Unsteady Dispersion of Nonconservative Pollutants in Natural Rivers

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Abstract

A numerical model is presented for the unsteady dispersion of nonconservative contaminants in natural streams. The model is based on a fractional-step finite difference method splitting the one-dimensional longitudinal dispersion equation for nonconservative substance into a set of three equations for pure advection, first-order decay, and pure diffusion, respectively. At each time step, the equations are solved successively over a 1/3 time step by the two-point fourth-order Holly-Preissmann scheme, a local analytic solution, and Crank-Nicholson schemes, respectively. The model is applied to hindcast the phenol spill accident which occurred in Nakdong River, South Korea in 1991. Sensitivities of the dispersion calculation to empirical equations for dispersion coefficient are analyzed. An optimization technique is used to calibrate the model parameters.

1. Introduction

A number of studies have been carried out on finite difference numerical methods for the longitudinal dispersion equation. However, most of the Eulerian methods do not adequately incorporate the hyperbolicity, or the directionality of the information propagation since they approximate partial derivatives with respect to time and space using fixed computational grid points. Consequently, they often accompany with numerical diffusion or numerical oscillations. Holly and Preissmann (1977) developed an explicit finite difference method, called Holly-Preissmann scheme, for pure advection equation, which takes the hyperbolicity of the equation by approximating the total derivative along the characteristic line. Since the characteristic line which passes through a grid point at current time level does not necessarily come from a grid point of the previous time level, it is needed to express the concentrations at any spatial points in

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terms of those at fixed Eulerian grid points. To do this they introduced a Hermite interpolating polynomial of the Courant number with coefficients expressed in terms of concentrations and their spatial derivatives at two adjacent grid points. They also extended the method to the advection-diffusion equation by approximating the diffusion term by the second-order partial derivative of the interpolating polynomial.

Holly and Usseglio-Polatera (1984) developed a split-operator method for two-dimensional advective diffusion equation. They decomposed the equation into pure advection and pure diffusion parts, and solved the advection equation using the Holly-Preissmann method with cubic interpolating polynomial, and solved the diffusion equation using the Crank-Nicholson scheme. One-dimensional version of their method is used as a numerical method for the longitudinal dispersion equation of the stream water quality model, CE-QUAL-RIV1 (WES, 1990), which is able to simulate the first-order decay of nonconservative substances as well.

In this study, the CE-QUAL-RIV1 model is modified to improve the numerical method of the first-order decay calculation. The modified model is tested using an analytic solution for the longitudinal dispersion of continuous source released into a nonuniform flow field. The 1991 phenol spill accident which occurred in Nakdong River, South Korea is hindcasted by the model.

2. Description of the Model

The model consists of two parts which are unsteady flow model and longitudinal dispersion model. The theoretical basis for each model are described briefly in the following.

2.1.Unsteady flow model

The flow model adopted here is extracted from the CHARIMA code (Holly et al., 1990) which was developed for the simulation of sediment transport in a looped-network channel system. The looped-network unsteady flow model is the most general one for it can also be applied to a single channel or branched-network systems. The model is composed of links, nodes, and computational points. The governing equations are one-dimensional St. Venant equations for links, and nodal continuity and energy equations.

The governing partial differential equations are discretized by the Preissmann's four-point implicit scheme (Liggett and Cunge, 1975; Cunge et al., 1980). The discretized equations together constitute a nonlinear system with stages and discharges at computational points and nodal water surface elevations unknown. Newton-Raphson method is used to solve the nonlinear system, and the resulting linear equations for the Newton-Raphson corrections can be solved with the least amount of calculation by applying the looped double sweep algorithm. The general double sweep solution algorithm comprises four phases for each iteration: link forward sweep, node matrix loading, node solution, and link backward sweep. Details of the solution algorithm can be found in many articles such as Cunge et al. (1980), and Holly et al. (1990).

From this flow model, the discharge and cross-sectional area of the flow can be computed for every computational point along the channels, and then used as the input to the dispersion model.

2.2. Longitudinal dispersion model

The equation for longitudinal dispersion of nonconservative contaminants in a channel can be expressed as

$$\frac{\partial(AC)}{\partial t}+\frac{\partial(UAC)}{\partial x}=\frac{\partial}{\partial x}\left[DA\frac{\partial C}{\partial x}\right]-kAC \qquad (1)$$

in which *C(x,t)* = mass concentration; *A(x,t)* = channel cross-section; *U(x,t)* = cross-sectional mean flow velocity; *D(x,t)* = longitudinal dispersion coefficient; *k* = first-order decay constant; *x* = spatial coordinate; and *t* = time. Using the equation of flow continuity, Eq. (1) can be reduced to the following form:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=D\frac{\partial^2 C}{\partial x^2}-kC \qquad (2)$$

where

$$u=U-\left[\frac{\partial D}{\partial x}+\frac{D}{A}\frac{\partial A}{\partial x}\right] \qquad (3)$$

The governing equation, (2) is classified as a parabolic partial differential equation, but it also implies hyperbolicity due to the advection term on the left hand side. These two types of equations have different characteristics from each other; and thus, appropriate numerical methods for each equation are quite different. Therefore, a fractional steps technique is used where the governing equation is time-split to separate the physical processes involved, i.e., the mean flow advection, first-order decay, and shear flow dispersion. Eq. (2) can be written as the set of equations

$$\frac{\partial C}{\partial t}+3\overline{u}\frac{\partial C}{\partial x}=0\,,\quad n\Delta t\le t\le(n+\frac{1}{3})\Delta t \tag{4}$$

$$\frac{\partial C}{\partial t}=-3kC,\quad (n+\frac{1}{3})\Delta t\le t\le(n+\frac{2}{3})\Delta t \tag{5}$$

$$\frac{\partial C}{\partial t}=3\overline{D}\frac{\partial^2 C}{\partial x^2}\,,\quad (n+\frac{2}{3})\Delta t\le t\le(n+1)\Delta t \tag{6}$$

where the upper bar denotes the average value between two time levels, n and n+1. The equations are solved separately in three 1/3 time steps to get from time level n to n+1. Note that Eqs. (4), (5), and (6) sum to give Eq. (2) over one time step. Eq. (4) contains three times of the advection effect concentrated over the first 1/3 time step; similarly, Eqs. (5) and (6) incorporate three times the first-order decay and diffusive effect, respectively, applied over the second and the last 1/3 of the step. Advantage of the fractional step method is that the most suitable numerical schemes for each equation can be applied to accurately simulate corresponding physical process. In particular, usual Eulerian schemes for the advection equation often accompany with numerical diffusion or oscillations (Noye, 1987) while they are widely used to solve the diffusion equation.

In this study, two-point fourth-order Holly-Preissmann scheme (Holly and Preissmann, 1977) is used to solve the advection equation, a local analytic solution for the first order decay equation, and Crank-Nicholson scheme for the diffusion equation. The procedure for the numerical solution is similar to that of CE-QUAL-RIV1 model, but a little modification is made. The following analytic solution is adopted to solve Eq. (5)

$$C_i^{n+2/3}=C_i^{n+1/3}e^{-k\Delta t} \tag{7}$$

while the Euler' s method is used in CE-QUAL-RIV1 model such that

$$C_i^{n+2/3}=(1-k\Delta t\,)C_i^{n+1/3} \tag{8}$$

Overall solution procedure can be found in WES (1990). The model has been tested using an analytic solution for the longitudinal dispersion of continuous source released into a nonuniform flow field(Yu and Jun, 1999).

3. Application of the Model

3.1 Application of the flow model

The model is applied to hindcast the phenol spill accident which occurred in Nakdong River, South Korea at March 14, 1991. Fig. 1 is a schematic representation of the study area. A 340 km reach of the Nakdong River is modeled. Upstream boundary is the Andong Dam, and the downstream boundary is Nakdong Estuarine Barrier where the discharge and water surface elevation, respectively, are known. There are nine water level recorders on the main stream. Water level observations at those stations are used for the calibration of the flow model. Among the thirteen tributaries discharges from four tributaries are known. The flow model consists of a total of 15 nodes located at the upstream and downstream boundary, and at the junctions of tributary inflows. A total of 744 computational points located at unequal intervals were used for the flow model. Average distance between computational points is 420 meters.

Records of the water surface elevations during the period of the accident were examined. It was found that both of the main stream and tributary water levels were fairly constant during the period. Since the discharge variations from the upstream dam were also negligible during the period, a steady flow condition was assumed. Tributaries were not simulated. To estimate the inflows from ungauged tributaries, it was assumed that the tributary inflow is proportional to the watershed area. The linear relation, $Q_t = 0.13A_d$, between the tributary inflow (Q_t) and the drainage area (A_d) was estimated by a regression analysis using the discharge records of the gauged tributaries (see Fig. 2).

The flow model was calibrated to determine Manning's roughness coefficient. The criterion used for the calibration is to minimize the sum of squares of the errors between the computed and the observed water levels. An optimization technique was used for the estimation of the model parameter. It is a modified Gauss-Newton method employing the scheme of Marquardt (1963). Details of the optimization procedures can be found elsewhere (Doherty et al., 1994; Hill, 1992).

3.2 Application of the dispersion model

The phenol spill accident occurred at about 10 p.m. on March 14, 1991. For the first eight hours thirty tons of phenol was discharged into the Nakdong River right upstream of the Geomho River, and it continued for about 5 days thereafter at the rate of 2.5 tons/day. Because the longitudinal dispersion model for the looped-network is not available at the current stage of study, a single channel model was used to hindcast the phenol spill accident.

The longitudinal dispersion model for nonconservative substances have two model parameters. One is the longitudinal dispersion coefficient D, and the other is the first-order decay coefficient k. There have been many studies to quantify the dispersion coefficient in terms of the channel dimensions and flow characteristics. Numerous empirical equations for D have been suggested. Eqs. (9)~(12) are those proposed by McQuivey and Keefer (1974), Liu (1977), Iwasa and Aya (1991), and Seo and Cheong (1998), respectively.

$$D = 0.058\frac{dU}{S} \tag{9}$$

$$D = \boldsymbol{b}\frac{U^2 W^2}{dU_*}, \ \boldsymbol{b} = 0.18(\frac{U}{U_*})^{1.5} \tag{10}$$

$$\frac{D}{dU_*} = 2.0(\frac{W}{d})^{1.5} \tag{11}$$

$$\frac{D}{dU_*} = 5.915(\frac{W}{d})^{0.620}(\frac{U}{U_*})^{1.428} \tag{12}$$

in which d = water depth, W = channel width, S = channel slope, and U_* = shear velocity. Dispersion coefficient can estimated from the channel geometry and flow conditions simulated by the flow model. Fig. 3 shows the dispersion coefficients estimated by Eqs. (9)~(12). It can be seen that dispersion coefficients estimated by McQuivey and Keefer's equation and those from Seo and Cheong's are relatively in good agreement with each other. The values calculated by Liu's equation are several order of magnitude larger than those from other empirical formulas.

Fig. 4 is the temporal concentration distributions at Susan (see Fig. 1) simulated by the model in which three different empirical equations for the dispersion coefficient are used. It is seen that the distribution from McQuivey and Keefer's equation agrees well with that from Seo and Cheong's. The first-order decay coefficient k was assumed to be null for the calculation. Also observed is that the arrival time is shorter if Liu's equation is used, and this makes sense for the dispersion coefficients from Liu's equation is generally larger than those from McQuivey and Keefer's or Seo and Cheong's. The time to peak concentration is different by about one day depending on the formula for the dispersion coefficient. Considering that the time to peak concentration is about 5 days for location, the difference of one day seems to be quite significant.

Fig. 5 is the concentration distributions for the same location simulated for k = 0.5 1/day. The dots in Figs. 4 and 5 present the observed concentration. Observations were made at eight different positions along the river. However, none of them were continuous observations. As it is seen in Figs. 4 and 5, if k = 0.5 1/day, the concentration distribution is reduced to about 10 % of that for k = 0. Although k does not affect the shape of the concentration distribution, the concentration values depend on the decay coefficient very significantly.

The decay coefficient was estimated using the observations. The performance criteria and method of the calibration are the same as those for the flow model. As it is well expected, the estimated *k* values were different depending on the empirical equation used for the dispersion coefficient. They ranged from 0.32 to 0.40

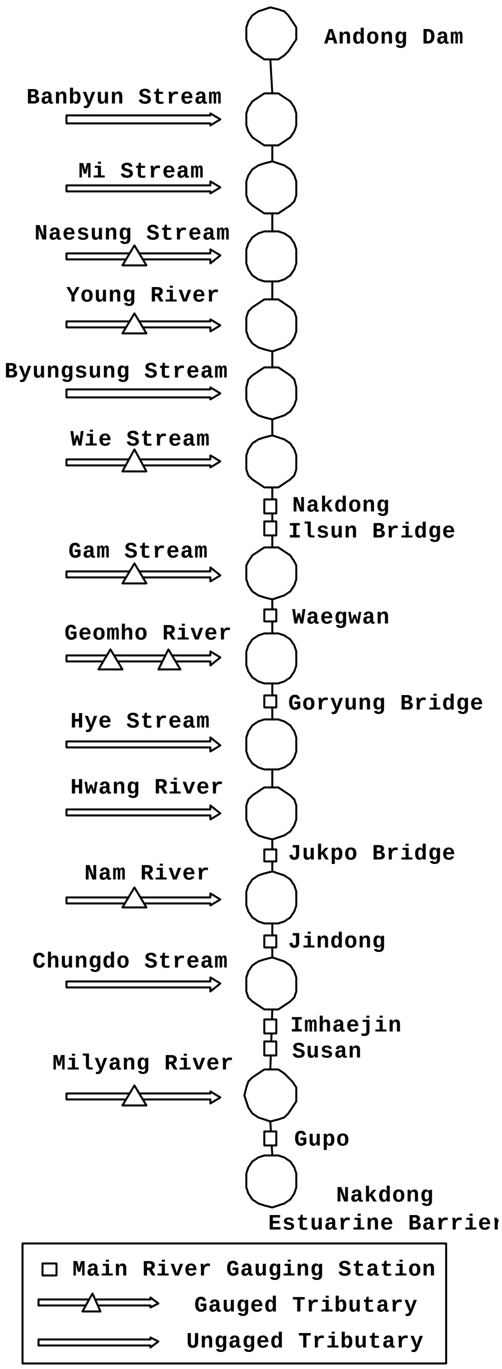

Fig. 1. Schematic View of the Study Area

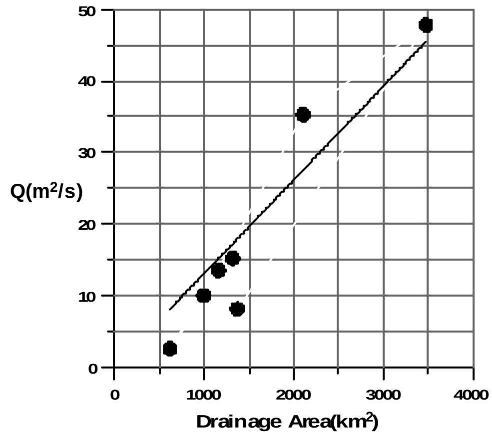

Fig. 2. Regression Analysis for the Estimation of Tributary Inflows.

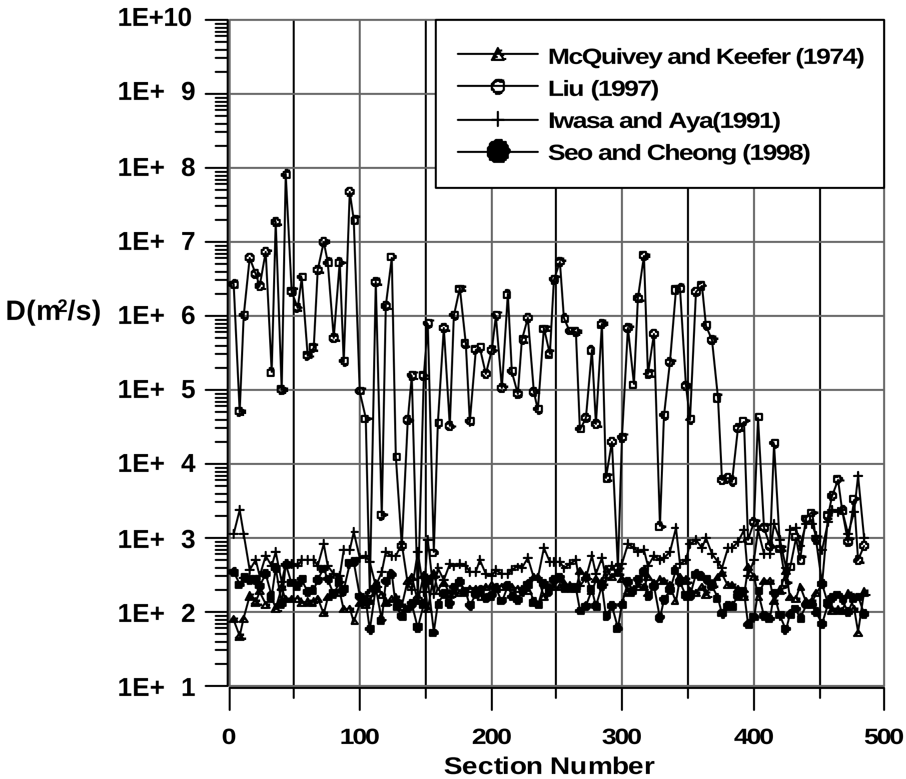

Fig. 3. Dispersion Coefficients along the Reach Estimated by Various Empirical Equations

4. Conclusions

A fractional-step finite difference model is presented for the unsteady dispersion of nonconservative contaminants in natural streams. The model is applied to hindcast the

1991 phenol spill accident which occurred in Nakdong River, South Korea. Calculated concentration distributions are sensitive to the decay coefficient as well as the empirical equations for dispersion coefficient. The calculated time to peak concentration is very sensitive to the formulas for dispersion coefficient while the magnitude of concentration to the first-order decay coefficient. This suggests that accurate modeling of dispersion in natural streams is hard to achieve due to the parameter uncertainty even though the numerical model produces accurate results.

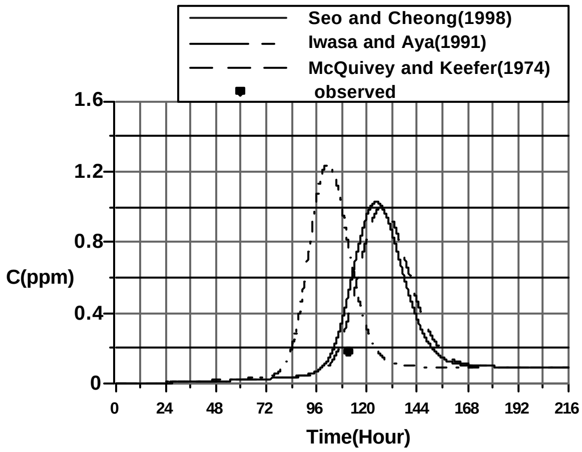

Fig. 4. Temporal Concentration Distribution at Susan Computed for k = 0

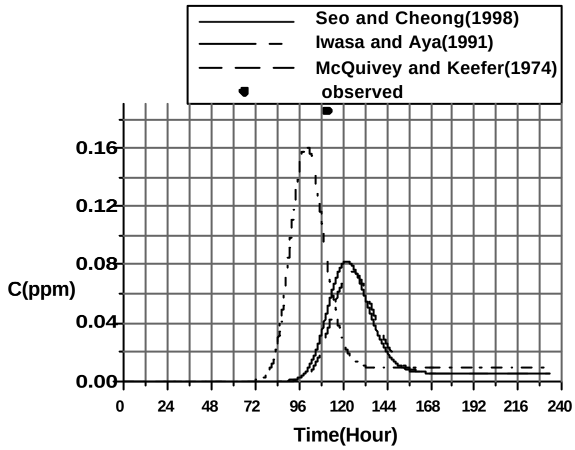

Fig. 5. Temporal Concentration Distribution at Susan Computed for k = 0.5 1/day

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