2.1. Synthetic Wastewater
For each experimental test, 13.5 L of synthetic wastewater were prepared. These samples were prepared by dissolving the substances according to the desired COD; according to Table 1, in drinking water contained in a polyethylene container. Then, to deoxygenate the samples, sodium sulfite and cobalt chloride (catalyst) were added, in amounts calculated with the oxygen concentration measured in each sample. Table 1 shows the concentrations of the substances used in the preparation of synthetic wastewater [7].

| Substances         | COD 400 ppm | COD 700 ppm |
|--------------------|-------------|-------------|
| Peptone (gr)       | 3.024       | 1.728       |
| Sucrose (gr)       | 0.728       | 0.416       |
| Starch (gr)        | 1.696       | 0.969       |
| Basic phosphate of Na (gr) | 0.072 | 0.041 |

2.2. Rotating Disc Contactor
The rotary disc contactor, its parts and the types of discs for experiments, are shown in Figure 1. The discs are fixed to the 16mm stainless steel axis. The engine with speed reducer has a power of 180 W. The dissolved oxygen sensor is optical type by fluorescence, the temperature sensor is resistive type (PT 100), and the data recorder brand NOVUS. Table 2 describes the main details of the container and discs made for the experiment.
Figure 1. Diagram of rotary disc contactor and disc types.

Table 2. Main characteristics of the container and the discs.

| Characteristics                        | Description                                      |
|----------------------------------------|--------------------------------------------------|
| Container material                     | Acrylic                                          |
| Total volume / dimensions (LxAxH)      | 16.5 L / 39.3 cm x 31 cm x 13.3 cm               |
| Volume of liquid per test              | 13.5 L                                           |
| Discs per test / Material/ diameter    | 04 units / PVC/ 25cm                             |
| Rotational speed of the discs           | 50 RPM                                           |
| Diameter of perforations in the discs  | 3mm                                              |

2.3. Modeling of the Mathematical Equation: Transfer of Oxygen Gas to Wastewater

2.3.1 Oxygen gas transfer rate. The oxygen transfer that occurs in the liquid layer that covers the moving disks, in figure 2 the oxygen transfer mechanism explained by the Lewis and Whitman theory is shown [4].

Figure 2. Oxygen transfer mechanism.
Lewis & Whitman [4] analysed transfer processes for three particular gas cases based on their solubility in liquids: highly soluble gases, poorly soluble gases, and intermediate solubility gases, with oxygen being a poorly soluble gas in water. Due to this behavior, the mass transfer rate of this gas is:

\[
\frac{dW}{Adt} = KL(Cs - CL) \tag{1}
\]

Where \( W \) - weight of solute (mg), \( t \) - time (min), \( \frac{dW}{Adt} \) - absorption rate (mg / min.cm²), \( A \) - area of the liquid-gas interface (cm²), \( KL \) - diffusion coefficient of liquid film, \( Cs \) - saturation concentration of solute in liquid film (mg / L), \( CL \) - oxygen saturation concentration in liquid (mg / L).

2.3.2. Dissolved Oxygen Concentration. Performing a mass balance for the oxygen dissolved in the liquid in the container, the mass flow of oxygen transferred at the air-water interface is equal to the rate of accumulation of oxygen dissolved in the liquid within the vessel:

\[
KL,A(C_s-C_L) = \frac{dc_L}{dt}V \tag{2}
\]

\[
\frac{dc_L}{dt} = KL,a(C_s-C_L) \tag{3}
\]

Where \( KL,a_T \) is the mass transfer coefficient at temperature \( T \) (min⁻¹), \( a \) - is the interfacial area per unit volume (cm²/L), \( CL \) - was considered to be constant throughout the volume, in an instant of time.

2.3.3. Mass Transfer Coefficient. Lee, 2017 is based on equations from HASLAM [8], the analysis of the phenomenon of oxygen absorption in water and proposes the following equation, in which temperature is considered:

\[
KL,a_T = KT^5 \frac{E \rho \sigma}{P_S} \tag{4}
\]

Where: \( T \) - is the absolute temperature of the liquid (°K), \( K \) - is a constant of proportionality (depends only on the geometric characteristics of the apparatus, and not on the temperature), \( E \) - is the modulus of elasticity of water at temperature \( T \) (kN/m²), \( \rho \) - is the density of water at temperature \( T \) (kg/m³), \( \sigma \) is the interfacial surface tension of water at temperature \( T \) (N/m) and \( P_S \) is the saturation pressure at the equilibrium position (atm).

2.3.4. Dissolved oxygen saturation concentration. The saturation concentration of oxygen is the solubility that this gas has in equilibrium, with the pressure that the gas exerts on the surface of the liquid. This solubility can be estimated with Henry's law, but it should be noted that this law is applicable only to ideal solutions, and for a real solution, the results are approximate. It is also limited to low solubility gases.

Lee [5] proposes a model that calls it oxygen solubility law, for the saturation concentration of oxygen in water (\( Cs \), mg/L), which is:

\[
Cs = Kcs \frac{P_S}{T^5 E \rho} \tag{5}
\]

Where: \( Kcs \) is the water solubility law constant and its value is 43.4 for the respective units of \( T \), \( P_S \) E and \( \rho \), indicated above.

The model that will be used to carry out the simulation results from combining equation 3, 4 and 5, generating the following:
\[
\frac{dC_L}{dt} = \left( KT^5 \frac{E \rho}{\rho_s} \right) \left[ K_{CS} \frac{P_S}{T^5 \rho E \rho} - C_L \right] \tag{6}
\]

\[
\frac{\Delta C_L}{\Delta t} = \frac{C_{Lt+1} - C_{Lt}}{\Delta t} = \left( KT_{FROM}^5 \frac{E \rho}{\rho_s} \right) \left[ K_{CS} \frac{P_S}{T_{FROM}^5 \rho E \rho} - C_{Lt} \right] \tag{7}
\]

Equation 7 is the result of expressing in finite differences equation 6. Where: \( \Delta C_L \) is the time that the oxygenation process takes for a finite change of oxygen concentration in the liquid (time interval) and \( T_{FROM} \), is the average temperature at which the liquid is found during \( \Delta t \).

The finite difference method is a tool that provides satisfactory results provided that \( \Delta t \) is small and, in that time, the changes in the variables involved in the process are small.

3. Results

3.1. Experimental Measurements

The measurements of dissolved oxygen concentration during testing are shown in Figure 3. The behavior of the evolution of this parameter is similar in all experiences. In addition, with repetitions a low dispersion is observed.

![Figure 3](image_url)

**Figure 3.** Evolution of dissolved oxygen in: a) disc type A and COD 400 ppm, b) disc type A and COD 700 ppm, c) disc type B and COD 400 ppm, c) disc type B and COD 700 ppm.
With type A disc, the time taken to increase the concentration from about 0.5 ppm to 6 ppm was 62 min. While, with type B disc, the approximate time is 54 min.

It was observed that the saturation concentration of oxygen in the synthetic wastewater is slightly lower than the saturation concentration in drinking water at the same pressure and temperature conditions. The ratio between the two oxygen saturation concentrations in synthetic sewage and drinking water varies from 0.945 to 0.98, for 700 and 400 ppm in COD respectively.

The temperature of synthetic sewage samples during testing decreases, as shown in Figure 4. This is due to the evaporative cooling that occurs in the layers of water that cover the moving discs. But, the temperature decrease does not exceed more than 1 °C in all cases.

![Figure 4](image-url)

**Figure 4.** Historical evolution of the residual water sample temperature in: a) disc type A with COD at 400 and 700 ppm, b) discs type B with COD at 400 and 700 ppm

### 3.2. Simulation

The simulation to estimate dissolved oxygen concentration was performed with equations 3 and 7. Equation 3 used $K_{L}a_{T}$ (was determined by adjusting the data to the linearized equation 3), and was considered constant, because the temperature of the liquid in the experiments does not vary by more than 1°C, as indicated above. Equation 7 used $K_{a}$, which was determined by better fit to experimental data.

Figure 5 shows the results of $K_{L}a_{T}$, which is the negative of the slopes in the equations in each graph. The results of the simulation are shown in Figure 6.

![Figure 5](image-url)

**Figure 5.** Historical evolution of the dissolved oxygen concentration in residual water sample in: a) disc type A with COD at 400 ppm, b) disc type A with COD at 700 ppm
Figure 5. $K_L a_T$ of synthetic wastewater samples in: a) Type A and DQO 400 ppm discs, b) Type A and DQO 700 ppm discs, c) Type B and DQO 400 ppm discs, d) Type B and DQO 700 ppm discs.

Figure 6. Results of the simulation of the oxygenation process of synthetic wastewater samples in: a) disc type A and 400 ppm COD, b) disc type A and 700 ppm COD, c) disc type B and 400 ppm COD, d) disc type B and COD 700 ppm.
4. Conclusions

The mathematical model that includes the mechanistic equations proposed by Lee, allows to estimate the concentration of dissolved oxygen in synthetic wastewater and its evolution over time. Comparing with the experimental measurements of oxygen concentration in the wastewater, it was shown that the type of disc, COD and the interaction of both, does not affect the estimation error presented by the model, which for these tests reaches a maximum of - 0.086 mg/L dissolved oxygen.

Future research aims to verify the validity of the model, increasing the amount of levels in both disc type, COD concentration of wastewater, and the temperature of the liquid. Also using other equipment to oxygenate, such as bubble diffusers, and apply them in real water treatment processes in continuous mode, in order to provide data to analyze the performance of the water purification system.

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