Modeling Dynamics of Nonconservative Pollutants in Streams with Pools and Riffles

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ABSTRACT

The complex nature of low flow transport and transformation of nonconservative pollutants in natural streams with pools and riffles has been investigated using a numerical solution of a proposed mathematical model that is based on a set of mass balance equations describing hydrodynamic processes (advection, dispersion, and mass exchange mechanisms in streams and in storage zones) and chemical processes (reaction or decay). In this study, a mathematical model (named "Storage-Transformation Model") has been developed to predict adequately the non-Fickian nature of mixing and transformation mechanisms for decaying substances in natural streams under low flow conditions. Comparisons between the concentration-time curves predicted using the proposed model and the measured stream data shows that the Storage-Transformation Model yields better agreements in the general shape, peak concentration and time to peak than the 1-D dispersion model. The result of this study also demonstrates the differences between transport in pool-and-riffle streams versus transport in more uniform channels. The proposed model shows significant improvement over the conventional 1-D dispersion model in predicting natural mixing and storage processes in streams through pools and riffles.

1. INTRODUCTION

Characteristics of low flows in natural streams are substantially different from those observed at bank-full or flood stages. Under low flow conditions, pollution problems are most acute. The water quality of streams receiving municipal, industrial, and agricultural return flow

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is further degraded when natural streamflow is low. Dilution of contaminants decreases as streamflow decreases; thus the hazard associated with an accidental spill may be much greater at low flow than at a higher flow. Variations in bed geometry such as pool and riffle structure, dominant channel features during low flow (Leopold et al., 1964), play their strongest role in affecting mixing characteristics of polluted releases in the channel. In recent years, the investigation of the low flow condition has become important as a means of determining critical levels of water pollution, aquatic habitat and instream flow needs. Seo (1990) and Seo and Maxwell (1992) have conducted important research on the transport and mixing characteristics for pollutants discharged into natural streams with pools and riffles. They showed that in natural channels under low flow conditions, the effect of storage induced by the pool-riffle sequences should be considered adequately in the modeling of transport and mixing of conservative solutes. Knowledge of transport and mixing characteristics for nonconservative pollutants as well as conservative pollutants are required to establish sound water pollution control and water resources management programs.

The one-dimensional (1-D) Fickian-type dispersion equation derived by Taylor (1954) has been widely used to give a reasonable estimate of the rate of longitudinal dispersion. The 1-D Fickian dispersion equation for nonconservative pollutants in which the decay term is modeled as a first-order function is

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = K \frac{\partial^2 C}{\partial x^2} - k_r C$$
 (1)

in which C = cross-sectional average concentration; U = cross-sectional average velocity; K = dispersion coefficient; $k_r = decay$ coefficient; t = time; and x = longitudinal distance.

The analytical solutions of Eq. 1 for limited period of injection of nonconservative pollutants can be derived using a Laplace transform technique and principle of superposition (Thomann and Mueller, 1987). Boundary and initial conditions of Dirichlet type are as:

$$C(t, 0) = C_0,$$
 $0 < t < \tau$ (2a)

$$C(t, 0) = 0,$$
 $t > \tau$ (2b)

$$C(0, x) = 0,$$
 $x > 0,$ (2c)

in which C_0 is the initial concentration injected, and τ is the period of injection. The solution of Eq. 1 for condition 2 is:

$$C(t, \mathbf{x}) = \frac{C_0}{2} \exp\left(-\frac{\mathbf{k_r x}}{U}\right) \left[G(t) \operatorname{erfc}\left(\frac{\mathbf{x} - Ut(1+H)}{\sqrt{4Kt}}\right) - G(t-\tau) \operatorname{erfc}\left(\frac{\mathbf{x} - U(t-\tau)(1+H)}{\sqrt{4K(t-\tau)}}\right) \right]$$
(3)

in which $H = 2k_rK/U^2$ and erfc(Z) is the complimentary error function which is defined by erfc(Z) = 1 - erf(Z). G(z) is the unit step-function which takes the values:

$$G(z) = 1, z > 0;$$
 (4a)

$$G(z) = 0, z < 0.$$
 (4b)

An immediate limitation is that the Fickian dispersion model cannot be applied until after the initial period, i.e., the model should be limited to locations far downstream from the source at which the balance between advection and diffusion assumed by Taylor is reached (Fischer et al., 1979). Literature describing the field studies including Zand et al. (1976) and Legrand-Marcq and Laudelot (1985) has indicated that concentration distribution data collected in natural streams seem to indicate non-linear behavior of the variance for times even beyond the initial period. Furthermore, most experimental studies in natural streams have produced concentration-time curves which are significantly more skewed than the concentration distribution predicted by the solution of the 1-D Fickian dispersion equation. These show that water and dye are retained in the regions having storage effects along the channel bed and banks and then released slowly after the main cloud has passed. Several researchers including Seo (1990), and Seo and Maxwell (1992) have suggested that a complete analysis must include the effect of channel storage zones.

The objective of the present study was to develop a mathematical model to predict adequately complex mixing characteristics of nonconservative pollutants in natural streams under low flow conditions. The predicted concentration-time curves were compared to the measured stream data.

2. MATHEMATICAL MODEL

2.1 Model Concept

The boundary geometry of natural streams is not smooth and regular. Under low flow conditions, irregularities and unevenness along the streams caused by pools and riffles can create storage zones that have significant storage effects. In this model a typical cross section

is considered to consist of two distinct zones, a flow zone and a storage zone. In the flow zone, the dominant mass transport mechanisms are longitudinal advection and dispersion. The storage zones are considered as regions having vortex or recirculating flow and having mass interchange with the main flow across the interface between the flow and the storage zones. The storage zones serve to retain part of the solute as the main cloud passes, and the solute is then slowly released back into the flow zone. It is assumed that mass is decaying in both zones. Among several conceptually different physical models of the transient storage of mass in the storage zone (Jackman et al. 1984), the exchange model assumes a different uniform concentration in each zone. Mass transfer at the interface between the zones is considered to be proportional to the difference in the average concentrations.

2.2 Governing Equations

The equations describing the Storage-Transformation Model are derived using conservation of mass. The mass balance equation in the flow zone for steady flow is

$$A_{f} \frac{\partial C}{\partial t} = -U_{f} A_{f} \frac{\partial C}{\partial x} + \frac{\partial}{\partial x} (K A_{f} \frac{\partial C}{\partial x}) + k P (S-C) - A_{f} k_{r} C$$
 (5)

in which A_f = cross-sectional area of the flow zone; U_f = flow zone velocity; P = wetted contact length between the flow zone and the storage zone in the transverse or vertical direction; k = mass exchange coefficient; and S = the concentration of mass in the storage zone. A mass balance equation describing S as a function of longitudinal position (x) and time (t) is

$$A_{S} \frac{\partial S}{\partial t} = -k P (S-C) - A_{S} k_{r} S$$
 (6)

in which A_s = cross-sectional area of the storage zone perpendicular to the general flow direction.

2.3 Numerical Modeling

An analytical solution of the given set of governing equations (Eqs. 5-6) corresponding to the initial and boundary conditions (Eq. 2) was not available because of the non-uniform parameters and the existence of the mass exchange terms in each equation. Therefore, numerical techniques were applied to solve the given set of governing equations. Based on the

preliminary numerical investigation (Seo 1990), among the various types of numerical schemes tested, the finite difference method (FDM) developed by Stone and Brian (1963) was selected to solve the given set of governing equations. This method, based on the Crank-Nicholson implicit approach, was considered to have no stability limitations as in the cases of other implicit schemes. The truncation error involved in this scheme was considered to be $O(\Delta t^2 + \Delta x^2)$, as in other Crank-Nicholson implicit approaches with the central difference approximation for space discretization, which is a higher-order than that of a fully implicit approach, $O(\Delta t + \Delta x^2)$. Δt is the time increment and Δx is the distance step.

The time derivative $\partial C/\partial t$ of the flow zone equation was represented by the spread form backward time difference approximation. The advective term was discretized by using the Crank-Nicholson approach, in which $\partial C/\partial x$ was centrally differenced. The dispersive term was also discretized by using the Crank-Nicholson type implicit method. Substituting each term into Eq. 5, and expanding the resulting equation for all the nodal points along the x axis, a set of simultaneous linear algebraic equations, of which the coefficient matrix is tridiagonal, can be obtained. The resulting system of algebraic equations was solved by using the Thomas algorithm, a variation of Gaussian elimination. The storage zone equation was also discretized by using the FDM developed by Stone and Brian similar to the flow zone equation. Because of the mass exchange terms in the mass balance equation for both flow and storage zones, another unknown term arises at the right hand side of the resulting system of algebraic equations for both flow and storage zones. So, additional iteration work was needed.

3. MODEL PREDICTIONS

3.1 Stream Data

The Storage-Transformation Model developed in this study was tested by using field data measured by Zand et al. (1976). This data was also used by Bencala (1983) for his solute transport model. Zand et al. described the dispersion study of nonconservative tracers in a small stream, Uvas Creek in California, U.S.A. The channel is highly irregular. It is composed of alternating pools and riffles and pool frequency ranges mostly 6 to 7 channel widths which falls into the range of that of the natural pool-riffle sequences studied by other investigators. The experiment was conducted in late summer during a period of low flow (Q = 0.0125 m³/s). The strontium tracer, as a nonconservative pollutant, was injected at a constant rate for three hours and reached a maximum concentration of 1.73 mg/l a short distance below the injection point. Background concentration was measured to be 0.13 mg/l.

3.2 Simulation Results

In the numerical model, the simplified geometric and hydraulic characteristics of the poolriffle sequences were used. The nonuniform hydraulic parameters, such as the flow depth and the storage zone area ratio, were considered to have single constant values at the pool and riffle, and then to vary linearly through the transition between the pool and the riffle. The mass exchange coefficient was also considered to follow the above assumption, but the dispersion and decay coefficients were assumed to be constant through the whole reach of pool-riffle sequences. The model parameters used for simulation are presented in Table 1.

TABLE 1.-Summary of the Model Parameters Used in the Simulation

A _s /A		Depth (m)		K k		(m/s) k _r	
Pool	Riffle	Pool	Riffle	(m ² /s)	Pool	Riffle	(1/s)
0.35	0.25	0.200	0.033	0.20	0.6*10-3	0.2*10-3	0.47*10-4

Comparisons of the concentration-time curves of the model simulations with those obtained in the stream experiments are depicted in Fig. 1. In general, in overall shape, the concentration-time curves given by the storage zone model better fit the measured concentration-time curves than those given by the 1-D dispersion model. The tails of the concentration-time curves by the storage zone model are quite close to those of the measured concentration-time curves, whereas those by the 1-D dispersion model fail to fit. The peak concentrations predicted by the Storage-Transformation Model are quite close to the experimental data. However, the 1-D dispersion model overestimated peak concentrations. More important, the times to peak concentration predicted by the 1-D dispersion model are inaccurate, whereas the storage zone model predicts the elapsed times to peak concentration very accurately.

In Fig. 2, concentrations are compared for simulations with parameters of pool-and-riffle streams and parameters of uniform channels in which average value of the parameters of the pool-and-riffle sequences are used. In overall shape and peak concentration, simulations with parameters of pool-and-riffle streams better fit the measured data than simulations with parameters of uniform channels. The result demonstrates the differences between transport in pool-and-riffle streams versus transport in more uniform channels.

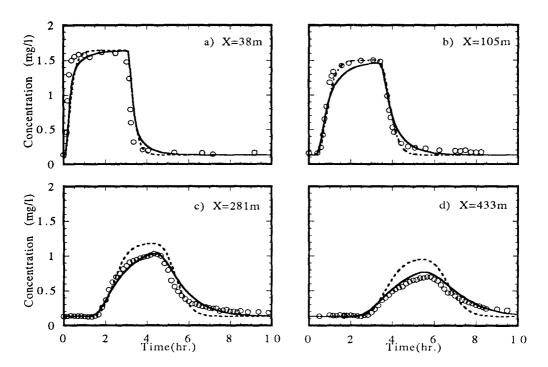


FIG. 1.-Concentration-Time Distribution of Observed Dispersion Data and Distributions Fitted by 1-D Dispersion and Storage-Transformation Models; — Observed Data; ---- 1-D Dispersion Model; ____ Storage-Transformation Model

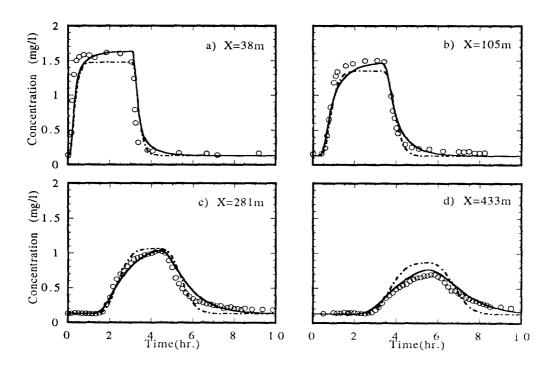


FIG. 2.-Concentration-Time Distribution of Observed Dispersion Data and Distributions Fitted by Storage-Transformation Models; — Observed Data; — - — Storage-Transformation Model with Parameters of Uniform Channels; _____Storage-Transformation Model with Parameters of Pool-Riffle Sequences

4. CONCLUSIONS

The comparison between measured and predicted concentration curves by the Storage-Transformation Model shows that there is a good level of agreement in the general shape, peak concentration and time to peak. The proposed model shows significant improvement over the conventional 1-D dispersion model in predicting natural mixing processes in natural channels with pools and riffles.

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