

An Alternative Mathematical Model for Oxygen Transfer Evaluation in Clean Water

Yanjun (John) He^{1*}, PE, BCEE

¹Kruger Inc., 4001 Weston Parkway, Cary, NC 27513

*Email: john.he@veolia.com

ABSTRACT

Energy consumption from aeration system is a biggest part of the total energy cost in wastewater treatment plant and account for as much as 60% of the energy consumption for the activated sludge process. Therefore, it is very important to know how effective the aeration system and significant attention has been paid to development and upgrade of standard method for quantifying oxygen transfer efficiency of the aeration system. In order to evaluate the performance of different types of aeration systems, the American Society of Civil Engineers (ASCE) and US EPA jointly developed a standard for the measurement of oxygen transfer in Clean Water in 1984. The Standard was subsequently improved, updated, and republished in 1991 and 2006. The focus of this paper has been to develop an alternative model which includes more parameters than the standard method. A new model would probably be a more accurate description of the aeration process and give more reliable oxygen transfer performance evaluation results.

KEYWORDS

Aeration, ASCE, SOTR, oxygen transfer, transfer coefficient, surface transfer, Model

INTRODUCTION

The ASCE Standard Method for the measurement of oxygen transfer in clean water, which has also been called the Nonlinear Regression Method, is based on the “unsteady-state” removal of dissolved oxygen (DO) by sodium sulfite followed by re-oxygenation back to “saturation” or steady-state conditions with accurate experimental measurement of the DO level over time. The results of the test are converted into the values at the standard conditions and the final results are expressed as standard oxygen transfer rate (SOTR) or standard oxygen transfer efficiency (SOTE), a hypothetical oxygen mass transferred per unit of time or fraction of oxygen in an injected gas stream dissolved in clean water when DO concentration is zero in the water volume, the water temperature is 20 °C, and the barometric pressure is 1.00 atm (101 kPa).

The following standard simplified mass transfer model is used to analyze DO measurement data to estimate volumetric mass transfer coefficient:

$$\frac{dC}{dt} = K_L \alpha \times (C_\infty - C_t) \quad (1)$$

Where $K_L \alpha$ is volumetric mass transfer coefficient (T^{-1}), C_∞ is the saturation or near saturation DO concentration at infinite time (mg/L), and C_t is the dissolved oxygen at time t .

Integration and re-arrangement of Eq. 1 gives:

$$K_L \alpha = \ln \left(\frac{C_\infty - C_0}{C_\infty - C_t} \right) \times \frac{1}{(t - t_0)} \quad (2)$$

Once $K_L \alpha$ value at site conditions is determined by Eq. 2, the SOTR can be readily calculated by the following equation:

$$\text{SOTR} = K_L \alpha \times \theta^{(20-t)} \times C_{s,20} \times V \quad (3)$$

Where Θ is the empirical temperature correction factor and V is liquid volume in the test tank with aerator.

Examination of Eq. 1 reveals that the standard model simply assumes the following: (1) water in the tank is completely mixed; (2) the overall oxygen transfer is only from air bubbles, oxygen transfer from water surface is not taken into consideration; (3) the equilibrium DO concentrations are the same everywhere in the tank, the DO equilibrium concentrations variation with water depth is also not taken into consideration. Since BIDs are won and lost by as little as 2 - 5% difference in oxygen transfers rates, it is important to know how accurate the standard method for quantifying oxygen transfer rate.

The paper reports how big the impact of oxygen transfer from the air is at the water surface in SOTR calculations. The paper also reports the effect of the equilibrium DO concentrations, which is also depending on the ratio of oxygen in the air bubble which varies with water depth in SOTR calculations.

METHODOLOGY

Modified Standard Method Model 1

When a submerged diffuser is operated, there are two main interfaces over which oxygen transfer occurs. Oxygen transfer occurs across the bubble interfaces as the bubbles rise through the water column. Oxygen transfer also occurs across the water surface where oxygen in the air dissolved into water. At the water surface, oxygen transfer is driven by the DO concentration gradient between gas-liquid films. The oxygen transfer across bubbles is driven by the DO concentration gradient between the equilibrium DO concentration and actual DO concentration in liquid phase.

In order to describe the oxygen transfers from the water surface and bubbles, we separate the total mass transfer into two different parts make it possible to evaluate the oxygen transfer from the air bubbles and at the water surface. The mass transfer coefficient for the air bubbles, $K_L \alpha$, is assumed to be present in the whole tank and the water is assumed to be completely mixed. $K_L \alpha_s$, which is the mass transfer coefficient at the water surface, is only present at the water surface. $K_L \alpha_s$ value depends on level of turbulence at water surface. The more turbulence at the water surface the more oxygen is transferred and $K_L \alpha_s$ increases (DeMoyer et al, 2003). How turbulent the water surface is can depend on the type of aeration system and the air flow rate.

$$\frac{dC}{dt} = K_L a \times (C_\infty - C_t) + K_{Ls} a_s (C_{SC} - C_t) \quad (4)$$

Where $K_L a_s$ is volumetric mass transfer coefficient (T^{-1}) at water surface, C_{SC} is the saturation concentration at site temperature and atmospheric, which is equal to C_∞ , and C_t is the dissolved oxygen at time t .

Integration and re-arrangement of Eq. 4 becomes:

$$\ln \frac{(C_t \times \lambda + \xi)}{(\xi + \lambda \times C_0)} \times \frac{1}{(t - t_0)} = \lambda \quad (5)$$

Where $\xi = K_L a \times C_{SC} + K_{Ls} a_s \times C_{SC}$, $\lambda = -K_L a - K_{Ls} a_s$, and C_0 is DO concentration at time zero. If the initial dissolved oxygen (D.O) concentration is 0 mg/L at time zero, Eq. 5 becomes:

$$\ln \frac{(C_t \times \lambda + \xi)}{\xi} \times \frac{1}{(t - t_0)} = \lambda \quad (6)$$

When system is at the steady state condition, $C_{(t)} \rightarrow C_{SC}$, Eq. 6 can be simplified as:

$$\ln \frac{2 \times K_L a_s}{K_L a + K_{Ls} a_s} = \lambda \times (t - t_0) \quad (7)$$

Because C_{SC} is DO saturation concentration at site conditions and can be calculated based on Henry's Law or can be found in the chemical engineering textbook or elsewhere (Lewis, 2006). $K_L a_s$ is the only parameter that must be evaluated. Once $K_L a_s$ is known, it is a simple matter to calculate $K_L a$ at site conditions and calculate the SOTR using Standard Method as discussed in preceding paragraph. a_s is ratio of total water surface area (A_s) to total tank volume (V), K_{Ls} is air-water transfer coefficient and it has been determined by a number of researchers (McWhirter and Hutter, DeMoyer, C.D. et al) under various test conditions. $K_L a_s$ could be also measured. The standard simplified mass transfer model as discussed in preceding paragraph is used to analyze DO measurement data to estimate volumetric mass transfer coefficient $K_L a_s$.

Modified Standard Method Model 2

Because the liquid phase equilibrium concentration of a given bubble is not only a function of temperature and atmospheric pressure, but also hydrostatic pressure and gas phase oxygen composition, oxygen transfer across bubbles as bubbles rise through the water column must include some additional considerations. First is that bubble-gas transfer of oxygen, nitrogen and some other trace gases occurs due to absorption process in the liquid phase. As a result, gas phase oxygen composition changes over the depth in the gas bubble. Second event that complicates the modeling of oxygen transfer is that DO equilibrium concentration also varies with water depth. According the Henry's law, the higher the pressure, the more oxygen can be dissolved in the water.

In order to describe the oxygen transfer behavior with considerations of oxygen transfer at water surface and the difference in equilibrium concentrations with depth, the following simplified mass transfer model that combine Standard Model and Modified Model 1 is used to analyze DO measurement data to estimate volumetric mass transfer coefficient:

$$\frac{dC}{dt} = \frac{K_L \alpha}{Z_d} \times (C_0^*(z) - C) dz + K_{L_s} \alpha_s (C_{SC} - C_t) \quad (8)$$

Where Z_d is side water depth to aeration system (L), Z is side water depth (L), and C_0^* is dissolved equilibrium concentration (mg/L). The DO equilibrium concentration, C_0^* can be estimated by following equation (McWhirter and Hutter, 1989):

$$C_0^*(z) = C_{SC} \times \left[\frac{P - P_{wv} + \frac{(Z_d - Z)}{10.33}}{1 - P_{wv}} \right] \times \frac{y}{0.266} \quad (9)$$

where y (kmol O_2 /kmol N_2) is gas-phase oxygen composition, which is the molar ratio of oxygen to nitrogen gas in the gas phase, P_{wv} (atm) is water vapor pressure, P (atm) is atmospheric pressure, 0.266 (kmol O_2 /kmol N_2) at $z = 0$ when the bubbles released from the diffusers.

Integration of Eq. 8 yields:

$$\frac{dC}{dt} = \frac{K_L \alpha}{Z_d} \int_0^z (C_0^*(z) - C_t) dz + K_{L_s} \alpha_s (C_{SC} - C_t) \quad (10)$$

In order to solve Eq. 10, C_0^* must be computed. Because y must be determined to be able to calculate C_0^* in Equation 8, and y is also depth dependent, it makes the computation of Eq. 10 extremely complicated. However, because at the steady state condition, $C_{(t)} \rightarrow C_{SC}$ and

$\frac{dC}{dt} \rightarrow 0$, Eq. 10 can be simplified as:

$$\frac{K_L \alpha}{Z_d} \int_0^z (C_0^*(z) - C_t) dz = 0 \quad (11)$$

Re-arrangement of Eq. 11 gives:

$$K_L \alpha = \int_0^z (C_0^*(z) - C_t) dz \times Z_d \quad (12)$$

The mass transfer model as discussed in preceding paragraph is used to determine $K_{L_s} \alpha_s$. $K_L \alpha$ can be easily calculated by Eq. 12. Once $K_{L_s} \alpha_s$ and $K_L \alpha$ are known, it is a simple matter to calculate the SOTR using Standard Method as discussed in Instruction paragraph.

RESULTS AND DISCUSSION

Fundamentals of K_La Prediction Using ASCE Standard Method

ASCE Standard Method (Figure 1) is based on a very simple model by assuming oxygen transfer only occurs across the bubbles and liquid water. The method requires measurement of DO over time and estimation of K_La by using nonlinear regression. Once K_La is determined, SOTR is calculated using the Eq. 3.

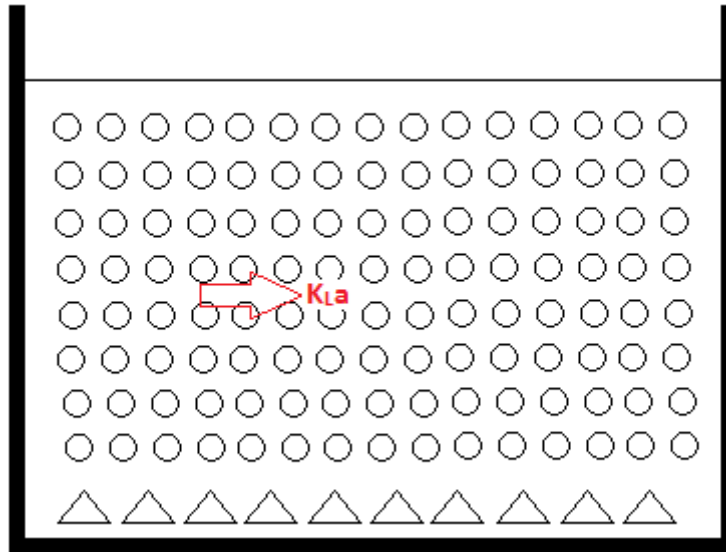


Figure 1. ASCE Standard Method Model Schematic Showing Oxygen Transfer Only Occurs across Air Bubbles and Bulk Liquid

Because ASCE Standard Method requires continuously recording DO values until DO concentration in the tank reaches at least 98% of the presumed steady state concentration, all measured DO concentrations over time are given in Table 1. Table 1 also lists the best estimates of three major parameters (K_La , DO saturation concentration, and initial DO concentration) that must be determined in the standard model. C_0 is the DO concentration at time zero, which is 0.04 mg/L. C_∞ is the saturation or near saturation DO concentration at infinite time (mg/L), this can be measured or calculated based on the equation in the ASCE standard. K_La values are calculated based on Eq. 2. Figure 2 shows re-aeration data and % of DO saturation concentration over time, plotted to conform to ASCE standard method. Table 2 shows estimated SOTR and SOTE values using K_La , tank volume, air flow rate, and diffuser submerged depth.

Table 1. Measured DO Data and Estimated Parameters for Standard Model

Time	DO	DO Saturation	Initial DO Conc.	% Cs	Log Deficit	K_La
(minutes)	(mg/L)	(mg/L)	(mg/L)	%	NA	hr ⁻¹
0.00	0.04	10.65	0.04	1%	0.01	NA
0.25	0.07	10.65	0.04	1%	0.01	1.58
0.50	0.12	10.65	0.04	1%	0.01	1.36
0.75	0.13	10.65	0.04	1%	0.01	0.98
1.00	0.15	10.65	0.04	1%	0.01	0.85
1.25	0.12	10.65	0.04	1%	0.01	0.54
1.50	0.14	10.65	0.04	1%	0.01	0.53
1.75	1.08	10.65	0.04	10%	0.11	3.66
2.00	1.95	10.65	0.04	18%	0.20	6.06
2.25	2.99	10.65	0.04	28%	0.33	8.77
2.50	4.00	10.65	0.04	38%	0.47	11.28
2.75	4.68	10.65	0.04	44%	0.58	12.60
3.00	5.34	10.65	0.04	50%	0.69	13.89
3.25	6.09	10.65	0.04	57%	0.85	15.62
3.50	6.53	10.65	0.04	61%	0.95	16.24
3.75	7.02	10.65	0.04	66%	1.07	17.18
4.00	7.52	10.65	0.04	71%	1.22	18.32
4.25	7.83	10.65	0.04	73%	1.32	18.70
4.50	8.18	10.65	0.04	77%	1.46	19.42
4.75	8.43	10.65	0.04	79%	1.56	19.74
5.00	8.68	10.65	0.04	81%	1.68	20.17
5.25	8.91	10.65	0.04	84%	1.80	20.62
5.50	9.15	10.65	0.04	86%	1.95	21.29
5.75	9.28	10.65	0.04	87%	2.04	21.30
6.00	9.39	10.65	0.04	88%	2.12	21.24
6.25	9.60	10.65	0.04	90%	2.30	22.11
6.50	9.67	10.65	0.04	91%	2.37	21.89
6.75	9.78	10.65	0.04	92%	2.49	22.12
7.00	9.89	10.65	0.04	93%	2.62	22.47
7.25	10.01	10.65	0.04	94%	2.79	23.09
7.50	10.06	10.65	0.04	94%	2.87	22.95
7.75	10.10	10.65	0.04	95%	2.94	22.74
8.00	10.18	10.65	0.04	95%	3.09	23.17
8.25	10.30	10.65	0.04	97%	3.37	24.54
8.50	10.29	10.65	0.04	96%	3.35	23.62
8.75	10.34	10.65	0.04	97%	3.49	23.93
9.00	10.38	10.65	0.04	97%	3.62	24.14
9.25	10.41	10.65	0.04	98%	3.73	24.21
9.50	10.49	10.65	0.04	98%	4.11	25.94
9.75	10.45	10.65	0.04	98%	3.90	24.01
10.00	10.48	10.65	0.04	98%	4.05	24.31
10.25	10.55	10.65	0.04	99%	4.53	26.49

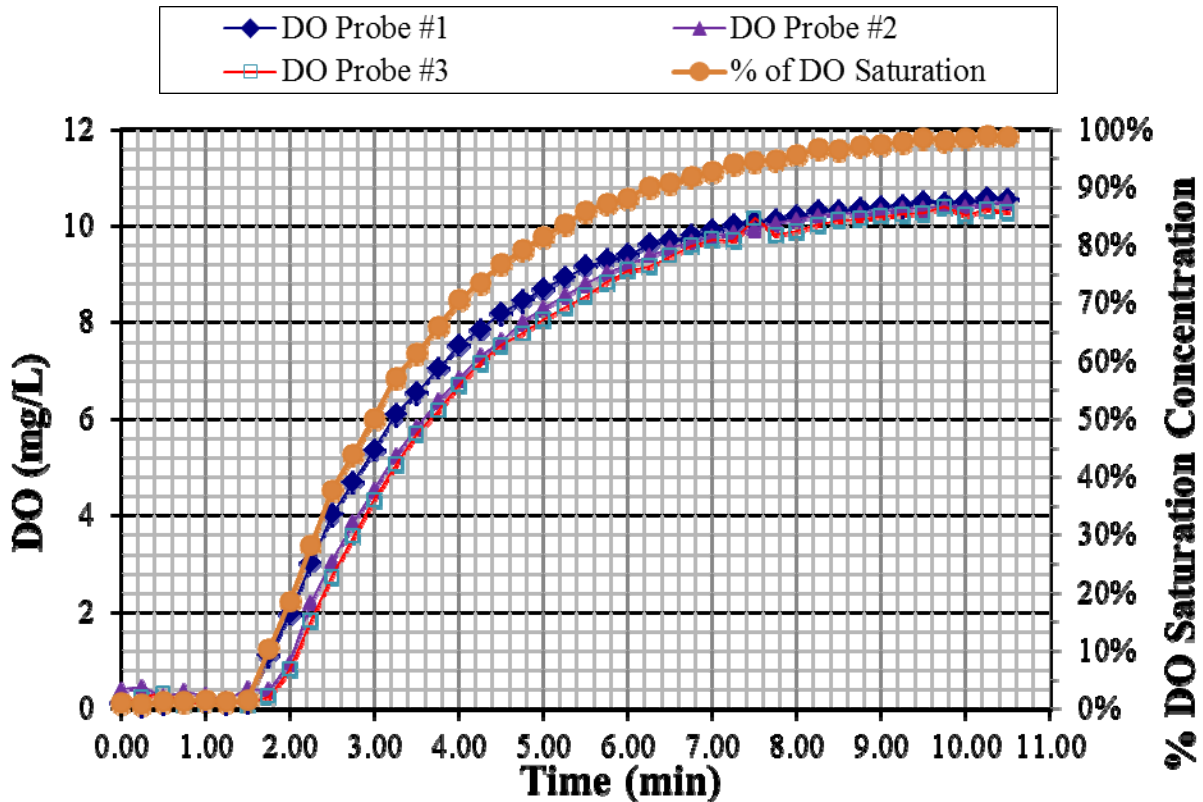


Figure 2. Measured DO Concentrations and % of DO Saturation over Time

Table 2: Standard Oxygen Transfer Rate and Efficiency Test Results Using ASCE Standard Model

Air Flow (SCFM)	Tank Volume (MG)	Diffuser Depth (ft)	K_{La} @ Site (hr^{-1})	K_{La} (20 °C) (hr^{-1})	SOTR (lbs/hr)	SOTE (%)	SOTE (%/ft)
3,500	0.333	16.45	26.49	26.62	809.44	22.34	1.36

Fundamentals of K_{La} Predication Using Modified Standard Model 1

As discussed in Methodology Section, there exist two difference mass transfer zones for oxygen transfer (Figure 3) in a diffused aeration system where the air is discharged into liquid on the bottom of the aeration tank and rise through liquid to the water surface. Because oxygen transfer rate consists of two terms: one from the air bubbles and the other from the water surface, $K_{La,s}$ must be determined to be able calculate K_{La} .

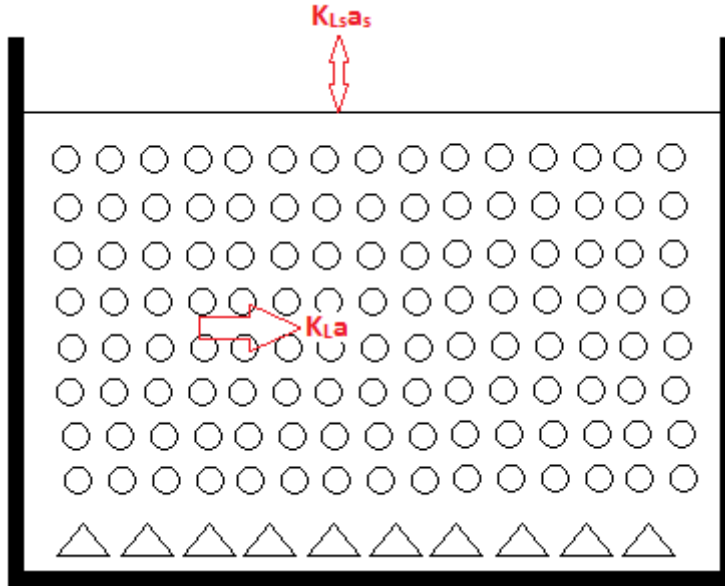


Figure 3. Modified Model 1 Schematic Showing Oxygen Transfer Only Occurs across Air Bubbles and Water Surface

Because a_s is ratio of total water surface area (A_s) to total tank volume (V), K_{Ls} is air-water transfer coefficient and it has been determined by a number of researchers (McWhirter and Hutter, DeMoyer, C.D. et al) under various test conditions, $K_{Ls} a_s$ calculation becomes very simple.

Once $K_{Ls} a_s$ is calculated, $K_L a$ can be calculated using the following equation:

$$SOTR = V \times [K_L \alpha \times (C_\infty - C_t) + K_{Ls} \alpha_s (C_{sc} - C_t)] \quad (13)$$

In order to use Eq. 7 to determine $K_L a$, an iterative approach must be used by assuming an arbitrary $K_L a$ value as an initial guess and repeat same calculation till values in two sides are equal. All estimated parameters using Modified Standard Model 1 are summarized in Table 3. As shown in Table 3, $K_{Ls} a_s$ value is relatively small in comparison to the total $K_L a$, this can be explained by bubble oxygen transfer is still the primary mode of oxygen transfer for aeration system in the deep aeration tank (17ft) in comparison with surface oxygen transfer.

Table 3. Standard Oxygen Transfer Rate and Efficiency Test Results Using Modified Standard Model 1

Air Flow (SCFM)	Tank Volume (MG)	Diffuser Depth (ft)	$K_L a$ (20 °C) (hr^{-1})	$K_{Ls} a_s$ (20 °C) (hr^{-1})	SOTR (lbs/hr)	SOTE (%)	SOTE (%/ft)
3,500	0.333	16.45	26.62	0.60	751	20.74	1.26

Fundamentals of $K_L a$ Predication Using Modified Standard Model 2

In this mass transport model, the air phase oxygen composition in the bubbles varies with depth. Air released from the diffuser contains an initial air phase oxygen composition (mole ratio) of 0.266 (0.21 O₂/0.79 N₂). At the same time, although solubility of nitrogen gas is almost twice as much as oxygen, the concentration gradient of nitrogen is significantly lower (DeMoyer et al). As a result, gas phase oxygen composition decreases over depth. K_{La_s} can be determined by the same method as discussed in preceding paragraph. C_0^* can be determined by Eq. 9. Once K_{La_s} and C_0^* are known, K_La can be determined by Eq. 12. All estimated parameters using Modified Standard Model 2 are summarized in Table 4. As shown in Table 4, the impact of oxygen transfer from the air is at the water surface in SOTR calculations can be significant (~10%). Meanwhile, the equilibrium DO concentrations and oxygen composition in gas bubble, which vary with water depth have a significant impact in SOTR calculations.

Table 4: Standard Oxygen Transfer Rate and Efficiency Test Results

Method	K_{La} (20)	K_{La_s}	SOTR	SOTE	SOTE/ft	K_{La} Difference
	hr ⁻¹	hr ⁻¹	lbs/hr	%	%	%
Standard	26.49	-	809.00	22.34	1.36	0.00
Modified 1	24.11	0.60	751.00	20.74	1.26	-7.7%
Modified 2	34.10	0.60	1000.00	28.90	1.76	19%

CONCLUSIONS

- Field oxygen transfer results presented in this paper supported the conclusion that standard method for oxygen transfer measurements oversimplified the oxygen transfer process by assuming surface oxygen transfer is negligible
- Field oxygen transfer results presented in this paper also supported the conclusion that standard method for oxygen transfer measurements oversimplified the oxygen transfer process by assuming the equilibrium DO concentrations are the same everywhere in the tank.
- Field oxygen transfer presented in this paper indicated oxygen transfer from water surface is around 10% of bubble transfer oxygen.
- Field oxygen transfer presented in this paper shown oxygen mass transfer efficient and SOTR measurement error could be up to 20% due to surface oxygen transfer and liquid-water DO equilibrium concentrations and gas phase oxygen composition variation over the depth.
- Standard method for oxygen transfer measurements dose not describe the whole aeration process, in order to get comparable results, all investigates must the method at the same conditions.

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