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A ONE DIMENSIONAL MASS TRANSPORT MODEL FOR NATURAL RIVERS*

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ABSTRACT

A numerical computer model is developed using the finite element method to analyze one dimensional transport of radioactive pollutants in natural rivers. The model generated includes some routines to predict the longitudinal diffusion coefficient as a default value, given some kinematic constants. Also, decay constants are generated as default value, given the specification of the radioactive material under study. The present paper summarizes the initial steps taken toward the goal of preparing a user-oriented computer model which will be available for use in cases of emergency, to predict the mass transport of pollutants in natural rivers with limited input data. Case studies analyzed indicate that quite accurate predictions can be made as initial estimates of the magnitude of concentration distribution as it varies through time by employing a model of this kind.

INTRODUCTION

In the course of time a number of methods and computational procedures have been developed to investigate and to predict mass transport in natural rivers. A literature review in this research area indicates that several Environmental Transport Models with varied degrees of complexity and different simulation objectives are available. A recent report by Little and Miller provides a rather complete listing of such studies as well as a critical review [1]. One major problem with these models is in part the inaccessibility of the generated

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computer code and in part, the specific, problem-oriented design employed. It is well known that model design, almost by definition, is a pragmatic process – the simulation objectives determine the basic form, usability, and generality of the model.

Model accuracy and reliability are two of the more important aspects of numerical modeling which should not be overlooked. If a numerical model is to be accepted as a reliable predictive tool, the numerical error bounds generated should be within acceptable limits, and the model should be validated regionally using available data. Proceeding in this direction, much of the recent work done in water quality modeling has been oriented towards improvement of models – towards incorporating better numerical solution techniques, the accuracy of which surpass by far the availability and accuracy of the field parameter data that have to be used with such models. Scarcity of such data, especially in surface water quality modeling, is well known to researchers and engineers working in this field.

Currently there is some disagreement among researchers as to whether higher priority should be placed on still further developments in model sophistication or on parameter prediction to improve accuracy. Naturally, improved sophistication of models is associated with increases in number of model parameters. Since it is likely that many of the additional parameters would be defined only in qualitative terms, a relatively more sophisticated model can be less reliable than a simpler version. On the other hand, however, some systems and some physical phenomena are so complex in nature that there is often little reason to believe that good simulations are possible with simplified representations. In such cases the need for more detailed and realistic models is clear. A simple and crude example can be found in the case of transport models for river systems. Given the current understanding and knowledge on turbulence characteristics, secondary currents, roughness concepts and sediment transport characteristics of natural rivers, it may be overly ambitious to attempt to develop a three-dimensional transport model for a river system just because it is possible numerically. Going to the other extreme, if in order to simplify such a model, that is, in order to reduce the model dependence on field parameters, one ignores the diffusive transport terms keeping the convective transport terms in the analysis, the reliability of the model becomes questionnable, at least for certain problem types like accidental spills of pollutants or daily cyclic variation of spills, as is the case in sewage output. In relation to the production of user-oriented models, the optimum solution lies between these two extremes.

In an attempt to achieve this goal, an initial effort is made in this study to analyze the one-dimensional mass transport equation, with the possibility of generating some default values for field parameters like the longitudinal diffusion coefficient and decay constants for several radioactive materials. Details of the computer code generated along with a users manual can be found in Aral et al. [2].

MATHEMATICAL MODEL

Transport of pollutants in natural rivers is a complex phenomenon, especially if an effort is made to cover all aspects of it. In an industrialized society, a great variety of pollutants can get mixed into surface waters. Dissolved matters such as chemicals, radioactive materials, and salt, solid matters such as sediments, and temperature gradients introduced by power plants may roughly describe the basic sources of pollution. Different models are needed to describe the transport characteristics of different pollutants. Thus, the choice of type of pollution is the first step to be considered. The stage of pollution transport is another variable, since mathematical models describing initial mixing zones are considerably different than mathematical models to be used for well mixed zones. The third variable is the choice of model dimensions. Given the present know-how in numerical methods, it is tempting to develop a three-dimensional model, with the assumption that the parameters needed in such a model are readily available. Thus, determination of physical and kinematic parameters is the fourth complexity encountered in the modeling of transport of pollutants in natural rivers. Parameters like longitudinal and transverse diffusion coefficients, decay of organic matter and other chemicals, heat transfer to atmosphere through water surface, erosion and deposition of sediments in natural environments have been studied by many researchers in the field, with no universal description of the phenomena involved. Keeping these complexities in mind, the boundaries of the model developed for this study are summarized below.

A one-dimensional model is used to describe the longitudinal transport of pollutants in natural rivers. Such an analysis is very useful in the study of accidental spills of pollutants from nuclear power plants or daily cyclic variations of output from sewage treatment plants. It is assumed that low concentration solutions of matter are transported with mean river velocity. Such an assumption helps to avoid the study of density currents which result in all cases of high concentration transport. It is assumed that dispersion is caused by uneven distribution of flow over a cross section, and dispersion effects due to overbank storage, tidal flows, and action of wind and waves are ignored. Further, the model does not describe the initial mixing stage of pollutant transport phenomena. Thus, transport of matter by such a mixing process including the molecular and turbulent diffusion effects, may be lumped into one term which is usually referred to as the longitudinal diffusion coefficient. Combining the definition of diffusive and convective transport of matter with the continuity equation for matter and river flow including the effects of decay for non-conservative substances, one may obtain the one-dimensional convective-dispersion equation as,

$$\frac{\partial \bar{C}}{\partial t} + \bar{u}\frac{\partial \bar{C}}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial \bar{C}}{\partial x}\right) + K\bar{C} = 0 \qquad (1)$$

in which A is the cross-sectional area of the river, K is the first order decay coefficient, $\overline{C}$ is mean concentration, $\overline{u}$ is mean velocity, D is the longitudinal dispersion coefficient, and (x) and (t) are space and time coordinates. Equation (1) is used to describe the time dependent one-dimensional transport of pollutants in natural rivers in this study. The reader is referred to Aral [2], Fisher [3], and Bird [4], for further details of the derivation of the above equation. In order to complete the mathematical description of the problem, an initial and two boundary conditions are required. The initial condition describes the concentration distribution along the river reach at the initial time t = 0

$$\overline{C}(x,0) = f(x) \tag{2}$$

Some typical examples of boundary conditions that can be used in the solution of Equation (1) can be given as:

a. The concentration at location x = a is a specified function of time or is given as a constant value, a Dirichlet boundary condition.

$$\overline{C}(a,t) = c_o(t) \quad \text{or} \quad \overline{C}(a,t) = c \tag{3}$$

b. There is no dispersive transport at the boundary x = a, a Neuman boundary condition.

$$\frac{\partial \overline{C}}{\partial x} = 0 \quad \text{at} \quad x = a \tag{4}$$

c. Supply of mass flux is specified at location x = a, a Mixed type boundary condition.

$$\lim_{x=a^-} \left[A\overline{u}\overline{C} - AD\frac{\partial \overline{C}}{\partial x} \right] - \lim_{x=a^+} \left[A\overline{u}\overline{C} - AD\frac{\partial \overline{C}}{\partial x} \right] = \overline{W} \tag{5}$$

where $\overline{W}$ is the supply of mass per unit of time at x = a.

The numerical model generated for this study is capable of analyzing any combination of these boundary conditions in a typical transport problem.

FIELD PARAMETERS

The one dimensional mass transport equation described earlier involves two important parameters, namely the longitudinal diffusion coefficient and the first order decay constant. There have been various efforts to estimate these parameters in natural rivers for different pollutants and different flow conditions, and a considerable volume of literature has accumulated over the years on this specific subject [3]. In what follows, a brief description of the equations used in this study to predict these constants is given. A chronological review of these predictive equations can be found in Aral [2].

Longitudinal Diffusion Coefficient

The first alternative that can be chosen to predict the longitudinal equation is the equation given by Fisher (1975). This equation can be stated as:

$$D = 0.011 \frac{\bar{u}^2 b^2}{dU_*} \tag{6}$$

in which $\bar{u}$ is the mean velocity, b is the width of the channel, d is the depth of flow, and U_* is the shear velocity. In order to use this equation to predict the longitudinal dispersion coefficient at a certain point in a river reach, the user must supply the variables $\bar{u}$, b, d, and U_* as data at a specific location. Equation (6) is incorporated into the transport model developed in this study as a first alternative.

The second alternative equation used in this model is the equation suggested by Liu [5], which is presented below:

$$D = \beta \frac{Q^2}{R^3 U_*} \tag{7}$$

in which β is a dimensionless coefficient for natural streams, Q is the discharge, U_* is the shear velocity and R is the hydraulic radius of the channel. The dimensionless coefficient β is given as

$$\beta = 0.18 \left(\frac{U_*}{\bar{u}}\right)^{1.5} \tag{8}$$

in which $\bar{u}$ is again the mean velocity.

A third alternative to Equations (6) and (7) is developed in this study as an extension of the equation suggested by Liu. The need for such an extension originated from the idea that sinuousity of river reaches, which plays an important role on the magnitude of the longitudinal dispersion coefficient, can be represented in a much better way if one introduces a parameter which reflects this effect better than the ratio $(U_*/\bar{u})$ chosen by Liu which mainly reflects the local resistance to flow.

The form of the predictive equation is assumed to be:

$$D = \alpha \left(\frac{U_*}{\bar{u}}\right)^{\beta} \left(\frac{L_r}{L_s}\right)^{\gamma} \left(\frac{Q^2}{R^3 U_*}\right) \tag{9}$$

which has essentially the same form as Equations (7) and (8) except the ratio (L_r/L_s) which is the ratio of the actual length of the river at the specific site considered, divided by the length of the straight line joining the two ends of the river reach for the same site. This ratio is chosen to reflect the sinuosity of the river reach as a first approximation although other more rigorous descriptions have been used in the literature earlier. A least squares curve fitting technique is used to arrive at the values of the coefficients, α, β, and γ. The resulting equation has the form as follows.

$$D = (0.0019)\left(\frac{U_*}{\bar{u}}\right)^{0.25}\left(\frac{L_r}{L_s}\right)^{4.56}\left(\frac{Q^2}{R^3 U_*}\right) \tag{10}$$

The field and laboratory data used in this curve fitting process is given in Aral [2] in detail. All three equations are incorporated into the computer model developed in this study. Thus, the choice between these three equations should be made by the user depending on the availability of data.

Decay Coefficient

In the case of radioactive spills the rate of decay of the radioactive material is an important aspect of the study especially for radionuclides with high rates of decay. The computer model generated in this study contains the half-lives of sixty-three radionuclides from which the decay constants can be generated. For any pure radioactive substance, the rate of decay is usually described by its half life Λ, i.e., the time it takes for a specified source material to decay to half its initial activity. Given this definition, the decay constant, K (sec^{-1}), can be given as:

$$K = \frac{Ln(2)}{\Lambda} \tag{11}$$

Thus, for a case study involving one of the sixty-three radionuclides the user only needs to identify the nuclide. The model automatically incorporates the decay constant into the analysis. List of radionuclides and associated half lives is obtained from Booth [6].

NUMERICAL MODEL

A one dimensional finite element model is used to approximate the mathematical model developed in the previous sections. The first step in such a discretization process is the division of the solution region into a finite number of subregions which are called elements. This process is dictated by the need to find an alternative form of the equilibrium equations which will be easier to solve than the governing equations of the continuum. The modified conceptualization of the system results in a set of simultaneous algebraic equations rather than differential equations, thus simplifying the solution considerably. The size and distribution of the elements and the approximation used in each element are arbitrary. Given the one dimensional nature of the problem analyzed, two nodal one dimensional linear elements are used in the solution process in this study. A summary of the steps involved in generating finite element matrix equations for the mathematical model studied is given below. A detailed description of finite element analysis can be found in Zienkiewicz [7].

A finite element approximation to Equation (1) can be obtained through a Galerkin approach. Over an element the residual, R, for Equation (1) can be given as follows.

$$R(C) = \frac{\partial C}{\partial t} + \bar{u}\frac{\partial C}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}\left\{AD\frac{\partial C}{\partial x}\right\} + KC \tag{12}$$

where C is considered to be an approximation to $\bar{C}$ which represents the exact value. Weighing the residual with respect to a weighing function N_m yields:

$$I^e = \int_{\ell^e} N_m \left\{\left(\frac{\partial}{\partial t} + \bar{u}\frac{\partial}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial}{\partial x}\right) + K\right) N_k C_k\right\} d\ell^e$$

$$m,k = 1, \ldots, n \tag{13}$$

where repeated indices indicate summation, n is the number of nodes, N_m is the weighing function which is chosen as the finite element shape functions in a Galerkin formulation and C_k is the nodal value of the dependent variable in an element. Equation (13) is written for a single element; however, it is understood that the same procedure is applied to the entire medium. The interpolation used to approximate $\bar{C}$ over an element can be given as:

$$\bar{C} = N_k C_k \quad k = 1, \ldots, n \tag{14}$$

where N_k is the interpolating polynomial used to approximate, $\bar{C}$, in an element. For a typical two nodal element these polynomials are given as:

$$\left.\begin{aligned} N_1(\xi_1,\xi_2) &= \xi_1 \\ N_2(\xi_1,\xi_2) &= \xi_2 \end{aligned}\right\} \tag{15}$$

where ξ_1, and ξ_2 are natural coordinate systems for a two nodal element defined as:

$$\xi_1 = \frac{\ell - x}{\ell}; \quad \xi_2 = \frac{x}{\ell} \tag{16}$$

where (x) is the local coordinate.

Integrating Equation (13) by parts and minimizing the residual leads to element equations in matrix form as:

$$[P^e]\left\{\frac{\partial C}{\partial t}\right\} + [S^e]\{C\} = \{F^e\} \tag{17}$$

where $\left\{\frac{\partial C}{\partial t}\right\}$ and $\{C\}$ are vectors of nodal time derivatives and nodal values of the dependent variable and $[P^e]$, $[S^e]$ are the local mass and stiffness matrices defined as:

$$[P^e] = \int_{\ell} N_m N_k d\ell^e \quad m,k = 1, \ldots, n. \tag{18}$$

$$[S^e] = \int_{\ell} \left[\bar{u}N_m\frac{\partial N_k}{\partial x} + D\frac{\partial N_m}{\partial x}\frac{\partial N_k}{\partial x} + KN_m N_k\right] d\ell^e$$

$$m,k = 1, \ldots, n \tag{19}$$

and $\{F^e\}$ is the local load vector defined by the boundary conditions of the associated problem.

Following formation of $[P^e]$, $[S^e]$ and $\{F^e\}$, a routine finite element assembly process yields, for the global system, a similar equation which can be given as:

$$[P] \left\{\frac{\partial C}{\partial t}\right\} + [S] \{C\} = \{F\} \tag{20}$$

Thus, the partial differential Equation (1) is reduced to a finite element matrix equation system through a finite element Galerkin process. An implicit time integration scheme can now be used to integrate Equation (20) step-by-step, as presented by Wilson [8]. This process leads to the matrix system:

$$\left(\frac{2}{\Delta t}[P] + [S]\right)\{C\}_{t+\Delta t} = \left(\frac{2}{\Delta t}[P] - [S]\right)\{C\}_t + 2\{F\} \tag{21}$$

Thus, the problem at this stage is reduced to the solution of a simultaneous algebraic system for the unknown nodal values of, C_k, at time $(t + \Delta t)$ starting from an initial condition on $\overline{C}$. Repeating the same process with increments of, Δt, yields an approximate solution for, $\overline{C}$, in time and space coordinates.

The finite element model generated above is coded in Fortran IV computer language. The complete listing of "Transport Model I" (TRMOD I) is given in Aral [2]. Several user oriented data generation routines are added to TRMOD I in order to simplify the data preparation process for the user.

NUMERICAL EXAMPLES

Numerical examples included here constitute the implementation and verification phase of the study. The patterns of dispersion observed by Godfrey and Frederick [9] at Clinch River, Speers Ferry, VA are compared with patterns predicted by the numerical model developed in this study.

The investigation, referred to above, approached the stream dispersion problem by conducting radiotracer tests in five reaches of natural channels and in one reach of a large irrigation channel. The purpose of these tests was to obtain data for an evaluation of the one dimensional approach to the description of dispersion in large open channels. Of the six reaches where experiments were conducted, Clinch River data was chosen arbitrarily for verification in this study. The alignment of this reach is described as straight with a total length of 5882(m). Six representative cross sections were chosen in each reach where multiple data collection was made in the same section. The tracer was injected in a line source across the stream either by wading or from a boat. The injection was made at a uniform rate over a one minute period. The concentration of radionuclide used in each test was proportional to the discharge, about two millicuries per cubic foot per second. Gold-198

was selected as the radiotracer because of high permissible concentrations, short half-life and low cost. The concentrations of the activity in the stream were observed by a scintillation detector with a one-by-one inch sodium iodide thallium-activated crystal. The concentrations were measured at or near the centerline of the stream. Detailed statistics of the experimental data for the Clinch River test can be seen in Table 1.

The data for the numerical model are generated using these base data. The reach is divided into seven subreaches with each subreach beginning and ending with the station location designated in the experimental setup. Each subreach is divided into smaller elements with (30), (40), (40), (50), (50), (60), and (10) elements, consecutively, from the point of injection to the extended end of the reach. This idealization resulted in (280) elements with (281) nodes. In each subreach the velocities and dispersion coefficients are assumed to be constant with varying magnitudes from subreach to subreach. Five computer runs are made for this set up in order to observe the behavior of different aspects of the model generated. In the first run, decay of tracer element is ignored and the longitudinal dispersion coefficient is introduced as input data using the value estimated in the experimental study. The longitudinal dispersion coefficient was predicted to be 11.0 m^2/sec for the Clinch River reach near Speers Ferry, VA. In Figure 1, observed time concentration data at five stations are plotted against the computed time concentration values at the same stations. The agreement between the model results and experimental data is excellent. Prediction of arrival time of peak concentrations at stations one, two, three, and four are excellent with a four minute lag in station five. The concentration intensities

Table 1. Channel Geometry, Flow Data and Statistical Parameters for Clinch River Test

Section	*1*	*2*	*3*	*4*	*5*	*6*
x (m)	688.84	1575.80	2490.22	3596.64	4663.44	5882.64
Width (m)	60.96	50.29	48.76	55.78	53.34	50.59
Depth (m)	1.74	1.62	1.98	2.26	2.25	2.72
R (m)	1.69	1.60	1.95	2.20	2.20	2.66
Fall (m)	0.70	1.25	1.42	1.62	1.98	2.24
Temp. °F	67.0	67.0	67.0	68.0	68.0	68.0
Q (m^3/s)	85.81	79.86	89.20	86.94	83.83	85.24
$\bar{u}$ (m/s)	0.81	0.98	0.92	0.68	0.70	0.62
$\bar{t}$ (sec)	684.00	1730.00	3070.00	4570.00	5740.00	8940.00
U* (m/s)	0.13	0.11	0.103	0.09	0.09	0.103

NOTE: $\bar{t}$: Elapsed time for the centroid of tracer cloud to move the distance (x) in seconds.

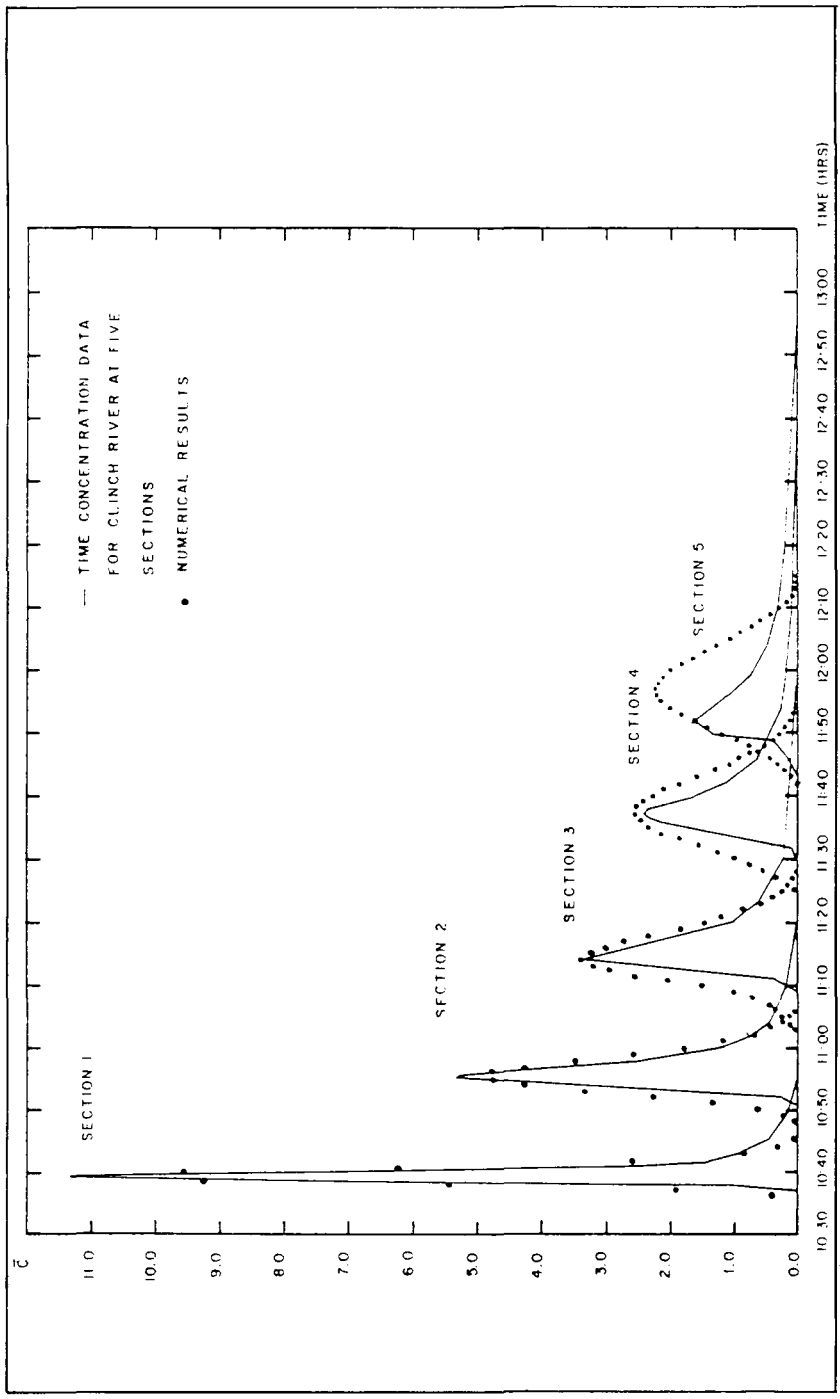

Figure 1. Time-concentration data and numerical results; D = 11m^2/sec as observed.

predicted by the model are within 3 per cent for the predicted peak concentration intensities at each station. The numerical results seem to diverge from the observed values as the tracer is transported in the downstream direction. This is expected however since decay of the Gold-198 element is not considered in this run. Overall results obtained in this run are satisfactory with the model yielding conservative estimates.

In order to observe the effects of decay of the tracer element used, this computer run is repeated including the decay of Gold-198 (half-life: 64h). Results are presented in Figure 2 in the same manner as before. The agreement between the numerical results and observed data for this case is excellent for peak concentrations. For both tails of the concentration distribution at a station, however, the model predicts much shorter durations with the difference becoming larger as the tracer is transported in the down-stream direction.

In the third, fourth, and fifth runs, the longitudinal dispersion coefficient is predicted in each subreach using the equations described earlier. The first prediction is done using Equation (10) which was developed in this study. Results obtained for each reach and predictions of time concentration values at each stations are given in Figure 3 comparatively with the observed data. Due to higher dispersion coefficients predicted in each reach, the tracer arrives more dispersed to the stations in downstream sections with lower peak values. Time of arrival of the peak is also shifted to the left indicating an early arrival. All these changes are expected numerically since higher longitudinal coefficients used in each reach would tend to distort the results in this manner. Once again this computer run stresses the importance of the longitudinal dispersion coefficient. In this and the following runs decay of the tracer element was ignored.

In the two remaining runs, the longitudinal dispersion coefficient was predicted using Equations (7) and (6). Since the resulting dispersion coefficients were larger for these cases the predicted values for concentration intensities were much more dispersed in comparison to the first case. Numerical results for these two runs are presented in Figures 4 and 5 comparatively with the observed data, indicating again the importance of the longitudinal dispersion coefficient.

CONCLUSION

The purpose of the model presented here is to obtain initial estimates of the concentration distribution of a pollutant, at the downstream sections of a river reach, following an accidental spill. Since one of the most important benefits of developing such a model involves its being used in emergency situations, the model should be well documented, readily available and should require a minimum data preparation effort for implementation. These considerations have dictated the direction of work on the model.

In its present form, the model developed here provides conservative, reliable and reasonable estimates of pollutant concentration intensities in field applications. The five computer runs presented here clearly indicate that the

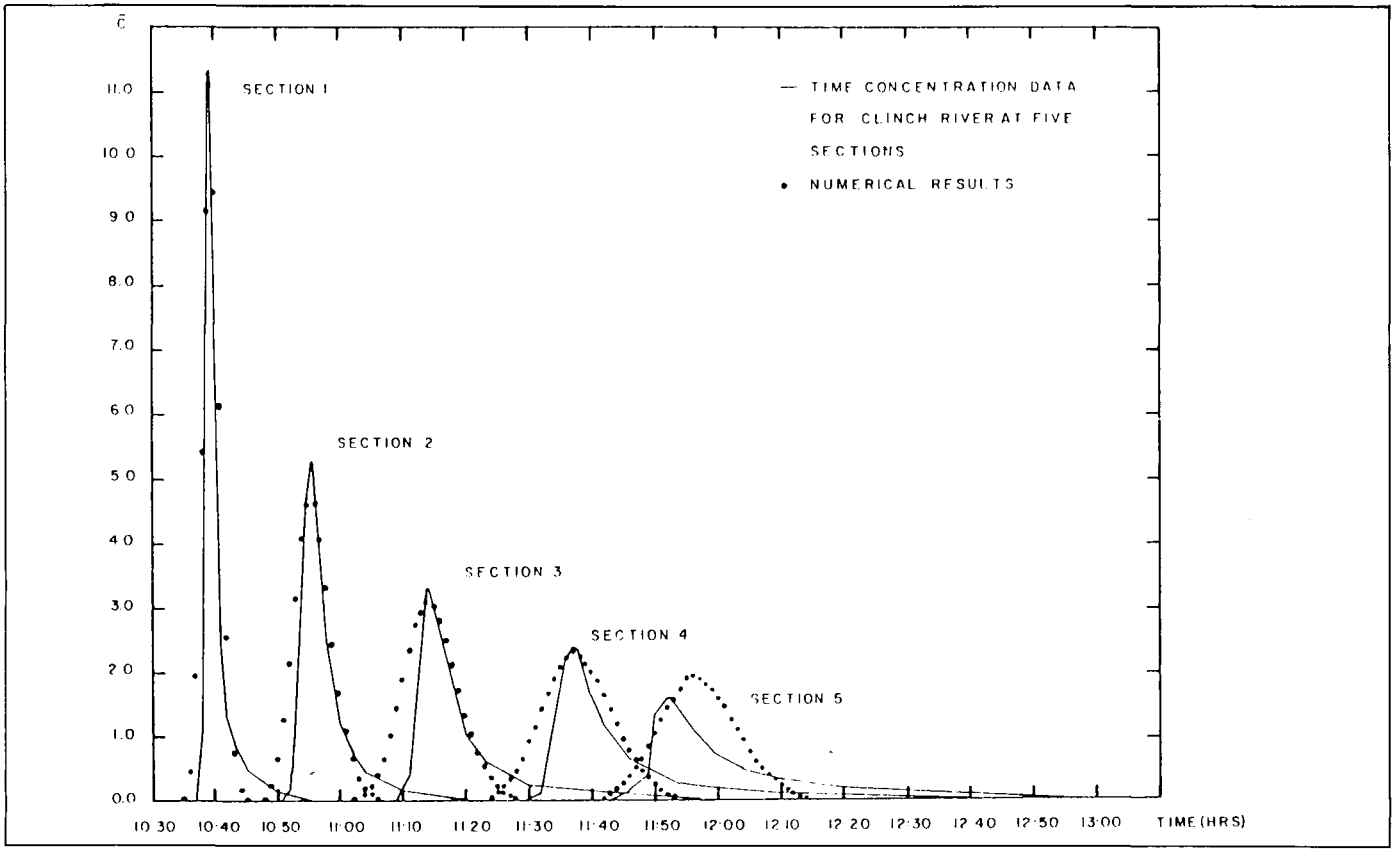

Figure 2. Time-concentration data and numerical results; D = 11 m^2/sec as observed with decay.

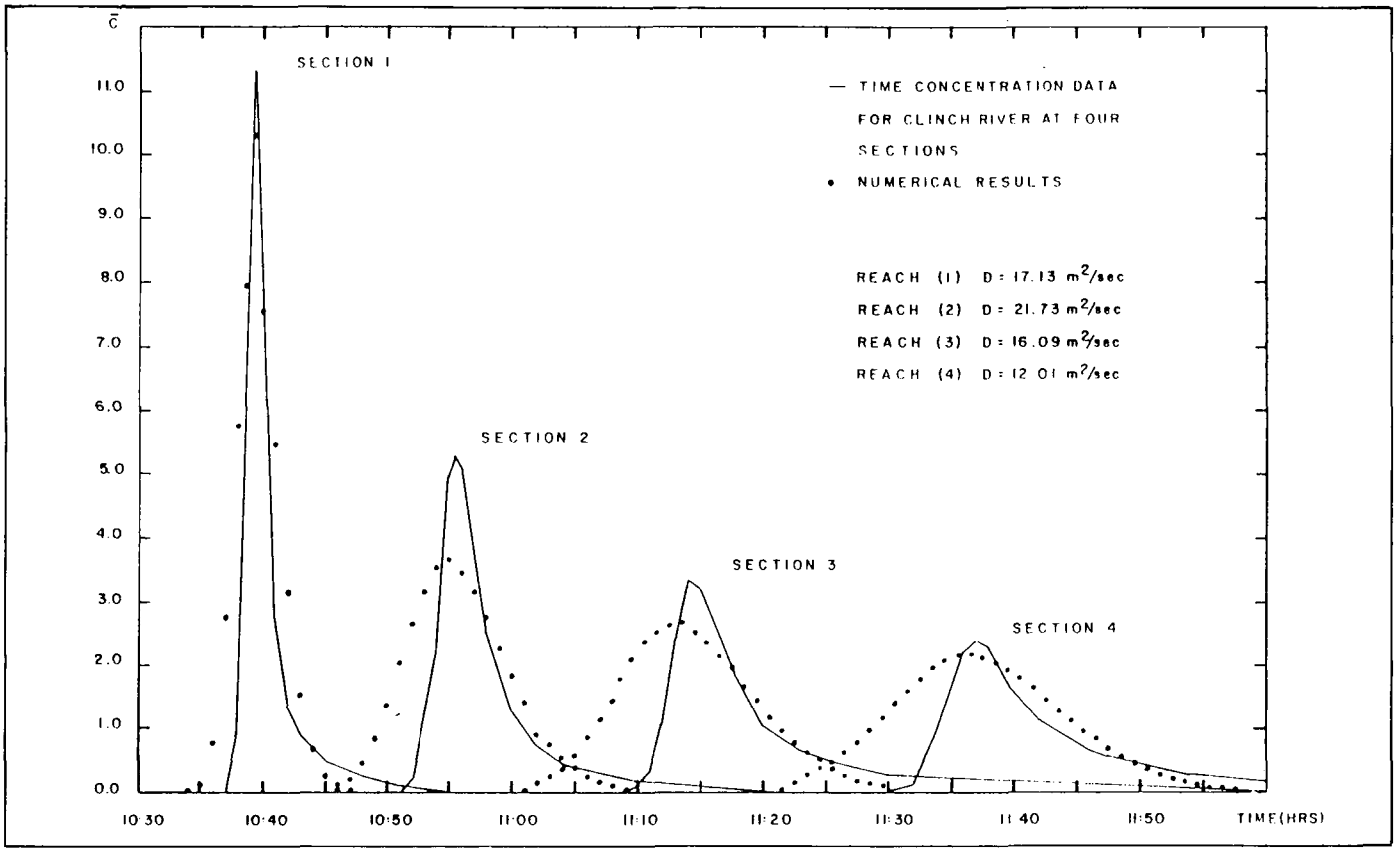

Figure 3. Time-concentration data and numerical results; D is generated from Equation (10).

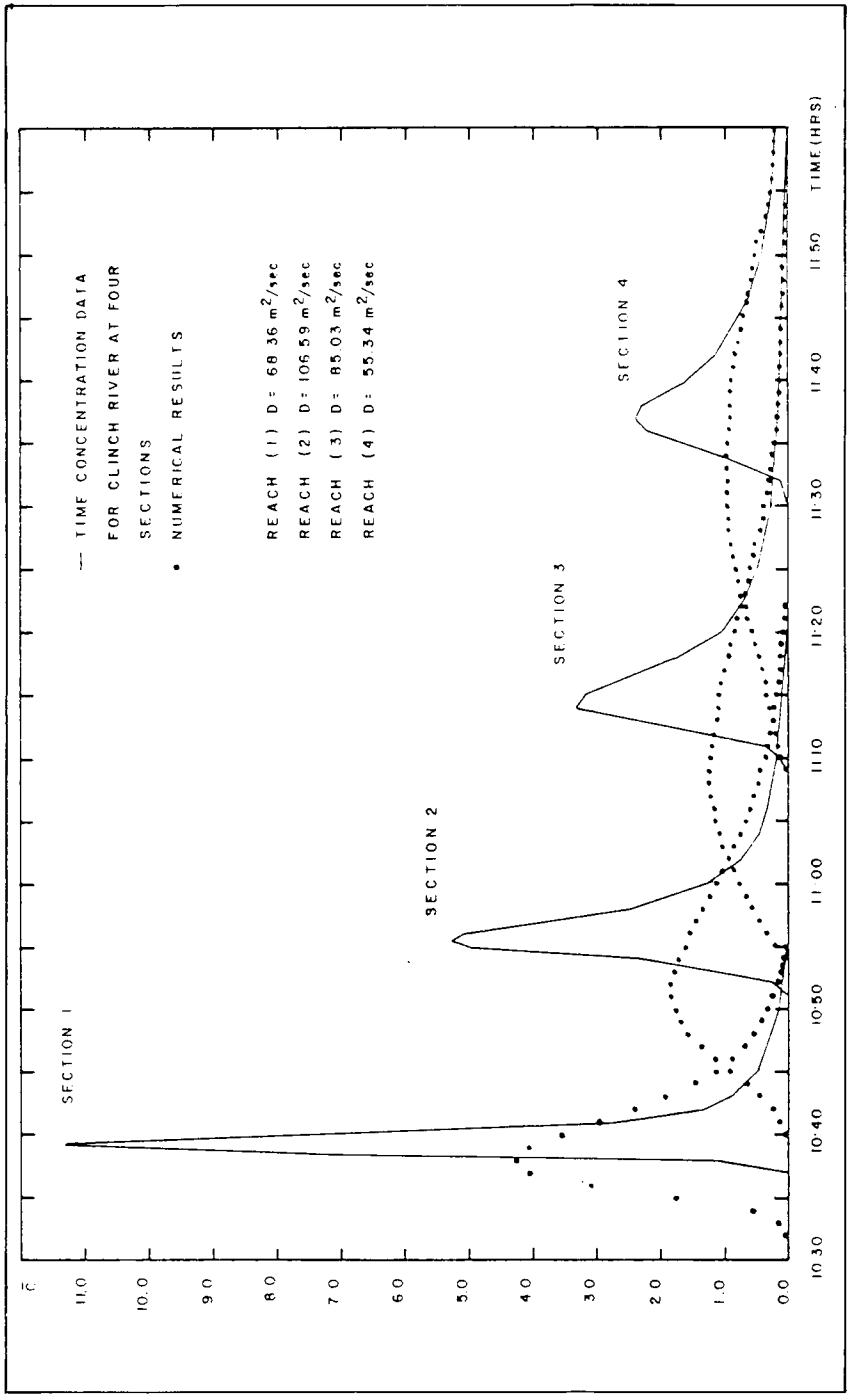

Figure 4. Time-concentration data and numerical results; D is generated from Equation (7).

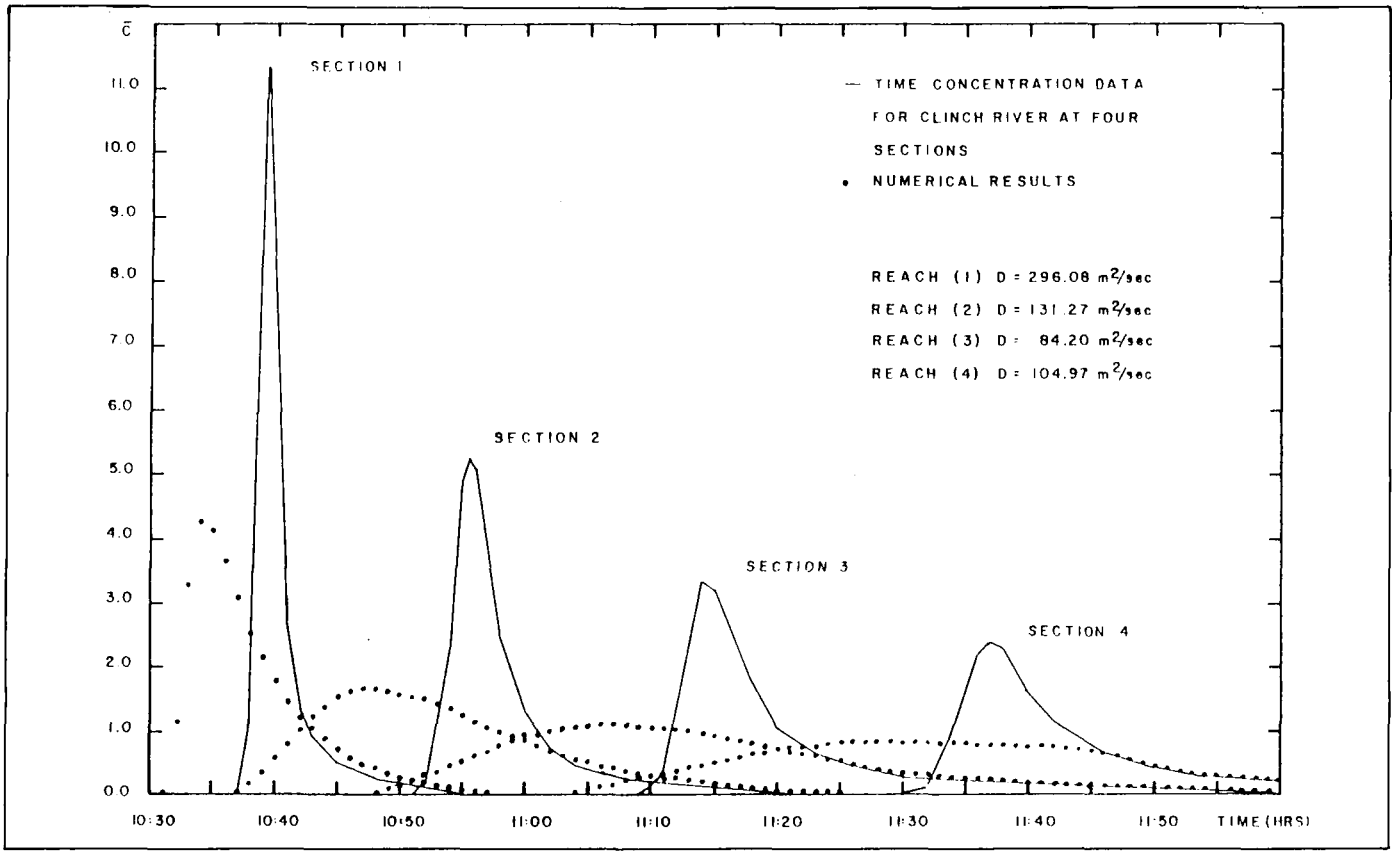

Figure 5. Time-concentration data and numerical results; D is generated from Equation (6).

model is capable of predicting mass transport in a natural river extremely accurately if proper values of field parameters are used as base data. The prediction of these field parameters, however, is crucial in such analysis and more detailed studies should be performed to arrive at better predictive equations. Equation (10) suggested in this study to estimate longitudinal diffusion coefficient definitely seems to be a better model than the other two which are obtained from most recent studies in the related literature.

To conclude, the results of this study clearly indicate that it is possible to generate regional package programs to predict pollution transport in a river reach. These package programs will provide sufficiently reliable initial estimates of concentration intensity in a sufficiently short time to be helpful for many environmental and health safety considerations. The potential utility of such package programs for the various purposes and needs of the various agencies involved in realted areas could not be exaggerated.

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