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DIFFUSIONAL MASS TRANSFER FROM BOTTOM SEDIMENT TO FLOWING WATER FOR SEDIMENT BED WITH STRIP ROUGHNESS

by

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SYNOPSIS

A model to estimate the release flux of dissolved substance from sediment to flowing water for a sediment bed with strip roughness has been formulated by applying analysis of gas transfer from vapor phase to solution phase. To examine the validity of this model, laboratory experiments were carried out to investigate how the diffusional mass transfer is affected by the flow velocity and roughness elements.

The experimental results show that release flux of dissolved substance increases with the increase in the flow velocity and that it decreases with the increase in the interval of roughness elements. These results suggest that the exchange between the water body near the sediment-water interface and the upper layer water becomes more frequent as the flow velocity increases or as the interval of roughness elements decreases. The release flux of dissolved substance estimated by the model is in fairly good agreement with the experimental values.

INTRODUCTION

The bottom sediment of rivers, reservoirs or lakes which contains a lot of organic compounds, nutrients, heavy metals and some chemical materials has often caused water quality problems. To take the effective measures for such problems, it is of great importance to clarify the mechanism of diffusional mass transfer at the sediment-water interface because the mechanism closely relates to dissolved oxygen (DO) consumption by bottom sediment and release of dissolved organic compounds or nutrients from the bottom sediment into the water.

Although most of the previous studies on diffusional mass transfer across the sediment-water interface were made from biological or chemical viewpoints, recently researchers are paying more attention to the effect of water flow on diffusional mass transfer, with a special focus on the evaluation of DO flux from water columns to sediment (SOD: Sediment Oxygen Demand) [1]. While all these researches were based on the assumption of a hydraulically smooth sediment surface, real bottom conditions are rugged and non-uniform and contain sand and gravel. Hence, diffusional mass transfer from the real sediment bed is considered to be influenced by the bed roughness. It seems that there are few reports dealing with the effect of bed roughness on diffusional mass transfer [2]. The authors have conducted a fundamental study on the effect of bed roughness on the release of dissolved substance from sediment to flowing water.

Near the sediment-water interface of the rough bed, flow regions with characteristics that are different from bulk flow are formed because of the wakes and vortices which form behind each roughness element. These locally disturbed flows influence the diffusional mass transfer across the interface as described below. The release flux of dissolved substance from sediment to flowing water is determined by the rate of exchange between water near the interface and the upper layer water. The rate of replacement of water bodies depends on the flow velocity and on parameters of roughness elements such as height, form and interval. Hence, we need to evaluate the exchange rate of water near the sediment-water interface as a function of flow velocity and of parameters of roughness elements in order to estimate the release flux for the rough-surface sediment bed.

We obtained a model for diffusional mass transfer in the region influenced by roughness elements near the sediment-water interface by applying gas transfer analysis from the vapor phase to the solution phase. Moreover, mass transfer in the upper water region was also analyzed by assuming that flow velocity and solute concentration have similar vertical profiles. By combining these two, a model to estimate the release flux from the rough-surface sediment bed was formulated. We conducted experiments to investigate the effect of roughness on the release flux of dissolved substance using kaolinite as the sediment, methylene blue as the dissolved substance and strip roughness as the roughness element. The validity of our formula for the release flux was examined by comparing the theoretical values with the experimental data.

FORMULATION OF DIFFUSIONAL MASS TRANSFER FROM SEDIMENT BED WITH STRIP ROUGHNESS

The flow structure and the process of dissolved substance release are schematically shown in Fig. 1. The strip roughness was used as roughness element in this study. The flow pattern near the sediment-water interface was divided into three zones. These were ① a zone upstream from the roughness element where the velocity profile is the same as the profile over a smooth bed, ② a zone where the velocity profile is different from the profile over a smooth bed due to the effect of roughness and ③ a reverse flow zone downstream from the roughness element.

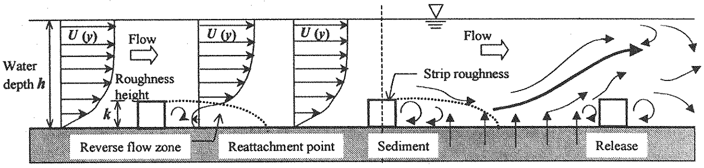

Fig.1 Flow structure and process of dissolved substance release.

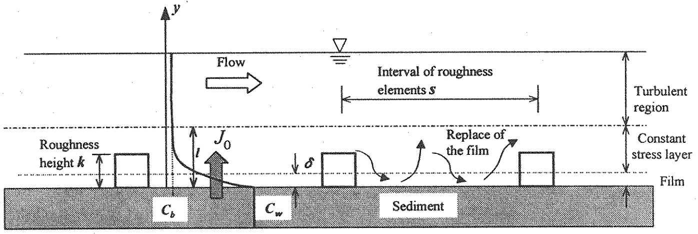

Fig.2 Modeling of dissolved substance release from bottom sediment to flowing water.

Since the solute concentration is a completely passive scalar for diffusional mass transfer from bottom sediment to flowing water, the release flux was estimated by solving the conservation equation of dissolved substance under given flow conditions. The flow structure near the bed was so complicated that diffusional mass transfer from the sediment bed with strip roughness needed to be simplified, and was thus modeled as shown in Fig. 2. It was assumed that there exists a film with thickness δ on the sediment surface, and this film is replaced repeatedly due to the near-bed turbulence, which results in migration of the dissolved substance.

In analyzing the process of diffusional mass transfer, the region above the interface is divided into two parts: the film mentioned above and the upper region where the solute concentration approaches the bulk concentration of solute C_b in Fig. 2. Moreover, the upper region is divided into a constant stress layer and a turbulent region. A model for the fully developed turbulent boundary layer was formulated under the following assumptions.

1) Any chemical reaction, microorganism metabolization or phenomena other than physical mass transfer are not considered.
2) The sediment surface where there is no strip roughness is hydraulically smooth, and

there is no erosion of sediment particles.

3) The flow velocity and solute concentration are uniform in the flow direction but have vertical profiles.
4) In the constant stress layer, the shear stress τ and the vertical flux of diffusional scalar J are equal to τ_0 and J_0 at the sediment-water interface, respectively.
5) In the turbulent region, the vertical profiles of flow velocity and solute concentration are similar, which leads to the following relationship: $\tau/J = \tau_0/J_0$.

A typical profile of solute concentration over the sediment bed with strip roughness is shown in Fig. 2. The vertical flux of the diffusional scalar and the shear stress are given as follows:

$$J = -(D + D_t)\frac{dC}{dy} \tag{1}$$

$$\tau = \rho(\nu + \nu_t)\frac{dU}{dy} \tag{2}$$

where J: vertical flux of the diffusional scalar (positive into water column), C: solute concentration, τ: shear stress, U: time-averaged velocity, D: molecular diffusivity, D_t: turbulent diffusivity, ν: kinematic viscosity, ν_t: kinematic eddy viscosity, ρ: fluid density, and y: vertical coordinate from the sediment-water interface (positive upward).

The boundary conditions are

$$C = C_w,\quad U = 0 \quad \text{at} \quad y = 0 \tag{3,a}$$

$$C = C_b,\quad U = \overline{U} \quad \text{at} \quad y = y_m \tag{3,b}$$

where C_w: solute concentration at the interface, C_b: bulk solute concentration, $\overline{U}$: mean velocity, and y_m: water depth where the flow velocity is equal to mean velocity $\overline{U}$.

When the Schmidt number Sc and the turbulent Schmidt number Sc_t are defined as

$$Sc = \frac{\nu}{D}, \qquad Sc_t = \frac{\nu_t}{D_t} \tag{4}$$

respectively, then the vertical profile of the solute concentration can be rewritten as follows:

$$dC = -\frac{J}{U_*}\frac{dy^+}{\frac{1}{Sc} + \frac{\nu_t^+}{Sc_t}} \tag{5}$$

In the above equation, y^+ and ν_t^+ are non-dimensionalized with respect to the friction velocity U_* and kinematic viscosity ν as:

$$y^+ = \frac{U_* y}{\nu}, \qquad \nu_t^+ = \frac{\nu_t}{\nu} \tag{6}$$

In addition, diffusional mass transfer is analyzed under the assumption that $Sc_t = 1$ in this study.

Mass transfer in the turbulent region

It is impossible to integrate Eq. (5) of y^+, because J is not constant in the turbulent region. By assuming a similarity in vertical profiles between the flow velocity and the solute concentration, we can express the difference in solute concentration $C_b - C_{l+}$ as a function of the boundary flux J_0 and the friction velocity $U_*(=\sqrt{\tau_0/\rho})$, where C_{l+} is solute concentration at $y^+ = l^+ = U_* l/\nu$ or $y = l$.

In Eqs. (1) and (2), D and ν are much smaller than D_t and ν_t, to the extent that they are negligible. From this, the following equation can be obtained.

$$\frac{\tau}{J} = \frac{\rho\nu_t \frac{dU}{dy}}{-D_t \frac{dC}{dy}} = \frac{\tau_0}{J_0} \tag{7}$$

Assuming Sc_t=1, Eq. (7) can be written as follows:

$$\frac{dC}{dy^+} = -\frac{J_0}{U_*}\frac{dU^+}{dy^+} \tag{8}$$

where $U^+=U/U_*$. By integrating Eq. (8) of y^+ from l^+ to y_m^+ ($=U_* y_m/\nu$), we can obtain the difference in solute concentration in the turbulent region as follows:

$$C_b - C_{l^+} = -\frac{J_0}{U_*}(\overline{U}^+ - U_{l^+}{}^+) \tag{9}$$

where $\overline{U}^+ = \overline{U}/U_*$, $U_{l+}{}^+=U_{l+}/U_*$, U_{l+} : velocity at $y^+=l^+$ or $y=l$.

Mass transfer in the constant stress layer

In the constant stress layer, the vertical flux of diffusional scalar J is assumed to be equal to J_0. Therefore, by integrating Eq. (5) of y^+ from δ^+ ($=U_*\delta/\nu$) to l^+, we can obtain the difference in solute concentration as follows:

$$C_{l^+} - C_{\delta^+} = -\frac{J_0}{U_*}\int_{\delta^+}^{l^+}\frac{dy^+}{\frac{1}{Sc}+\nu_t{}^+} \tag{10}$$

where $C_{\delta+}$: solute concentration at $y^+=\delta^+$ or $y=\delta$.

A vertical profile for eddy viscosity $\nu_t{}^+$ is required when we integrate Eq. (10) of y^+. The eddy viscosity is given by the turbulent kinetic energy balance [2] as follows:

$$\nu_t{}^+ = \frac{\kappa y^+ - 2 + \sqrt{(\kappa y^+ - 2)^2 - 4}}{2} \qquad (10 \leqq y^+) \tag{11}$$

$$\nu_t{}^+ = \left(\frac{y^+}{10}\right)^3 \qquad (0 \leqq y^+ < 10) \tag{12}$$

where κ: von Karman's universal constant (=0.4) for water.

Mass transfer in a film near the sediment-water interface

Diffusional mass transfer in the region near the sediment-water interface caused by roughness elements was modeled as shown in Fig. 2. We assumed that there exists a film with thickness δ on the sediment-water interface. This film is replaced repeatedly due to the near-bed turbulence. The mean rate of production of fresh film is constant and is denoted by r. The surface-age distribution $F(t)$ is given as a function of r as follows [4], [5]:

$$F(t) = re^{-rt} \tag{13}$$

Taking $F(t)$ into account, we obtained the following equation for the mean release rate of dissolved substance N from the sediment to the overlying water:

$$N = -\int_0^\infty D\left.\frac{dC}{dy}\right|_{y=0} F(t)dt = -Dr\int_0^\infty e^{-rt}\left.\frac{dC}{dy}\right|_{y=0} dt$$

$$= -\frac{DU_*}{\nu}\cdot\frac{d}{dy^+}\left.\mathcal{L}(C(t,y^+))\right|_{y^+=0} \tag{14}$$

where $\mathcal{L}(C(t,y^+))$: Laplace transformation of $C(t, y^+)$.

On the other hand, the solute concentration C should satisfy the following equation.

$$\frac{\partial C}{\partial t} = \frac{DU_*{}^2}{\nu^2}\frac{\partial^2 C}{\partial y^{+2}} \tag{15}$$

Since U_* and ν do not depend on y^+, $DU_*{}^2/\nu^2$ is independent of y^+ in the above equation.

When the boundary conditions are given as follows:

$$C=C_w \quad \text{at} \quad t \geqq 0,\ y^+=0 \tag{16,a}$$

$$C=C_{\delta+} \quad \text{at} \quad t>0,\ y^+=\delta^+ \tag{16,b}$$

the solution of Eq. (15) is expressed by Eq. (17):

$$\mathcal{L}(C(t,y^+)) = \frac{C_{\delta^+}}{r} + \frac{C_w - C_{\delta^+}}{r} \cdot \frac{e^{-\sqrt{\frac{r}{D'}}(y^+-\delta^+)} - e^{\sqrt{\frac{r}{D'}}(y^+-\delta^+)}}{e^{\sqrt{\frac{r}{D'}}\delta^+} - e^{-\sqrt{\frac{r}{D'}}\delta^+}} \tag{17}$$

where $D'=DU_*/\nu$ (const.).

When $d\mathcal{L}(C(t, y^+))/dy^+$ obtained from Eq. (17) is substituted into Eq. (14), the mean release rate of dissolved substance N, i.e., release flux J_0 is given as follows:

$$J_0 = \sqrt{Dr}\,\coth(\sqrt{\frac{r}{D'}}\delta^+)\cdot(C_w - C_{\delta^+}) \tag{18}$$

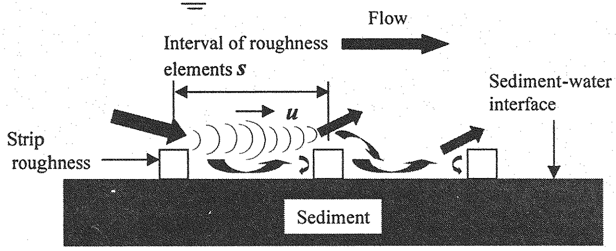

Fig.3 Schematic illustration of replacement of the water body near the sediment-water interface.

In order to evaluate the effect of roughness on diffusional mass transfer, it is necessary to formulate r and δ^+ in Eq. (18) as a function of the parameters of roughness elements such as height, form and/or interval. It is considered that r is related to the detention time of a water body in a gap between two strips as shown in Fig. 3. Thus, we expressed the velocity scale u for the water body near the interface by using the kinetic energy of the turbulent motion K $(=1/2\overline{u'_i{}^2})$ as follows:

$$u = c\sqrt{K} \tag{19}$$

where c: numerical constant. The relationship between K and Reynolds stress $-\overline{u'v'}$ is expressed by the following empirical formula for a fully-developed turbulent boundary layer in a two-dimensional shear flow.

$$\left|-\overline{u'v'}\right| / K = 0.3 = \text{const.} \tag{20}$$

On the other hand, because shear stress is constant in the logarithmic region over the film (i.e., $-\overline{u'v'} = U_*{}^2$), u can be expressed as follows:

$$u = c\sqrt{K} = \frac{c}{\sqrt{0.3}}U_* = c'U_* \tag{21}$$

In the above equation, c' is replaced with c.

$$u = cU_* \tag{22}$$

The detention time scale of the water body which travels in the flow direction at the velocity u in the gap between strips is defined by $T=s/u$, where s is the interval of roughness elements. Then, r is expressed by using the detention time scale T as follows:

$$r \propto \frac{1}{T} = \frac{u}{s} = \frac{cU_*}{s} \tag{23}$$

By substituting Eq. (23) into Eq. (18), we can obtain $C_{\delta+}$-C_w as a function of J_0, U_*, Sc, k and s as follows:

$$C_{\delta^+} - C_w = -\frac{J_0}{U_*} \cdot \frac{1}{\sqrt{c \cdot \frac{1}{Sc} \cdot \frac{1}{Re_*} \cdot \frac{k}{s}}\,\coth(\sqrt{c \cdot Re_* \cdot Sc \cdot \frac{k}{s}}\,\frac{\delta}{k})} \tag{24}$$

where $Re_*(=U_*k/\nu)$: roughness Reynolds number.

Derivation of a formula to estimate the release flux

The region above the sediment-water interface was divided into three zones as shown in Fig. 2. The mass transfer in each zone was modeled as mentioned above. Then, the differences in solute concentration in each zone were expressed using the release flux J_0. On the other hand, because the profile of the solute concentration is continuous at $y^+=l^+$ and $y^+=\delta^+$, a difference in solute concentration between the sediment-water interface and the bulk solute concentration C_b - C_w can be obtained from Eqs. (9), (10) and (24). Finally, the following formula can be obtained with respect to the release flux.

$$J_0 = -\frac{1}{F(Sc, Re_*, s/k)} U_*(C_b - C_w) \tag{25}$$

where

$$F(Sc, Re_*, s/k) = \overline{U}^+ - U_{l^+}{}^+ + \int_{\delta^+}^{l^+} \frac{dy^+}{\frac{1}{Sc} + \nu_t{}^+} + \frac{1}{\sqrt{c \cdot \frac{1}{Sc} \cdot \frac{1}{Re_*} \cdot \frac{k}{s}} \coth(\sqrt{c \cdot Re_* \cdot Sc \cdot \frac{k}{s}} \frac{\delta}{k})} \tag{26}$$

LABORATORY EXPERIMENT

Experimental apparatus

Laboratory experiments dealing with dissolved substance which is released from sediment bed with strip roughness were performed in an open channel of acrylic resin which was 650 cm long, 20 cm wide, 20 cm deep and which had a 1/650 slope. As shown in Fig. 4, square rods of stainless steel (k=5 mm) were placed at constant intervals on the channel bed as roughness elements. A sediment bed which was 5 cm deep was installed about 4 m down from the upstream end of the channel. The sediment bed was filled with a mixture of kaolinite and methylene blue solution which was prepared to a given ratio of water content. Water samples were collected at the downstream end of the channel under various flow velocity conditions, and the absorbance was measured with a spectrophotometer. The concentration C_{obs} of methylene blue in each sample was calculated from a calibration curve for concentration against absorbance obtained in advance. With the calculated value of C_{obs}, J_0 can be obtained from the

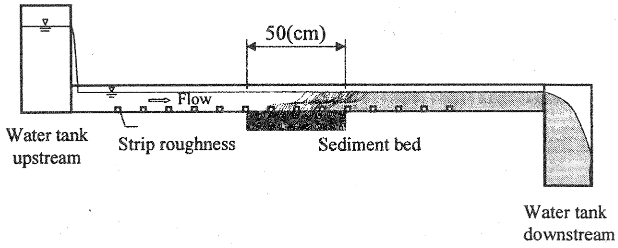

Fig.4 Schematic view of experimental setup.

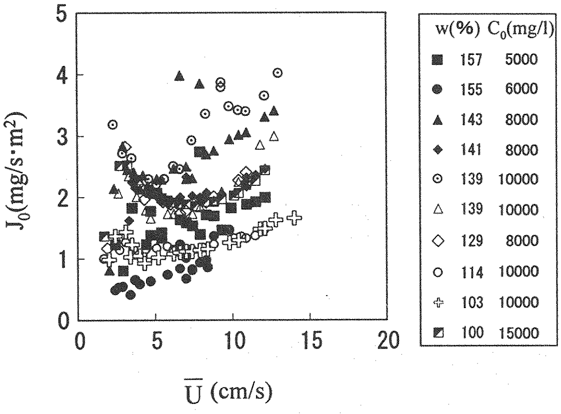

Fig.5 Relationship between release flux of dissolved substance J_0 and mean velocity $\overline{U}$.

following equation:

$$J_0 = QC_{\mathrm{obs}}/A \tag{27}$$

where Q: flow discharge, and A: area of sediment bed. The flow depth was determined as the distance between the sediment bed and the water surface at the center of the channel.

In order to investigate the influence of roughness on diffusional mass transfer, experiments were performed for various conditions, such as three intervals of roughness elements [i.e., s/k=8 (Case 1), s/k=16 (Case 2) and s/k=32 (Case 3)], different methylene blue concentrations and different amounts of kaolinite.

Effect of flow velocity on release flux

Figure 5 shows the dependence of the release flux J_0 on mean velocity $\overline{U}$ in Case 2. This figure shows that J_0 increases as $\overline{U}$ increases under almost all conditions, which is similar to the results of the experiments for a smooth bed [3]. These results suggest that the release flux increases when exchanges between the water body near the sediment-water interface and the upper layer water are encouraged by the increase in mean velocity.

Effect of interval of roughness elements on release flux

Figure 6 shows the relationship between the Sherwood number Sh and the Reynolds number Re in Cases 1, 2 and 3 with experimental data from a smooth bed [3]. The definitions of Sh and Re are as follows:

$$Sh = \frac{J_0}{C_w - C_b} \cdot \frac{R_H}{D} \tag{28}$$

$$Re = \frac{\overline{U}R_H}{\nu} \tag{29}$$

where R_H: hydraulic radius. In evaluating Sh in the experiments, we approximated the value of C_w as the solute concentration in pore water. In other words, C_w (mg/l) was calculated from Eq. (30) using the initial methylene blue concentration C_0 (mg/l) and water content of the sediment w (%). Moreover, C_b is approximated by the experimental value C_{obs}.

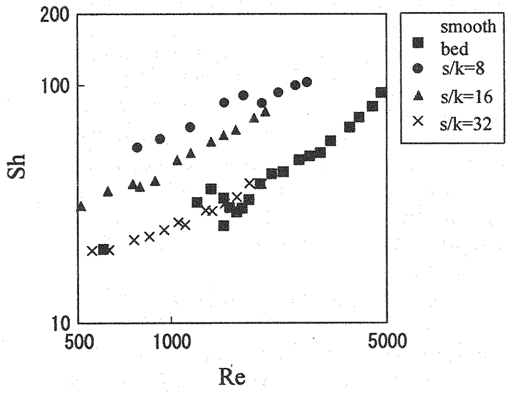

Fig.6 Effect of interval of roughness elements on the release flux.

$$C_w = \frac{-g(C_0, w) + \sqrt{\{g(C_0, w)\}^2 + 4.22C_0}}{4.22} \tag{30}$$

where

$$g(C_0, w) = 1 + \frac{1.07 \times 10^6}{w} - 2.11C_0 \tag{31}$$

We found in our previous study that the release flux was influenced by the water content of the sediment [3]. Therefore, we used experimental values for sediment beds with a constant water content ($w \cong 140\%$) for plotting rough and smooth bed cases as shown in Fig. 6. This figure shows that the values of Sh for the longest interval (i.e., s/k=32) are always small for given Re values, and Sh for given Re tends to be larger as the interval of roughness elements decreases. These results suggest that the release flux increases when exchanges between the water body near the sediment-water interface and the upper layer water are encouraged by the increase in disturbance due to the decrease in the interval of the roughness elements.

ESTIMATION OF RELEASE FLUX FOR SEDIMENT BED WITH STRIP ROUGHNESS

The release flux for the sediment bed with strip roughness is given by Eqs. (25) and (26) as described above. When Eq. (25) is non-dimensionalized, the Stanton number *St* (i.e., non-dimensional release flux) defined by Eq. (32) is given as Eq. (33).

$$St=\frac{J_0}{\overline{U}(C_w-C_b)} \tag{32}$$

$$St=\sqrt{\frac{f}{8}}\cdot\frac{1}{F(Sc,Re_*,s/k)} \tag{33}$$

The friction factor *f* in Eq. (33) is given by the following equation.

$$\frac{\overline{U}}{U_*}=\sqrt{\frac{8}{f}}=5.75\log_{10}\frac{R_H}{k_s}+6.25 \tag{34}$$

where k_s: equivalent sand roughness. Experiments were performed under the condition of completely rough bed because the values of $Re_*'(=U_*k_s/\nu)$ where k_s was calculated by Eq. (34) were larger than 70 in almost all experiments.

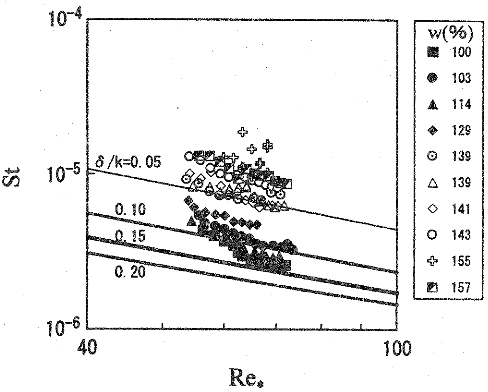

Fig.7 Comparison of experimental results and estimated values from the model (Case 2).

To verify the validity of Eq. (33), the estimation by the model was compared with the experimental results. The values of *St* estimated by Eq. (33) with varied non-dimensional film thickness δ/k and numerical constant *c* of 0.001 are shown together with the experimental values in Fig. 7 (Case 2). In the calculation of *St* in Eq. (33), *Sc* was assumed to be constant, i.e. *Sc*=4500, although it varied from 4000 to 5500 in the experiments.

On the other hand, to calculate the experimental values of *St*, C_w was approximated by the solute concentration in the pore water; i.e., C_w was calculated from Eq. (30) with C_0 and *w*.

In Fig. 7, the experimental values are plotted downward when the water content of the sediment decreases, and they are plotted upward when the water content of the sediment increases. The influence of the water content is thought to be due to mass transfer with adsorption and desorption in the sediment. In other words, the adsorption-desorption processes between the solute and sediment particles are related to the spatial concentration of sediment particles (i.e. the number of sediment particles per unit volume of sediment) which varies with the water content of the sediment.

Figure 7 also shows that the estimated values of larger δ/k tend to agree fairly well with the experimental values for sediment with a lower water content, and that the estimated values of smaller δ/k agree more or less with the experimental values for higher water content. In addition, the erosion of the sediment bed might influence the experimental values for higher water content which are larger than the estimated values.

Consequently, by adjusting the non-dimensional film thickness δ/k for sediment with a given water content, the release flux estimated by the model agrees well with the experimental values.

CONCLUSION

Three important findings in this study can be summarized as follows:

1) The diffusional mass transfer in the region influenced by strip roughness near the sediment-water interface was modeled by applying gas transfer analysis from the vapor phase to the solution phase. Under the assumption that the vertical profiles of flow velocity and solute concentration were similar over the region near the interface, a model to estimate the release flux from sediment bed with strip roughness was formulated.
2) The release flux of dissolved substance varies in accordance with the mean flow velocity on the sediment, the interval of roughness elements and the water content of the sediment. The influence of mean flow velocity and the roughness strip interval on the release flux reflects the frequency of replacement of the water body in the gaps between the strips. In addition, the influence of the water content of the sediment on the release flux is caused by mass transfer with adsorption and desorption in the sediment.
3) When the non-dimensional film thickness δ/k is correctly determined for sediment with a given water content, the release flux of dissolved substance estimated by our model agrees fairly well with the experimental values.

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APPENDIX-NOTATION

The following symbols are used in this paper :

J = vertical flux of diffusional scalar ;

J_0 = vertical flux of diffusional scalar at the sediment-water interface ;

C = solute concentration ;

τ_0 = boundary shear stress ;

τ = shear stress ;

U = time-averaged velocity ;

ρ = fluid density ;

D = molecular diffusivity ;

D_t = turbulent diffusivity ;

ν = kinematic viscosity ;

ν_t = kinematic eddy viscosity ;

C_w = solute concentration at sediment-water interface ;

C_b = bulk solute concentration ;

Sc = Schmidt number ;

Sc_t = turbulent Schmidt number ;

U_* = friction velocity ;

f = friction factor ;

$\overline{U}$ = mean velocity ;

κ = von Karman's universal constant (=0.4) for water ;

K = kinetic energy of turbulent motion ;

k = roughness height ;

s = interval of roughness elements ;

Q = flow discharge ;

A = area of sediment bed ;

w = water content of the sediment ;

Sh = Sherwood number ;

Re = Reynolds number ;

k_s = equivalent sand roughness ;

δ = film thickness ;

$Re_*(=U_*k/\nu)$ = roughness Reynolds number ;

$Re'_*(=U_*k_s/\nu)$ = roughness Reynolds number ; and

St = Stanton number.

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