Integration of Impact Factors of Gas-Liquid Transfer Rate

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ABSTRACT

The gas transfer rate at air-water interface (reaeration rate) has significant impact on surface water quality. The gas transfer rate is affected by multiple factors including stream, wind, wave breaking, etc. When wind is blowing over water, the turbulence generated at the air-water interface is the predominant factor impacting reaeration. A number of empirical relationships have been established for the gas transfer rate as a function of wind speed. A theoretical model of the wind reaeration rate has also been developed by O'Connor. However, in addition to wind-induced turbulence in an "unbroken" water surface, wave breaking is predominant factor impacting reaeration in the "broken" water surface, where the reaeration is driven by the bubble-mediated gas transfer. In this paper, a relationship is developed to integrate the effects of wave breaking and wind on the rate of reaeration.

Keywords: Models, Surface Water, Water Quality

Introduction

The distribution of the constituents in aquatic ecosystems is significantly affected by the transfer of sparingly soluble gases such as dissolved oxygen across the air-water interface. Many factors such as wind, wave breaking, bubbles, etc. affect the gas-liquid transfer rate. Some studies (Broecker et al. 1978; Jahne et al. 1979; Liss and Merlivat 1986; Wanninkhof 1992; Wanninkhof and McGillis 1999) have focused on the effects of wind; some studies (Boettcher et al. 2000; Peirson et al. 2003; Woolf 1997; Zappa 2001) on the effects of wave breaking; and some other studies (Broecker and Siems 1984; Eckenfelder 1959; Memery and Merlivat 1983; Thorpe 1982 and 1986; Woolf and Thorpe 1991) on the effects of bubble-mediated gas-liquid transfer rate. Only a few studies (Asher and Farley 1995) were on the combined effects of wind, wave breaking and bubbles, in which basically empirical formulae were used for the calculation of the total gas-liquid transfer rate. In this study, an integrated gas-liquid transfer rate formula is developed, in which the majority components are theoretical. It will have wider application ranges as its majority is theoretical.

Wind-driven gas-liquid transfer rate

Wind has significant effects on gas-liquid transfer rate in many water bodies such as estuaries, lakes, oceans, etc. A theoretical wind-stream-driven gas-liquid transfer rate has been developed (Duan et al. 2007). It incorporates the combined effects of both wind and stream on gas-liquid transfer rate. By setting the stream velocity to be zero, a theoretical wind-driven gas-liquid transfer rate formula was obtained

(Duan and Martin 2007) as:

$$\text{when } 0 \le u_{*_1} \le \left(\frac{g\upsilon}{\lambda_1 \alpha}\right)^{\frac{1}{3}}, \tag{1}$$

$$K_L = \frac{1}{\dfrac{\left(\Gamma - \dfrac{1}{\lambda_1}\right)\nu}{D\sqrt{\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}} + \sqrt{\dfrac{121.5\nu}{D\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}}} W = C_1 W$$

$$\text{when } \left(\frac{g\upsilon}{\lambda_1 \alpha}\right)^{\frac{1}{3}} \le u_{*_1} \le \left(\frac{\Gamma g\upsilon}{\alpha}\right)^{\frac{1}{3}},$$

$$K_L = \frac{1}{\left(\dfrac{\Gamma\nu}{D\sqrt{\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}} + \sqrt{\dfrac{121.5\nu}{D\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}}\right) W^{-1} - \dfrac{\alpha\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}{Dg} W^2} = \frac{1}{C_{21}W^{-1} + C_{22}W^2}$$

$$\text{when } u_{*_1} \ge \left(\frac{\Gamma g\upsilon}{\alpha}\right)^{\frac{1}{3}},$$

$$K_L = \sqrt{\frac{D\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}{121.5\nu}} W = C_3 W$$

where C_1 = coefficient of wind-driven gas-liquid transfer rate in segment 1; C_{21}, C_{22} = coefficient of wind-driven gas-liquid transfer rate in segment 2; and C_3 = coefficient of wind-driven gas-liquid transfer rate in segment 3. The wind-driven gas-liquid transfer rate formula is reasonable as a specific case of the wind-stream-driven gas-liquid transfer rate formula which has been successfully tested. In this study, the wind-driven gas-liquid transfer rate formula is considered as applicable for non-breaking wave gas-liquid transfer rate.

Wave breaking gas-liquid transfer rate

When wind speed is large enough and wave breaking occurs, the gas-liquid transfer rate is significantly increased. The gas transfer dominated by breaking wave is proportional to fractional whitecap coverage. The coefficient is based on the calculations of bubble-mediated transfer, and therefore depends on the solubility of the gas. A simple formula, appropriate for CO_2 at 20°C, is given by (Woolf 1997):

$$K_L = 850W \tag{2}$$

where K_L = gas-liquid transfer rate induced by breaking wave in cm/hr; W = wind speed, m/s.

Different research areas focus on the gas-liquid transfer processes of different gases; e.g. dissolved oxygen is the major concern in environmental engineering and carbon dioxide is the major concern in oceanography. The similarity of the transfer processes of different low solubility gases allows the conversion of transfer rates among different low solubility gases. The related conversion relationships are described with Schmidt number:

$$K_{La} = K_{Lb}\left(\frac{Sc_a}{Sc_b}\right)^x \tag{3}$$

where K_{La} = gas-liquid transfer rate of gas a, m/s; K_{Lb} = gas-liquid transfer rate of gas b, m/s; Sc_a = Schmidt number of gas a; Sc_b = Schmidt number of gas b; and x = Schmidt number dependence that is -2/3 for smooth surfaces and -1/2 for rough surfaces (Donelan, et al. 2001). The Schmidt number (Sc) is a dimensionless number which equals to *v*/D, with *v* as kinematic viscosity, a property of the material. The Schmidt number is used to characterize fluid flows with convection processes caused by simultaneous momentum and mass diffusion (Munson, 1994).

With this relationship, the transfer rates of different gases including oxygen, carbon dioxide, PCBs, etc. are related. With the transfer rate of one gas, the rates of other gases can be calculated by this relationship. Thus, Substitution of Eq.2 into Eq.3 yields the wave breaking gas-liquid transfer rate for dissolved oxygen as:

$$K_{Lbw} = 850W\left(\frac{Sc_a}{Sc_b}\right)^x = C_{bw}W \tag{4}$$

where K_{Lbw} = breaking wave gas-liquid transfer rate, m/s; and C_{bw} = coefficient of breaking wave gas-liquid transfer rate.

Bubble-mediated gas-liquid transfer rate

Bubble-mediated gas transfer is an important part of the total gas transfer especially during wave breaking, dropletss, etc. It was reported that dissolved oxygen will be supersaturated by deep bubble clouds (Thorpe 1982 and 1986; Woolf and Thorpe 1991). The breaking waves entrain bubbles at high wind speeds, which increase the gas-liquid transfer rate (Memery and Merlivat, 1983; Broecker and Siems, 1984). The bubbles entrained by breaking waves were observed to greatly enhance the gas-liquid transfer rate (Farmer et al. 1993). But some studies indicated that the bubble-mediated gas transfer was at most 7% of the total gas transfer in wind-driven turbulence (Komori and Misumi 2001).

Eckenfelder (1959) described the oxygen transfer in terms of Sherwood number, Reynolds number and Schmidt number:

$$\frac{K_L d_B}{D} = F(\frac{d_B U_B}{\nu})(\frac{\nu}{D}) \qquad (5)$$

where U_B = bubble velocity, m/s; ν = kinematic viscosity, m^2/s; $K_L d_B/D$ = Sherwood number (Sh); $d_B u/\nu$ = Reynolds number (Re); ν/D = Schmidt number (Sc); and F = bubble-mediated gas-liquid transfer rate constant coefficient.

Integration of impact factors of gas-liquid transfer rate

Asher and Farley (1995) showed that gas-liquid transfer rate KL could be partitioned into several components: near-surface turbulence generated by currents and non-breaking wave (KLnw), turbulence generated by breaking waves (KLbw), and bubble-mediated transfer (KLB). If the gas concentration grade is large, the total gas-liquid transfer rate is given by:

where Wc = fractional area of whitecap whitecap coverage.

$$K_L = [K_{Lnw} + Wc(K_{Lbw} - K_{Lnw})] + WcK_{Lb} \qquad (6)$$

In this study, Eq.1 is used for the calculation of KLnw; Eq.4 is used for the calculation of KLbw; and Eq.5 is used for the calculation of KLb. Substitution of Eq.1, Eq.4 and Eq.5 into Eq.6 yields the integrated gas-liquid transfer rate for the combined effects of wind, wave breaking, and bubbles as Eq.7-10 (Eq.10 has three segments) show:

$$K_L = \left(K_{Lnw} + Wc\left(K_{Lbw} - K_{Lnw}\right)\right) + WcK_{Lb} \tag{7}$$

$$\frac{K_{Lb} d_B}{D} = F\left(\frac{d_B U_B}{\nu}\right)\left(\frac{\nu}{D}\right) \tag{8}$$

$$K_{Lbw} = C_{bw} W \tag{9}$$

(10)

$$0 \le u_* \le \left(\frac{g\upsilon}{\lambda_l \alpha}\right)^{\frac{1}{3}} \qquad K_L = \frac{1}{\dfrac{\left(\Gamma - \dfrac{1}{\lambda_l}\right)\nu}{D\sqrt{\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}} + \sqrt{\dfrac{121.5\nu}{D\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}}} W = C_1 W$$

$$\left(\frac{g\upsilon}{\lambda_l \alpha}\right)^{\frac{1}{3}} \le u_{*1} \le \left(\frac{\Gamma g\upsilon}{\alpha}\right)^{\frac{1}{3}} \qquad K_L = \frac{1}{\left(\dfrac{\Gamma\nu}{D\sqrt{\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}} + \sqrt{\dfrac{121.5\nu}{D\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}}\right)W^{-1} - \dfrac{\alpha\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}{Dg}W^2} = \frac{1}{C_{21}W^{-1} + C_{22}W^2}$$

$$u_{*1} \ge \left(\frac{\Gamma g\upsilon}{\alpha}\right)^{\frac{1}{3}} \qquad K_L = \sqrt{\frac{D\dfrac{\rho_a}{\rho_w}\dfrac{C_{f1}}{2}}{121.5\nu}} W = C_3 W$$

Conclusions

An integrated gas-liquid transfer rate formula was developed in this study for the combined effects of wind, wave breaking and bubbles. The wind-driven gas-liquid transfer rate formula was used for the calculation of the non-breaking wave component K_{Lnw}. A breaking wave gas-liquid transfer rate formula was developed for the calculation of the breaking wave component K_{Lbw}. The bubble-mediated gas-liquid transfer rate formula developed by Eckenfelder (1959) was used for the calculation of the bubble-mediated component K_{Lb}. All of the components except the wave breaking one are theoretical formulae. Thus, the integrated gas-liquid transfer rate formula has wide application ranges since its majority is theoretical. For further study, a theoretical wave breaking gas-liquid transfer rate formula needs to be developed. The experimental data for the combined effects of wind, wave breaking and bubbles need to be conducted to test the integrated gas-liquid transfer rate formula.

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