ISSN: 2996-2498

Research Article,

Environmental Science and Climate Research

An Enhanced Oxygen Transfer Model for Water Treatment

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Submitted: 2026, Mar 10; **Accepted**: 2026, Apr 21; **Published**: 2026, Apr 30

Citation: L, J., Catano-Lopera, Y. A. (2026). An Enhanced Oxygen Transfer Model for Water Treatment. *Env Sci Climate Res, 4*(1), 01-11.

Abstract

The oxygen transfer efficiency of an aeration device based on a clean water test is defined by a standard specific baseline parameter for the mass transfer coefficient (KLa0) that exemplifies the effect of gas depletion in oxygen transfer. The baseline is defined as the oxygen transfer rate coefficient at zero depth. The purpose of the work is to propose an enhanced oxygen transfer equation that would more accurately estimate the device performance in the field using the procedures as stipulated in the ASCE/EWRI standards. The enhanced model is applied to wastewater through an alpha factor (α) that pertains particularly to the wastewater characteristics. The paper argues that the alpha factor (the ratio of mass transfer in process water versus clean water) is independent of microbial activity. The theoretical baseline is a groundbreaking development in physics that can be used to derive the KLa for different heights and wastewater compositions. In this study, a new equation to estimate KLa is presented to unify all the standards applicable not only to clean water but also to most types of respiring systems. The proposed modified mass balance equation, where the consumption rate due to microbial respiration in the activated sludge should be considered twice as high as in conventional models to account for the impact of microbial resistance is a key finding. Based on case studies found in the literature, the parameter KLa is expected to be estimable with the help of computational fluid dynamics (CFD) and experimental testing in future studies. One key point is that the effect of gas-side oxygen depletion effects on C (the saturation concentration) more than on the KLa coefficient, that without this understanding CFD or other modeling work cannot be successfully applied.*

Keywords: Wastewater Treatment, Activated Sludge, Mathematical Modelling, Oxygen Transfer, Standards, CFD, Experiments

1. Introduction

Oxygen transfer measurement in wastewater treatment is usually based on the two-film theory of mass transfer of oxygen from gas to liquid phase [1]. Because of the complexity of the topic, testing is first done using clean water, whereas the fundamental equation describing the oxygen transfer process is given by,

$$dC/dt = K_L a\ (C^* - C) \quad (1)$$

where C is the dissolved oxygen (DO) concentration, t is time, and C^* is the saturation concentration. In the conventional model, $K_L a$, and C^* are treated as independent of time so that Equation 1 can be integrated to yield,

$$C = C^* - (C^* - C_0) exp\,(-K_L a \times t) \quad (2)$$

where C_0 is the concentration at the beginning of the test. Equation 1 is applicable only to a particular point in a water body. In order to apply this expression to a macroscopic domain such as an aeration tank, it is necessary to integrate it over the tank volume, V, yielding,

$$\int_V \frac{dC}{dt} dV = \int_V K_L a(C^* - C) dV \quad (3)$$

According to the two-film theory combined with Henry's Law, C^* becomes the saturation concentration for the DO in equilibrium with the partial pressure of oxygen in the gas phase. For submerged bubble aeration, the partial pressure of oxygen in a rising air bubble changes with depth and time. This happens with or without any oxygen depletion in the bubble due to microbial or biological respiration. Therefore, strictly speaking, C^* shall not be considered as constant in Equations 1, 2 and 3. Consequently, the term C^* (or C^*_f in a non-clean water test), cannot be taken out of the integrand while solving for Equation 3.

As hinted above, Equations 1 and 2 have been traditionally applied to describe oxygen transfer phenomena in a macroscopic situation, while treating K_La and C^* as constants. Most analyses of non-steady state submerged aeration have applied the relationship in Eq. (1) by considering C^* as constant and equal to the average saturation concentration attained at infinite time, C^*_∞ where C^*_∞ is the determination point value of the steady-state DO saturation concentration as time approaches infinity. Note, however, that C^* clearly increases during the course of a non-steady state test as the oxygen content of the exit gas increases. It is worth pointing out that C^* and K_La vary with temperature, with K_La exhibiting a strong dependency on hydraulic conditions such as flow velocity, water depth, and turbulence dissipation rate. Furthermore, these parameters are further impacted by the microbial respiration rate in wastewater treatment systems.

Reported that field K_La [in units of /hr] values are dependent on the biological oxygen uptake rate (OUR) [in units of kg O_2/ hr] and increases as the OUR increases [2]. Herein, however, we postulate that the relationship trend is decreasing rather than increasing, with a fixed gas supply. By separating the effect of microbial respiration from the hydraulic conditions, we assert that the true oxygen transfer equation can be adopted to yield a more accurate outcome. This can be validated via CFD modeling and experimental tests [3]. One such confirming experiment has already been conducted [4]. The test results from such work are reproduced in Figure 1. The data reveals an inconsistency in the oxygen uptake rate determined by a "dynamic method" and the conventional "process" uptake rate determination [4]. The OUR based on the "dynamic method" [essentially an in-situ "BOD" bottle OUR where aeration is stopped and then measuring rate of change of O2 vs. time] is about half the "process" method of fitting the DO vs. time data to the conventional oxygen transfer model, presumably to the data collected during re-aeration and then calculating OUR based on the fitted K_La_f and C data.

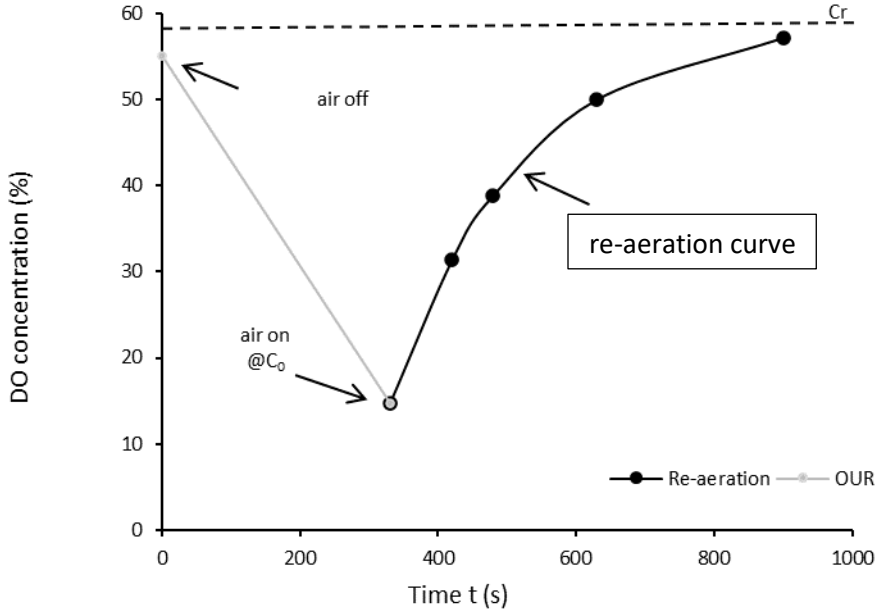

Figure 1: Dynamic Measurement of OUR and K_La [4]

The air-on/air-off is done while biological fermentation continues with feed and that there is a turbine mixer to provide mixing when air is off. The "process" OUR = $K_La_f\,(C^*_{\infty f} - C_R)$ at steady state; whereas it becomes OUR = $K_La_f\,(C^*_{\infty f} - C) - dC/dt$ at non-steady state, based on the conventional oxygen transfer model in a respiring system. The "dynamic" OUR equals 0.125 %/second while the OUR based on the process modeled data is 0.256 %/ second, an obvious inexplicable anomaly with the conventional equation. To reinforce the discrepancy, it seems the best way to determine OUR is through an off-gas measurement. Knowing the input air flow rate (can be measured accurately) and off-gas oxygen content, the calculation is straightforward and has good accuracy assuming conditions are close to steady state. [We could do that on an existing aeration tank, say 3 m or so, or on an experimental column as per ASCE 18-18.].

A non-steady state test (switching from air to pure oxygen, for example or perhaps a reduction in DO by switching from air to nitrogen to de-aerate to a low DO, but still positive to avoid impacting the biology) followed by resumption of the usual air-based aeration to steady state (C_R) will yield a K_La_f value that would be the same K_La_f value according to either the conventional or the proposed derivations. [This is similar to Garcia's experiment.] Then, plugging in the values of OUR (from off-gas) into both equations will verify which is correct. Mixed liquor at endogenous respiration conditions (i.e., no external substrate) provides a pretty constant OUR and would be a good respiring system for testing.

The deficiency of an incomplete model is most apparent when attempting to use CFD to model activated sludge systems because of the alpha-factor, even though it can be quite easily modeled

in clean water, as alpha is highly sensitive to local and dynamic conditions that simplified models often ignore [5,6]. Alpha is the ratio of the K_La of clean diffusers in process water to their KLa in clean water, and can range from approximately 0.1 to greater than 1.0 [7-14]. Since the impacts of biochemical reactions on the parameters are different from the impact of contaminants, the former is related to the OTR (oxygen transfer rate or oxygen dissolution rate) which is more related to the driving force, and the latter is an impact on K_La which is more related to the transfer efficiency of the aeration device, the modelling equations would necessarily change to reflect this modified concept in any attempt to use CFD to eliminate the alpha-uncertainty based on the conventional equations.

2. Resistance in Oxygen Transfer

Figure 2 shows a conceptual representation of the mechanism in which gas transfers into a typical liquid cell. In this figure, the thick line represents the energy grade line for a fixed energy input representing the evolution of the oxygen energy potential as a function of the energy transport length, *Ci* being the interfacial DO concentration and, C^*_f is the saturation concentration in the field. The difference between the oxygen content of the feed and exit gas is termed the "exit gas depletion". This difference between the input feed gas and the exit gas is the net gas supply rate (m_0). When m_0 matches the oxygen demand R, then $m_0 = R$, in terms of per unit volume. The topic of R measurement is covered and a more precise method for measuring R using various methods including a dilution method that avoids shaking up a collected MLSS sample are presented in [15,16]. In the transport of the DO molecules, one could say there is a resistance force against the eventual oxygen saturation of water.

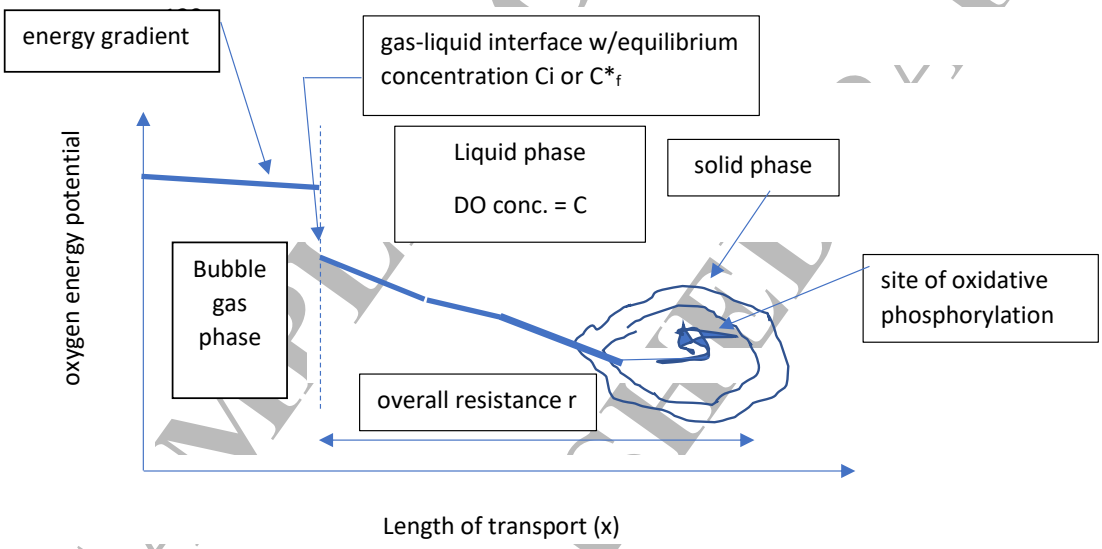

Figure 2: Conceptualization of the Energy Gradient from Gas to Liquid and to Cell

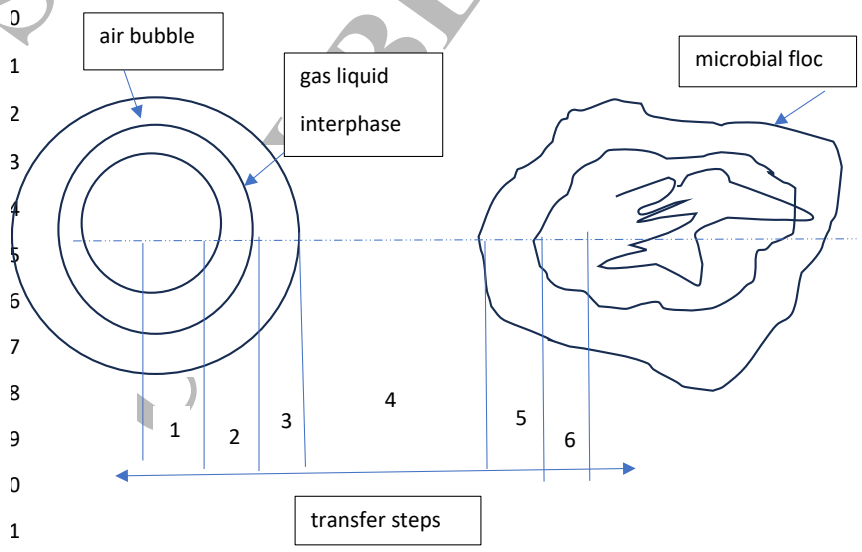

Figure 3: Oxygen Transport and uptake in a Three-Phase Biological Reactor [17],

We posit that dissolved oxygen transfer in natural water bodies or any liquid body is not an energyless process. The total energy *E* within the bubble gas phase is used to overcome resistance "r" of flow through the broth and the liquid boundary layer of the cells [18]. But according to one critic, which the authors have disputed:

"Assuming that the energy required will reduce substantially the mass of oxygen transferred during a given time is either fully erroneous or a revolutionary idea. Generations of physicists and chemists have studied the processes of mass transfer and diffusion, since the 19th century, and I have never heard of a latent heat of diffusion, which would be similar to the latent heat of vaporization. Of course, I am not a physicist, …. so, if Mr Lee considers that energy "r" should be included in the mass transfer equations, he should submit his work to a more appropriate journal. However, I would suggest him to prepare a very strong background, based on two centuries of literature, much stronger than a simplistic reference to pipe hydraulics, as in the current version of his manuscript."

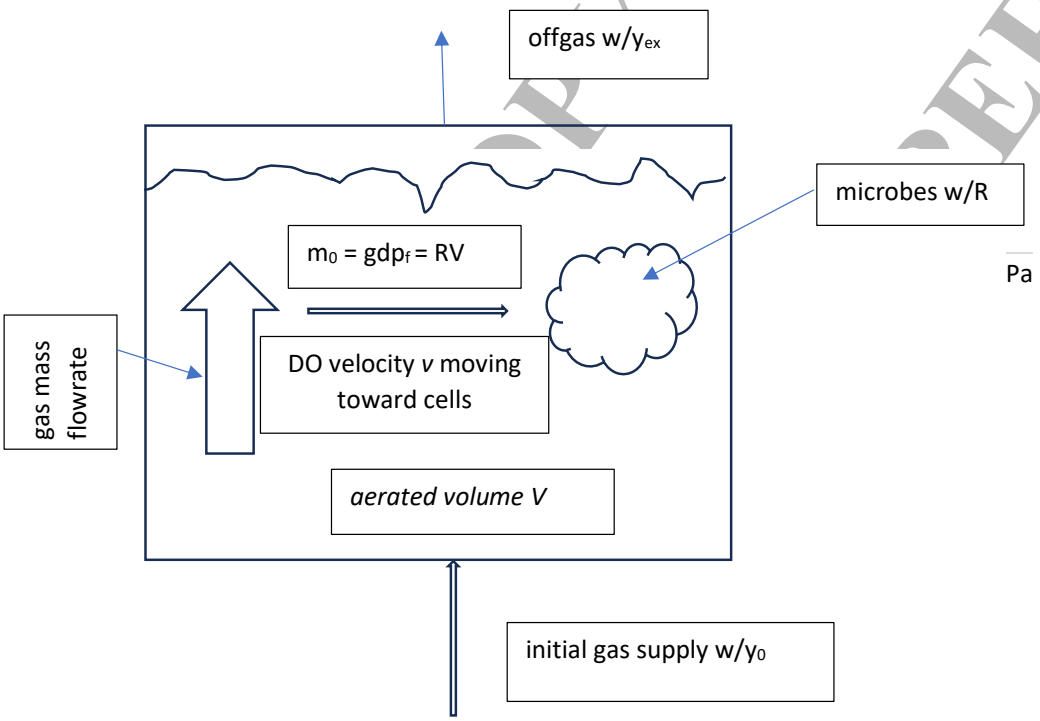

Figure 4: Detailed Schematic of step 4

In the event where the transfer rate is zero at this state, (i.e., the consumption rate is also zero), the oxygen transfer rate in terms of kg O_2/hr (*OTR*) or (m_0) = K_La (C^*_∞ - *C*), during the unsteady state before reaching the steady state [19].

Fig. 3 gives a schematic of the transfer mechanism illustrating the six steps (without the details) based on Campbell 2020 to make the conceptual illustration intuitive and system-specific. Fig. 4 gives a schematic showing the mechanism of the oxygen transfer in step 4.

Conversely, when there is microbial demand causing a loss of energy, the effect is a reduction of the OTR. Therefore, $OTR = K_La\ (C^*_\infty - C) - R$, because m_0 is reduced if the energy supplied is kept constant. Note that the gas-side oxygen depletion rate (gdpf) and the net gas supply rate m_0 are the two sides of the same coin, so that m_0 is reduced when *R* increases. Then the gas-phase mass flowrate or the exit gas increases for the same initial gas supply rate as shown in Fig. 4. The gdp_f can be measured to be exactly the same as *R* when the system is at a steady state [20].

According to Henry's Law, at constant temperature, the concentration of oxygen molecules in the [treated] water column is proportional to the solubility and partial pressure of the oxygen. Once the oxygen molecule has migrated into the water phase, the conventional assumption is that the oxygen molecules become instantaneously and homogeneously diffused and/or mixed throughout the water column. Strictly speaking, this assumption is incorrect since the diffusion process, although considered spontaneous, is a time-consuming process and therefore, far from being instantaneous. Showed that multi-phase flows with bubbles entrained in water are energy processes [21]. In another paper a new parameter is proposed to determine the type of air-water mass transfer interface [22]. On this basis, developed a supersaturated TDG (total dissolved gas) mass transfer model suitable for the whole process of spillway discharge [23]. The Volume of Fluid (VOF) method which is a CFD technique used to simulate oxygen transfer by tracking the sharp interface between gas bubbles and liquid is used to calculate the aeration concentration, which has limitations for the water surface breakage [24]. Therefore, the

latest aeration simulation methods such as water surface breakage aeration can be introduced in the future to integrate the bubble mass transfer results and improve the accuracy of supersaturated TDG mass transfer simulation [23]. Similarly, the influence of microbial respiration can be introduced in the future to integrate the bubble mass transfer simulations if the underlying mechanism in a respiring system is known. The impact of gas depletion rate (*gdp*) must always be considered in any gas-liquid transfer calculations. The bottleneck must be in the bulk liquid. But since all the motions (from point A at the interface to point B at the cell surface) are in series, this bottleneck transfer rate in the liquid must also affect and also be identical to the transport rate at the oxygen-liquid interface, which changes the equilibrium concentration *C** but still allowing the gas-side driving force to have a vertical distribution, from both hydrostatic pressures affecting the saturation DO and gas depletions reducing the % oxygen during the vertical rise of the bubbles. The gas depletion in the gas phase applied to the dissolved gas being transferred to microbial cells can be explained by Einstein's mass-energy equivalence principle [25]. Using a Taylor expansion, one obtains the kinetic energy expressed in terms of m_0 where v is the velocity of flow of the DO molecules. Therefore, $m_0 = 2E/v^2$ and from it, one concludes that the net gas supply m_0 is equivalent to the kinetic energy loss due to the mass transfer to the microbial cells, and is 221 symbolized as m_0.

The above argument challenges the conventional thinking on oxygen transfer in the presence of microbial oxygen consumption. Therefore, a correction to the conventional equation $OTR = K_L a_f (C^*_{\infty f} - C)$, with, $K_L a_f = \alpha \times K_L a$, and $C^*_{\infty f} = \beta \times C^*_{\infty}$, [where, α and β are correction factors] is necessary. By subtracting the OTR in the absence of microbial respiration by *R*, the mass-energy equivalence principle is satisfied. The equation then becomes $OTR = K_L a_f (C^*_{\infty f} - C) - R$. Relying on first principle arguments, the following equation is derived,

$$\frac{dC}{dt} = OTR - R \qquad (4)$$

Note that for the transfer equation $OTR = dC/dt = K_L a (C^* - C) - R$, $K_L a$ is an empirical value that must be estimated or experimentally assayed (typically in an abiotic setting) [26]. Inaccurate values of $K_L a$ may lead to considerable errors when estimating mass transfer rates in biological systems because biological activity directly affects the properties of the aqueous system through, for example, the release of biosurfactants and other metabolites. It can be argued that effects such as gas-phase oxygen depletion due to oxygen consumption are predominantly more pronounced on *C** than the surfactant effects on $K_L a$. Therefore, after incorporating the effect of gas-side oxygen depletion in a non-steady state, the mass balance equation becomes,

$$\frac{dC}{dt} = K_L a_f \left(C^*_{\infty f} - C\right) - gdp_f - R \qquad (5)$$

The above equation can be used to determine gdp_f since, when the system reaches steady state saturation conditions, $dC/dt = 0$ and $C = C_R$, leading to,

$$gdp_f = K_L a_f (C^*_{\infty f} - C_R) - R \qquad (6)$$

After substituting equation 6 into equation 5, it yields,

$$dC/dt = K_L a_f (C_R - C) \qquad (7)$$

Equation 7 is exactly identical to the experimental equation under a respiring system; where, C_R is the equilibrium or saturation concentration for such a system. Many investigators have found that C_R is a function of *R* for a fixed gas flow rate and substrate. An example is given in [27]. In the above equation (Eq. 7), the apparent saturation concentration as given by ßC* which would be equivalent to *CR* in a respiring system, is indeterminate as opposed to $ßC^*_{\infty}$ that is only measurable for non-respiring waters. In the case of a respiring system, superimposing the bio-chemical process over the non-respiring transfer at any value of *C* may be a significant tendency toward undersaturation, i.e., $C_R \ll C^*_{\infty}$. The apparent saturation concentration will be lower than $ßC^*_{\infty}$ (non-respiring saturation) due to oxygen depletion in the gas bubble.

The sewage flow in the aeration basins typically requires proper design criteria predicated on bench or pilot plant scale tests [28,29]. It is not possible to always test a system at full-scale, largely because full-scale is not available prior to a design. Therefore, the drawback of the current standards lies in the difficulty to facilitate testing under a reduced scale, and the lack of experimental procedures necessary for such formulations. Solving this scale problem requires derivation from first principles as it will be shown below.

3. The Submerged Oxygen Transfer Mechanism

One of the major conflicts between the ASCE standard and the European standards is the mathematical treatment of *C** in the clean water test (CWT). Clean water is usually taken to be equivalent in quality to a potable public water supply. The unsteady-state clean water test is occasionally conducted with detergent added to simulate municipal wastewater. stipulates volumetrically and depth-wise representative sampling as the only method for arriving at the global saturation value, a procedure further supported by Jiang and [30,31]. Proposes the effective depth ratio $e = d_e/Z_d$, where d_e is the effective saturation depth and Z_d is the diffuser depth, to be 50% for a theoretical calculation of the saturation concentration to avoid the need for accurate DO probe calibration, if agreed upon between the parties concerned [32]. While referring to this put forward d_e/Z_d from 40% to 50%, unless the depth is greater than 7 m, for which 33% is stated [33]. For a 6 m diffuser submergence, assuming 50%, and where 33% would be detected by testing, an overestimate of the standard oxygen transfer rate (SOTR) by 8% results, a considerable bias. The SOTR is the standard oxygen transfer rate in clean water at 20 0C, barometric

pressure of 101.3 kPa, and dissolved oxygen of 0 mg/L, in kg/h. By convention, the oxygen transfer capacity of an oxygenation system is usually expressed as the rate of oxygen transfer predicted by the model at zero DO under standard conditions. The empirical approach in the ASCE standard is pretty much the only reasonable way to obtaining the global saturation value, or equivalently, d_e [34]. Unfortunately, the equilibrium concentration under a respiring setting cannot be easily determined through experiments. The parameters K_La and C^* are in fact intimately related. They are inversely proportional to each other under controlled conditions [35]. A simple experiment in a beaker of well-mixed water under aeration would illustrate the fact. If the beaker is initially devoid of dissolved oxygen when subjected to oxygen dissolution by diffusion, the amount of oxygen transfer is the product of K_La and C^* over the beaker volume. This product is a constant no matter how the intermolecular forces change, as can be illustrated by changing the water temperature, within the normal working range, that would affect the kinetic energy that would change the forces [36,9,37,38].

The initial rate of transfer is therefore given by $dC/dt = \underline{C^*}$ K_La. This is the standard model of oxygen transfer in its most elementary form. In all cases, except where a slow chemical reaction is involved, the rate of absorption is controlled by the rate of diffusion through the surface films at the gas-liquid boundary [39]. However, the microbial consumption is a slow chemical reaction, and so the rate of absorption is controlled by the mass-energy equivalence principle rather than the rate of diffusion, as the reaction occurs downstream of the gas-liquid interface within the bulk liquid. The biochemical reactions are usually governed by a low Hatta number which suggests the reaction is slow, and the reaction occurs in the bulk liquid, beyond the liquid film. If this is the case, first the oxygen will be consumed from the liquid phase before it is then transferred from the gas bubble to the liquid phase [40]. However, this mechanism may turn out not be completely accurate. As the dissolved oxygen content builds up in an aeration basin, this build-up of dissolution gas in the aqueous solution exerts a counter-force in favor of diffusing of the DO molecules from the liquid back to the gas phase. This can be written as $dC/dt = K_La$ $(C^* - C)$, as in Equation 1, assuming the liquid film coefficient does not change regardless of whether the gas molecules are going into or out of the bubble, and both C^* and C are time-dependent variables. An exhaustive study of the problem of variable C^* is given who showed that C^* is indeed a function of time as well as space [41].

4. Le Chatelier's Principle Applied to Gas Transfer

Le Chatelier's principle states that the process in the context of a bubble containing oxygen and rising through water with a dissolved-oxygen deficit, relative to the composition of the bubble, would seek equilibrium via the net transfer of oxygen from the bubble to the water [42].

At steady state, equilibrium is typically defined as a state where the gas flowing into the bulk liquid equals the gas flowing out of the bulk liquid. In contrast to clean water, the oxygen mole fraction (the ratio of the oxygen mass content to the entire mass content of a bubble) varies with the bubble location in a wastewater aeration basin, and will not reach equilibrium even at steady state, as it would be represented by a different curve for process water. Steady-state (SS) does not mean equilibrium, but equilibrium does imply SS. The standard mass transfer model for a bulk liquid aeration under constant gas flow rate has been theoretically derived shown below as Eq. (8) [43],

$$\frac{dC}{dt} = K_La\,(C^*_\infty - C) \tag{8}$$

Lee (2018) defined a baseline oxygen mass transfer coefficient (K_La_0) as the oxygen transfer rate coefficient at zero liquid depth and described a model relating K_La to the baseline K_La_0 (Eq. 9 318 below) as a function of temperature, system characteristics (e.g., the gas flow rate, the diffuser depth), and oxygen solubility [44].

$$K_La = \frac{1 - exp(-\Phi Z_d . K_La_0)}{\Phi Z_d} \tag{9}$$

where $\Phi = x(1 - e)$, x = HR'T/Ug, with Ug being the height-averaged superficial gas velocity; H is Henry's Law constant; R' is the specific gas constant of oxygen (note: a different symbol is used to distinguish it from R); T is the water temperature in Kelvin. Furthermore, a model has been developed for the mole fraction variation curve and is defined as the Lee-Baillod model [43]. The model, and the subsequent integrated form, was based on a constant bubble volume and was therefore named the constant bubble volume model (CBVM). For the more general case, where the bubble size is a variable, exacerbated by gas-side gas depletion, the mole 328 fraction variation curve is based on the generalized Lee-Baillod equation, which was derived by assigning calibration factors (n, m) according to,

$$y = \frac{C}{nHP} + \left(\frac{Y_0\,P_d}{P} - \frac{C}{nHP}\right)\exp(-xK_La_0 . mz) \tag{10}$$

Eqs. (9) and (10) can be utilized to formulate five simultaneous equations for solving the unknown parameters (n, m, K_La_0, y_e, Z_e) as described [43]. Hence, the basic transfer equation for the non-steady state clean water test as given above by Eq. (8), is proven valid for the general case (non-constant bubble volume) as well, where K_La and C^*_∞ are obtainable by solving the above set of equations when the baseline K_La_0 is known. When only the baseline is known, one more equation is needed. This additional equation can be obtained by applying Eq. 336 (18) derived in the next section. The concept of a baseline or a benchmark for the mass transfer 337 coefficient was given [43,45,46].

Based on the depth ratio concept above, for a very shallow tank ($Z_d \approx 0$), the transfer equation is again applicable, hence, the following equation applies,

$$\frac{dC}{dt} = K_L a_0 \, (C_S - C) \quad (11)$$

where *Cs* is the handbook solubility value at the atmospheric pressure and water temperature at testing. By comparing Eq. (8) with Eq. (11), it follows that the two mass transfer coefficients are not the same, since the former has incorporated the effect of gas depletion as seen in the derivation, whereas in the latter equation, gas depletion is non-existent because of the hypothetical zero depth [43]. However, for tank aeration with gas depletion, Eq. (8) can be modified to 346 yield,

$$\frac{dC}{dt} = K_L a_0 (C^*_{\infty 0} - C) - gdp_{cw} \quad (12)$$

where the subscript cw refers to clean water and $K_L a_0$ is the baseline as calculated by Eq. (9) thru Eq. (10). In a CWT, the parameters $K_L a_0$, $K_L a$ and $C*_\infty$ can be determined.

$C*_{\infty 0}$ is a parameter that would have existed without the gas depletion, and gdp_{cw} is the overall gas depletion rate during a clean water test. This equation (Eq. 12) is based on overlapping of two functions: the transfer rate as if *gdp* does not exist, and the actual gas depletion rate which is a negative quantity. $C*_{\infty 0}$ cannot be the same as *Cs* because the latter is the oxygen solubility under the condition of one atmosphere pressure only, while $C*_{\infty 0}$ should correspond to the saturation concentration of the bulk liquid under the bulk liquid equilibrium pressure, but minus the gas depletion (this of course is not allowed, since without gas depletion there can be no oxygen transfer). The hypothetical $C*_{\infty 0}$ must, consequently, be greater than $C*_\infty$ which is greater than Cs since the former corresponds to a pressure Pe which is the pressure at the equilibrium level de while the latter corresponds to Pa (e.g., 1 atm). The hypothetical saturation concentration is not determinable, but this method of reasoning allows solving for the transfer from the baseline mass transfer coefficient as shown in Eq. (12). Since $K_L a$ is a function of gas depletion, and since every test tank may have different water depths and different environmental conditions, their gas depletion rates are not the same; hence, they cannot be compared without a baseline [43]. Furthermore, by introducing the term gdpcw, the oxygen transfer rate based on the fundamental gas transfer mechanism (the two-film theory) can be separated from the effects of gas depletions on $K_L a$.

5. Theoretical Translation of Clean to Dirty Water Oxygen Transfer Rates

The gas depletion rate gdp_{cw} cannot be determined experimentally, since *gdp* varies with time throughout the test. Demonstrated the varying nature of the exit gas, which is directly related to the *gdp* if the gas feed is constant, during a non-steady state clean water test [31]. Therefore, the only equation that can be used to estimate the parameters is still Eq. (8).

Note that Eq. (8) is essentially equivalent to Eq. (12) but expressed differently ($K_L a$ *vs.* $K_L a_0$). Therefore, for in-process water without any microbes, Eq. (12) can be expressed as,

$$\frac{dC}{dt} = K_L a_{0_f} \left(C^*_{\infty 0_f} - C \right) - gdp_{ww} \quad (13)$$

where the subscript *f* refers to the dirty water in the field, and subscript *ww* stands for wastewater or the reactor solution without the microbes. In the presence of microbes with a respiration rate *R,* based on the same mathematical development, the following equation results,

$$\frac{dC}{dt} = K_L a_{0_f} \left(C^*_{\infty 0_f} - C \right) - gdp_{ww} - gdp_f - R \quad (14)$$

where gdp_f is the gas side gas depletion due to the microbes only, or when expressed differently as before, Eq. (5) previously derived from the mass-energy equivalence principle is obtained.

Note that in this equation, gdp_f is identical in magnitude to *R*, where *C* becomes a constant, 382 usually denoted by C_R. However, even if *C* varies, as long as it remains above a critical value, *R* 383 will not change and gdp_f remains constant [16]. If the CWT is performed at 20 0C, the average value of SOTR shall be calculated by averaging the values at each of the *n* determination points by,

$$\text{SOTR} = \frac{V}{n} \sum_{i=1}^{n} (K_\text{L}\text{a})_{20i} \, (C^*_\infty)_{20i} \quad (15)$$

from

$$\text{SOTR} = \frac{1}{n} \sum_{i=1}^{n} \text{SOTR}_i \quad (16)$$

and

$$\text{SOTR}_i = (K_\text{L}\text{a})_{20i} (C^*_\infty)_{20i} V \quad (17)$$

In the case of bubble aeration, if the oxygen saturation was not measured at the test, it can be estimated by the following equation to make a correction for the higher hydrostatic pressure, this equation is based but slightly revised to account for the oxygen depletion at the equilibrium level d_e, and is similar to Appendix F when Y_e approaches Y_0, [47,30].

$$C^*_\infty = \frac{(r_w \, d_e + P_a - P_{vt}) C^*_{sT}}{P_a - P_{vt}} \times \frac{Y_e}{Y_0} \quad (18)$$

where Y_e is oxygen mole fraction at equilibrium level d_e, Y_0 is initial mole fraction at diffuser = 0.21, C_s*_T = tabular value of DO surface saturation concentration, at the test temperature, a standard total pressure of 1.0 atm (101.3 kPa), and 100% relative humidity

in units of mg/L [14]. $C^*_{\infty f}$ can then be calculated by using the correction factor ß, resulting in $\boldsymbol{C}^*_{\infty f} = \beta \times C^*_{\infty}$.

The entire proposed aeration design process is written [48]. For design, the conventional approach has been to calculate the required OTR_f using factors for carbonaceous oxygen demand, nitrogenous oxygen demand, denitrification credit if applicable, and so forth. Once OTR_f is determined, a value for alpha is selected, or several depending on the bioreactor configuration. The *SOTR* needed to obtain the design OTR_f is calculated. Once the *SOTR* is known, design proposals from several aeration equipment manufacturers are requested. The aeration system technical specification is then prepared that would include conducting clean water tests in accordance with the ASCE Standard. The equipment manufacturers' proposals are then evaluated to come up with the guaranteed performance requirements presented in the technical specification. One can argue that it is not possible to select an alpha factor that would satisfy all conditions in the field.

The enhanced approach advocated here is that *R* be measured, and the *SOTR* needed to obtain the design OTR_f is calculated by Eq. (5) above. Note that Eq. (5) translates, given that $gdp_f = R$, into the following amendment $dC/dt = K_L a_f (C^*_{\infty f} - C) - 2R$.

If the handbook data of oxygen solubility at various temperatures, also known as surface saturation, together with the physical properties of water at various temperatures is plotted against the inverse of the temperature correction function affecting solubility as derived, the straight-line linear plot as depicted is as shown in Fig. 5 and the equation gives the solubility directly and is expressed by [30,40,35].

$$C^*_{sT} = 43.457 \times \frac{Ps}{(T^5 E_m \rho)} \quad (19)$$

where *Ps* is the standard barometric pressure, 1 atm (101.3 kPa), E_m is the modulus of elasticity, *T* is water/wastewater temperature in Kelvin, ρ is the liquid density.

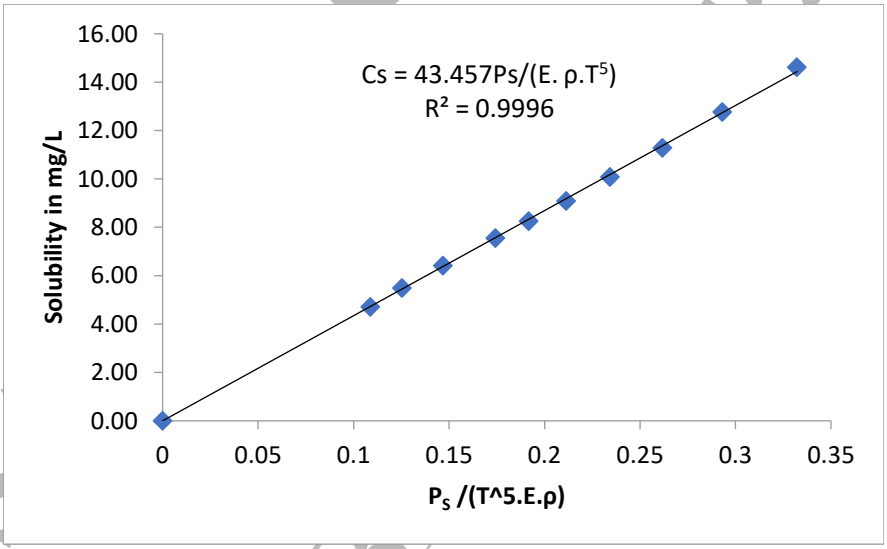

Figure 5: Solubility Plot for Water Dissolving Oxygen at Ps = 1 atm

Henry's Law is applicable only to ideal solutions and for an imperfect liquid subject to changes in physical state, at extreme temperatures between 273 K and 373 K, it is only approximate and limited to gases of slight solubility in a dilute aqueous solution with any other dissolved solute concentrations not more than 1 percent [50]. Since in Henry's Law, the solubility Cs is proportional to the partial pressure, the Henry's Law constant would be given by $H = 43.457/(T^5 E_m \rho)/y_0$, where y_0 is the mole fraction of the solute in air and equates to 0.21 for oxygen. It should also be adjusted for the vapor pressure P_{vt} [35]. In a mixed liquor (MLSS), the liquid density may depart from that of clean water significantly, and so the sample should be measured for its density using a hygrometer to measure the humidity and a hydrometer to measure the relative density, when applying Eq. (18) and Eq. (19). While the modulus of elasticity of pure water is relatively consistent, the presence of various contaminants in wastewater can alter its mechanical properties, potentially increasing or decreasing its stiffness, thus its modulus of elasticity should be measured separately.

6. Measurement and Application of Alpha, α

The alpha factor is influenced by a great number of process conditions, including surfactants, turbulence, power input per unit volume, geometry, scale, bubble size, sludge age, degree of treatment, and other wastewater characteristics. Several studies have described small-scale tests for measurement of the alpha factor, such as [12]. To circumvent the above uncertainties, the following procedure is recommended to be used in the bench-scale determination of the relative oxygen transfer coefficient, α.

A vessel similar to that shown can be used [51]. For the diffused

system, where the gas-side gas depletion effect is significant and testable, an air measuring rotameter can be installed for recording the gas flow rate. Clean water tests can then be performed with tap water as per until a reproducible K_La is obtained and re-aeration curves can be plotted, and the important parameters K_La and C^*_∞ can then be estimated using the non-linear least squares (NLLS) method as described in the standard [30]. If wastewater is used in the test, the procedure should come after the clean water test, and should be repeated using the same volume of wastewater as the previous clean water test. As the test results would depend on the microbial respiration rate, as previously described, every effort should be made to eliminate the influence of the microbial respiration. This can be achieved by killing off all live microbes, such as using a sulphamic acid455 copper sulphate solution, or if a bench scale biological reactor has been used, the effluent from the reactor should be used for the test when a completely mixed system is contemplated either in the 457 entire aeration basin, or a section of the basin where complete mixing is envisaged.

If the latter method is used, the biological solids should be filtered out to prevent any microbial oxygen uptake that remains during the test period. The respective K_La values determined from the two tests (clean water vs. wastewater) can then be compared at the same temperature, pressure and mixing conditions, and α can be calculated in accordance using the following equation,

$$\alpha = (K_La_f \text{ wastewater}) / (K_La \text{ clean water}) \quad (20)$$

In the application for wastewater treatment, using the transfer of oxygen to clean water as the datum, the equivalent bench-scale oxygen transfer coefficient (K_La_{0f}) for a wastewater system can be determined, and the ratio of the two coefficients can then be used as a correction factor to be applied to fluidized systems treating wastewaters via aerobic biological oxidation, where microbial respiration has a significantly different contribution to gas depletion compared to clean water.

Before any mass balance equations can be used to evaluate this difference in the gas depletion rates, it is paramount to determine α, the correction factor 470 given also by [52,53],

$$\alpha = \frac{K_La_{0f}}{K_La_0} \approx \frac{K_La_f}{K_La} \quad (21)$$

It is postulated that α can be determined by bench scale experiments or by pilot tests as mentioned above. It is hypothesized that this alpha value is not dependent on the liquid depth and geometry of the aeration basin and the model developed that relates K_La to depth then allows the alpha value to be used for any other depths and geometry of the aeration basin where the mass transfer coefficient can be generically represented by a function K_{LB} (the average K_La for the entire basin) 477 as shown which shows exactly what found in his experiments [43,54]. That is, that K_La_f decays with respect as the depth of the immersion vehicle of gas supply increases.

Therefore, using Equations 20 and 21, and after incorporating **α** into Eq. (9) for in-process water, 480 the mass transfer coefficient in in-process water K_La_f would be given by,

$$K_La_f = \frac{1 - \exp(-\Phi Z_d . \boldsymbol{\alpha} K_La_0)}{\Phi Z_d} \quad (22)$$

Where symbols are as previously defined. By plotting K_La_f against the function ØZd for when the baseline is unity for various α values, K_La for any test conditions can be found. If K_La_f is measured at full-scale as in, then the baseline can be calculated by rearranging Eq. (22) to yield [9],

$$K_La_0 = \frac{\ln(1 - \emptyset \boldsymbol{\alpha} K_La)}{(-\emptyset \boldsymbol{\alpha} Z_d)} \quad (23)$$

where, $K_La_f = \boldsymbol{\alpha} K_La$. The full-scale measured K_La_f that is measured in accordance to ASCE standards should then match up with the K_La_f (Eq. 22) calculated from the baseline K_La_0 (Eq. 23) as determined from the CWT.

7. Conclusion

In this manuscript, the author postulates that the true OTR_f for a batch process is given by K_La_f 492 ($C^*_{\infty f}$ -C) -R, so that the standards ASCE/EWRI 02-22 and ASCE/EWRI 18-18 should be 493 amended as follows:

- The oxygen transfer efficiency based on the oxygen transfer rate by a prescribed CWT for a fixed gas supply is uniquely defined by a standard specific baseline value K_La_0 [43].
- A new mathematical model for the gas depletion rate (*gdp*) has been derived namely, in Equations 9 and 10, which were verified by testing under a variety of water depths for clean water [55,56,43]. This model is shown to be applied to wastewater through an alpha factor (α) that pertains specifically to wastewater characteristics as shown in Equation 21.
- The respiration rate produces additional resistance to oxygen transfer in the system resulting in a loss of *gdp,* that would lead to an increase in the exit gas oxygen content compared to the CWT at the process DO level, and therefore must be accounted for in the mass balancing equations [10].
- The difference in gdp_f due to the microbial cells that affect oxygen transfer is precisely R itself based on all the test results in the literature, and therefore is important for the revising of the ASCE equations [36,57,58,45].
- Using the α value would now require revising the design equations to include the gas depletion effect as evidenced in this manuscript; otherwise, α would become highly unpredictable [52,53,59].
- The oxygen transfer equation in this research aims to decouple biological effects due to bacterial activity from physical ones to achieve more reliable and consistent aeration system designs and operations. The enhanced equation should be given by Eq. (5) which translates, given that $gdp_f = R$, into the following amendment $dC/dt = K_La_f(C^*_{\infty f} - C) - 2R$. The effects of temperature in the selection of a proper value for the temperature correction parameter Θ, and the

effect on $K_L a$ due to geometry and wastewater characteristics (Eqs. 20 thru 23) have been covered in this and previous manuscripts [38,35,43].

Data Availability Statement

All data, models, and code generated or used during the study appear in the submitted article.

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