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Original Research

Mathematical Modeling of Oxygenation Capacity in Wastewater Based on Air Diffuser Type

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ABSTRACT

The oxygenation capacity in wastewater directly impacts the performance of biological treatment systems. In this context, this study develops a mathematical model describing this capacity as a function of the aeration system used. Three configurations were evaluated: fine bubble, coarse bubble, and extra coarse bubble, through experimental tests measuring dissolved oxygen concentration, saturation time, and the overall mass transfer coefficient (kLa). The data generated models with high fit levels (R^2 between 0.9988 and 1), supporting their validity in representing the observed behavior. The fine bubble system showed the highest initial oxygenation capacity, reaching a rate of 1.28 mg/L·s^{-1}, though it decreased significantly over time by 96.09%. Overall, the results quantitatively characterize the dynamics of each diffuser type, providing relevant technical criteria for the design and selection of wastewater treatment systems.

INTRODUCTION

Wastewater contains a wide range of contaminants, such as organic matter, nutrients, heavy metals, toxic chemicals, and pathogens, which, if not effectively treated, pose a potential threat to aquatic ecosystems, water quality, and human health (Dey et al., 2022; Xu & Xu, 2022). Physical, chemical, and biological processes are employed for their removal (Pang et al., 2020).

Among these, biological methods like aeration offer a more sustainable and efficient alternative compared to physical and chemical treatments, which often involve higher operational costs and generate unwanted by-products. This treatment is particularly suitable for small- and medium-scale domestic wastewater treatment plants. It operates by supplying oxygen to the wastewater through pipes that release air bubbles, promoting mass transfer at the air-water interface. As a result, aerobic microorganisms can effectively degrade the present organic matter (Cheng et al., 2016; Dyagelev et al., 2021; Lebrun et al., 2022).

However, despite its wide applicability, significant gaps remain in understanding the factors affecting its efficiency. Aspects such as system geometry, diffuser type, bubble size, dissolved oxygen concentration, and dynamic flow conditions can significantly influence process performance. Mathematical modeling emerges as a key tool to address these limitations, enabling the simulation of system behavior under different scenarios without costly or hard-to-control physical tests (Cao et al., 2017; Farazaki & Gikas, 2019; Hocaoglu et al., 2011; Ma et al., 2017).

These predictive models allow the analysis of critical variables, optimization of operational parameters, and improvement of system design. However, many remain generalized and require specific validations for conditions (Arora-Jonsson, 2023; Levitsky et al., 2022; Lu et al., 2021).

In this context, this study aimed to model the oxygenation capacity in domestic wastewater, considering three key variables: diffuser type, overall mass transfer coefficient, and aeration time. The results can be applied to both the design of new treatment plants and the optimization of existing facilities, contributing to improved energy efficiency and treated effluent quality in urban and rural settings.

2. MATERIALS AND METHODS

2.1 Components of the Experimental Unit and Sample Preparation

Data collection involved oxygenation tests on synthetic domestic wastewater samples using a specially designed experimental unit. The system included an air compressor as the primary oxygen source, connected via a 10 mm inner diameter transparent plastic hose. A pressure regulator and a 1/4” needle valve was incorporated to precisely control the flow rate.

For monitoring relevant variables, a PT100 temperature sensor (measurement range: -50 °C to 150 °C, accuracy: ±0.1 °C) and a dissolved oxygen sensor (range: 0 to 20 ppm, accuracy: ±0.1 ppm) were integrated. A 1" ball valve was installed at the bottom of the container to facilitate drainage and cleaning between tests (Figure 1).

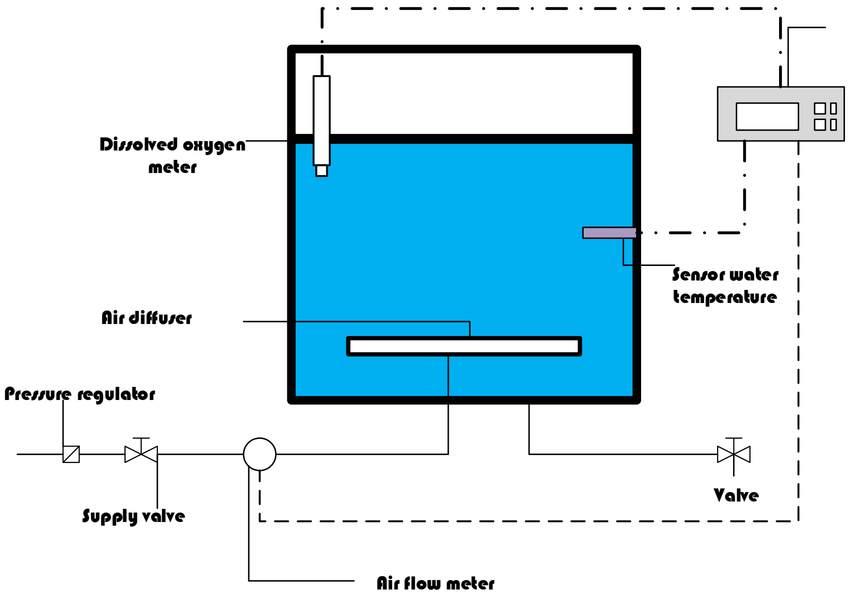

Fig. 1: Schematic of the experimental unit used for oxygenation tests in synthetic wastewater

Once assembled, 36 liters of domestic wastewater were prepared. For this, 5 g of peptone were added to provide organic nitrogen, peptides, and amino acids for protein synthesis and cell development. As the primary energy source, 1.2 g of sucrose was incorporated, while 2.8 g of starch provided sustained carbon release. Additionally, 1 g of soybean oil was added to supply lipids and essential fatty acids for cell membrane formation. The inclusion of 0.6 g of ammonium sulfate covered inorganic nitrogen requirements, favoring amino acid synthesis. Finally, 0.12 g of tribasic sodium phosphate was added as a pH regulator and phosphorus source, a key element in metabolic and structural functions.

2.2 Wastewater Deoxygenation

To begin the experiments, sodium sulfite (Na_2SO_3) and its catalyst, cobalt chloride ($CoCl_2$), were added to reduce the dissolved oxygen concentration to zero, according to the following reaction:

$$Na_2SO_3 + \frac{1}{2}O_2 \underset{\rightarrow}{CoCl_2} Na_2SO_4$$

Considering the stoichiometric ratio:

$$\frac{Na_2SO_3}{\frac{1}{2}O_2} = \frac{126{,}043\,\frac{g}{mol}}{32\,\frac{g}{mol}} = 3.94$$

Based on this value, the required amount of Na_2SO_4 was calculated, applying a 20% excess to ensure complete dissolved oxygen removal. The mixture was stirred for 5 minutes with a stainless-steel rod to ensure homogeneous reagent distribution. The compressor was then activated to begin the oxygenation process, essential for adequate oxygen transfer. This procedure was repeated for each evaluated air diffuser type.

2.3 Calculation of Mass Transfer Coefficient and Oxygenation Capacity

The volumetric mass transfer coefficient ($k_L a$) required a mathematical approach based on the temporal behavior of dissolved oxygen concentration.

2.4 Oxygen Transfer Equation (Exponential Model)

This dynamic was described using an exponential model proposed by Levitsky et al. (2022), expressed by Equation (1):

$$C_L = C_S - (C_S - C_O).e^{-K_L a.(t_2 - t_1)} \quad \ldots (1)$$

Where C_L represents dissolved oxygen concentration at time t; C_S the saturation concentration; C_O the initial concentration; and $K_L a$ the mass transfer coefficient. Expressed differentially, Equation (2) is obtained:

$$\frac{dc}{dt} = k_L a(C_s - C) \quad \ldots(2)$$

Rearranging the above expression yields an integrable form facilitating experimental calculation of $k_L a$, presented in Equation (3):

$$\frac{dc}{(C_s - C)} = k_L a(d_t) \quad \ldots (3)$$

2.5 Integration of the Equation to Obtain $k_L a$

To determine $k_L a$, the oxygen transfer differential equation (Equation 3) was used. Considering that at t = 0, oxygen concentration is C_i, and at time t, it increases to C_t, both sides of the equation were integrated:

$$\int_{C_i}^{C_t} \frac{dc}{C_s - C_L} = \int_0^t k_L a(dt) \quad \ldots (4)$$

This expression allows solving for the coefficient $k_L a$ as a function of time and initial and final dissolved oxygen concentrations, yielding the following logarithmic relation (Equation 5):

$$\ln\left[\frac{C_s - C_i}{C_s - C_t}\right] = k_L a.t \quad \ldots(5)$$

Rearranged equivalently:

$$\ln[C_s - C_t] = \ln[C_s - C_i] - k_L a.t \quad \ldots(6)$$

Thus, $k_L a$ was determined via linear regression of experimental data.

2.6 Relation to Oxygenation Capacity

Oxygenation capacity represents the amount of oxygen transferred per unit volume and time, calculated using Equation 7:

$$N = k_L a(C_s - C_L) \quad \ldots(7)$$

Where N is oxygenation capacity (mg O_2/L min); $k_L a$ is the mass transfer coefficient (min^{-1}), C_S is oxygen saturation concentration in the system (mg/L), and C_L is dissolved oxygen concentration at time t.

2.7 Data Processing

Measurements were organized by bubble type: fine, coarse, and extra coarse. Interpolation and surface fitting techniques were applied to construct a 3D mesh representing the combined behavior of time, mass transfer coefficient (k_La), and oxygenation capacity.

For visualization, R programming was used with libraries for 3D graphics. Response surfaces were color-coded by bubble type: red, yellow for fine bubbles, blue, yellow for coarse bubbles, and purple-green-yellow for extra coarse bubbles. The graph featured three axes: x-axis for time (minutes), y-axis for mass transfer coefficient (kLa), and z-axis for oxygenation capacity (mg/L).

R was also used for linear regression to calculate mass transfer coefficients (k_La), polynomial model fitting by diffuser type and operation time, and ANCOVA to statistically evaluate bubble type, time, and their interaction on system efficiency. To ensure the statistical reliability of the results, each experimental run for the different diffuser configurations was performed in triplicate

3. RESULTS AND DISCUSSIONS

3.1 Dissolved Oxygen Concentration

Figure 2 shows dissolved oxygen concentration evolution over time at 0.5-second intervals. The fine bubble diffuser reached saturation in 18.5 minutes, while coarse and extra coarse bubble diffusers took 72 and 64 minutes, respectively. Global average temperature was 16.1 °C ±0.249. ANOVA by diffuser type showed significant differences favoring fine bubble diffusers in average time to maximum oxygen concentration (ANOVA $p < .001$, Shapiro normality test $p < .001$).

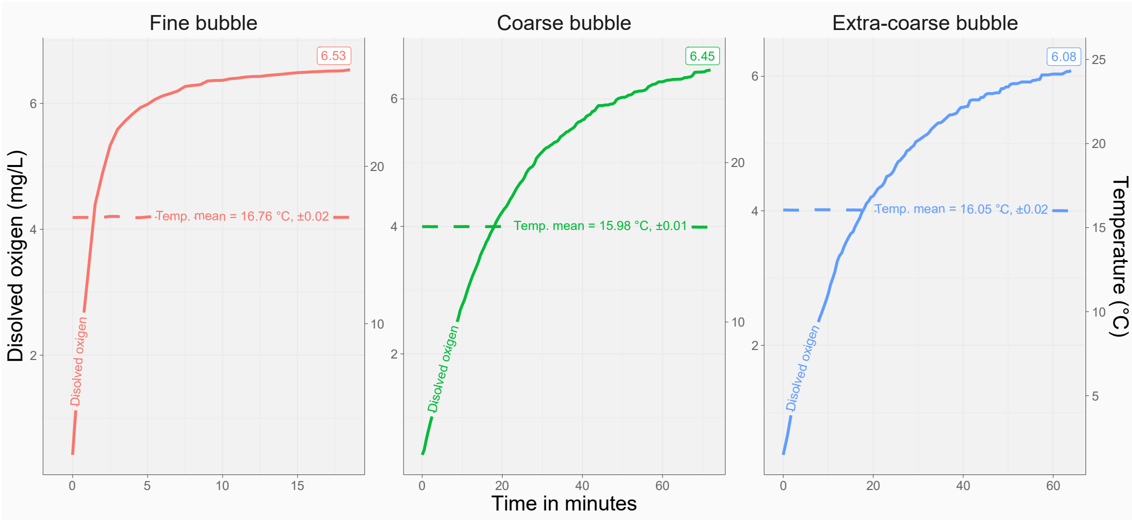

Fig. 2: Dissolved oxygen concentration

Note. Maximum time FB = 18.5 min, CB = 72 min, ECB = 64 min. ANOVA p < .001. Global average maximum dissolved oxygen = 6.36 ±0.24. Global average temperature = 16.1 °C ±0.249.

The fine bubble diffuser achieved saturation faster than coarse or extra coarse bubble diffusers, aligning with prior studies reporting higher efficiency in oxygen transfer per unit time (Newbry, 1998; Rosso & Stenstrom, 2006). Herrmann-Heber et al. (2021) recorded 98% dissolved oxygen concentration in 10.25 minutes under constant flow, while unagitated liquid systems may require significantly longer equilibration times (Ghodke & Vishal Reddy, 2023).

3.2 Mass Transfer Coefficient ($k_L a$)

Figure 3 presents $k_L a$ values adjusted per Equation (5): 0.25 for fine bubbles, 0.049 for coarse bubbles, and 0.056 for extra coarse bubbles.

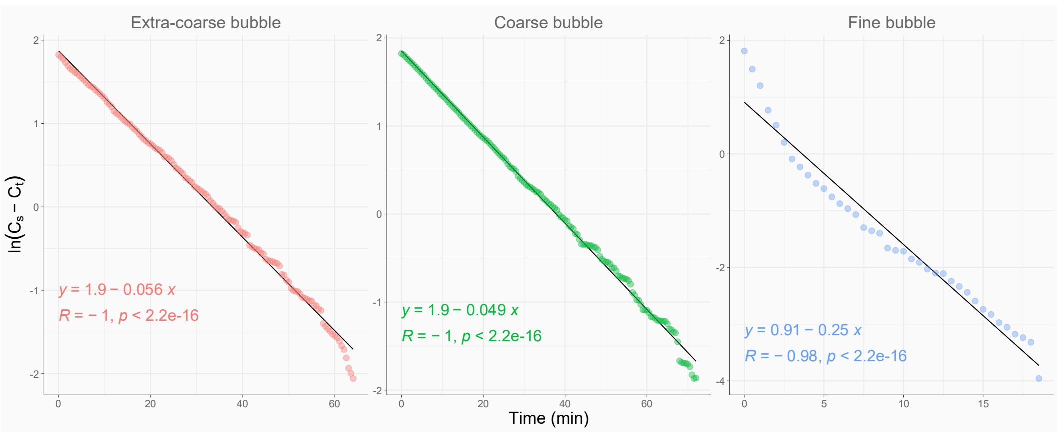

Fig. 3. Regression curves for determining $k_L a$

Higher kLa values for fine bubbles align with literature, where smaller bubbles generate greater gas-liquid interfacial area, enhancing oxygen transfer efficiency (Asselin et al., 1998; Gillot et al., 2005; Skouteris et al., 2020). Elevated kLa indicates better medium oxygenation (Reshma et al., 2021).

It is important to note that the oxygen transfer rate is directly influenced by the surface area to volume (S/V) ratio of the system. While this study did not explicitly calculate the gas-liquid interfacial area, the superior performance of the fine bubble diffuser is qualitatively consistent with this principle. The generation of smaller bubbles creates a significantly larger total surface area for a given volume of air, thereby increasing the S/V ratio and enhancing the driving force for mass transfer. The consistent experimental geometry (36 L volume and 35 cm liquid depth) ensures that the observed differences are primarily attributable to the diffuser characteristics. This is a key factor that should be quantitatively explored in future studies.

While this study did not implement an airlift recirculation system, its potential for future applications is noteworthy. Such systems can increase activated sludge concentration and improve suspended solids distribution, potentially boosting dissolved oxygen by 15% and mass transfer reactions by 11.8% (Khalil & Sharshir, 2022). Industrial studies show fine-slot disc diffusers can triple oxygen transfer efficiency in saline media compared to conventional configurations (Behnisch et al., 2022), suggesting relevant improvements for aeration systems like this study's.

3.3 Oxygenation Capacity

Oxygenation capacity (OC) was calculated using Equation 7, generating curves describing OC behavior by diffuser type over time t (Figure 4). Curves showed a descending trend as OC decreases toward oxygen saturation, indicating higher efficiency in early minutes. The fine bubble diffuser achieved maximum OC of 1.28 mg/L, significantly outperforming coarse (0.30 mg/L) and extra coarse (0.34 mg/L) diffusers.

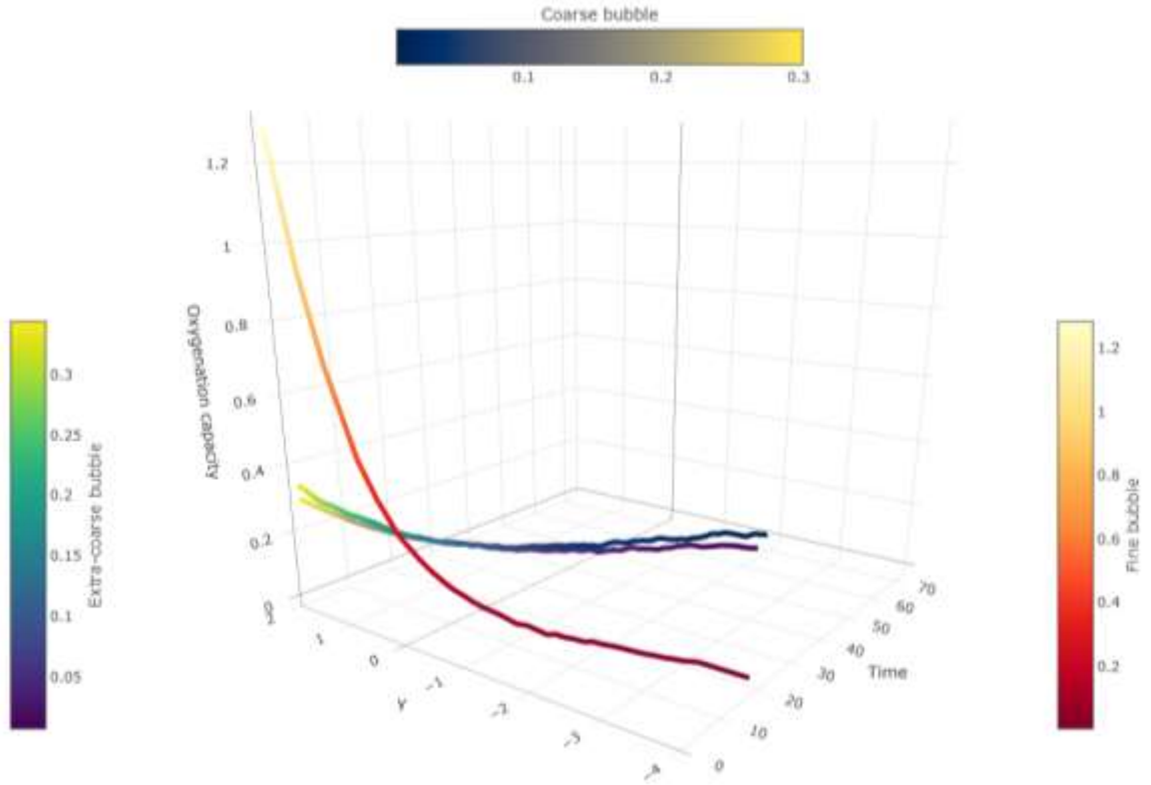

Fig. 4: Oxygenation capacity vs time. y = ln (Cs - Ct)

Between 5-10 minutes, values approached 2.0 mg/L, representing the optimal operation range before stabilization. Color transition (red, yellow) visually reinforces this trend. Extra coarse bubbles showed flatter, lower surfaces (purple, green), evidencing low efficiency, not exceeding 0.8 mg/L even at process end, suggesting limited oxygen transfer over time.

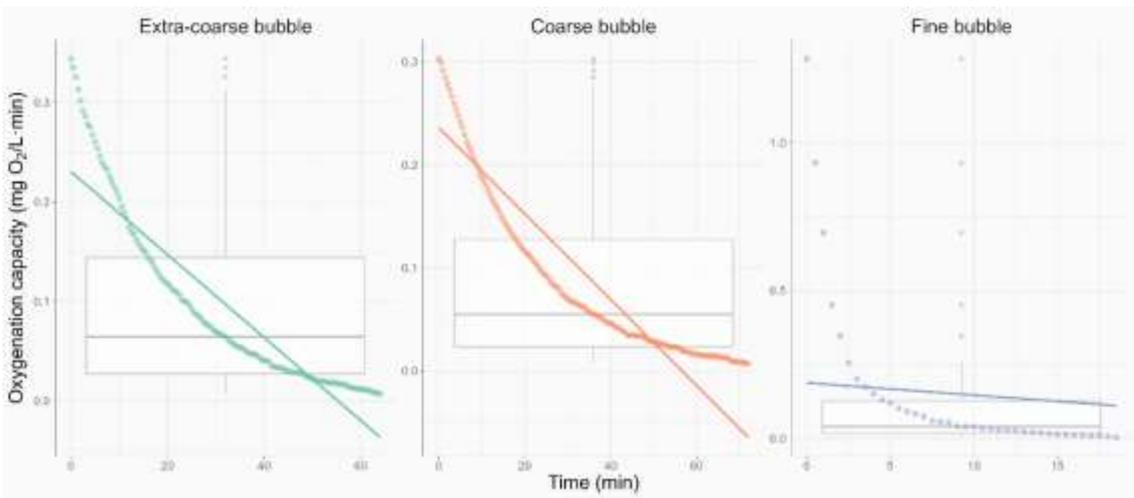

Fig. 5. Oxygenation capacity differences by time and diffuser type

Figure 5 and Table 1 show time and diffuser type interactions on OC. ANCOVA showed significant OC differences by diffuser type (Table 1, $p < .001$), demonstrating OC's dependence on time and diffuser type.

Table 1. Covariance analysis results

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Time	1	1.970035	1.970035	342.0105	8.70E-52
Diffuser type	2	0.05783	0.028915	5.019829	0.00716
Time:Diffuser	2	0.984258	0.492129	85.43674	3.31E-30
Residuals	306	1.762609	0.00576		

3.4 Polynomial Model Fitting

To characterize OC evolution over time, polynomial models were fitted for each diffuser type, with time as the independent variable. The fine bubble model fit a sixth-degree polynomial with $R^2 = 1$, indicating perfect experimental data correspondence (Table 3).

Table 2. Polynomial regression equations by diffuser type

Diffuser Type	Mathematical Model	R^2
Fine bubble	$y = 1.2781 - 0.81339x + 0.22821x^2 - 0.03277x^3 + 0.0025x^4 - 9.61937E\text{-}5x^5 + 1.47022E\text{-}6x^6$	1
Coarse bubble	$y = 0.30323 - 0.01496x + 3.64529E\text{-}4x^2 - 5.29557E\text{-}6x^3 + 4.36382E\text{-}8x^4 - 1.57334E\text{-}10x^5$	0.999
Extra coarse bubble	$y = 0.33975 - 0.01607x + 2.90008E\text{-}4x^2 - 1.89363E\text{-}6x^3$	0.998

The use of a high-degree polynomial for the fine bubble system, resulting in an R^2 value of 1, warrants a discussion on model validity. While this indicates an excellent descriptive fit for the collected data within our controlled experimental setup, it also raises concerns about potential overfitting. A model that perfectly fits the training data may not generalize well to new, unseen data. For future studies, it would be beneficial to apply techniques such as cross-validation or to evaluate alternative, less complex models (e.g., exponential or mechanistic models) to ensure the development of a robust predictive tool that avoids overfitting.

Nonlinear responses, especially for fine bubbles, relate to complex, unstable bubble dynamics in liquid, causing abrupt oxygenation rate variations. Coarse bubble models showed more regular, predictable behavior, suggesting factors like mixing regime and residence time maintain steadier oxygen transfer rates (Herrmann-Heber et al., 2020).

Extra coarse diffusers, though less efficient than fine bubble diffusers, slightly outperformed coarse bubble diffusers, suggesting variables like bubble dispersion patterns, diffuser geometry, or liquid contact time significantly influence oxygen transfer efficiency. This highlights the importance of viable technological alternatives given operational or economic constraints.

5. CONCLUSIONS

Mathematical modeling of the oxygenation capacity in wastewater, considering air diffuser type, enabled accurate representation of the temporal evolution of dissolved oxygen through polynomial models fitted to experimental data. These models highlighted key influences on the oxygenation process. Fine bubble diffusers demonstrated significantly higher oxygen transfer efficiency due to the greater gas-liquid contact area they produce, making them particularly suitable for aqueous environments. However, coarse and extra-coarse bubble diffusers, while slower in performance, provided more stable and predictable results, which can be advantageous in systems where operational stability is a priority. Statistical analysis of diffuser type time interactions revealed that the type of diffuser plays a particularly important role during the initial stages of the oxygenation process. This underscores the need to consider both diffuser type and process duration when designing efficient oxygenation systems, as both factors significantly interact to influence overall treatment performance. This study acknowledges certain limitations that open avenues for future research. The experiments were conducted using synthetic domestic wastewater to ensure controlled and reproducible conditions. However, performance in real wastewater may differ due to the presence of contaminants such as surfactants and suspended solids, which can alter bubble coalescence and surface tension, thereby affecting the mass transfer coefficient. Furthermore, the long-term potential for biofilm formation on diffuser surfaces in a real-world setting could impact performance over time. Future work should aim to validate these models using real wastewater and investigate the long-term operational stability of each diffuser type. This approach lays a foundation for future research aimed at exploring additional factors affecting oxygen transfer, such as environmental conditions or the physicochemical properties of water.

Author Contributions: A.L.: Conceptualization, Methodology, Formal analysis, Investigation, writing original draft, writing review & editing; O. S.: Validation, Data curation, Writing review & editing, Visualization; Methodology, Software, Validation, Formal analysis; J.C.: Investigation, Resources, Supervision, Project administration ; E.C.: Funding acquisition, Supervision, Software, Data curation, Visualization.

Conflicts of Interest: The authors declare no conflicts of interest.

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