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2-D Non-Fickian Dispersion Model for the Initial Period of River Mixing

Il Won Seo, Inhwan Park
Department of Civil and Environmental Engineering, Seoul National University
Seoul, Korea

ABSTRACT

The non-Fickian dispersion model which was available both in the initial and Taylor periods was developed using the physical interpretation of shear dispersion theory and particle tracking method. The proposed model treated the diffusive mass flux term using the sequential calculations of shear advection and vertical diffusion instead of implementing the dispersion coefficients. The simulation results of the non-Fickian dispersion model show that the concentration curves have the skewed distribution in the initial period and gradually changed to the symmetric distribution likewise the Fickian dispersion model. Also, the skewness coefficients of concentration curves were similar with the theoretical formula.

KEY WORDS: Non-Fickian dispersion model; Initial period; Taylor period; Skewed concentration curve; Shear dispersion

INTRODUCTION

Simulation of the pollutant mixing in shallow water flow has been conducted using the depth-averaged advection-dispersion equation. In the process of depth-averaging, the diffusive mass flux induced by the velocity deviations in vertical direction is treated using the Fick's law in which the concentration flux is assumed to be proportional to the concentration gradient (Taylor, 1954). The model applying the Fick's law is named as the Fickian dispersion model, and the proportional coefficient is called the dispersion coefficient. However, the proportionality is attained only after the Taylor period where the balance is achieved between the shear advection and vertical diffusion (Fischer et al., 1979). Also, the initial period is not short enough to be neglected, and the mixing properties have differences from the Taylor period (Chatwin, 1973). Therefore, the alternative model is necessary to analyze the pollutant mixing in the initial period.

The aim of this study is to develop the non-Fickian dispersion model for analysis of the pollutant mixing both in the initial and Taylor periods, and the mixing properties were analyzed by using the simulation results. The new model was developed using the particle tracking method, and the step-by-step calculation method to calculate pollutant mixing in the initial period instead of using the Fick's law. Also, the simulation results were compared with the Fickian dispersion model, and the solute mixing in the initial period was analyzed.

MIXING PROPERTIES IN THE INITIAL PERIOD

The shear dispersion is occurred by the interaction between the shear advection and vertical diffusion. Contaminants introduced in rivers are translated by the shear flow. The stretched pollutant cloud induced by the velocity deviations is well mixed in vertical by the turbulent fluctuations. In the Fickian dispersion model, the aforementioned shear dispersion is treated using Eq. 1 according to the Taylor's analysis (Taylor, 1954).

$$-\frac{1}{h}\int_0^h u_i'(z)c'(z)\,dz = D_{ij}\frac{\partial \overline{c}}{\partial x_j} \tag{1}$$

where h is the water depth; u_i' is the velocity deviations which is defined as $u_i - \overline{u}_i$; u_i is the vertical velocity profile; $\overline{u}_i$ is the depth-averaged velocity; $\overline{c}$ is the depth-averaged concentration; c' is the concentration deviation between c and $\overline{c}$; D_{ij} is the dispersion coefficient. However, Eq. 1 can be applied after the initial period. Chatwin (1970) presented the initial period as Eq. 2.

$$t_I = \frac{0.4h^2}{\varepsilon_z} \tag{2}$$

where t_I is the initial period; ε_z is the vertical diffusion coefficient. t_I was calculated using the hydraulic properties summarized by Jeon et al. (2007), and the change of t_I was plotted against h and u^* in Fig. 1. From the calculation results, t_I was maintained for 0.2 ~ 9.1 min which was increased in the deep water. Thus, the initial period would be expected to be increased in large rivers.

The pollutant mixing in the initial period is also different with the mixing in Taylor period. Rutherford (1994) reported that the cloud of contaminants is negatively skewed due to the velocity distributions. Thus, the skewness coefficient is abruptly increased after the pollutant injection and then slowly decreased. The change of skewness coefficient was presented by Nordin and Troutman (1980) as follow.

$$\xi = 3\sqrt{\frac{2K}{Ux}} \tag{3}$$

where ξ is the skewness coefficient; K is the longitudinal dispersion coefficient; U is the section-averaged velocity. According to Eq. 3, the skewness coefficient converges to 0 at the far away. Furthermore, during the initial period, the variance of concentration curves is non-linearly increased with time due to the imbalance between shear advection and vertical diffusion. After the initial period, the increase of variance has the linear relation with time. The Fickian dispersion model would not be reproduced the aforementioned mixing properties of contaminants in the initial period which maintained quite long period.

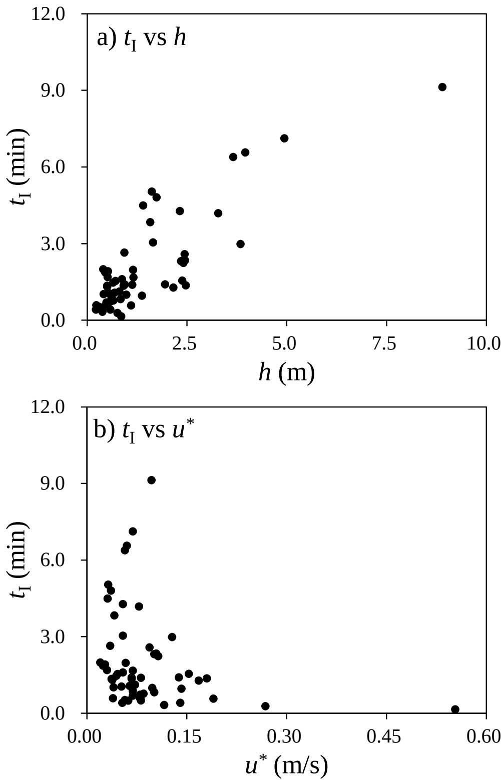

Fig. 1 Change of the initial period according to the hydraulic properties

DEVELOPMENT OF THE 2-D NON-FICKIAN DISPERSION MODEL

For the simulation of pollutant mixing in the initial period, the 2-D non-Fickian dispersion model was developed using the sequential calculation of the shear dispersion process and the particle tracking method. In the particle tracking method, an individual particle can be traced using Eq. 4.

$$\Delta x_i = A_i \Delta t + B_{ij} \Delta W_j \tag{4}$$

where Δx_i is the displacements; A_i is the drift term; B_{ij} is the diffusion term; ΔW_j is the Wiener process defined as $R\sqrt{\Delta t}$; R is the random number which follows the normal distribution. The particle position has the stochastic properties, and it has the conditional probability density, p which follows the Fokker-Plank equation in Eq. 5 (Gardiner, 1985).

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}\left(A_i p\right) = \frac{1}{2}\frac{\partial^2}{\partial x_i \partial x_j}\left(B_{ik} B_{jk} p\right) \tag{5}$$

In the 2-D mixing, A_i and B_{ij} can be determined from the mathematical analogy with the depth-averaged advection-dispersion equation as follow.

$$p = \bar{c} h \tag{6a}$$

$$A_i = \bar{u}_i + \frac{1}{h\bar{c}}\int_0^h u_i' c' \, dz \tag{6b}$$

$$B_{ij} = \varepsilon_h \tag{6c}$$

where ε_h is the horizontal diffusion coefficient. Eq. 6 was substituted into Eq. 4, and the particle position was calculated using Eq. 7 without applying the Taylor's analysis.

$$\Delta x_i = \left(\frac{1}{h}\int_0^h \frac{c}{\bar{c}} u_i \, dz\right)\Delta t + R\sqrt{\varepsilon_h \Delta t} \tag{7}$$

Eq. 7 consists of the deterministic translation by shear flow and the random translation by the isotropic homogeneous turbulence. In the deterministic translation, the pollutant column is transported by the skewed vertical velocity profiles, and the translated pollutant cloud was well mixed in vertical. Also, in the random translation, the pollutant particles were displaced by the turbulent fluctuations in the horizontal plane.

The non-Fickian dispersion model was developed using Eq. 7, and Eq. 7 was calculated using the step-by-step calculations which calculates the continuous physical process using the discontinuous computation step (Fischer, 1968). The computation procedures were divided into the shear advection and vertical diffusion steps as shown in Fig. 2. In the shear advection step, displacements of pollutant particles by the vertical velocity profiles and the turbulent fluctuations were calculated using Eq. 8.

$$x_i\left(z_k, t_s\right) = x_i\left(z_k, t\right) + u_i\left(z_k\right)\Delta t + R\sqrt{2\varepsilon_h \Delta t} \tag{8}$$

where t_s is the time after the shear advection. In this study, the shear flows were reproduced using the vertical velocity formulas. The stream-wise velocity was assumed to have the logarithmic distribution in Eq. 9a (Rozovskii, 1959), and the span-wise velocity was generated using the linear profile in Eq. 9b (Odgaard, 1986).

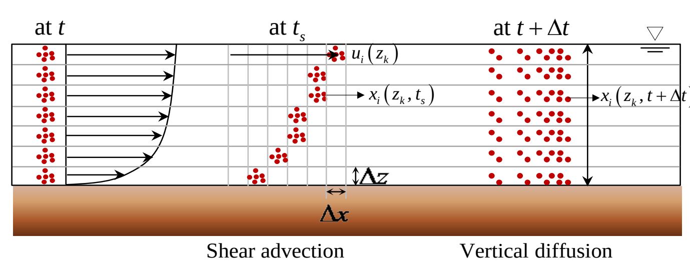

Fig. 2 Computation procedures of the non-Fickian dispersion model

$$u_s\left(z_k\right) = \bar{u}_s\left[1 + \frac{1}{m}\left(1 + \ln\frac{z_k}{h}\right)\right] \tag{9a}$$

$$u_n\left(z_k\right) = \bar{u}_n + 2\left(\bar{u}_s \frac{2m+1}{2\kappa^2 m}\frac{h}{r_c}\right)\left(\frac{z_k}{h} - \frac{1}{2}\right) \tag{9b}$$

where u_s^k, u_n^k is the vertical velocity profiles in stream-wise and span-wise directions, respectively; $\bar{u}_s$, $\bar{u}_n$ is the depth-averaged velocity in stream-wise and span-wise, respectively; z_k is the vertical position on k th layer; κ is the von Karman constant; $m = \kappa C_h / \sqrt{g}$; C_h is the Chezy coefficient. In the vertical diffusion step, the translated particles were rearranged in vertical using Eq. 10.

$$x_i\left(z_k, t+\Delta t\right) = x_i\left(z_k + h/L, t_s\right) \quad (10a)$$

$$x_i\left(z_k, t+\Delta t\right) = x_i\left(z_k + R\sqrt{2\varepsilon_z \Delta t}, t\right) \quad (10b)$$

where L is the number of vertical layer. As shown in Fig. 2, pollutant particles were evenly distributed on each vertical layer using Eq. 10a. However, if Δt is shorter than the time for vertical mixing completion (t_m), some part of pollutant particles would not be fully mixed. Thus, only α% of particles which was defined as $\alpha = \Delta t / t_m$ was fully mixed using Eq. 10a and the remained particles were randomly mixed in vertical using Eq. 10b. The developed model would be applied both in the initial and Taylor period since the model doesn't implement the Taylor's analysis.

SIMULATION RESULTS

The solute transport simulation was conducted in the straight channel using the 2-D non-Fickian dispersion model. Also, the simulation results were compared with the Fickian dispersion model. As shown in Table 1, the section-averaged velocity (U) was 1 m/s and the water depth was 0.3 m. For the simulation of non-Fickian dispersion model, 10,000 particles which has 1 kg total mass (M) were introduced at the center of channel and the number of vertical layers was set as 100. The Fickian dispersion model were calculated using Eq. 11.

$$\bar{c}\left(x, y, t\right) = \frac{M/h}{4\pi t\sqrt{D_L D_T}} \exp\left[-\frac{\left(x-\bar{u}t\right)^2}{4D_L t} - \frac{\left(y-\bar{v}t\right)^2}{4D_T t}\right] \quad (11)$$

where D_L, D_T is the longitudinal and transverse dispersion coefficient, respectively. In Eq. 12, D_L/hu^* was 5.93 as presented by Elder (1959) in the assumption of logarithmic velocity profile, and D_L/hu^* was 0.15 according to the study of Fischer et al. (1979).

Table 1. Simulation conditions for the solute transport

	U (m/s)	h (m)	W (m)	$\frac{D_L}{hu^*}$	$\frac{D_T}{hu^*}$	n
Fickian dispersion model	1.0	0.3	4.0	5.93	0.15	-
Non-Fickian dispersion model				-	-	10,000

Simulation results of the non-Fickian dispersion model were plotted in Fig. 3. In the hydraulic conditions in Table 1, t_I was maintained for 18.6 sec, and the particle distribution at $t = 12$ sec shows the pollutant cloud in the initial period. In the initial period, the pollutant particles were accumulated at the front of the cloud of contaminant due to the imbalance between the shear advection and vertical diffusion. However, during the Taylor period, the peak value was moved to the center of pollutant cloud which shows the symmetric distribution. Fig. 4 shows the concentration-distance curves which were plotted with the Fickian dispersion model. The results of non-Fickian dispersion model has the asymmetric distribution in the initial period, whereas the Fickian dispersion model generates the symmetric concentration curve. After the initial period, the concentration curve of non-Fickian dispersion model changed to the Gaussian distribution and the results were similar with the Fickian dispersion model.

The skewness coefficient of concentration curves were calculated from the simulation results of non-Fickian dispersion model. Table 2 shows the calculation results of the skewness coefficient using the simulation results and Eq. (3). After pollutant injection, the concentration curves have the asymmetric distribution and ξ was increased to 0.71. Also, ξ

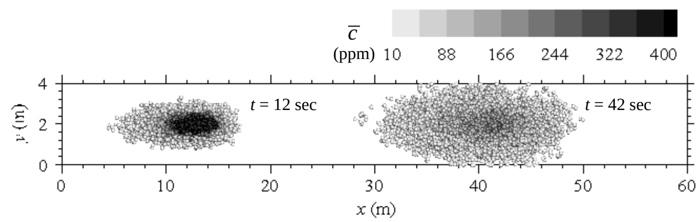

Fig. 3 Simulation results of the 2-D non-Fickian dispersion model

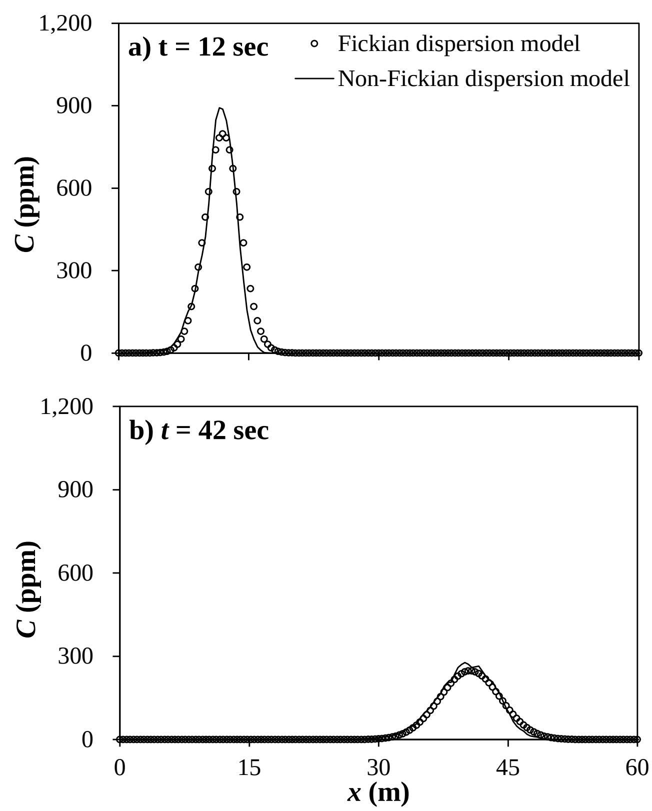

Fig. 4 Comparison of the concentration-distance curves

Table 2. Change of the skewness coefficient

ξ	t (sec)				
	6	18	30	42	54
Nordin and Troutman (1980)	0.79	0.46	0.35	0.30	0.26
Non-Fickian dispersion model	0.71	0.53	0.40	0.32	0.28

was gradually decreased to 0.28 in which the concentration curves were approached to the Gaussian distribution. The change of ξ with time show similar results with the theoretical value presented by Nordin and Troutman (1980). Thus, the non-Fickian dispersion model would be properly reproduced the interaction between the shear advection and vertical diffusion.

From the simulation results of the non-Fickian dispersion model, the longitudinal dispersion coefficient was calculated using the moment method. Fig. 5 shows the time evolution of D_L / hu^* . In the initial period, the variance of concentration curve was abruptly increased and slowly converged to the value of 6.0 which was similar with the proposed value by Elder (1959). These results indicate that the Fickian dispersion model which use the invariant value of dispersion coefficient would not be appropriate to use in the initial period. Also, the simulation results using the non-Fickian dispersion model were provided similar results with the Fickian dispersion model during the Taylor period.

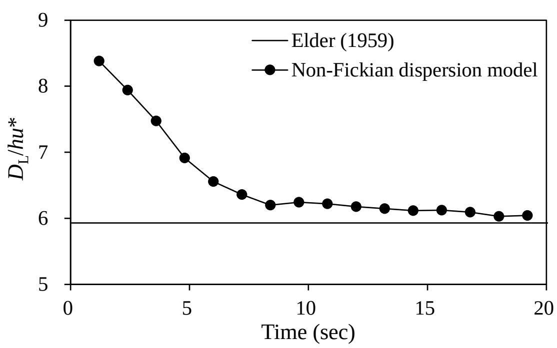

Fig. 5 Change of the longitudinal dispersion coefficient with time

CONCLUSIONS

In this study, the 2-D non-Fickian dispersion model was developed for the simulation of solute transport both in the initial and Taylor periods. The new model was adopted the particle tracking method and the step-by-step calculation to reproduce the physical mixing process by shear dispersion. The computation procedures consist of the shear advection and vertical diffusion steps. In the shear advection step, the introduced particles were transported by the vertical velocity profiles in the stream-wise and span-wise directions. After the horizontal translations, the particles were redistributed in vertical during the vertical diffusion step and the 2-D mixing was completed. The non-Fickian dispersion model can be applied in the initial period because the model avoided to use the Taylor's analysis.

The non-Fickian dispersion model was applied in the straight channel and compared the simulation results with the Fickian dispersion model. The concentration curves of the non-Fickian dispersion model show the asymmetric distribution in the initial period, whereas the Fickian dispersion model shows the symmetric distribution. In the Taylor period, the breakthrough curves of non-Fickian dispersion model were slowly changed to the symmetric distribution which produced similar results with the Fickian dispersion model. The calculation results of skewness coefficients were similar with the results of theoretical formula suggested by Nordin and Troutman (1980). Furthermore, the calculation results of dispersion coefficient during the Taylor period show the similar value with the Elder's study. Thus, the non-Fickian dispersion model properly reproduced the solute transport in the initial and Taylor periods.

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