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Effect of hydrodynamic characteristics on reaeration process

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Abstract: The equilibrium-perturb technique was used in the flume reaeration experiment. The interfacial mass transfer coefficients of DO were obtained by implementation of the oxygen-flux theory in the study. The turbulence characteristics of the flow field were investigated by numerical simulation approach. The expression of interfacial mass transfer coefficient related with velocity and turbulence kinetic energy was built. Examination with the experimental datum of different cases showed the validation of the expression.

Keywords: reaeration: hydrodynamic characteristics

Introduction

The reaeration process plays an important role in degradation of organic pollutants and self-purification process of water body. The previous studies show that flow field and its turbulence characteristics have strong influence on dissolved oxygen (DO) distribution in water (Li, 2000a; 2000b). There are many empirical and semi-empirical formulas for calculation of reaeration coefficients of natural streams. As the formulas were based on approximate descriptions of flow field and cannot reveal the mechanism of reaeration process, they are usually case dependent and have poor accuracy.

Based on turbulence and gas-liquid mass transfer theories, the reaeration process with both of theoretical analysis and experiments was studied. The 3-D turbulence numerical simulation approach was adopted and the reaeration coefficient which considered the effect of hydrodynamic characteristics was developed.

1 The flume experiment on turbulent reagration

Many previous studies showed that flow field has strong impact on reaeration process. The concentric cylinder reaeration experiment confirmed the close relationship to a reaeration process with the turbulence kinetic energy (Li, 2000a). Due to the difference of flow field characteristics between the concentric cylinder experiment and natural rivers, the relations between flow field and reaeration was not studied enough in the concentric cylinder experiment. So, the flume experiment on turbulent reaeration was carried out.

The experiment was completed in a concrete flume with 280 meters long, 0.4 meters wide and 0.5 meters high. The slope of the flume was 1%. The equilibrium-perturb technique was adopted. The temperature of the inlet water was 20 °C and its DO concentration was saturated. In order to obtain the oxygen deficit condition during experiment, the sodium sulfite and cobalt were introduced at the inlet to consume out of the initial DO. The DO concentrations were monitored at upstream station (X = 5m) and downstream station (X = 275 m) respectively. The setup of the experimental flume is shown in Fig. 1.

The velocity was measured with the computer-controlled velocimeter and its monitoring section is located in the middle of the flume (X = 140m). The DO concentration was measured with a dissolved oxygen meter(model YSI52).

38 experiment cases were accomplished. The experimental water depths ranged from 3.09 cm to

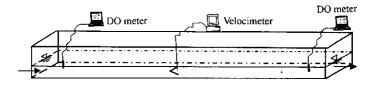


Fig.1 Setup of the flume experiment

14.55 cm, and the velocities between 25.92 cm/s to 65.53 cm/s.

2 Numerical simulations for the experimental flow field

The three dimensional mathematical k- ϵ turbulence model was used to investigate the flow field. The governing equations of the model are as follows:

Continuity equation:

$$\frac{\partial U_i}{\partial X_i} = 0. (1)$$

Momentum equation:

$$\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial X_i} (U_i U_j) = -\frac{1}{\rho} \frac{\partial P}{\partial X_i} + \frac{\partial}{\partial X_i} \left[(\nu + \nu_i) \left(\frac{\partial U_i}{\partial X_i} + \frac{\partial U_j}{\partial X_i} \right) \right]. \tag{2}$$

k equation:

$$\frac{\partial k}{\partial t} + U_i \frac{\partial k}{\partial X_i} = \frac{\partial}{\partial X_i} \left(\nu + \frac{\nu_i}{\sigma_k} \frac{\partial k}{\partial X_i} \right) + G - \varepsilon, \tag{3}$$

where G is the production term, $G = \nu_i \left(\frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i} \right) \frac{\partial U_i}{\partial X_j}$.

ε equation:

$$\frac{\partial \varepsilon}{\partial t} + U_i \frac{\partial \varepsilon}{\partial X_i} = \frac{\partial}{\partial X_i} \left[\left(\nu + \frac{\nu_t}{\sigma_{\varepsilon}} \right) \frac{\partial \varepsilon}{\partial X_i} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} G - C_{2\varepsilon} \frac{\varepsilon^2}{k}. \tag{4}$$

The wall function implied the roughness effect was bounded on the wall boundary condition of the flume. The function can be written as:

$$\frac{U_p}{U_*} = \frac{1}{\kappa} \ln \left(\frac{E \rho y_p U_*}{\mu} \right) - \Delta B. \tag{5}$$

Where U_p is the velocity at near wall grid p; U, is the friction velocity; y_p denotes the distance from grid p to the wall; k is the Von Karman's constant (k = 0.42); E is an empirical constant (E = 9.8); and ΔB is the roughness function and given by:

$$\Delta B = \frac{1}{\kappa} \ln(1 + c_{k}k_{\star}^{\dagger}), \qquad (6)$$

in which c_k is the roughness constant and was taken to be 0.5 in the model, k_i^+ is the roughness height and the value of 0.009 was adopted.

Slip wall boundary condition was applied for the water surface.

The flow field and turbulence kinetic energy distribution were obtained by the numerical solution from the above model. The velocity magnitude distribution on the downstream DO monitoring section of case 1 is plotted in Fig.2. Fig.3 shows the turbulence kinetic energy distribution on the same section. The values of the free surface-averaged turbulence kinetic energy of cases 1—38 are represented in Fig.4.

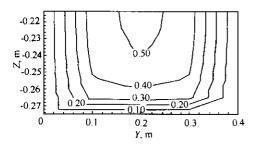


Fig. 2 The velocity magnitude distribution on the downstream section of case 1 (m/s)

-0.22 -0.23 E-0.24 N -0.25 -0.26 -0.27 0 0.1 0.2 0.3 0.4 Y, m

Fig. 3 The turbulence kinetic energy distribution on the downstream section of case 1 (m/s)

3 Calculation of the interfacial mass transfer coefficient

The flume experimental datum indicated that the dissolved oxygen distributed uniformly on cross sections, so the relation between reaeration coefficient, k_2 , and interfacial mass transfer coefficient, K_L , satisfies the following expression: $k_2 = K_L/H$ (Li, 2000b), where H stands for the water depth. Hence, under the experimental conditions, the 1-D equation for dissolved oxygen can be established as:

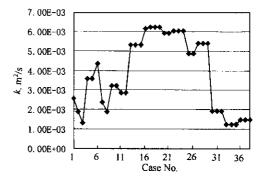


Fig. 4 The averaged turbulence kinetic energy

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = \frac{\partial}{\partial x} \left(D_m \frac{\partial C}{\partial x} \right) + k_2 (C_s - C). \tag{7}$$

The DO distribution reached steady state after a period of experiment time, then the Equation (7) is reduced to:

$$U\frac{\partial C}{\partial x} = \frac{\partial}{\partial x} \left(D_m \frac{\partial C}{\partial x} \right) + k_2 (C_s - C). \tag{8}$$

The diffusion term in Equation (8) can be neglected under experimental conditions and Equation (8) becomes:

$$U\frac{\partial C}{\partial x} = k_2(C_* - C). \tag{9}$$

As DO concentration changes linearly in longitudinal direction, the expression for the reaeration coefficient is obtained by discretization of the Equation (9):

$$k_2 = \frac{U(C_d - C_u)}{(C_s - (C_u + C_d)/2)\Delta x},$$
(10)

where C_u , C_d are the upstream and downstream DO concentrations respectively, Δx stands for the distance between the upstream and downstream monitoring sections.

The interfacial mass transfer coefficients for each experimental cases can be calculated by the use of the expression: $K_L = k_2 H$. Their values are listed in Table 1.

In previous studies (Atkinson, 1995; Satoru, 1982), many empirical and semi-empirical formulas for reaeration coefficient were provided. Seven typical formulas for natural streams are listed in Table 2. The Fig.5 compares the reaeration coefficients obtained in the flume experiment with those calculated with formulas.

Table 1 The reaeration coefficients and interfacial mass transfer coefficients for each case													
Case No.	1	2	3	4	5	6	7	8	9	10	11	12	13
k ₂ ,10 ⁻⁴ s ⁻¹	1.615	1.972	2.304	1.450	1.946	1.743	1.684	2.126	1.796	1,483	1.986	1.884	1.547
K_L , 10^{-5} s $^{-1}$	0.996	0.864	0.712	1.254	1.683	1.774	0.923	0.931	1.389	1.146	1.349	1.279	1.851
Case No.	14	15	16	17	18	19	20	21	22	23	24	25	26
$k_2, 10^{-4} s^{-1}$	1.566	1.397	1.472	1.604	1.534	1.368	1.672	1.466	1.244	1.414	1.278	1.705	1.547
K_L , $10^{-5}\mathrm{s}^{-1}$	1.873	1.671	1.970	2.170	2.075	1.851	2.174	1.906	1.810	2.058	1.859	1.916	1.739

Fig. 5 reveals that the reaeration coefficient in the flume experiment is larger than those calculated by the formulas. It is believed that the formulas were obtained from natural streams, and then the degradation or deposition actions in natural minify reaeration streams may the coefficients. In other words, the k_2 in Table 2 was not a pure reaeration

Table 2 Empirical formulas for reaeration coefficient

NO.	Formula	Researcher					
1	$k_2 = 0.175 \overline{U}^{0.5} H^{-1.5}$	O'Connor-Dobbins					
2	$k_2 = 8.15 (\overline{U}S)^{0.408} H^{-0.66}$	Krenkel-Orlob					
3	$k_2 = 8.70(\overline{U}S)^{0.5}H^{-1}$	Cadwallader-McDonnell					
4	$k_2 = 6.38\overline{U}S$	Tsivoglou-Wallace					
5	$k_2 = 0.235 \overline{U}^{0.969} H^{-1.673}$	Churchill, Elmore, Buchkingham.					
6	$k_2 = 0.325 \bar{U}^{0.73} H^{-1.75}$	Owens, Edwards, Gibbs					
7	$k_2 = 1.17(1 + F_r^{0.5}) \overline{U} H^{-1}$	Thackston-Krenkel					

coefficient, which may included DO consumption in natural environment. The water depth difference between the experiment and a natural stream played some role in the discrepancy as well.

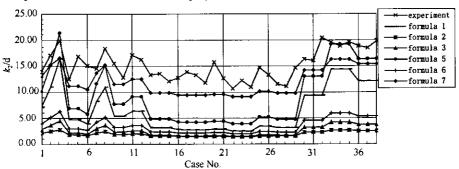


Fig. 5 Comparison of reaeration coefficients

4 The expression for interfacial mass transfer coefficient

Take velocity \overline{U} , turbulence kinetic energy k and oxygen deficit D as the base physical quantities, the oxygen flux through the gas-liquid interface contributed by turbulence can be written as:

$$F_{\epsilon} = f(\overline{U}, k, D). \tag{11}$$

Where \overline{U} is the flow velocity, k is the turbulence kinetic energy, D is the oxygen deficit.

According to dimensional analysis, the following expression is obtained:

$$[F,] = [\overline{U}]^* [k]^{\gamma} [D]^z.$$
 (12)

Take [M], [L] and [T] as the base dimensions, reached:

$$[ML^{-2}T^{-1}] = [LT^{-1}]^{x}[L^{2}T^{-2}]^{y}[ML^{-3}]^{z}.$$
 (13)

Solve the equations about x, y and z, the following expressions for oxygen flux and interfacial mass transfer coefficient are derived:

$$F_{t} = c_{1} \overline{U}^{x} k^{(1-x)/2} D, \qquad (14)$$

$$K_{t,t} = c_1 \, \overline{U}^x k^{(1-x)/2} \,, \tag{15}$$

in which c_1 is an undetermined constant.

The dimension for $K_{L,\iota}$ is m/s. Including the mass transfer coefficient for non turbulence water K_{L0}

 $(3.9 \times 10^{-7} \text{ m/s})$ into $K_{L,t}$, and the mass transfer coefficient for turbulent water body (Li, 1999) is rewritten as:

$$K_L = c_1 \overline{U}^* k^{(1-x)/2} + K_{t0}.$$
(16)

According to the interfacial mass transfer coefficients of experimental cases 1—26 and the turbulence kinetic energy obtained by 3-D numerical simulation, the constant c_1 in Equation (16) is found to be 0.00012 and x is 1/3 by mean of the least square method. Thus the expression for interfacial mass transfer coefficient in terms of velocity and turbulence kinetic energy is as follows:

$$K_L = 0.00012 \overline{U}^{1/3} k^{1/3} + 3.9 \times 10^{-7}$$
 (17)

The square of correlation coefficient, R^2 is 0.9585. It indicates that the interfacial mass transfer coefficient has good relativity with velocity and turbulence kinetic energy.

5 Validation of the turbulent reaeration theory

The turbulent reaeration theory was examined with the experimental datum of cases 27-38.

5.1 Validation for K_L

The interfacial mass transfer coefficients of cases 27—38 were calculated with the expression (17) by use of velocity and turbulence kinetic energy obtained in previous flow field studies. The calculated values were compared with the experiments in Fig. 6. The difference is small enough to support the expression (17) for interfacial mass transfer coefficient.

5.2 Validation for DO concentration

The DO concentration equation was derived from the three-dimensional k- ε numerical turbulence model:

$$\frac{\partial C}{\partial t} + U_i \frac{\partial C}{\partial X_i} = \frac{\partial}{\partial X_i} \left[\left(\nu + \frac{\nu_i}{\sigma_C} \right) \frac{\partial C}{\partial X_i} \right]. (18)$$

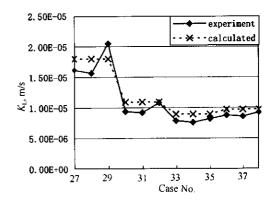


Fig. 6 Comparison of K_L

The following oxygen flux was applied on the free surface: $F = (0.00012 \overline{U}^{1/3} k^{1/3} + 3.9 \times 10^{-7}) (C_s - C). \tag{19}$

The inlet DO concentration was assumed to be the measured concentration at the upstream section.

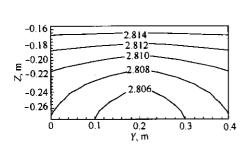


Fig. 7 The calculated DO distribution on the downstream section of case 27 (mg/L)

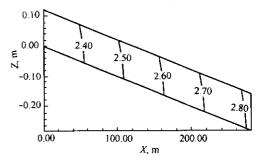


Fig. 8 The calculated DO distribution on the longitudinal section of case 27 (mg/L)

The reaeration processes for each case were simulated with the model. Fig. 7 shows the DO distribution on the downstream monitoring section in case 27. The calculated section-averaged DO is 3.811 mg/L and the measured value is 3.80 mg/L. The relative error is less than 0.3%. The maximum relative

error in other cases is less than 0.8%.

The DO distribution on the middle longitudinal section is depicted in Fig. 8. It reveals that the dissolved oxygen on each cross-section distributed approximately uniformly. The results were fitted with the experiment well.

6 Conclusion

The oxygen flux theory was implemented in the study on the turbulent reaeration process and the oxygen transfers contributed by molecular diffusion and turbulent diffusion were treated separately. The flume experiment was performed and the expression for interfacial mass transfer coefficient in terms of velocity and turbulence kinetic energy was built at the first time.

The expression for interfacial mass transfer coefficient provided fully understanding to flow field and turbulence characteristics. It makes the reaeration formula more delicate and reasonable, and is important to the study on vertical distribution of DO. As turbulence kinetic energy is a physical quantity often needed to be determined in numerical turbulence simulation, the expression for interfacial mass transfer coefficient is easy of use for numerical simulators. Some empirical approaches to calculate the turbulence intensity of a river, for example, the Prandtl's mixing length theory, could be used to give out a river's interfacial mass transfer coefficient in engineering site. The authors will evaluate the practical approach of the interfacial mass transfer coefficient of a natural water body in the future's investigation.

The dissolved oxygen distribution is not only related with the reaeration rate at the gas-liquid interface, but also with the turbulence characteristics inside water body. So both the interfacial characteristics at the gas-liquid interface and the turbulence characteristics inside the water body need to be studied simultaneously when the reaeration process is investigated in the future, especially for the situation when water depth can not be ignored.

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