WIND EFFECTS ON GAS TRANSFER AT AIR-WATER INTERFACE

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INTRODUCTION

Gas transfer plays an important role in many environmental phenomena such as the reaeration of polluted streams, the fate of volatile toxic pollutants, the water contamination caused by atmospheric pollutants transferred through the air-water interface, etc. Because of its impact on environmental pollution, water quality, and climate changes, it has recently become an important subject.

Natural water bodies (streams, lakes, ponds, reservoirs, seas) are exposed to wind. The presence of wind makes the gas transfer process a complicated phenomenon. The air and water flows above and below the air-water interface are dynamically coupled. Also, the interface is a moving boundary which is governed by the coupled dynamics. There is considerable exchange of momentum and energy at the interface. If the water is initially at rest, then due to the wind action, surface waves will be generated (Miles 1957; Phillips 1957), and in the meanwhile, a surface drift will also be present (Wu 1975). The initiation of the motion of the water body will in turn significantly affect the air flow. The interface dynamics is itself a subject currently under study. The related gas transfer process is even more complicated. Simply speaking, the flow conditions of the water surface layers, the wind conditions, and the bubble dynamics play roles in the gas transfer process (Kanwisher 1963). Because of the complexity of the problem, needless to say, certain simplifications are needed. Experimental and field studies have been conducted to investigate how the transfer coefficient is affected by the wind action. For example, through their experimental study, Merlivat and Memery (1983) found the linear correlation between the gas transfer coefficient and the representative wind wave speed. Jahne et al. (1985) concluded from their large wind wave facility experiments that the wave characteristics must be included as parameters to describe the gas transfer process. To add to the complexity of the problem, Jahne et al. (1987) further revealed from their wind wave tunnel experiments the change of the gas transfer coefficient dependency on the Schmidt number (Sc=\nu/D). On the modeling aspect, the interface has been traditionally regarded as a fixed smooth boundary. Only recently, effort has been made to include the effect of wave motion. For instance, Coantic (1986) considered the capillary wave effect in his model and evaluated the resulting transfer coefficients under different assumptions of the hydrodynamic conditions. Using oxygen as the transferred gas, Daniil and Gulliver (1991) conducted experimental studies to investigate the breaking wave effects on the gas transfer coefficients. By assuming that the enhanced gas flux at higher wind speeds results from bubble entrainment in small scale breaking waves, Kerman (1984) tried to correlate the enhanced gas transfer to the group wave characteristics. The effect of the surface drift, however, is still not included. The present investigation will include the surface drift and wave affects on the gas transfer process in the simple mathematical model.

BASIC TRANSFER MECHANISM

When both air and water are still, the rate of transfer is governed by the equation

$$\frac{dC}{dt} = k_a (C_s - C) \tag{6}$$

where t is time, C and C_s are the actual (volume) concentration and the saturation (volume) concentration, respectively, and k_a is a constant related to given physical conditions. The absorption of the gas occurs when $C < C_s$, while the desorption of the gas occurs when $C > C_s$. The magnitude of k_a depends on the temperature of the system, the interfacial area available for gas transfer, and the resistance to movement from one phase to the other.

The resistance to movement between the two phases is traditionally explained by the two-film theory of mass transfer initially postulated by Lewis and Whitman in 1924 (Peavy, Rowe, and Tchobanoglous 1985). According to this theory, the air-water interface is composed of two distinct films, one on the gas side and one on the water side, that serve as a barrier between the bulk phases. Figure 1 schematically illustrates the directions of the gas transfer.

The saturation concentration C_s is related to the solubility of a gas in equilibrium with a liquid and is governed by Henry's law which can be expressed as

$$x_e = \frac{P}{H} \tag{2a}$$

in which x_e is the equilibrium mole fraction of the dissolved gas at 1 atm or

$$x_e = \frac{moles\ of\ gas(n_g)}{moles\ of\ gas(n_g) + moles\ of\ liquid(n_l)} \tag{2b}$$

and P is the pressure of the gas above the liquid, H is the coefficient of absorption, also called Henry's coefficient, which is unique for each gas-liquid system. The relation between the volume saturation concentration C_s and the gas solubility x_s can be written as

$$C_s = \frac{\rho_l w_g x_e}{\rho_l w_g x_e + \rho_g w_l (1 - x_e)} \tag{3}$$

where ρ_g and ρ_l are the density of the gas and the density of the liquid, respectively; w_g and w_l are the molecule weight of the gas and molecule weight of the liquid, respectively.

Equation (1) can be solved to yield

$$C = C_s + (C_0 - C_s)e^{-k_a t} \tag{4}$$

in which C_0 is the initial gas concentration in the water. Since in stagnant situations (air and water are still), movement of gas molecules to and away from the interface depends totally on diffusion, k_a is very small, so the process is very slow. When wind is present, however, the situation changes and the process becomes fast, as will be analyzed below.

EFFECTS OF INTERACTION AT INTERFACE

When the wind blows over the water surface, water surface waves and surface drift are generated. The generation of waves is itself a subject under study. From his experiments, Wu (1975) reported that the relation between the surface drift u_s and the friction velocity u_* of the air flow can be approximately written as

$$u_s = 0.55 u_* \tag{5}$$

Since u_* is proportional to the magnitude of the representative wind speed, so Equation (5) indicates that the drift velocity is also proportional to the magnitude of the wind speed, which further implies that the existence of the surface drift is inevitable. Recently Zhou and Mendoza (1993) showed that the surface drift plays an important role in the wind wave generation process. The effect of surface drift on the gas transfer process is yet to be studied.

The effect of wind on gas transfer is directly reflected on the transfer coefficient k_l. Laboratory and field data indicated that the presence of wind makes k_l at least one order of magnitude larger than that without wind, and k_l is related to u_* in the following manner (Coantic 1986)

$$k_l = m_1 u_* Sc^{m_2} \tag{6}$$

where m_1 and m_2 are constants, $Sc = \nu/D$ is the Schmidt number (ν is the kinematic viscosity of the water, D is the Fick diffusion coefficient). If the interface is treated as rigid surface for simplicity, the constants m_1 and m_2 approximately take the typical values: m_1=1/12.5, m_2=-2/3 (Coantic 1986).

Since both u_s and k_l are proportional to u_* as suggested by Equations (5) and (6), so Equations (5) and (6) imply that, under wind wave conditions, k_l is proportional to u_s. This means that the larger the surface drift, the larger the gas transfer coefficient. The effect of wind on the gas transfer process displays itself in two ways: first, increasing k_l is equivalent to making the effective diffusion process faster; second, the presence of surface drift will add advection to the diffusion process, thus helping the transport faster in the related flow direction. This mechanism is the basis of the modeling to be introduced next.

GENERAL FORMULATION

When wind exists, the general equation governing the gas transfer takes the form

$$\frac{\partial C}{\partial t} + U_j \frac{\partial C}{\partial x_j} = D \frac{\partial^2 C}{\partial x_j^2} + k_a (C_s - C) \tag{7}$$

where $k_a = k_l/h$, h is the thickness of the liquid film, and k_l is called the (gas) transfer coefficient which has the same dimension as velocity. In Equation (7), U_j is the water flow velocity just beneath the interface, the related term displays the advection effect; D is the Fick diffusion coefficient, and the associated term represents the Fick diffusion; the last term in the Right-hand side is the source term.

In general, the water flow field composing of surface waves and surface drift is two and even three dimensional, and the diffusion can be longitudinal, vertical, and lateral. In this study, however, only the longitudinal transport is considered, since the effect of the surface drift on the transfer is maximum in this direction. Under this assumption, C is then only a function of time t and the coordinate x_1, where x_1 is in the wind direction (Figure 2), and Equation (7) is reduced to

$$\frac{\partial C}{\partial t} + U_1\frac{\partial C}{\partial x_1} = D\frac{\partial^2 C}{\partial x_1^2} + k_a(C_s - C) \qquad (8)$$

Introducing the new variable *tilde* $C = C - C_s$, it is clear that Equation (8) can be written as

$$\frac{\partial \tilde{C}}{\partial t} + U_1\frac{\partial \tilde{C}}{\partial x_1} = D\frac{\partial^2 \tilde{C}}{\partial x_1^2} - k_a\tilde{C} \qquad (9)$$

In the following analysis the notation $x \equiv x_1$ will be used for convenience.

FINITE ELEMENT MODELING

Finite element technique is used to numerically solve Equation (9). Specifically, *tilde* C is expressed as

$$\tilde{C} = \sum_{i=1}^{n} \tilde{C}_i \phi_i(x) \qquad (10)$$

in which $\phi_i(x)$ is the Lagrange quadratic shape function given by

$$\phi_1(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)}$$
$$\phi_2(x) = \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)}$$
$$\phi_3(x) = \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)}$$

The use of quadratic shape function is to suitably reflect the effect of the diffusion term in Equation (9). The Galerkin formulation is adopted in the finite element analysis, the backward finite difference method is employed for the time marching scheme, and the Gaussian elimination technique is used to solve the system of the linear algebraic equations. For the numerical results presented in this paper, a total of 10 to 30 elements were used for a distance of 10m.

A case of the following boundary condition and initial condition is considered:

$$C(x,t) = C_0, \quad x<0 \qquad (11)$$

$$C(x,t=0) = \begin{cases} 0, & x>0 \\ C_0, & x<0 \end{cases} \qquad (12)$$

In the simulation, C_0=0.01, C_s=0.03 are taken. The thickness of the liquid film is taken as h=4cm, the transfer coefficient used is k_f=4 x 10^{-5}m/s for the stagnant conditions, and k_f=4 x 10^{-4}m/s for the presence of wind. Figure 3 shows the simulation results of the stagnant condition. Figure 4 shows the simulated gas transfer process when surface waves and surface drift exist. The results shown in Figure 4 are corresponding to a typical drift velocity U_1=0.01m/s. The simulation indicates that there is a big difference in the time scales for the concentration to reach its saturation limit. Specifically, the gas transfer process with the presence of wind is about 10 times faster than that without wind effect.

DISCUSSION

In the present simulation the water flow velocity below the thin film is assumed to be stationary. In the case of the presence of the current, such as the stream condition, the flow velocity in the liquid film is the vector sum of the current velocity and the surface drift.

Gas transfer is a complicated process. The interface dynamics plays an important role in enhancing the gas transfer. Therefore, understanding the dynamic process at the interface is essential to the successful modeling and prediction of the gas transfer process. In particular, the dynamic processes stated below needs special attention.

Wave breaking. Wave breaking involves the significant air entrainment, which will greatly enhance the gas transfer. The experiments of Daniil and Gulliver (1991) showed that the transfer coefficient increases with the increment of the wave variable 2Af, where A is the wave amplitude before breaking, and f is the associated wave frequency. However, since wave breaking is a local phenomenon how to model its effect on the transfer process depends on the successful modeling of the wave breaking process.

Wave-structure interaction. The presence of structures in the water affects the wave field and will also directly or indirectly influence the gas transfer process. In the event of breaking waves, significant air entrainment and air bubbles are generated (Zhou, Chan, and Melville 1991). It is found that the presence of bubbles in the water also affects the gas transfer (Kanwisher 1963). Again, a successful modeling of the phenomenon is largely dependent upon the progress on the modeling of the bubble dynamics and the detailed dynamic process of the wave-structure interaction.

Turbulence. The presence of turbulence affects the gas transfer. The laboratory experiments of Dickey et al. (1984) indicated that the gas transfer coefficient is proportional to $D^{1/2}\varepsilon^{1/4}$, where ε is the turbulent dissipation rate. How to model the effect of turbulence on the gas transfer process is a topic in need of study. In the presence of turbulence, the concentration field C and the flow field U_i can be separated into

$$C = \bar{C} + \check{C} + C' \tag{13a}$$

$$U_i = \bar{U}_i + \check{U}_i + U'_i \tag{13b}$$

where the overbar denotes the Reynolds-averaged mean part, the symbol ˇ represents the associated wave part, and the prime stands for the turbulent part, respectively. Substituting Equation (13) into Equation (7) and then taking ensemble average over it produces

$$\begin{aligned}\frac{\partial \bar{C}}{\partial t} + \bar{U}_j \frac{\partial \bar{C}}{\partial x_j} &= D\frac{\partial^2 \bar{C}}{\partial x_j^2} + k_a(C_s - \bar{C}) \\ &+ \frac{\partial}{\partial x_j}(-\overline{\check{U}_j\check{C}} - \overline{U_j'C'})\end{aligned} \tag{14}$$

in which $\overline{\check{U}_j\check{C}}$ represents the wave effect, while $\overline{U_j'C'}$ stands for the turbulence effect. They are generally unknown and, as a result, certain closure schemes are needed in order to solve the equation.

Energy transfer process. In the initial period when wind starts to blow over the water surface, surface waves are generated and waves grow subsequently. The wave growth will cause the difference in the wave correlation term in Equation (14). The wave growth mechanism is governed by the energy transfer process. For instance, in the initial period, the energy transfer rate is proportional to the square of wave amplitude (Zhou and Mendoza 1993). Therefore, modeling the gas transfer process is related to understanding and modeling of the wind energy transfer to waves. When waves grow to their limit, wave breaking occurs. A complete model, therefore, must identify the different periods and include the effects.

CONCLUSIONS

From the context of the coupled dynamics of the air flow and the water flow at their interface, the effects of wind on the gas transfer process is explored. A simple numerical model is developed to illustrate the wind effects on the gas transfer process. It is clear that the presence of wind greatly enhances the transfer. Specifically, the diffusion process is significantly accelerated due to the dynamic interaction at the air-water interface, and the surface drift results in advection that helps the faster transfer process in the wind direction. Dynamic processes affecting the transfer are also discussed for improvement of numerical models.

REFERENCES

Coantic, M. 1986. A model for gas transfer across air-water interfaces with capillary waves. J. Geophys. Res. 91(C3), 3925-3943.

Daniil, E.I., and Gulliver, J.S. 1991. Influence of waves on air-water gas transfer. J. Environment Eng. ASCE, 117(5), 522-540.

Dickey, T.D., Hartman, B., Hammond, D., and Hurst, E. 1984. A laboratory technique for investigating the relationship between gas transfer and fluid turbulence, Gas transfer at water surfaces. W. Brutsaert and G.H. Jirka, eds., Reidel Publishing Co., Dordercht, Holland, 93-100.

Jähne, B., Münnich, K.O., Bösinger, R., Dutzi, A., Huber, W., and Libner, P. 1987. On the parameters influencing air-water gas exchange. J. Geophys. Res. 92(C2), 1937-1949.

Jähne, B., Wais, T., Mémery, L., Caulliez, G., Merlivat, L., Münnich, K.O., and Coantic, M. 1985. He and Rn gas exchange experiments in the large wind-wave facility of IMST. J. Geophys. Res. 90(C6), 11989-11997.

Kanwisher, J.W. 1963. On the exchange of gases between the atmosphere and the sea. Deep-Sea Res. 10, 195-207.

Kerman, B.R. 1984. A model of interfacial gas transfer for a well-roughened sea. J. Geophys. Res. 89(D1), 1439-1446.

Merlivat, L., and Mémery, L. 1983. Gas exchange across an air-water interface: Experimental results and modeling of bubble contribution to transfer. J. Geophys. Res. 88, 707-724.

Miles, J.W. 1957. On the generation of surface waves by shear flows. J. Fluid Mech. 3, 185-204.

Peavy, H.S., Rowe, D.R., and Tchobanoglous, G. 1985. Environmental Engineering. McGraw-Hill, New York.

Phillips, O.M. 1957. On the generation of waves by turbulent wind. J. Fluid Mech. 2, 417-445.

Wu, J. 1975. Wind-induced drift currents. J. Fluid Mech. 68, 49-70.

Zhou, D., Chan, E.S., and Melville, W.K. 1991. Wave impact pressure on vertical cylinders. Applied Ocean Research. 13(5), 220-234.

Zhou, D., and Mendoza, C. 1993. Surface drift effect on wind energy transfer to waves. J. Geophys. Res. 98(C8), 14527-14543.

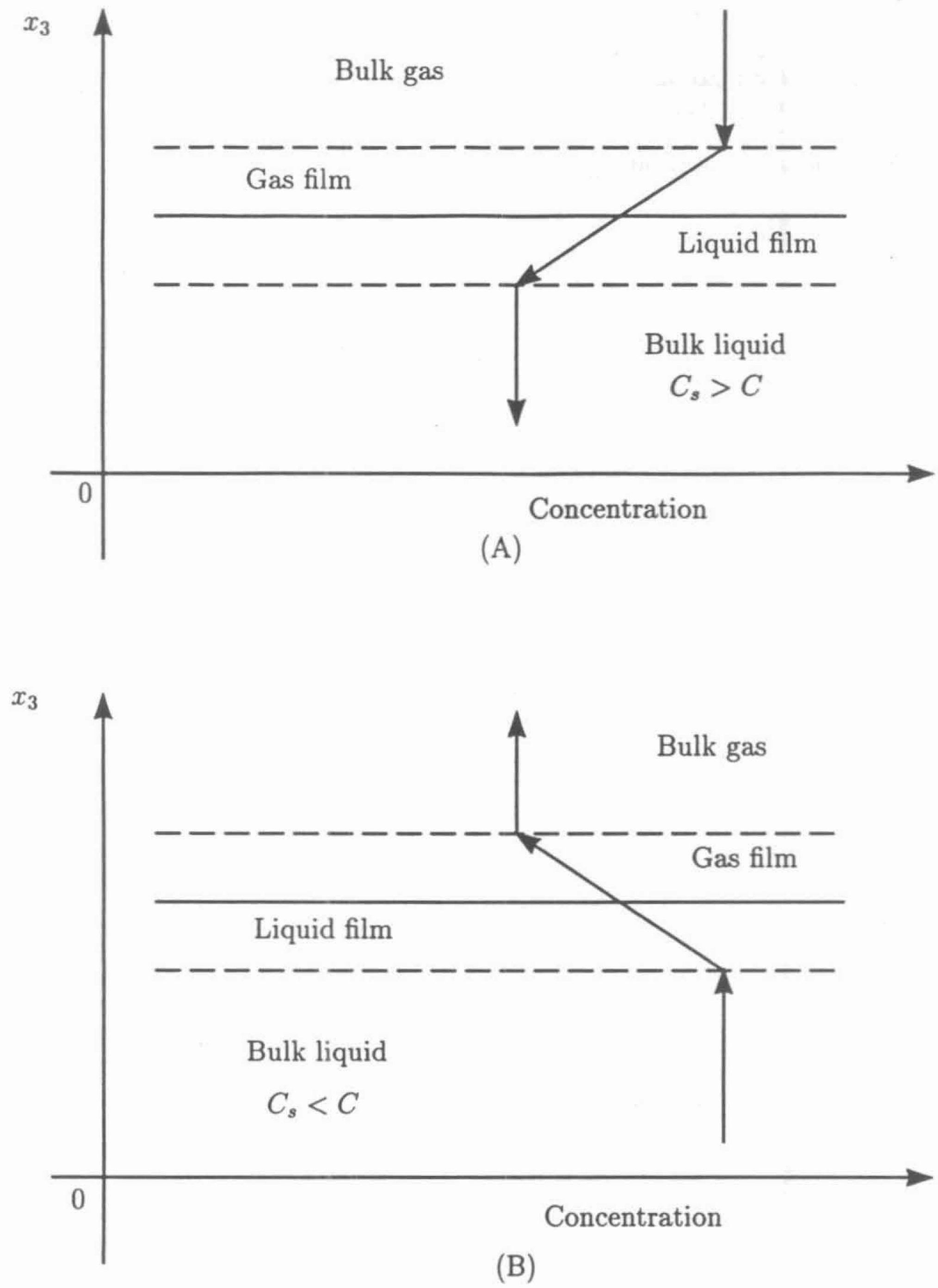

Figure 1. Two-film model of the interface between gas and liquid: (A) absorption mode and (B) desorption mode.

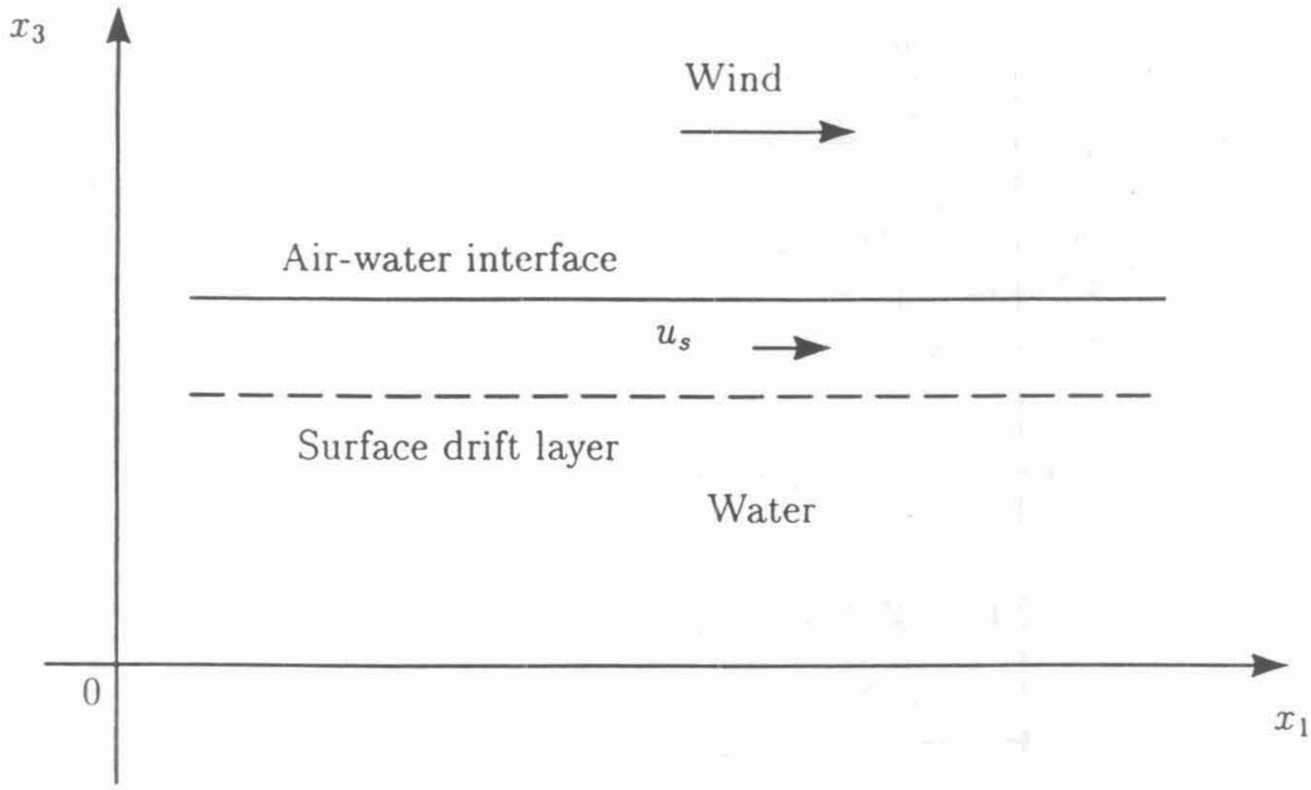

Figure 2. Definition Sketch

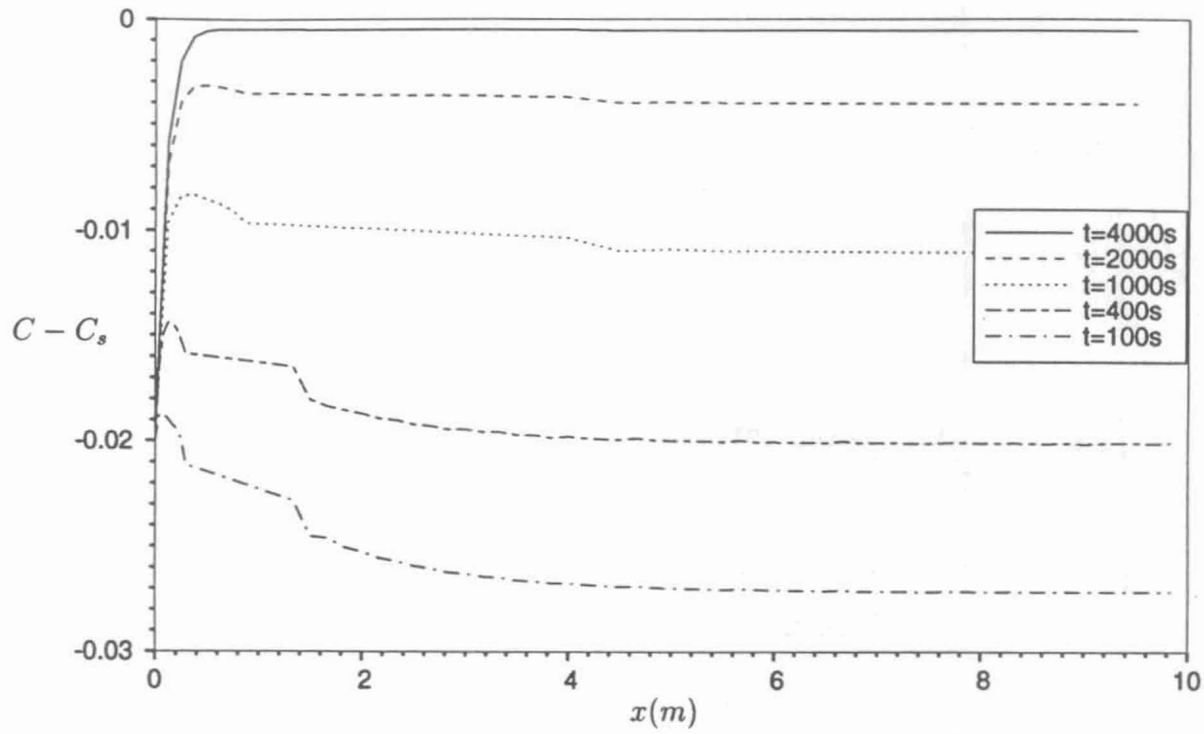

Figure 3. Simulated gas transfer process without wind effect

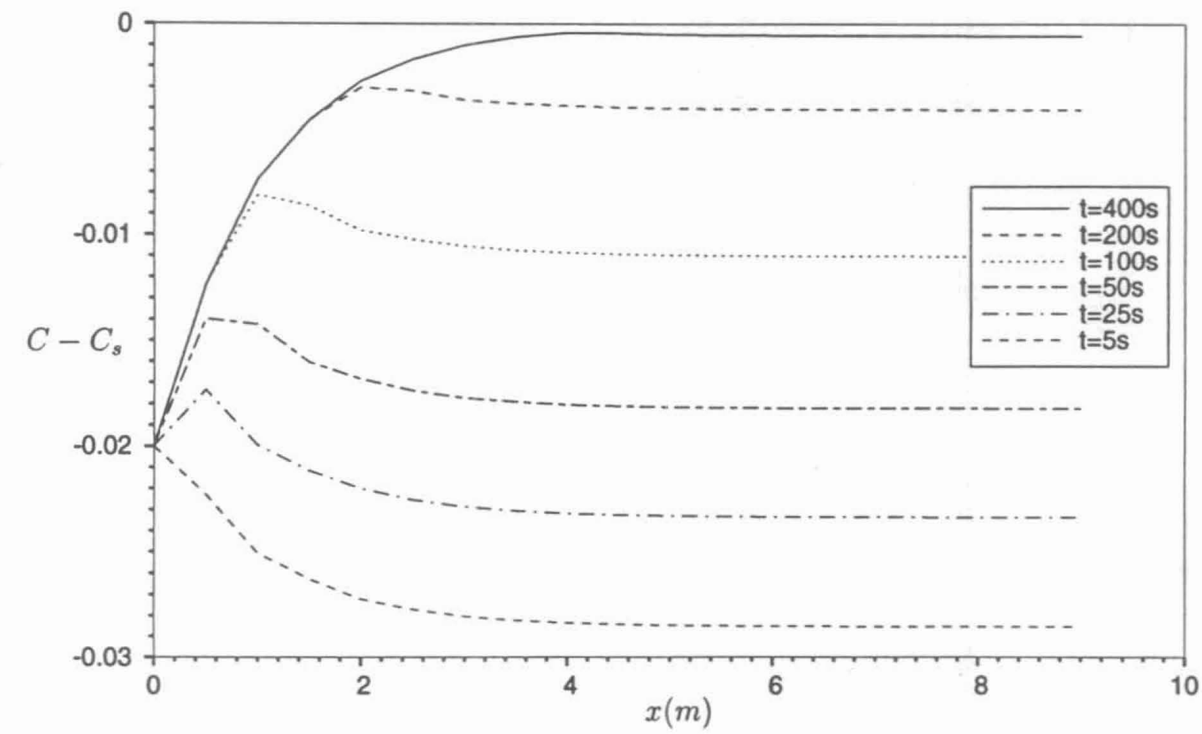

Figure 4. Simulated gas transfer process with wind effect