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Development of Mathematical Model for Overall Oxygen Transfer Coefficient of an Aerator and Comparison with CFD Modeling

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***Abstract*—**The value of overall oxygen transfer Coefficient (K_La), which is the best measure of oxygen transfer in water through aeration, is obtained by a simple approach, which sufficiently explains the utility of the method to eliminate the discrepancies due to inaccurate assumption of saturation dissolved oxygen concentration. The rate of oxygen transfer depends on number of factors like intensity of turbulence, which in turns depends on the speed of rotation, size, and number of blades, diameter and immersion depth of the rotor, and size and shape of aeration tank, as well as on physical, chemical, and biological characteristic of water. An attempt is made in this paper to correlate the overall oxygen transfer Coefficient (K_La), as an independent parameter with other influencing parameters mentioned above. It has been estimated that the simulation equation developed predicts the values of K_La and power with an average standard error of estimation of 0.0164 and 7.66 respectively and with R^2 values of 0.979 and 0.989 respectively, when compared with experimentally determined values. The comparison of this model is done with the model generated using Computational fluid dynamics (CFD) and both the models were found to be in good agreement with each other.

***Keywords*—**CFD Model, Overall oxygen transfer coefficient, Power, Mathematical Model, Validation.

I. Introduction

THE rotor is rotated to create turbulence in the water body so that the aeration takes place through interface of atmospheric oxygen and the water surface1[1]. The rate of oxygen transfer depends on number of factors like intensity of turbulence, which in turns depends on the speed of rotation, size, and number of blades, diameter and immersion depth of the rotor, and size and shape of aeration tank, as well as on physical, chemical, and biological characteristic of water [2]-[3]. The aeration process generally depends on three types of variables, namely geometric, physical and dynamic variables. Based on this the mathematical model is formulated.

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II. Mathematical Model

Using Buckingham's $\boldsymbol{\pi}$ theorem [4] the model is formulated which states that "If there are n variables (dependent and independent variables) in a dimensionally homogeneous equation and if these variables contain m fundamental dimensions (such as M,L,T, etc), then the variables are arranged into (n - m) dimensionless terms. These dimensionless terms are called as $\boldsymbol{\pi}$ – terms".

The variables which can influence the oxygen transfer coefficient K_La, for a given shapes of aeration tanks is given by.

$$K_La = f\left(A, D, l', l, b, h, n, N, g, \rho_a, \rho_w, \nu, d, c, V, \alpha\right)$$

Where,

A – Cross sectional area of aeration tank (m^2).
D – Diameter of the rotor. (m).
l' - Horizontal projection of bent length of curved blade (m).
h – Submergence of the rotor. (m).
l – Length of blade (m).
b – Breadth of blade (m).
n – Number of blade on rotor
d – Distance between the rotors (m).
c - Clearance between rotor and O.D walls (m).
V- Volume of the tank. (m^3)
u – Velocity of flow in the O.D.(m/s)
N – Rotational speed of rotor (min^{-1}).
K_La – Oxygen transfer coefficient (min^{-1})
α – Curved angle of the blade aerator (degree).
ρ_w – Density of clear water.(kg/ m^3)
ρ_a – Density of air.(kg/ m^3)
ν – Kinematic viscosity (m^2/s)

Above equation can be written as,

$$f_1\left(K_La, A, D, l', l, b, h, n, N, g, \rho_a, \rho_w, \nu, c, d, \alpha, V\right) = 0$$

For dimension analysis, units for each and every parameter are given as follow.

$$K_La = T^{-1}, l' = L, A = L^2, D = L, l = L, b = L, h = L$$
$$n = M^o L^o T^o, N = T^{-1}, g = L^2 T^{-1}, \rho_a = ML^{-3}, \rho_w = ML^{-3}$$
$$\nu = L^2 T^{-1}, d = L, C = L, \alpha = M^o L^o T^o, V = L^3$$

According to Buckingham's $\boldsymbol{\pi}$ theorem,

Total numbers of variable = 17.
And number of π terms those will be formed =
n - m = 17 - 3 = 14.

Selecting the repeating variable as D, N, ρ_w. Because according to Buckingham's **π** theorem, the repeating variables should be chosen in such a way that one variable contains Geometric property, other variable contains flow property and the third variable contain fluid property.

1) Geometric property – D.
2) Flow property - N.
3) Fluid property - ρ_w.

K_La is a dependent variable & should not be selected
Once all the 14 Pi- terms are formed,We know that by Buckingham π theorem.

$$f_1(\pi_1\pi_2,\pi_3,\pi_4,\pi_5,\pi_6,\pi_7,\pi_8,\pi_9,\pi_{10},\pi_{11},\pi_{12},\pi_{13},\pi_{14})=0$$

Substituting the value of π_1 to π_{14} in above equation.

$$f_1\left(\frac{K_La}{N},\frac{A}{D^2},\frac{l'}{D},\frac{h}{D},\frac{l}{D},\frac{b}{D},n,\frac{g}{N^2D},\frac{\rho_a}{\rho_w},\frac{\nu}{ND^2},\frac{d}{D},\frac{C}{D},\alpha,\frac{V}{D^3}\right)=0$$

Or,

$$K_La=f\left[\frac{A}{D^2},\frac{l'}{D},\frac{h}{D},\frac{l}{D},\frac{b}{D},n,\frac{g}{N^2D},\frac{\rho_a}{\rho_w},\frac{\nu}{ND^2},\frac{d}{D},\frac{C}{D},\alpha,\frac{V}{D^3},N\right]$$

In above equation

$\frac{g}{N^2D}$ – F (Froude Number)

$\frac{\nu}{ND^2}$ – R (Reynolds number)

The above equation can be written as

$$K_La=f\left[\frac{A}{D^2},\frac{l'}{D'},\frac{h}{D},\frac{l}{D},\frac{b}{D},n,\frac{\rho_a}{\rho_w},\frac{d}{D},\frac{C}{D},\alpha,\frac{V}{D^3},F,R,N\right]$$

ρ_a/ρ_w, is non influencing parameters and can be taken as constant. Therefore equation reduces to

$$K_La=f\left[\frac{A}{D^2},\frac{l'}{D'},\frac{h}{D},\frac{l}{D},\frac{b}{D},n,\frac{d}{D},\frac{C}{D},\alpha,\frac{V}{D^3},F,R,N\right]$$

Where,
F – Froud number
R – Reynolds number.
N – Rotational speed of rotor (T^{-1}).
K_La – Overall Oxygen transfer coefficient (T^{-1})
α – Curved angle of the blade aerator.

From the equation

$$K_La=\phi\left[\frac{A}{D^2},\frac{l'}{D},\frac{l}{D},\frac{h}{D},\frac{b}{D},n,\frac{d}{D},\frac{C}{D},\alpha,\frac{V}{D^3},F,R,N\right]$$

Now $\left[\frac{A}{D^2},\frac{l'}{D},\frac{l}{D},\frac{b}{D},n,\frac{d}{D},\frac{C}{D},\frac{V}{D^3}\right]$ are const.

Therefore the above equation reduce to

$$K_La=\phi\left[N,\frac{h}{D},\alpha,F,R\right]$$

From above equation it can be seen that F (Froude number) and R (Reynolds number) cannot be considered as design parameters but its influence on K_La is discussed later on. Now, the above reduces to

$$K_La=\phi\left[(N)\left(\frac{h}{D}\right)(\alpha)\right]$$

for solving by linear multiple regression method it can be written as,

$$y=[(X_1)^{a1},(X_2)^{a2},(\alpha)^{a3}]$$

Or

$$y=\varphi\left[(X_1)^{a1},(X_2)^{a2},(\alpha)^{a3}\right] \quad (1)$$

Solving equation (1) by multiple linear regression method (A program developed in CPP) we get,
ϕ (Const.) = 0.000746,

a_1 = 1.768, Where X_1 = N
a_2 = 1.038, X_2 = h/D
a_3 = 0.031 X_3 = α
y = K_La.

Substituting the value of 'y', 'X_1', 'X_2', 'X_3' & 'a_1', 'a_2', 'a_3' In equation 45, the equation becomes.

$$K_La=0.000746\left[(N)^{1.768},\left(\frac{h}{D}\right)^{1.038},(\alpha)^{0.031}\right] \quad (2)$$

A. Modified Equation Showing the Relationship Between K_La, α, F and R

A dimensionally homogeneous equation showing the influence of blade tip angle, Froude number and Reynolds number is developed and is given as,

$$K_L a = \phi\left[N, \frac{h}{D}, \alpha, F, R\right]$$

Eliminating the N, h / D, the equation reduces to,

$$K_L a = \phi[\alpha, F, R]$$

Which can be written in linear form as follows

$$y = [(X_1)^{a1}, (X_2)^{a2}, (\alpha)^{a3}]$$

Or

$$y = \varphi\left[(X_1)^{a1}, (X_2)^{a2}, (\alpha)^{a3}\right] \quad (3)$$

Again solving equation (4) by multiple linear regression analysis method the values of indices obtained are, ϕ(constant) = 0.00419
a_1, a2 and a3 equals to -0.003, -0.8586 and 0.0456 respectively
where, y is equal to K_La and X1, X2, X3 are α, F and R respectively.

Therefore substituting the values of y, X1, X2,and X3 in (4) we get,

$$K_L a = 0.00419\left[(\alpha)^{-0.003}(F)^{-0.8586}(R)^{0.0456}\right] \quad (4)$$

B. Mathematical Model for Power Required For CBR:

The power consumption P of given CBR aerator is, generally dependent upon the same parameters as that of the term K_La [5].

Therefore the relationship between dependent and independent parameter can be expressed as

$$P = f\left(K_L a, A, l', D, l, b, h, n, N, g, \rho_a, \rho_w, \nu, d, c, V, \alpha\right)$$

Or

$$f\left(P, K_L a, A, l', D, l, b, h, n, N, g, \rho_a, \rho_w, \nu, d, c, V, \alpha\right) = 0$$

Or

$$f\left(\frac{P}{N}, \frac{K_L a}{N}, \frac{A}{D}, \frac{l'}{D}, \frac{l}{D}, \frac{b}{D}, \frac{h}{D}, h, \frac{g}{N^2 O}, \frac{\rho_a}{\rho_w}, \frac{\nu}{D^2 N}, \frac{d}{D}, \frac{C}{D}, \alpha, \frac{V}{D^3}\right) = 0$$

$$\frac{P}{N} = \phi\left[\frac{K_L a}{N}, \frac{A}{D}, \frac{l'}{D}, \frac{l}{D}, \frac{b}{D}, \frac{h}{D}, \frac{g}{N^2 D}, \frac{\nu}{D^2 N}, \frac{d}{D}, \frac{C}{D}, \alpha, \frac{V}{D^3}\right]$$

Solving the above equation as discussed in 3.2 and eliminating the constant terms, the equation reduces to

$$P = \varphi\left[N, \frac{h}{D}, \alpha, k_L a\right] \quad (5)$$

P – Power in watt
K_La – per min.
N – rpm (per min).

$$y = \varphi\left[(X_1)^{a1}, (X_2)^{a2}, (X_3)^{a3}, (X_4)^{a4}\right] \quad (6)$$

Solving the equation by multiple linear regression method the indices, we get

ϕ = 0.0694	where X_1 = N
a_1 = 2.062	X_2 = h/D
a_2 = 1.14	X_3 = α
a_3 = 0.194	X_4 = K_La
a_4 = -0.1729	y = P.

Substituting the value of ϕ, a_1, a_2, a_3 & a_4 in equation (7)
We get

$$P = 0.0694\left[(N)^{2.062}, \left(\frac{h}{D}\right)^{1.1412}, (\alpha)^{0.1942}, (K_L a)^{-0.1729}\right] \quad (7)$$

Therefore three different BFMM mathematical models are developed, which are then validated by the data generated by the experimental observations.

III. CFD Model

The computational fluid dynamic model of an aerator used for treatment of waste water in oxidation ditch is a crucial part of this study [6]. The results of this phase have a huge impact on the quality of the results obtained by experimental setup and the mathematical model developed. The main problem to solve was to model the geometry of the aerator and the oxidation ditch. Actually the CFD part of this study is only to find out the correlation between the experimentally observed data and data generated by the CFD model and if the CFD model thus developed establishes good correlation with the observed data, it could be used to analyze the various parameters of the said system without fabricating the physical model. It is relatively trivial to draw the aerators in Gambit, but the problem is the overall number of elements. A single aerator has a number of groups with 12 blades each. Going further with the computation it can be seen that in the oxidation ditch there are 2 aerators with 14 groups of 12 blades each. Overall it is about 350 elements. For computation ANSYS Fluent post version 1.2 is used and the source of momentum in the ditch is the rotating aerators. To model the aerators the moving mesh option in fluent is used and the part of aerator that is submerged in the water is created.

A. Modeling the Aerator:

The aerator is modeled in few different ways. The one that is finally used is the one phase, 3D model. To model the moving wall in fluent a volume with the shape of aerator is created and to define the constant velocity of it a user defined function is used. This way the cells that were source of momentum and were working like moving wall were created. It is hard to say if this solution is modeling the pressure and turbulence correctly but even though it is gross simplification, the results were looking plausible. There are low and high pressure regions before and after the rotor's blades respectively, while a strong turbulence is created by the blades. Because it was decided to use a one phase model, instead of creating the whole aerator, only the part of the aerator under water level is used.

B. Computational Domain:

The model dimensions are 32 x12 x 4.3 cm (length x width x height). In the top part it is the aerator. Only the part of the aerator that is submerged in the water is modeled. The sides of the model are symmetry boundary conditions. That way we represent a number of groups of rotating blades. After meshing 2, 40,000 cells were created.

Setting up Fluen:t
Solver: 3 D, Pressure based, steady state
Viscous: Standard k–ε (k-epsilon) fluid model
Material:
Water: Density 998.2 kg/m^3
Viscosity 0.001003 kg/m-s
Operating conditions: Gravity OFF

IV. Result And Discussion

The calculated values using above models yielded good coefficient of correlation (R^2) with the experimentally observed values as well as are in good agreement with standard error of estimation. A program in CPP is developed to inter relate the various influencing parameters mentioned above and are solved by multiple linear regression analysis method. Fig 1 and Fig 2 are the plots between experimentally determined values and calculated values from the model formulated for K_La and power respectively. It has been estimated that the simulation equations (2) and (7) predicts the values of K_La and power with an average standard error of estimation of 0.0164 and 7.66 respectively and with R^2 values of 0.9797 and 0.9892 respectively, when compared with experimentally determined values. Thus equations (2) and (7) are justifiable by taking into consideration all of the experimental errors themselves. Therefore above equations may be used with confidence for predicting the K_La and power (P) and can be considered as design equations for CBR aerator.

The influence of Frouds number and Reynolds number together with the blade tip angle can also be predicted on K_La by using equation (4). Fig 3 is the plot between experimentally determined values and calculated values from the model formulated for K_La with respect to α, F and R. The R^2 value of 0.9606 is obtained in this case, which indicates that a the values are in good agreement with each other. In the present study, an attempt is made to correlate the data generated in the laboratory with the model developed using Computational Fluid Dynamics.

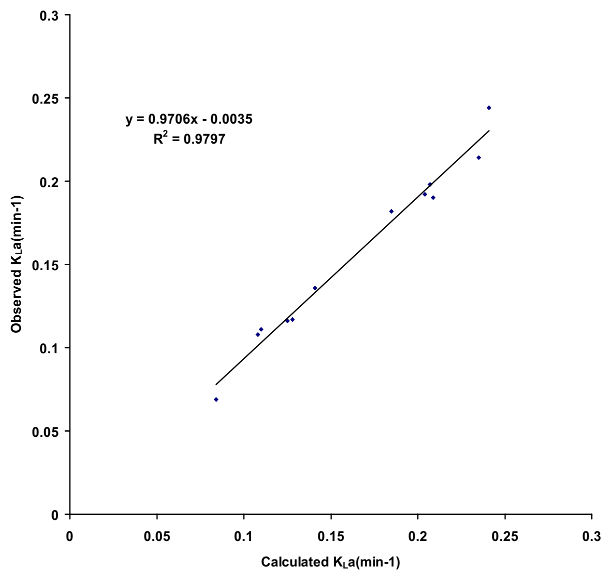

Fig. 1 Relationship between Observed Overall Transfer coefficient (KLa) & Calculated Overall Transfer coefficient (KLa).

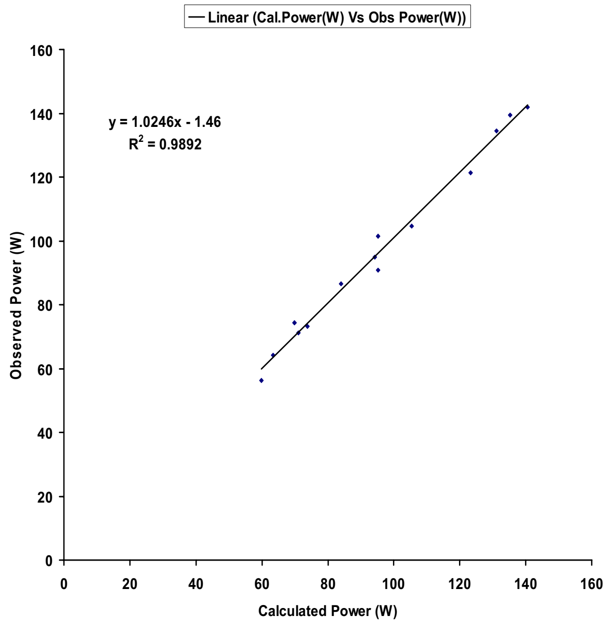

Fig. 2 Relationship between Observed power values(W) & Calculated power values(W)

A series of simulation experiments were carried out on the CFD model developed. (Software ANSYS - FLUENT POST 1.2). Fig 4. Shows, the variation in the oxygen transfer in different zones. It is clearly visible from the figure that oxygen transfer in the immediate vicinity of aerators is quite predominant than that of in other parts of the ditch.

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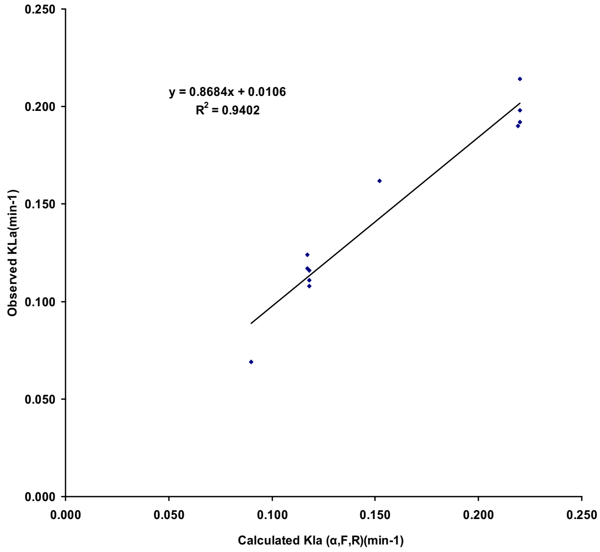

Fig. 3 Relationship between Observed Overall Transfer coefficient (K_La) & Calculated Overall Transfer coefficient (K_La) w.r.t (α,F,R)

It can concluded that the trend followed by results obtained with CFD simulation is same as that of obtained with experimentally observed values.

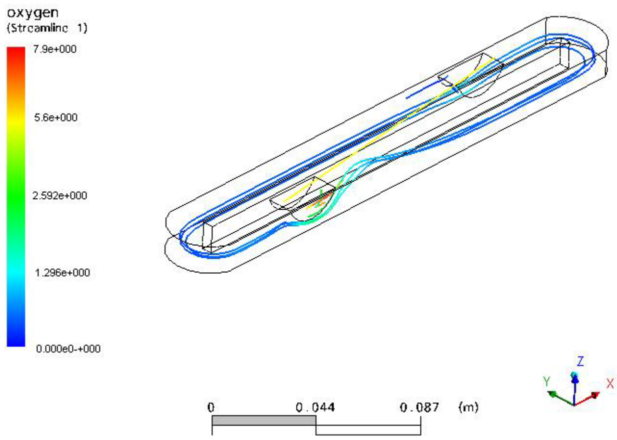

Fig. 4 Streamlines of Oxygen Transfer in the water present in Oxidation Ditch

Fig 5, Illustrates the relationship between the observed values of K_La and K_La values obtained from CFD model simulation. The R^2 value of 0.9609 is obtained by plotting the above values against each other and with standard error of estimation of 5.858, which suggests that the CFD model developed and the simulation values thus generated are in good agreement with the experimental model and the observation recorded therein.

V. Conclusion

i) A simplified simulation equations (2),(4) and (7) are developed, which can be used to calculate the values of K_La and power, for given diameter of aerator (D), depth of immersion (h), blade tip angle (α).

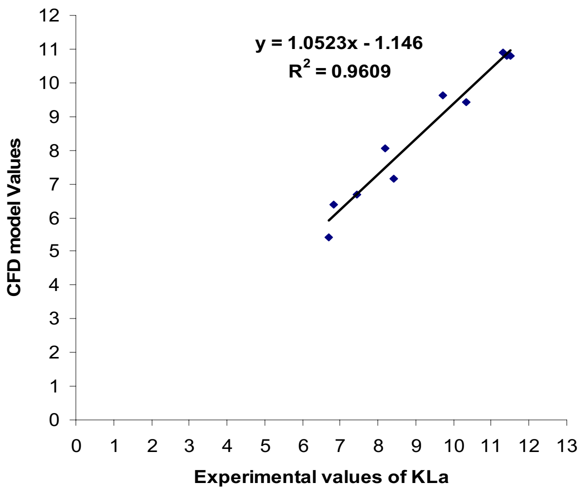

Fig. 5 Relationship between Experimental values and CFD Model values

It has also been estimated that the simulation equation (2), (4) and (7) predicts the values of K_La and power with an average standard error of estimation of 0.0164 and 7.66 respectively and with R^2 values of 0.9797 and 0.9892 respectively, when compared with experimentally determined values. Thus equations (2), (4) and (7) are justifiable by taking into consideration all of the experimental errors themselves. Therefore above equations may be used with confidence for predicting the K_La and power (P) and can be considered as design equations for CBR aerator.

ii) A CFD model is developed, which shows a good coefficient of correlation (R^2 = 0.9609) with the experimentally observed values, standard error of estimation of 5.858 and proves to be best fit model with respect to its validation.

Finally, it can be concluded that aeration can be made more effective by selecting appropriate configuration of aerator and optimizing the various factors affecting it viz, speed of aerator, depth of immersion, blades angles. Also, overall oxygen transfer coefficient, K_La gives an excellent measure of oxygen transfer efficiency in conjunction with power required.

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