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EFFECTS OF DISPERSION ON NONCONSERVATIVE SUBSTANCES



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PREFACE

For more than 70 years, since the early work by Harold Streeter and Earle Phelps on the Dissolved Oxygen of the Ohio River, decision makers, engineers, scientists have continued to seek more rigorous means for assessing the effectiveness of environmental control actions. Many solutions have come out and control strategies have improved a lot. Despite of that, problems of water pollution in the developing countries like ours are still unmanageable. Population dynamics may be one of the problems, however, the other major problems are ignorance, unscientific management of pollution and lack of adequate awareness/knowledge about the consequences of pollution.

River is the major sources of water in our Country for various designated uses , on the other side, it is also the main carrier of pollution originates from municipal and industrial sources. Most of the major rivers in the Country are victim of pollution, the status of some of them are serious in nature. If the problems of water pollution are not well taken within the appropriate time frame and managed scientifically, the problem will be more worse and may lead to the scarcity of water.

Movement of pollutants in a river follows specific guidelines govern by the river hydraulics. Researchers have described the transport processes for a control system by the Advection-Dispersion equation. Because of the local complexities of the problem, the propagation of pollutants in a real stream is complex in nature and needs thorough understanding and better representation for accurate prediction and forecasting.

As a scientific programme of the Environmental Hydrology Division for the year 1995-'96, the basic research carried out by **Shri N.C. Ghosh, Scientist "E"** under the title "Effects of Dispersion on Nonconservative Substances" is a significant and mentionable contribution to that direction. The study is assisted by Shri Om Prakash, Research Assistant of the Division.


(S. M. Sethi)
Director

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LIST OF SYMBOLS

Symbols have been defined properly wherever they have appeared first. However, the most commonly used symbols are defined below:

$A_1, A_2, A_3 \dots A_n$:	Cross Sectional area of the Stream tubes perpendicular to the direction of flow, (L^2).
$A_{I,J}$:	Cross Sectional area of the Ith segment and Jth Stream tube perpendicular to the direction of flow, (L^2).
$B_{I,J}$:	Distance between the centre of Ith segment and Jth Stream tube along the transverse direction, (L).
C_0	:	Concentration of pollutants at time, $t=0$, ($M.L^{-3}$).
C_t	:	Concentration of pollutants at time, t , ($M.L^{-3}$).
$C_{I,J}$:	Concentration of pollutants in the Ith segment and Jth stream tube, ($M.L^{-3}$).
$C_{I,J,K}$:	Concentration of pollutants in the Ith segment and Jth stream tube after the time step K, ($M.L^{-3}$).
d	:	Depth of flow, (L).
E_t	:	Transverse Dispersivity coefficient for the river, ($L^2.T^{-1}$).
E_x	:	Longitudinal Dispersion coefficient, ($L^2.T^{-1}$).
E_y	:	Transverse Dispersivity coefficient for the stream tube, ($L^2.T^{-1}$).
$H_{I,J}$:	Area of the Ith segment and Jth Stream tube along the transverse direction, (L^2).
I	:	Segment numbered along flow direction.
J	:	Stream tube numbered along transverse direction.
K	:	First order decay coefficient, (T^{-1}).
M	:	Number of segments.
$M(X_n)$:	Mass of pollutants at any location, (M)

N	:	Number of stream tubes.
Q	:	Flow in the stream, ($L^3.T^{-1}$).
R	:	Sources/sinks of pollution, ($M.T^{-1}$).
t	:	Time, (T).
U	:	Average cross sectional velocity, (LT^{-1}).
u^*	:	Shear velocity, ($L.T^{-1}$).
U'_j	:	Relative velocity in the Jth stream tube, ($L.T^{-1}$).
U_j	:	Velocity factor, dimensionless term.
UR_j	:	Local velocity in the Jth stream tube, ($L.T^{-1}$).
W	:	Width of the river/stream, (L).
W_I, W_J	:	Coefficients of the finite difference matrices.
X	:	Longitudinal distance, (L).
X_d	:	Distance require for decay of the substances, (L).
X_m	:	Mixing length, (L).
X_I, X_J	:	Coefficients of $C_{I-1,J,K+1}$ and $C_{I,J-1,K+1}$ respectively obtained from the finite difference matrices.
Y_I, Y_J	:	Coefficients of $C_{I,J,K+1}$ obtained from the finite difference matrices.
Z_I, Z_J	:	Coefficients of $C_{I+1,J,K+1}$ and $C_{I,J+1,K+1}$ respectively obtained from the finite difference matrices.
Δt	:	time step, (T)
$\Delta x, \Delta y, \Delta z$:	Dimensions of elementary strip in three cartesian coordinates, (L).
ΔM	:	Difference of mass transported in two adjacent layers, (M).
δc	:	Difference of concentration of pollutants transported in the two adjacent layers, ($M.L^{-3}$).
ξ	:	Pre-assigned convergence factor.
$\alpha \ \& \ \beta$:	Weightage

ABSTRACT

A common practice in modeling of water quality of a river is to assume immediate cross sectional mixing and to neglect longitudinal dispersion; for example, the derivation of the widely used Streeter-Phelps equation. Researchers had explained that the propagation of pollutants in a moving water is because of the differential advection and cross sectional dispersion and, thus represented by the Advection-Dispersion equation.

For nonconservative or decaying substances, the spatial distribution of pollutants are usually estimate considering the equation which represents Advection-Dispersion-Decay of pollutants. Most of the water quality models have thus been developed assuming pollutants are completely mixed just after the point of release and neglecting the effects of dispersion.

Points arise; i) could pollutants reach to the other bank (if release is at the one bank) at the point of discharge ? ii) since the decay of nonconservative substances depends upon the incoming pollution load at any point [expression being, $C_t/C_0 = \exp(-K.t)$; C_t = concentration at any desire time, C_0 = incoming concentration of pollution, K = decay coefficient, t = time], would the estimate give the correct picture when it is assumed pollutants are completely mixed at the point of release ?

Literatures reveal that once the pollutants are completely mixed, the first order decay dominates the concentration profiles more than the longitudinal dispersion coefficient. And the effect of longitudinal dispersion could then be neglected. But in the initial period both decay and cross sectional dispersivity govern the concentration distribution. Analytical solution of pollutants transport for the initial period is difficult. A numerical analysis could be a best alternative.

A "Numerical Model" using the finite difference technique for the conceptualized stream tubes generated on the basis of the equi-velocity lines , has been developed, and solved forming the tridiagonal matrices considering Alternate Direction Implicit Explicit (IADIE) technique. Two types of convergence criteria ; i) convergence w.r.t. IADIE, ii) convergence w.r.t. time have been used for obtaining the spatial distribution of pollutant's concentration. The factors which govern the stability of the solution are; i) size of the segment, ii) selection of time step, ii) dispersivity coefficient, and iii) transverse velocity profile.

For given cross sectional and vertical velocity distribution at a specific width and depth respectively, and with a pre-determined dispersivity coefficient, the model can be used for estimating the concentration profile at any time step and at any location within the initial period. The model has been verified with published data and found satisfactory results. The results reported in this study are based on the continuous release of pollutants at one bank. Further study assuming centre line injection of pollutants and with different dispersivity coefficients are suggested for generalization of the solution. The report also addresses a comparative pictures of effects of dispersion on conservative and nonconservative substances.

1.0 INTRODUCTION

Irrespective of any biological and/or biochemical reactions that may occur, it is axiomatic that polluting solutes which enter water courses are transported and dispersed downstream, where they affect the environment in various ways. The ability to describe and predict the effects of the transport processes on the distribution of pollutant concentration is, therefore, of great importance for the investigation of problems such as; estimating the assimilative capacity of rivers receiving urban and industrial effluents; assessing the ecological impact of the discharge of cooling water from power stations and predicting the passage of pollutant clouds through river systems.

Observations reveal that, as a pollutant cloud is carried downstream in a water course, so it disperses, with the cloud steadily lengthening and peak concentrations decreasing as the pollutant is distributed in the ever-increasing volume of water. These effects are the result of a number of particular flow and mixing mechanisms, they are caused primarily by the interaction of two basic phenomena : differential advection and cross sectional diffusion.

Open channel flows are shear flows, i.e., they support lateral and vertical gradients of longitudinal velocity. Therefore, pollutant is differentially advected downstream at the local flow velocity, with pollutant in the faster-moving water is carried downstream faster than pollutant in the slower-moving water. At the same time, pollutant is continually being distributed within the flow cross section via transverse and vertical processes, such as diffusion.

After a tracer has become adequately mixed across the cross section, the final stage in the mixing process is the reduction of longitudinal gradients by longitudinal dispersion. If an effluent is discharged at a constant rate into a river whose discharge is also constant, it is apparent from the under mentioned discussion that there is no need to be concerned about longitudinal dispersion. However, a common practice in Sanitary Engineering has been to assume immediate cross sectional mixing

and to neglect longitudinal dispersion. Question, however, persists about the accountability of decay/growth of substance concentrations within the mixing length (Ghosh, 1993). The mixing length which largely depends upon the width of the river, cross sectional and vertical velocity distribution increases with increasing river width and non-uniform velocity distribution. For small stream, the magnitude of decay/growth within the mixing length may be small thus ignorance of this aspect may lead to small error in computation, however, for large river width this magnitude may be higher. These eventually call upon for a study to ascertain the effect of dispersion both in the mixing length and after the complete mixing of pollutants specially for the nonconservative substances.

This study highlights the effects of dispersion on nonconservative substances both in the "initial period" (defined later on) and the period after the complete mixing of substances. A Numerical model for the initial period of pollutant's transport developed based on the finite difference approach and solved using IADIE (Iterative Alternate Direction Implicit and Explicit) method, is also addressed in this report.

2.0 NONCONSERVATIVE SUBSTANCES

Nonconservative Substances or Decaying substances are those for which the mass changes as a function of time. For most water quality applications, the time rate of change of concentration or mass of nonconservative substances is described by either first order kinetics or kinetics of the Michaelis-Menten type. In the first order kinetics, the time rate of change of concentration of a substance is described as proportional to the concentration, C, present at time, t, as follows:

$$\frac{dC}{dt} = KC \dots \dots \dots (1)$$

Integrating this expression, we have, $C_t = C_0 e^{Kt}$

where

C_t = concentration of substance at time t, M/L³

C_0 = initial concentration of substance at t = 0, and

K = first order rate coefficient, T⁻¹.

For decaying substances (decrease of concentration with respect to time), K is algebraically negative, and for growth (

increase with respect to time), K is algebraically positive.

3.0 BASIC SYSTEM CHARACTERISTICS

The one dimensional mass balance equation which describes the behaviour of a substance in a waterbody in which concentration is affected by the dispersion, advection, growth or decay, and other sources or sinks can be written as :

$$(Adx) \frac{\partial C}{\partial t} = \frac{\partial (AE_x \frac{\partial C}{\partial x})}{\partial x} dx - \frac{\partial (A\bar{U}C)}{\partial x} dx \pm (Adx) \frac{dC}{dt} \pm R \dots \dots \dots (2)$$

- where
- C = concentration of substance, M/L³
 - x = distance along the direction of flow, L
 - t = real time, T
 - A = cross sectional area perpendicular to x, L²
 - E_x = longitudinal dispersion coefficient, L²/T
 - \bar{U} = avg. stream velocity along flow direction, L/T
 - R = source or sink of substances, M/T

dc/dt = growth or decay of substances as given in Eq.(1).

The left hand side of Eq.(2) represents the local derivative of substance concentration, whereas the right hand side respectively represents the behaviour of substances for; dispersion, advection, growth or decay and other sources or sinks.

A solution to this equation would typically yield a relationship expressing the dependent variable, C, as a function of the independent variables, x and t. To get the solution, the other variables, E_x, \bar{U} , R, and A need to be expressed by appropriate expression, in which they are expressed as functions of C, x, t and constant terms and coefficients. For example, A is a function of x and t; \bar{U} is a function of x and t, sources and sinks are functions of C, x and t; and E_x may be constant.

For steady state system, the local derivative $\partial C / \partial t = 0$, i.e., the left hand side of Eq.(2) becomes zero.

3.1 SYSTEM CHARACTERIZED BY ADVECTION AND DISPERSION

Before explaining the effect of dispersion on non-conservative substances, the phenomenological characteristics of advection and dispersion need to be understood.

The combined effects of advection and dispersion can be

illustrated by the following schematic diagram;

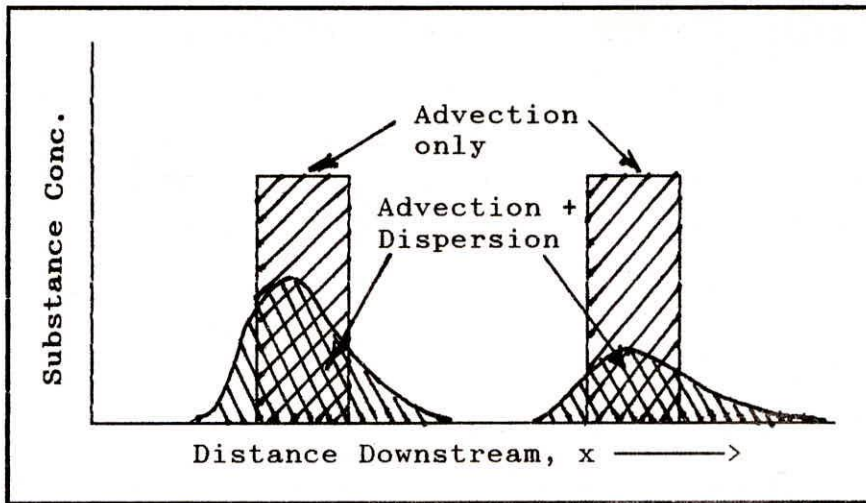


Figure 1: Effects of Advection and Dispersion on concentration profiles resulting from the introduction of a Slug of conservative substance into a stream.

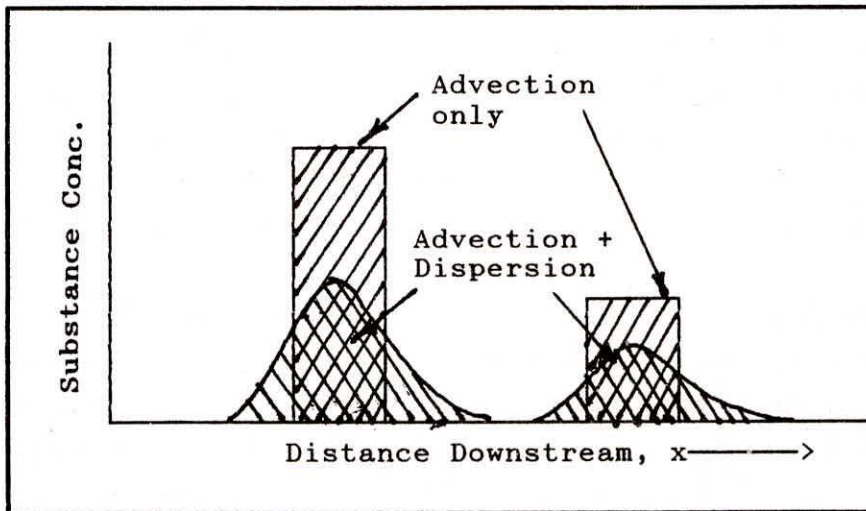


Figure 2 : Effects of Advection and Dispersion on concentration profiles resulting from the introduction of a slug of nonconservative substance into a stream.

Figures 1 & 2 respectively describe the behaviour of conservative and nonconservative substances after its discharge into a receiving stream under the following set of conditions: a) the substance is discharged at a constant rate over a finite time, b) downstream from the discharge, all properties of the stream, such as flow rate and velocity, are constant, c) the stream is one dimensional, d) net velocity is positive in the

flow direction, e) nonconservative substance decays as a function of time, while conservative does not.

The total mass of substances initially released and the area under the concentration profile curves represent the total mass present at the corresponding time after release. The effect of advection is reflected by the displacement downstream of the concentration profiles. The effect of dispersion is reflected by the spreading of the concentration profiles and by the lowering of the peak concentrations. The combined effects of advection and dispersion are reflected in the skewness of the concentration profiles in the downstream direction.

The effects of substance decay are reflected by comparison of corresponding areas under the concentration profile curves between Figures 1 and 2, and by the equalities and inequalities shown.

Figures 3 and 4 schematically represent instream concentration profiles resulting from continuous point source discharge releases at a constant rate at $x=0$ of a conservative and nonconservative substance respectively.

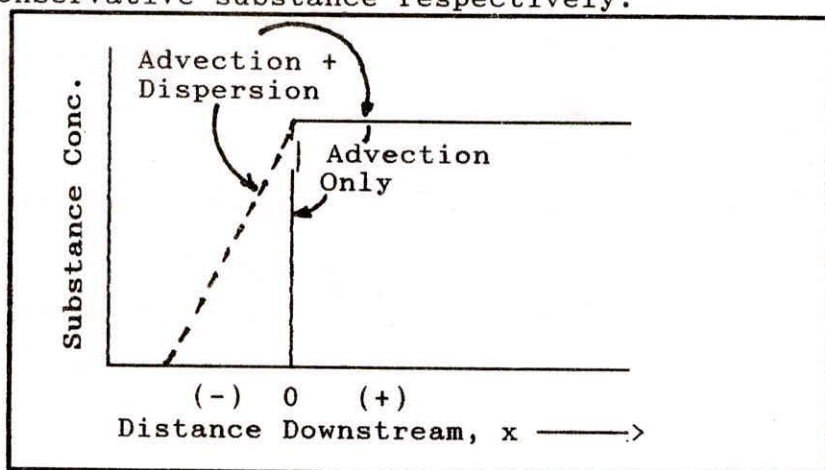


Figure 3: Effects of Advection and Dispersion on concentration profiles resulting from a constant continuous discharge of conservative substance.

For conservative substance, (Fig.3) the effect of dispersion is to produce a concentration profile upstream from the discharge point, while identical concentration profiles are produced downstream from the discharge point for both advection only and for advection and dispersion. For a nonconservative substance (Fig. 4) the effect of dispersion also produces an upstream

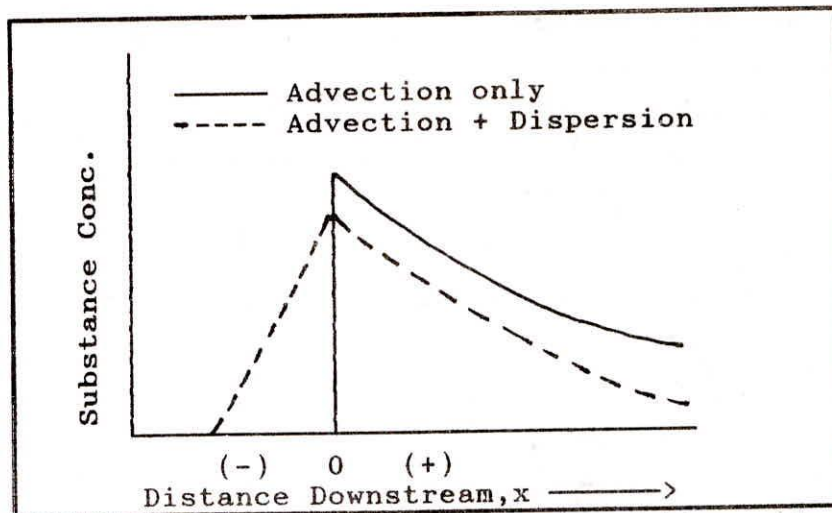


Figure 4 : Effects of Advection and Dispersion on concentration profiles resulting from a constant continuous discharge of nonconservative substance.

concentration profile, but is diminished by decay as compared with Fig. 3.

However, for the nonconservative substance the maximum concentrations (at $x=0$) and the shapes of the downstream concentration profiles are not same for the advection only and advection plus dispersion cases. These are both a function of the dispersion coefficient.

3.2 DISPERSION OF DECAYING SUBSTANCES

Supposing a substance whose rate of decay in a stagnant water body is given by the Eq.(1), and supposing that M units of mass per unit time of this substance are discharged into a river whose discharge is, say, Q . Downstream of the initial mixing zone the diffusion equation becomes;

$$U \frac{\partial C}{\partial X} - E_x \frac{\partial^2 C}{\partial X^2} - KC \dots \dots \dots (3)$$

where, \bar{U} = average cross sectional velocity, L/T
 E_x = longitudinal dispersion coefficient, L^2/T

with a boundary condition that $C \rightarrow 0$ as $x \rightarrow \infty$. The solution of the Eq.(3) is;

$$C = C_0 \exp\left(-\frac{Kx}{U}\right) \left[\frac{2}{\alpha} (\sqrt{\alpha+1} - 1) \right] \dots \dots \dots (4)$$

$$-C_0 \exp\left[-\left(\frac{Ux}{2E_x}\right)(\sqrt{\alpha+1}-1)\right], \dots \text{where, } \alpha = \frac{4E_x K}{U^2} \dots (4a)$$

where, C_0 is a constant of integration. $\alpha = 0$ corresponds to neglecting the dispersion term in the equation, because for tending to zero the quantity forming the exponential term in Eq. (4) tends to one, and the solution is that for simple first-order decay.

The constant of integration can be determined from the condition that the rate at which mass entering the stream must equal the rate at which it is being removed by decay. If the source is located at $x=0$ and the initial mixing distance has length X_m , we can write for the reach in which the one dimensional equation applies that;

$$\int_{X_m}^{\infty} K \cdot C \cdot A \cdot dx = M(X_m) \dots \dots \dots (5)$$

where C is given by the Eq.(4) and $M(X_m)$ is the mass transported through a cross section at $x = X_m$. Substitution of Eq.(4) into Eq.(5) permits computation of C_0 for given $M(X_m)$; however, $M(X_m)$ is not the same as the rate of release of mass at the source because some decay occurs during the initial mixing process. The magnitude of decay can only be computed from a detailed investigation of the concentration distribution in the initial zone. For most practical purposes, the problem is handle by neglecting the existence of the initial zone, in effect setting $X_m=0$ in Eq.(5). The integration then gives;

$$C_0 = \frac{M}{Q} \left[\frac{2}{\alpha} (\sqrt{\alpha+1}-1) \right] \dots \dots \dots (6)$$

For steady flow in a river, the distance required for cross sectional mixing, X_m , is approximately;

$$X_m = \frac{0.4 U W^2}{E_t} \dots \dots \dots (7)$$

where, W = width of the stream, E_t = cross sectional diffusivity,

The distance required for decay of the substance, X_d , to a factor of e^{-1} is

$$X_d = u/K$$

and the ratio is $X_d/X_m = 2.5 \cdot E_t / K W^2$. The quantity α may be

written approximately, using $E_x = 0.011 u^* \cdot W^2 / d \cdot u^*$, [d = depth of flow; u^* = shear velocity] as;

$$\alpha = \frac{4 \cdot E_x \cdot K}{U^2} = \frac{0.024 W^2 K}{E_t} \dots \text{where, } E_t = 1.83 \cdot d \cdot u^*$$

which means that in order for the decay distance to exceed the cross-sectional mixing distance ($X_d > X_m$) must be less than approximately 0.06. The corresponding value of the bracketed term in Eq.(4) is 0.985, which means that the solution is almost exactly that for first order decay neglecting longitudinal dispersion. Thus there are two possibilities: either the material decays before it mixes across the cross section, in which case Eq.(3) is not a suitable model, or else the longitudinal dispersion term in Eq.(3) has a negligible effect and can be dropped. If the former, $X_d < X_m$, the concentration distribution must be computed numerically. If $X_m < X_d$, and if the river and effluent discharges are steady as assumed in dropping the time derivative from Eq.(3), the downstream concentration in that case is reasonably well given by the first-order decay solution $C = (M/Q) \exp(-K \cdot x/u)$. It should be noted, however, that effluent discharges are hardly ever steady. The typical daily fluctuation in output from a sewage treatment plant leads to gradients of concentration of the discharged material along the river, and these gradients are subsequently levelled out by the process of longitudinal dispersion. Although unsteady solutions of the one dimensional diffusion equation are available, practical problems involving daily variations are usually handled most easily by numerical models.

It is apparent from the above discussion that in case of nonconservative substances, once the pollutants are completely mixed over the entire cross section the factor longitudinal dispersion coefficient, E_x , has very little effect on the downstream concentration of pollutants. The occurrence and concentration of pollutants in the downstream locations, in that case, are governed by the first order decaying coefficient. The distribution and the effect of dispersivity of pollutants are mainly dominant in the initial period of pollutants transport. One of the approaches for estimating the concentration of pollutants in the initial period is Numerical Analysis of the

pollutants cloud; that has been described below.

4.0 NUMERICAL MODELING OF INITIAL PERIOD OF POLLUTANTS TRANSPORT

The "initial period" is defined as the period in which longitudinal dispersion is not properly described by the one dimensional diffusion equation. The time required from injection and to become the pollutants completely mixed is called as mixing time and the distance corresponding to this time scale is termed as mixing length or initial reach. In the initial reach, slug discharge is transformed into a longitudinally skewed concentration distribution by the combined action of transverse mixing and longitudinal advection. This reach has been defined approximately by $0 < X' < 0.4$, where, $X' = x W^2 / U E_t$ (Fischer, 1968) [where, x = observation point along flow direction, W = width of the stream, U = average stream velocity, and E_t = transverse dispersivity coefficient). In the initial period, the cloud of pollutants is first advected by the local velocity in the direction of flow and thereafter disperses by the cross sectional diffusivity. Because of the nonuniform velocity distribution across the width faster moving water carry pollutants downstream at a faster rate than the pollutants in the slower moving water. Thus, one dimensional dispersion equation can not be applied over the entire reach considering the total width as an unit. A numerical approach would, therefore, be needed for better representation of pollutants movement and estimation of concentration of pollutants.

4.1 THE MODEL

In the initial period of moving pollutants, the effect of longitudinal dispersivity, E_x , can be ignored assuming Taylor's concept of balancing advection and diffusion. On the contrary, because of sectional variability of velocity of flow, the propagation of pollutants in the perpendicular direction of flow, dominates by the cross sectional dispersivity, E_y . It can be better explained by the following example;

Let us suppose that at some initial time, $t = 0$, a line source of tracer is injected in the flow. The actual initial distribution of the tracer does not much matter, but could

visualize in the form of a line source. Initially, the line source is advected and distorted by the velocity profile. At the same time, the distorted line source begins to diffuse across the cross section at the rate of the potentiality of transverse diffusivity, E_y . During this period, the advection and diffusion are by no means in balance. If we wait a much longer time, it could observe that cloud of tracer extends over a long distance in the x- direction, the average concentration of pollutants, C , in that case varies slowly along the flow direction, and $\partial C/\partial x$ is essentially constant over a long period of time. C' then becomes small because cross sectional diffusion evens out cross sectional concentration gradients. Once the balance is established further longitudinal spreading follows at the rate as depicted in Eq.(2) whose solution after sufficiently long time is a normally distributed cloud moving at the mean speed u , and continuing to spread.

Therefore, the mathematical treatment of the transport processes can be considered with the assumption of the conservation of mass of a pollutants within an infinitesimally small control volume (Fischer et al., 1979). If it is assumed that pollutants are completely mixed over the small elementary strip and transport of pollutants are governed by the advection (along the direction of flow) and transverse dispersivity (along the other direction), the mass balance equation in the differential form into a control volume as shown in Fig. 5 can be written as:

$$\begin{aligned}
 \Delta x \cdot \Delta y \cdot \Delta z \frac{\partial C}{\partial t} &= \bar{U} \cdot C \cdot \Delta y \cdot \Delta z - \bar{U} \cdot C \Delta y \cdot \Delta z - \frac{\partial}{\partial x} [\bar{U} \cdot C \cdot \Delta y \cdot \Delta z] \Delta x \\
 -E_y \cdot \Delta x \cdot \Delta z \cdot \frac{\partial C'}{\partial y} &+ E_y \cdot \Delta x \cdot \Delta z \cdot \frac{\partial C'}{\partial y} + \frac{\partial}{\partial y} [E_y \cdot \Delta x \cdot \Delta z \cdot \frac{\partial C'}{\partial y}] \Delta y \\
 &+ K \cdot C \cdot \Delta x \cdot \Delta y \cdot \Delta z + R \dots \dots \dots (8)
 \end{aligned}$$

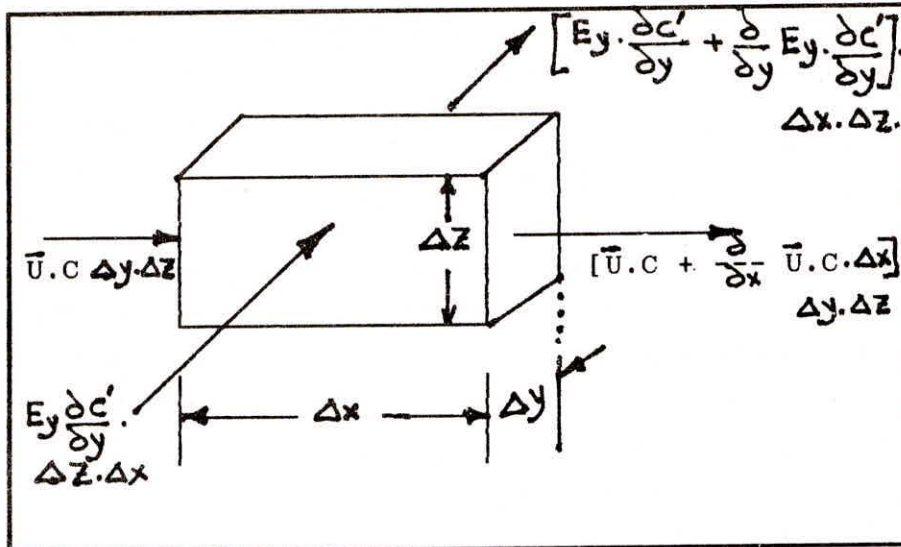


Figure 5 : Definition Sketch

Simplifying equation (8) :

$$\frac{\partial C}{\partial t} - \frac{\bar{U} \cdot \Delta y \cdot \Delta z}{\Delta x \cdot \Delta y \cdot \Delta z} \frac{\partial C}{\partial x} \Delta x + \frac{E_y \cdot \Delta x \cdot \Delta z}{\Delta x \cdot \Delta y \cdot \Delta z} \frac{\partial}{\partial y} \left[\frac{\partial C'}{\partial y} \right] \Delta y + K \cdot C \pm \frac{R}{\Delta x \cdot \Delta y \cdot \Delta z} \dots (9)$$

where

$\Delta x, \Delta y, \Delta z$ = dimensions of elementary strip in three coordinates i.e., along the flow direction, transverse direction, and depth wise respectively.

E_y = transverse dispersion coefficient, L^2/T

\bar{U} = average velocity in the elementary strip, L/T

K = first order growth or decay coefficient, T^{-1}

C = concentration of pollutants in the elementary strip, $M L^{-3}$

C' = concentration of pollutants moving in and out of the elementary strip along the transverse direction, $M L^{-3}$

R = source or sink of pollutants, M

Assuming, uniform velocity and uniform mixing over the depth, the initial period can be modeled applying the Finite Difference scheme for the equation (9).

To apply the finite difference scheme, following concepts are applied :

i) Dividing the total flow by vertical lines into n stream tubes of Area A_1, A_2, \dots, A_n , based on equi-velocity lines along the

depth, as shown in Fig. 6. Each stream tube is assigned a relative velocity, u_1', u_2', \dots, u_n' (Figs. 7(a) & 7(b)), based on the actual velocity measurement, care being taken that

$$\sum_{j=1}^n u_j' \cdot A_j = 0 \dots \dots (10)$$

ii) A computer mesh for concentration values $C_{I,J}$ is established as shown in Fig. 8, [where, I refers to longitudinal distance in a coordinate system moving at the mean flow velocity and J refers to the Jth stream tube]. A time step Δt is selected subject to condition given below; the computer longitudinal distance step is taken as

$$\Delta x = u_{j_{\max}} \Delta t \dots \dots (11)$$

in which, u'_j is the mean velocity of the jth stream relative to a coordinate system moving at the overall cross-sectional mean velocity. Thus, the average flow in the stream tube of maximum relative velocity $u'_{j_{\max}}$ is moving at plus or minus one computer mesh point per time step as shown in Fig. 7(b).

iii) Each time step is assumed to consist of two parts: first, the concentration distribution within each stream tube is advected up or downstream according to the velocity of that tube, second, transfer is accomplished between adjoining stream tubes according to the given mixing coefficients.

iv) In the advective part, an entire set of mesh point values $C_{I,J,K+1}$, is generated from the values of $C_{I,J,K}$, where K indicates values at the beginning of each time step Δt . The advective velocities are converted to units of mesh points per time step by the relation

$$U_j = u'_j \left(\frac{\Delta t}{\Delta x} \right) \dots \dots (12)$$

The concept of transport of pollutants in the stream tube having nonuniform velocity can also be explained as; withdrawal and addition of pollutants in each segment depending upon positioning of local velocity with reference to the average cross sectional velocity. That means, if the velocity in a stream tube is less than the average cross sectional velocity, pollutants mass

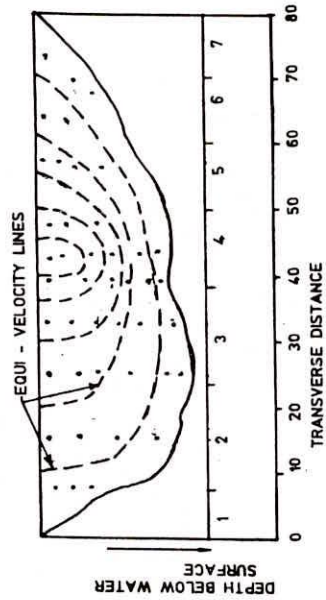


FIG. 6 THE CROSS SECTIONAL VELOCITY DISTRIBUTION

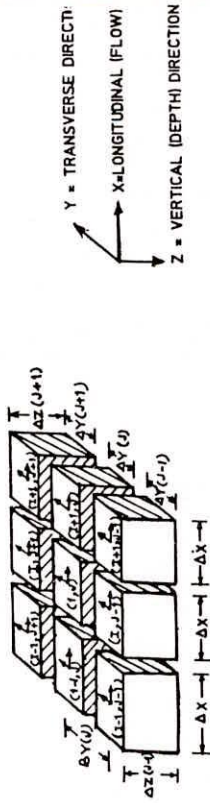


FIG. 8: CONCEPTUALIZED FINITE DIFFERENCE SCHEME OF THE POLLUTANTS MOVEMENT.

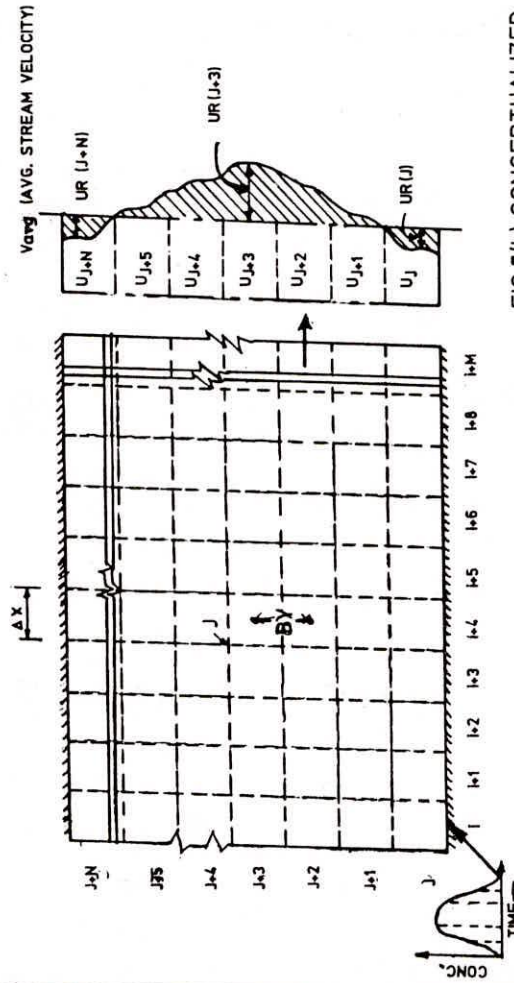


FIG. 7(b) CONCEPTUALIZED VELOCITY-DISTRIBUTION ALONG THE TRANSVERSE DIRECTION

FIG. 7 (a) CONCEPTUALIZED COMPUTER MESH OF THE STREAM.

equivalent to the mass less advected because of difference in velocities are withdrawn from that stream segment, and for reverse condition pollutants' mass equivalent to the mass more advected because of difference in velocities are added to that stream segment. However, selection of stream tubes and size of segment are the two important factors responsible for the stability of the solution.

4.2 FORMULATION OF FINITE DIFFERENCE SCHEME

The finite difference scheme of equation (9) is written in the following form :

$$\begin{aligned}
 & C_{I,J,K+1} - C_{I,J,K} - U_{I,J} \cdot U_{I,J} [\alpha_{I,J} C_{I,J,K+1} - \beta_{I,J} C_{I+1,J,K+1}] \\
 & + U_{I,J} \cdot U_{I,J} [\alpha_{I,J} C_{I-1,J,K+1} - \beta_{I,J} C_{I,J,K+1}] + \left(\frac{E_{Y(I,J+1)} \cdot H_{I,J+1}}{B_{I,J+1}} \right. \\
 & \left. [(C_{I,J+1,K} - U_{I,J+1} \cdot U_{I,J+1} [\alpha_{I,J+1} C_{I,J+1,K+1} - \beta_{I,J+1} C_{I+1,J+1,K+1}] \right. \\
 & \left. + U_{I,J+1} \cdot U_{I,J+1} [\alpha_{I,J+1} C_{I-1,J+1,K+1} - \beta_{I,J+1} C_{I,J+1,K+1}]) \right. \\
 & \left. - (C_{I,J,K} - U_{I,J} \cdot U_{I,J} [\alpha_{I,J} C_{I,J,K+1} - \beta_{I,J} C_{I+1,J,K+1}] + \right. \\
 & \left. U_{I,J} \cdot U_{I,J} [\alpha_{I,J} C_{I-1,J,K+1} - \beta_{I,J} C_{I,J,K+1}]) \right] + \\
 & - \frac{E_{Y(I,J-1)} \cdot H_{I,J-1}}{B_{I,J-1}} [(C_{I,J,K} - U_{I,J} \cdot U_{I,J} [\alpha_{I,J} C_{I,J,K+1} - \beta_{I,J} C_{I+1,J,K+1}] \\
 & + U_{I,J} \cdot U_{I,J} [\alpha_{I,J} C_{I-1,J,K+1} - \beta_{I,J} C_{I,J,K+1}]) - (C_{I,J-1,K} \\
 & - U_{I,J-1} \cdot U_{I,J-1} [\alpha_{I,J-1} C_{I,J-1,K+1} - \beta_{I,J-1} C_{I+1,J,K+1}] + U_{I,J-1} \cdot U_{I,J-1} \\
 & [\alpha_{I,J-1} C_{I-1,J-1,K+1} - \beta_{I,J-1} C_{I,J-1,K+1}]) \left] \frac{\Delta t}{A_{I,J}} - K \cdot C_{I,J,K+1} \Delta t + \frac{R \cdot \Delta t}{\Delta X \cdot \Delta Y \cdot \Delta Z} \dots (13)
 \end{aligned}$$

where $U_{I,J} = \frac{U'_{I,J} \cdot t}{x}$; $J = 1, 2, 3, \dots, n$
 $\frac{U'_{I,J}}{\bar{U}}$ = relative velocity = $UR_J - \bar{U}$
 \bar{U} = average stream velocity.
 $U_{I,J}$ = dimensionless velocity factor (+ve or -ve).
 UR_J = local velocity in the stream tube.
 α, β = weightage
 when $U_{I,J} = +ve$, $\alpha = 1$ & $\beta = 0$

when $U_{I,J} = -ve$, $\alpha = 0$ & $\beta = 1$.

4.3 FORMULATION OF THE PROBLEM

The Finite Difference schemes for each segment can be written in the algebraic form mentioned above. For M number of segments and N number of stream tubes there will be (M x N) number of algebraic equations. Using IADIE (Iterative Alternate Direction Implicit Explicit) solution techniques the algebraic equations can be solved to obtain the concentration of pollutants at each segment after every time step.

Explicit solution implies - solving of linear algebraic equation for the unknowns for the spatial derivatives written at the beginning of the time step. It does not ensure stability and convergence unconditionally.

In Implicit scheme, the spatial derivatives are written at the end of the time step. Since the number of unknowns become more than the number of equations, it is difficult to solve and will require prohibitively large memory requirement for solution.

Implicit -Explicit on ADIE (Alternate Direction Implicit-Explicit) scheme implies writing of spatial derivative implicitly for one direction and explicitly in the other direction. This is used for two dimensional equations where both 'x' and 'y' directions are involved. These types of schemes lead to determinate system of linear equation with known boundary conditions.

4.4 ITERATIVE ALTERNATE DIRECTION IMPLICIT EXPLICIT (IADIE) SCHEME

Alternate direction means - firstly writing the different coefficients of the tridiagonal matrices implicitly along the row treating the diagonal element of the explicit direction as implicit (in order to make diagonal element strong to behave well) and then writing the coefficients implicitly along columns treating the diagonal element of the explicit direction as implicit. This process is repeated (iterated) till the specified

convergence criteria is satisfied.

The equation for any segment written implicit along row is given by :

$$X_J \cdot C_{I,J-1,K+1} + Y_J \cdot C_{I,J,K+1} + Z_J \cdot C_{I,J+1,K+1} = W_J \dots\dots(14)$$

where, X_J , Y_J , and Z_J are the coefficients of tridiagonal matrix and are also the coefficients of concentration of pollutants at (J-1)th, Jth and (J+1)th stream tubes. W_J is a constant.

So, there will be NC (number of columns) number of equations.

Similarly the equation for any segment implicit along column can be written in the form :

$$X_I \cdot C_{I-1,J,K+1} + Y_I \cdot C_{I,J,K+1} + Z_I \cdot C_{I+1,J,K+1} = W_I \dots\dots(15)$$

where, A_I , B_I and Z_I are the coefficients of the tridiagonal matrix and are also the coefficients of concentration of pollutants at the (I-1)th, Ith, and (I+1)th row. W_I is a constant.

4.5 FORMULATION OF X,Y,Z AND W MATRICES

The matrices X,Y,Z, and W are formulated for defining spatial and temporal derivatives appearing in equation (13) by finite differences for the following conditions :

Interior Segments

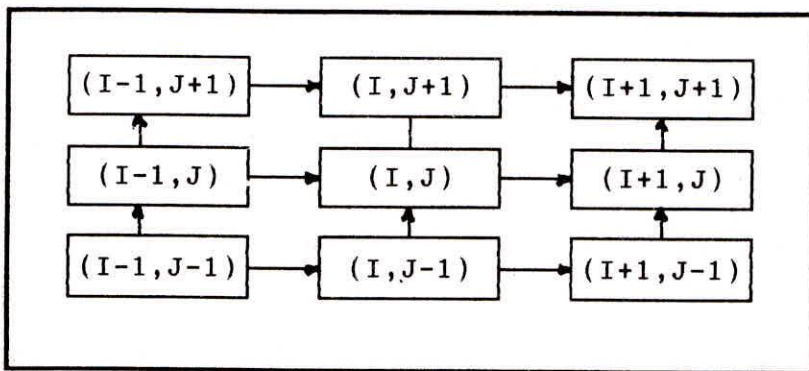


Figure - 9 : Linkages of Segments for Interior Segments.

Writing the equation (13) in Finite Difference form for the Fig.9 given above:

4.5.1 Column-wise Solution

Separating the coefficients of $C_{I,J-1,K+1}$, $C_{I,J,K+1}$ and $C_{I,J+1,K+1}$; we have:

$$\begin{aligned}
& C_{I,J-1,K+1} U_2 \cdot F_3 [\alpha_{I,J-1} + \beta_{I,J-1}] + \\
& C_{I,J,K+1} (1.0 + F_2 [\alpha_{I,J} + \beta_{I,J}] \cdot (1.0 - L_1 - L_2) + K \Delta t) + \\
& C_{I,J+1,K+1} U_1 \cdot F_1 [\alpha_{I,J+1} + \beta_{I,J+1}] \\
& - C_{I,J,K} [1.0 - L_1 - L_2] + C_{I,J+1,K} \cdot L_1 + C_{I,J-1,K} \cdot L_2 + C_{I+1,J+1,K+1} \cdot L_1 \cdot F_1 \cdot \beta_{I,J+1} \\
& + C_{I+1,J,K+1} \cdot F_2 \cdot \beta_{I,J} \cdot [1.0 - L_1 - L_2] + C_{I+1,J-1,K+1} \cdot L_2 \cdot F_3 \cdot \beta_{I,J-1} \\
& + C_{I-1,J+1,K+1} \cdot L_1 \cdot F_1 \cdot \alpha_{I,J+1} + C_{I-1,J,K+1} \cdot F_2 \cdot \alpha_{I,J} \cdot [1.0 - L_1 - L_2] \\
& + C_{I-1,J-1,K+1} \cdot L_2 \cdot F_3 \cdot \alpha_{I,J-1} + \frac{R \cdot \Delta t}{\Delta X \cdot \Delta Y \cdot \Delta Z} \dots \dots (16)
\end{aligned}$$

where,

$$F_1 = U_{I,J+1} \cdot U_{I,J+1} ; F_2 = U_{I,J} \cdot U_{I,J} ; F_3 = U_{I,J-1} \cdot U_{I,J-1}$$

$$L_1 = \frac{E_{Y(I,J+1)} \cdot H_{I,J+1} \cdot \Delta t}{A_{I,J} \cdot B_{I,J}}$$

$$L_2 = \frac{E_{Y(I,J-1)} \cdot H_{I,J-1} \cdot \Delta t}{B_{I,J} \cdot A_{I,J}}$$

$$H_{I,J+1} = \Delta X \cdot \Delta Z_{J+1}$$

$$H_{I,J-1} = \Delta X \cdot \Delta Z_{J-1}$$

$$A_{I,J} = \Delta Y_J \cdot \frac{\Delta Z_J + \Delta Z_{J+1}}{2}$$

$$B_{I,J+1} = \frac{\Delta Y_J + \Delta Y_{J+1}}{2}$$

$$B_{I,J-1} = \frac{\Delta Y_{J-1} + \Delta Y_J}{2}$$

The coefficients of the matrix are;

$$X_{J-L_2} F_1 [\alpha_{I,J-1} + \beta_{I,J-1}] \quad Y_{J-1} \cdot 0 + F_2 \cdot [\alpha_{I,J} + \beta_{I,J}] (1 \cdot 0 - L_1 - L_2) + K \cdot \Delta t$$

$$Z_{J-L_1} \cdot F_1 [\alpha_{I,J+1} + \beta_{I,J+1}]$$

$$W_J = C_{I,J,K} (1 \cdot 0 - L_1 - L_2) + C_{I,J+1,K} \cdot L_1 + C_{I,J-1,K} \cdot L_2 + C_{I+1,J+1,K+1} \cdot L_1 \cdot F_1 \cdot \beta_{I,J+1}$$

$$+ C_{I+1,J,K+1} \cdot F_2 \cdot \beta_{I,J} (1 \cdot 0 - L_1 - L_2) + C_{I+1,J-1,K+1} \cdot L_2 \cdot F_3 \cdot \beta_{I,J-1}$$

$$+ C_{I-1,J+1,K+1} \cdot L_1 \cdot F_1 \cdot \alpha_{I,J+1} + C_{I-1,J,K+1} \cdot F_2 \cdot \alpha_{I,J} \cdot [1 \cdot 0 - L_1 - L_2]$$

$$+ C_{I-1,J-1,K+1} \cdot L_2 \cdot F_3 \cdot \alpha_{I,J-1} + \frac{R \cdot \Delta t}{\Delta X \cdot \Delta Y \cdot \Delta Z} \dots (17)$$

Row-wise Solution

Separating the coefficients of $C_{I-1,J,K+1}$, $C_{I,J,K+1}$, and $C_{I+1,J,K+1}$; i.e. to ascertain the elements X_I , Y_I , Z_I , and W_I , we have;

$$C_{I-1,J,K+1} (-F_2 \cdot \alpha_{I,J} [1 \cdot 0 - L_1 - L_2]) + C_{I,J,K+1} (1 \cdot 0 + F_2 \cdot [\alpha_{I,J} + \beta_{I,J}]$$

$$(1 \cdot 0 - L_1 - L_2) + K \cdot \Delta t) + C_{I+1,J,K+1} (-F_2 \cdot \beta_{I,J} \cdot (1 \cdot 0 - L_1 - L_2))$$

$$C_{I,J,K} [1 \cdot 0 - L_1 - L_2] + C_{I,J+1,K} \cdot L_1 + C_{I,J-1,K} \cdot L_2$$

$$+ C_{I+1,J+1,K+1} \cdot L_1 \cdot F_1 \cdot \beta_{I,J+1} + C_{I+1,J-1,K+1} \cdot L_2 \cdot F_3 \cdot \beta_{I,J-1}$$

$$+ C_{I,J+1,K+1} (-L_1 \cdot F_1 \cdot [\alpha_{I,J+1} + \beta_{I,J+1}]) + C_{I,J-1,K+1} (-L_2 \cdot F_3 \cdot [\alpha_{I,J-1} + \beta_{I,J-1}])$$

$$+ C_{I-1,J+1,K+1} (L_1 \cdot F_1 \cdot \alpha_{I,J+1}) + C_{I-1,J-1,K+1} (L_2 \cdot F_3 \cdot \alpha_{I,J-1}) + \frac{R \cdot \Delta t}{\Delta X \cdot \Delta Y \cdot \Delta Z} \dots (18)$$

In which, the coefficients; X_I , Y_I , Z_I and W_I are;

$$X_I = (-F_2 \cdot \alpha_{I,J} \cdot [1.0 - L_1 - L_2]) \quad Y_I = (1.0 + F_2 \cdot [\alpha_{I,J} + \beta_{I,J}] \cdot (1.0 - L_1 - L_2)) + K.$$

$$Z_I = (-F_2 \cdot \beta_{I,J} \cdot (1.0 - L_1 - L_2))$$

$$W_I = C_{I,J,K} [1.0 - L_1 - L_2] + C_{I,J+1,K} \cdot L_1 + C_{I,J-1,K} \cdot L_2$$

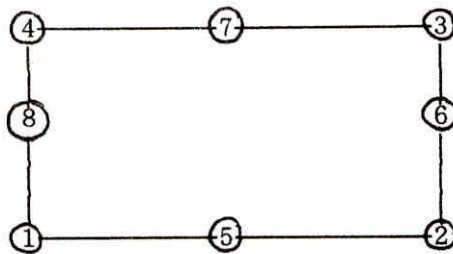
$$+ C_{I+1,J+1,K+1} \cdot L_1 \cdot F_1 \cdot \beta_{I,J+1} + C_{I+1,J-1,K+1} \cdot L_2 \cdot F_3 \cdot \beta_{I,J-1}$$

$$+ C_{I,J+1,K+1} (-L_1 \cdot F_1 \cdot [\alpha_{I,J} + \beta_{I,J}]) + C_{I,J-1,K+1} (-L_2 \cdot F_3 \cdot [\alpha_{I,J-1} + \beta_{I,J-1}])$$

$$+ C_{I-1,J+1,K+1} (L_1 \cdot F_1 \cdot \alpha_{I,J+1}) + C_{I-1,J-1,K+1} (L_2 \cdot F_2 \cdot \alpha_{I,J-1}) + \frac{R \cdot \Delta t}{\Delta X \cdot \Delta Y_J \cdot \Delta Z_J} \cdot (19)$$

4.6 Neuman Boundary Segments

The matrices X, Y, Z, and W for boundary segments are formulated on the basis of the mass balance within the segment discretized by the boundary segment, accounting for the known input/output concentration. The types of boundary segments are described in the figure below;

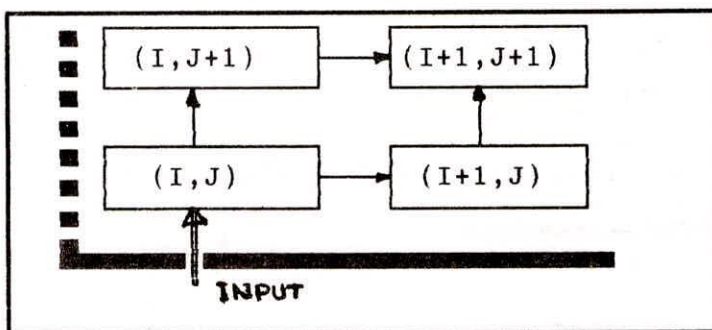


1. L.H.S. bottom corner segment.
2. R.H.S. bottom corner segment.
3. R.H.S. top corner segment.
4. L.H.S. top corner segment.
5. Bottom middle segment.
6. Vertical far segment.
7. Top middle segment.
8. Vertical near segment.

Applying the mass balance equations for each segment as follows;

Inflow of pollutants - Outflow of pollutants
= Change of concentration within the control volume.

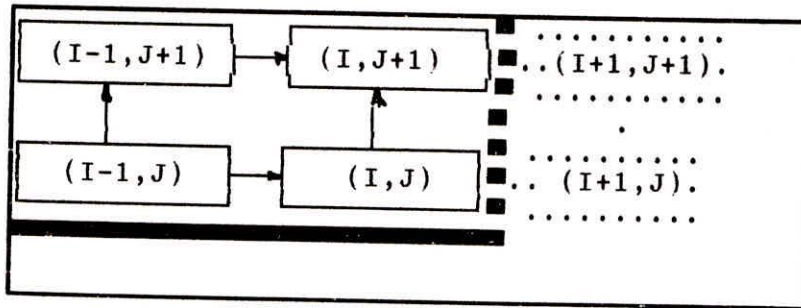
4.6.1 L.H.S. Bottom Corner Segment (Input receiving segment)



where,

$$\begin{aligned} X_J &= 0.0 \\ U_{I,J-1} &= 0.0 \\ H_{I,J-1} &= 0.0 \\ C_{I-1,J-1,K+1} &= 0.0 \\ C_{I,J-1,K+1} &= 0.0 \\ C_{I+1,J-1,K+1} &= 0.0 \\ C_{I-1,J,K+1} &\& \\ C_{I-1,J+1,K+1} &= 0.0 \end{aligned}$$

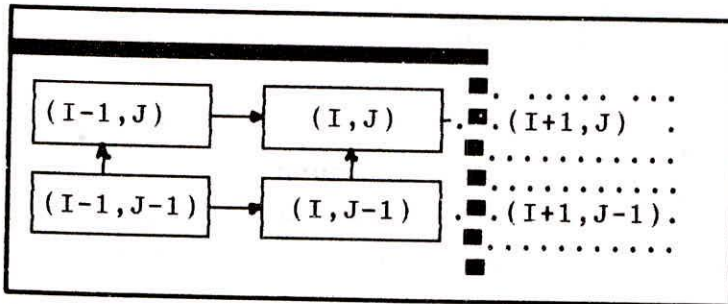
4.6.2 R.H.S. Bottom Corner Segment.



Where,

$$\begin{aligned}
 X_J &= 0.0 \\
 U_{I, J-1} &= 0.0 \\
 H_{I, J-1} &= 0.0 \\
 C_{I, J, K+1} &= C_{I+1, J, K+1} \\
 C_{I, J+1, K+1} &= C_{I+1, J+1, K+1} \\
 C_{I-1, J-1, K+1} &= C_{I, J-1, K+1} \\
 &= C_{I+1, J-1, K+1} = 0.0
 \end{aligned}$$

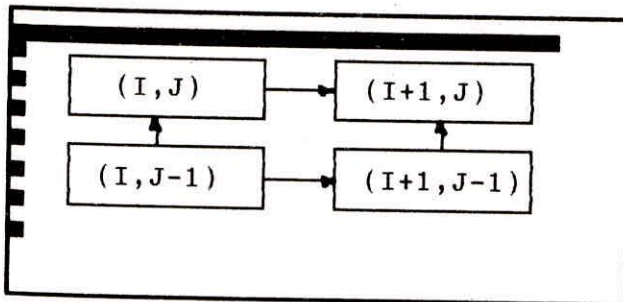
4.6.3 R.H.S. Top Corner Segment



Where,

$$\begin{aligned}
 Z_J &= 0.0 \\
 U_{I, J+1} &= 0.0 \\
 H_{I, J+1} &= 0.0 \\
 C_{I+1, J, K+1} &= C_{I, J, K+1} \\
 C_{I+1, J-1, K+1} &= C_{I, J-1, K+1} \\
 C_{I-1, J+1, K+1} &= C_{I, J+1, K+1} \\
 &= C_{I+1, J+1, K+1} = 0.0
 \end{aligned}$$

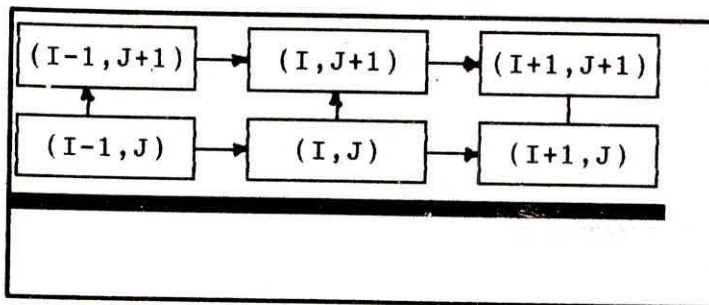
4.6.4 L.H.S. Top Corner Segment



Where,

$$\begin{aligned}
 Z_J &= 0.0 \\
 U_{I, J+1} &= 0.0 \\
 H_{I, J+1} &= 0.0 \\
 C_{I-1, J+1, K+1} &= C_{I-1, J, K+1} \\
 &= C_{I-1, J-1, K+1} = 0.0 \\
 C_{I, J+1, K+1} &= C_{I+1, J+1, K+1} \\
 &= 0.0
 \end{aligned}$$

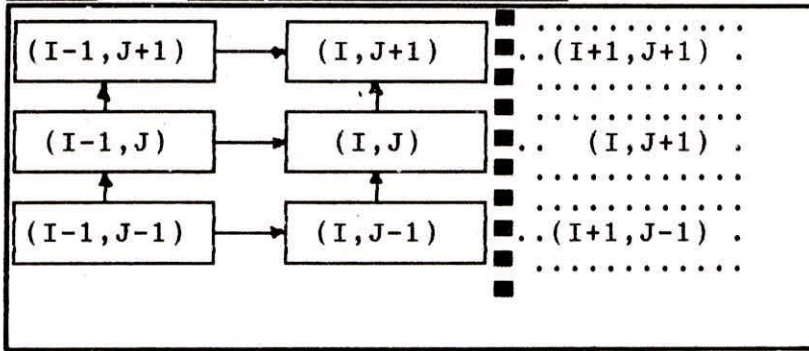
4.6.5 Bottom Middle Segments



Where,

$$\begin{aligned}
 X_J &= 0.0 \\
 U_{I, J-1} &= 0.0 \\
 H_{I, J-1} &= 0.0 \\
 C_{I-1, J-1, K+1} &= C_{I, J-1, K+1} \\
 &= C_{I+1, J-1, K+1} = 0.0
 \end{aligned}$$

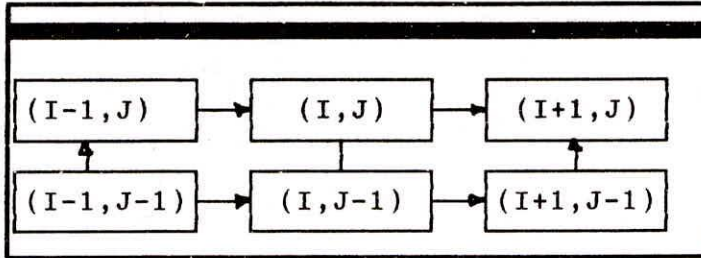
4.6.6 Vertical Far Segments



Where,

$$\begin{aligned} C_{I+1, J+1, K+1} &= C_{I, J+1, K+1} \\ C_{I+1, J, K+1} &= C_{I, J, K+1} \\ C_{I+1, J-1, K+1} &= C_{I, J-1, K+1} \end{aligned}$$

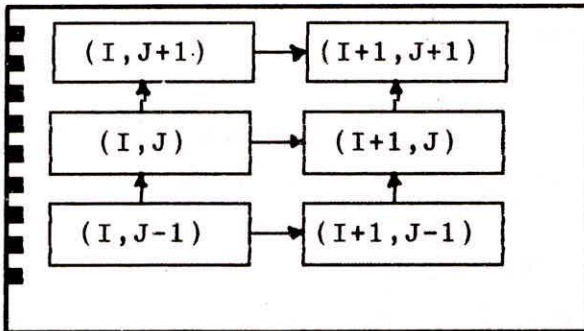
4.6.7 Top Middle Segments



Where,

$$\begin{aligned} Z_J &= 0.0 \\ U_{I, J+1} &= 0.0 \\ H_{I, J+1} &= 0.0 \\ C_{I-1, J+1, K+1} &= C_{I, J+1, K+1} \\ &= C_{I+1, J+1, K+1} = 0.0 \end{aligned}$$

4.6.8 Vertical Near Segments



Where,

$$\begin{aligned} C_{I-1, J+1, K+1} &= 0.0 \\ C_{I-1, J, K+1} &= 0.0 \\ C_{I-1, J-1, K+1} &= 0.0 \end{aligned}$$

5.0 SOLUTION TECHNIQUES

5.1 FORMATION OF TRIDIAGONAL MATRICES

A matrix is called a tridiagonal matrix if it has all its nonzero elements on the principal diagonal and in the positions immediately adjacent to the principal diagonal.

Tridiagonal systems arise when differential equations are finite differenced. The system of equations which form the tridiagonal matrix can be written as;

$$\begin{array}{rcl}
 Y_1 \cdot C_1 + Z_1 \cdot C_2 & & = W_1 \\
 X_2 \cdot C_1 + Y_2 \cdot C_2 + Z_2 \cdot C_3 & & = W_2 \\
 & X_3 \cdot C_2 + Y_3 \cdot C_3 + Z_3 \cdot C_4 & = W_3 \\
 & \cdot & \cdot \\
 & \cdot & \cdot \\
 & \cdot & \cdot \\
 & X_{N-1} \cdot C_{N-2} + Y_{N-1} \cdot C_{N-1} + Z_{N-1} \cdot C_N & = W_{N-1} \\
 & X_N \cdot C_{N-1} + Y_N \cdot C_N & = W_N
 \end{array} \dots (20)$$

This can also be written as;

$$A \cdot C = W \dots (21)$$

where, A is the tridiagonal matrix; C and W are the vectors and can be represented by:

$$\begin{bmatrix}
 Y_1 & Z_1 & & & & \\
 X_2 & Y_2 & Z_2 & & & \\
 & X_3 & Y_3 & Z_3 & & \\
 & \cdot & \cdot & \cdot & & \\
 & \cdot & \cdot & \cdot & & \\
 & X_{N-1} & Y_{N-1} & Z_{N-1} & & \\
 & & X_N & Y_N & & \\
 \end{bmatrix}
 \begin{bmatrix}
 C_1 \\
 C_2 \\
 C_3 \\
 \cdot \\
 \cdot \\
 C_{N-1} \\
 C_N
 \end{bmatrix}
 =
 \begin{bmatrix}
 W_1 \\
 W_2 \\
 W_3 \\
 \cdot \\
 \cdot \\
 W_{N-1} \\
 W_N
 \end{bmatrix} \dots (22)$$

5.2 CONVERGENCE CRITERIA

Two types of convergence criteria have been used in the model to be fulfilled before computing concentration of pollutants. They are :

- i. convergence with respect to IADIE
- ii. convergence with respect to time steps.

5.2.1 Convergence with respect to IADIE

In the alternate direction implicit explicit scheme, the final target is to get nearly true implicit solution.

Mathematically this can be written as:

$$\sum C_{I,J,K+1}(m) - C_{I,J,K+1}(t) \dots (23)$$

$$m \rightarrow \infty$$

where, $C_{I,J,K+1}(t)$ is the true implicit solution.

In order to terminate the number of iterations, some pre-decided convergence factor is assigned. If the sum of the difference of concentration between the current and preceding iteration is less than or equal to the convergence factor

assigned, the convergence level with respect to IADIE is said to be achieved. This can be explained mathematically as :

$$\sum_{I=1}^{NR} \sum_{J=1}^{NC} |C_{I,J,K+1}(M) - C_{I,J,K+1}(M-1)| \leq \xi \dots (24)$$

where, ξ : Pre-decided convergence factor.

- NR & NC : Number of rows and number of columns.
- $C_{I,J,K+1}(m)$: Concentration of pollutants in the current iteration w.r.t. ADIE.
- $C_{I,J,K+1}(m-1)$: Concentration of pollutants in the preceding iteration w.r.t ADIE.

5.2.2 Convergence with respect to time steps

A time step is divided into increasing number of subtime steps for IADIE solution, till the desired convergence level is achieved, i.e.,

$$\sum_{I=1}^{NR} \sum_{J=1}^{NC} |C_{I,J,K+1}(KK+1) - C_{I,J,K+1}(KK)| \leq \xi_1 \dots (25)$$

where,

- $C_{I,J,K+1}(KK+1)$: Concentration of pollutants at the end of the current time step estimated by dividing the time step into KK+1 number of subtime steps.
- $C_{I,J,K+1}(KK)$: Concentration of pollutants at the end of the previous time steps.
- ξ_1 : Pre-decided convergence level.

6.0 Analysis of Results and Discussion

The combined effects of advection and dispersion govern the transport of pollutants in a moving water. Advection is mainly responsible for displacement of pollutants in the direction of flow, while dispersion is responsible for spreading of pollutants along the three cartesian coordinates.

It is apparent from the discussions made in sections 3.1 and 3.2 that in case of nonconservative substances, once the substances are completely mixed over the entire cross section, the effect of longitudinal dispersion is so small in comparison to the decay of substances that the term of dispersion can be

overlooked and the downstream concentration profile can then be conceptualized by the first order decay as given by Eq.(1). The effects of dispersivity are mainly dominant in the initial period of pollutants transport because of the differential advection and cross sectional diffusion. Alternately, because of the concentration gradients between the adjacent layers the cross sectional dispersivity due to the transverse diffusion coefficient propagates the spreading of pollutants toward the otherside of river bank. The decay and transport of non-conservative substances, in that case, depend upon the travel time of pollutants cloud within water body. The "travel time" is defined as the time taken by a pollutant to reach from the point of injection upto the point of complete mixing. The concentration of pollutants thus at any point would be equal to the exponential decay of the term $(K.t)$ [where, K = first order decay coefficient, T^{-1} ; t = travel time, T].

In order to assess the concentration of pollutant's cloud over different space and time in the initial period of pollutant transport, a "Numerical Model" using the finite difference schemes on one dimensional Advection-Dispersion-Decay-Sources equation has been conceptualized and described in section 4.1. It is assumed in the model that; i) transport of pollutants along the flow direction is due to the differential advection and depend upon the magnitude of local velocities of flow, while ii) spreading of pollutants in the other direction is due to the transverse diffusivity.

For given velocity fields of a particular flow at any river cross section, the equi-velocity lines of any desired magnitude if drawn, will represent flow through number of stream tubes. If the river bed effects on velocity are ignored, and vertical lines are drawn based on the magnitude of velocity to form n number of stream tubes of area $A_1, A_2, A_3, \dots, A_n$, and a relative velocity respectively of; $u'_1, u'_2, u'_3, \dots, u'_n$ are assigned in each stream tubes such that summation of total flow for the stream tubes is zero, the problem can then be solved forming the finite difference schemes for each segments formed dividing the total length into number of equal segments. The "relative velocity", here is defined as the difference of local velocity and the average cross sectional velocity. Thus, the average flow in the

stream tube may be moving at plus or minus for each time step in comparison to the other stream tube. Selection of the width of stream tubes which form the size of segment is an important factor to obtain the stability of solution and to get the accuracy of solution. Larger the dimensions of stream tube means commitment of more error in the solution. Alternately, more number of stream tubes and segments would lead to better approximation of the velocity field and for that matter well conceptualization of transport process. The length of the segment is determined from the eq.(11), in which the time step, Δt , determines the length of segment and the advective velocities accordingly converted to units of mesh points per time step as depicted by the expression given in eq.(12). The mixing coefficient, E_y , is also governed by the time step. Thus, selection of time step is an important factor. Selection of excessive higher/lower time step may lead to the unstability of solution. The physical significance of time step may be defined as; for example, if a higher time step is selected for a particular set of mesh points and for a given hydraulic conditions, the transverse mixing of pollutants due to the cross sectional diffusivity may be underestimated than the actual situation, in otherwords, the length of the initial period will be over estimated. For the smaller time step, it would be just opposite. It has been shown (Fischer, 1968) that a stable solution could be obtained if, for all stream tubes,

$$\frac{E_{y_{I,J}} \cdot \Delta t}{(B_{I,J})^2} < 0.5 \dots \dots (26)$$

It was suggested by Fischer (1968) that in practice it is well to keep this ratio less than approximately 0.2.

The concept derived in section 4.1 can be explained as :

The mass transport between stream tubes per time step is computed by assuming that for the duration of the step the concentration gradient at the dividing surface equals the difference in convected concentrations at the mesh points divided by the distance between them; that is

$$\Delta M_{I,(J,J+1)} = \frac{H_{I,J} \cdot E_{y_{I,J}} \cdot \Delta C_{I,J} \cdot \Delta x \cdot \Delta t}{B_{I,J}} \dots \dots (27)$$

Where, $\Delta C_{I,J}$ is the difference in concentration between stream tubes J and J+1, i.e., $[C_{I,J+1} - C_{I,J}]$.

Since the mesh-point concentration is meant to represent the concentration within the entire stream tube, the change in concentration $\delta C_{I,J}$ at mesh point (I,J) is given by;

$$\delta C_{I,J} = \frac{1}{A_{I,J} \Delta X} [\Delta M_{I,(J,J+1)} - \Delta M_{I,(J-1,J)}] \dots \dots (28)$$

where,

$$\delta C_{I,J} = \frac{[C_{I,J+1} - C_{I,J}]}{\Delta t}$$

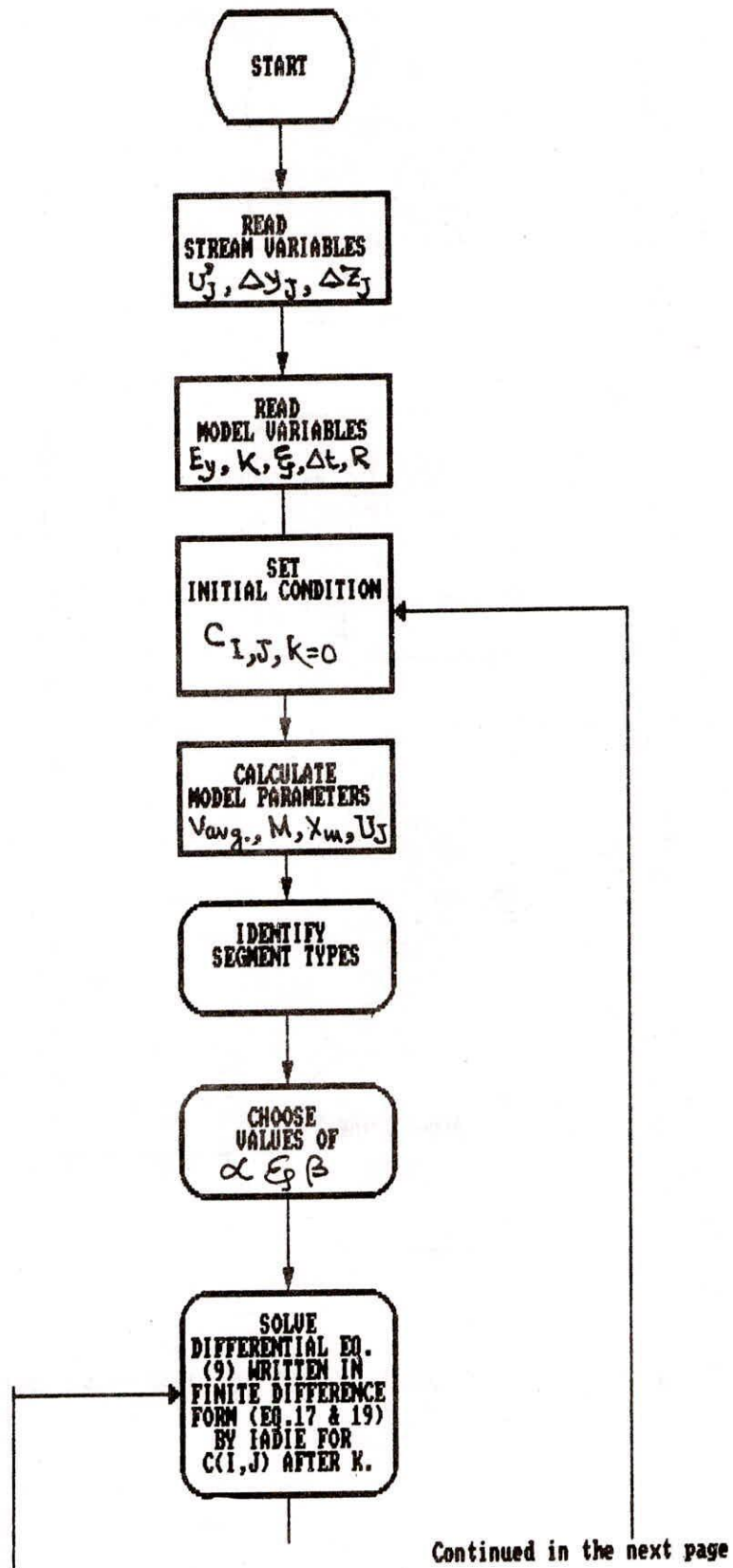
From the Eq.(28) a new set of mesh points for the next time step is estimated from the previous time step using Eq.(13).

one advective step followed by one diffusive step completes the computation for one time step. The method can be applied for any desired initial distribution; for example, a slug source can be modeled by setting all initial concentrations equal to zero except for one, a plane source can be modeled by setting all initial concentrations zero except for the concentrations on one line, which are all set to some constant value. A constant or variable rate of discharge can also be modeled.

Based on the above concept a computer model has been developed, which is capable of demonstrate the spatial distribution of concentration of pollutants for varying input conditions. A flow chart of the computer program is given in Figure 10. For given initial conditions and assumed boundary values, the problem is solved forming tridiagonal matrices as described by eqs. (21 & 22) with pre-decided convergence factors having convergence with respect to IADIE and convergence with respect to time steps.

The model has been verified with the published data of the river Green-Duwamish at USA reported in the book "Mixing in Inland and Coastal Waters" (Fischer et al., 1979). The cross sectional velocity distribution and the contours of constant velocity for the river at Renton junction were given. The cross sectional velocity distribution and other hydraulic data are reproduced in Fig. 11.

[Units shown in Fig. 11 and mentioned in Table-1 are in F.P.S. system. The conversion factor is; 1 inch = 2.54 cm]



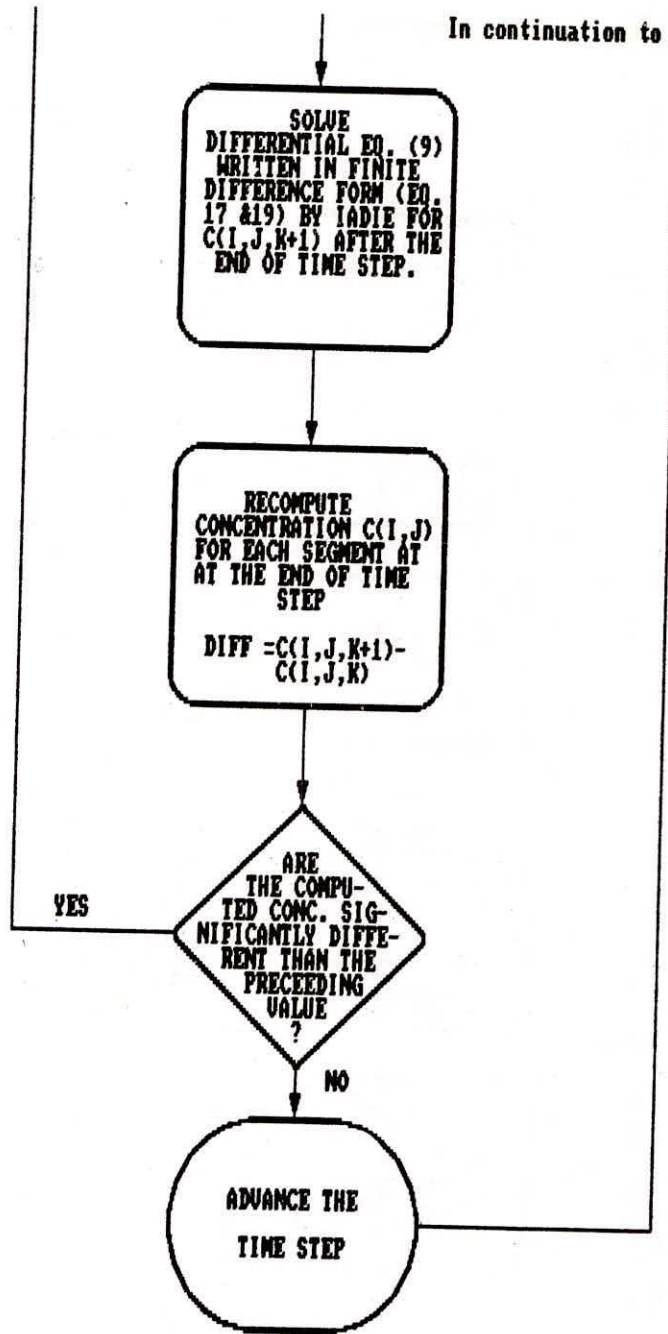


Figure-10 : FLOW CHART OF THE MODEL

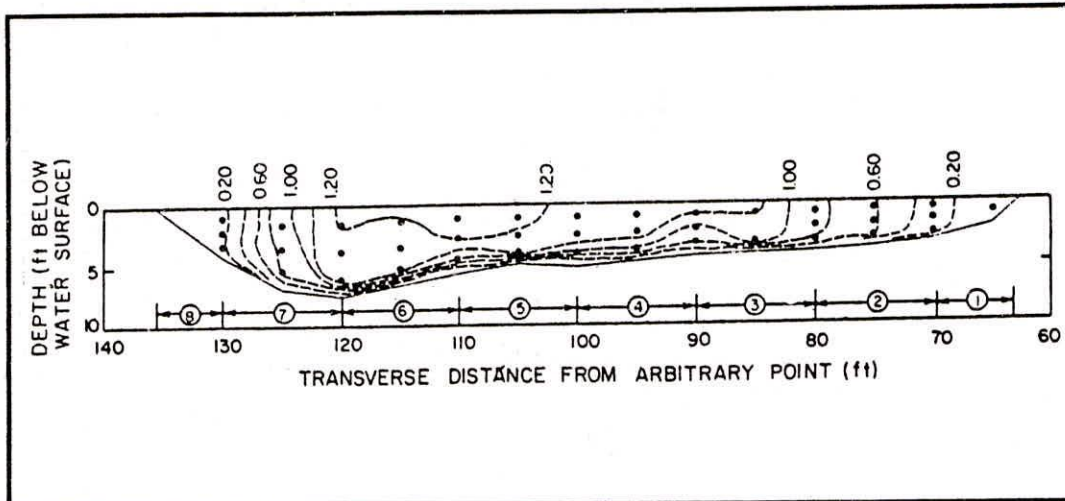


Figure 11: The cross sectional velocity distribution at Renton Junction in the Green-Duwamish River, USA (Source: Fischer et al., 1979).

The hydraulic data of the river are given in Table - 1.

Table I : Hydraulic Data of the Green-Duwamish River, USA (Source : Fischer et al, 1979)

Subarea no.	Depth range (ft)	width (ft)	Mean Velocity in subarea (ft/sec)	Mean velocity in subarea relative to mean x-section velocity (ft/sec)
1	0.0 - 3.9	6.5	0.105	-0.799
2	3.9 - 4.48	10.0	0.526	-0.378
3	4.48- 4.50	10.0	0.986	0.082
4	4.50- 5.16	10.0	1.091	0.187
5	5.16- 5.28	10.0	1.196	0.292
6	5.28- 8.00	10.0	1.148	0.244
7	8.00- 4.72	10.0	0.766	-0.138
8	4.72- 0.00	5.0	0.067	-0.837

Total area = 339.25 sq. ft.

Assuming the value of transverse mixing coefficient, $E_y = 1.40 \text{ ft}^2/\text{sec}$ ($7.98 \text{ m}^2/\text{min}$) and using the hydraulic data mentioned in Table-1 and other values as given below, the model is tested for the input conditions as shown in Fig.12.

$$\Delta t = 0.25 - 1.0 \text{ min}, \dots \Delta x = U_{J_{max}} \cdot \Delta t$$

$$K = 0.25 - 0.75 \text{ day}^{-1}.$$

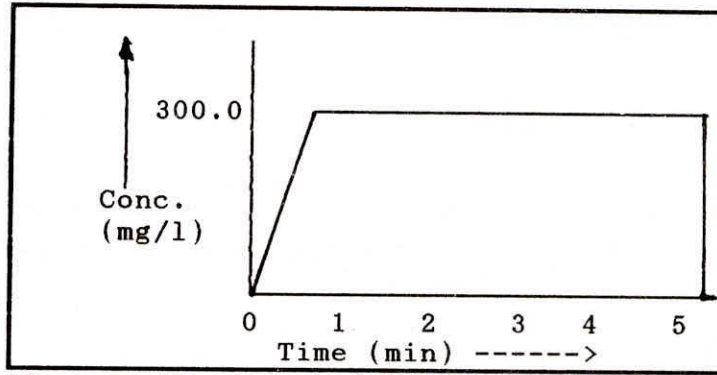


Figure -12: Input Pollution Load Considered for Verification of the Model.

Number of segments have been determined finding out the mixing length from the following expression (Eq. 29) and dividing the mixing length by the pre-determined length of the segment obtained from the Eq.(11).

$$X_m = \frac{L_c \cdot U \cdot W^2}{E_y} \dots \dots (29)$$

- where,
- X_m = mixing Length.
 - L_c = a coefficient, value ranges 0.2 - 0.5.
 - W = width of the river.
 - $\frac{E_y}{U}$ = transverse mixing coefficient.
 - U = average stream velocity.

The number of segment (M), thus;

$$M = \frac{X_m}{\Delta X} \dots \dots (30)$$

The termination criteria is considered, assuming the appropriate value from the range of values of 0.05 -0.5% and comparing with the sum of the difference of values of previous and current iteration ,if the difference is less than or equal to the pre-decided convergence factor, the values determined in the previous iteration are taken as the desired concentration of pollutants for that particular set of loading condition. Else, either iteration numbers are to be increased or a higher value of convergence factor is to be assumed. A convergence factor, $\epsilon = 10^{-3}$ and 10 number of iterations are used in this study. A constant pollution load at a rate equal to 25920 Kg/day

representing the concentration of pollutants 300 mg/l. [for an assume input flow rate of $1.0 \text{ m}^3/\text{sec.}$] for a duration of 5 minutes as depicted in Figure-12 is considered as input to the right bank of the river at the first segment, i.e., $I = 1$ and $J = 1$. A time step of 0.25 min. and 0.50 min. (15 sec. & 30 sec.) are considered for the iteration. Results of time step = 0.25 min. and dispersivity coefficient, $E_y = 7.98 \text{ m}^2/\text{min}$ are shown in Figures -13 & 14.

Figures-13(b,c,d) and 14 (a,b,c,d) respectively represent plots of concentration profiles along the direction of flow, and at different locations in the transverse direction within the mixing length for the above mentioned loading and input conditions. It is apparent from Figures-13(b,c,d) which represent plots of concentration profile along flow direction respectively for the bank receiving the pollution load (as depicted in Figure-13(a)), at the centre of the river and, for the other bank of the river, that location of release of pollutants and transverse velocity dictate the concentration profiles along the flow direction. While from Figures -14 (a,b,c,d) which indicate concentration profiles along the transverse direction at downstream locations of 25 meter, 50 meter, 100 meter and 150 meter from the point of release, it could be observed that advective velocity coupled with dispersivity and fluctuation of transverse velocity w.r.t. average stream velocity govern the mixing of pollution. Thus, one can easily say that river hydraulics such as; transverse velocity, whether magnitude plus or minus w.r.t. cross sectional velocity, depth of flow, river width, and transverse mixing coefficient, are the important parameters that dictate the mixing and transport of pollutants in the initial period. It is estimated that pollutants cloud travel a maximum time of 35 min. in the initial period before arriving at the complete mixing. Within the travel time, pollutants of nonconservative nature get about 0.75% -2.0% decay for the assumed values of $K = 0.25 - 0.75 \text{ day}^{-1}$.

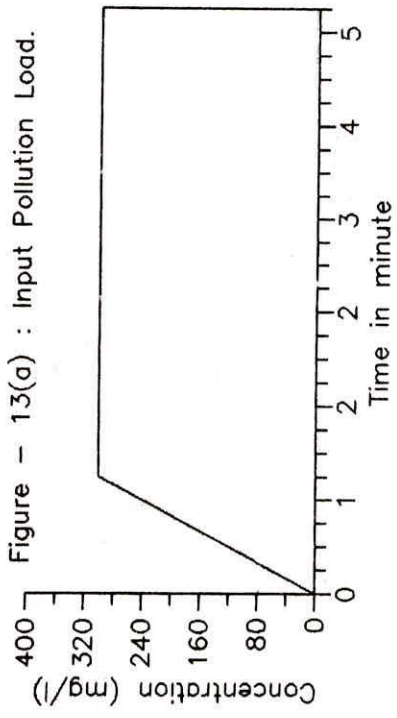


Figure - 13(a) : Input Pollution Load.

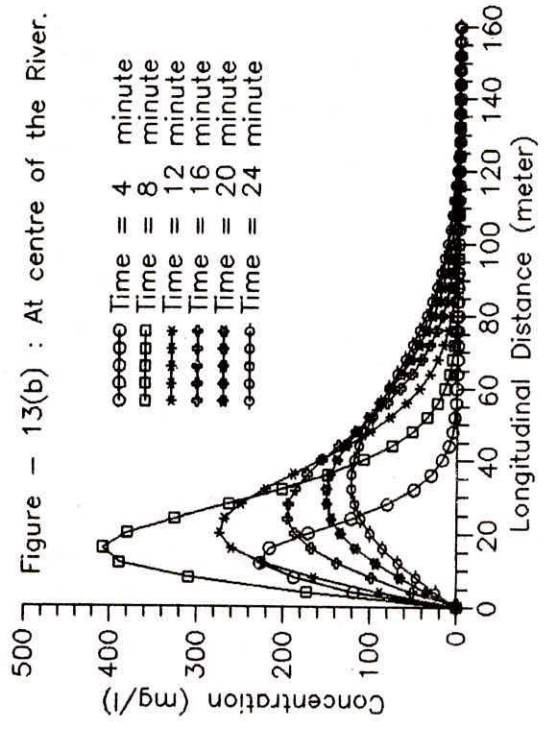


Figure - 13(b) : At centre of the River.

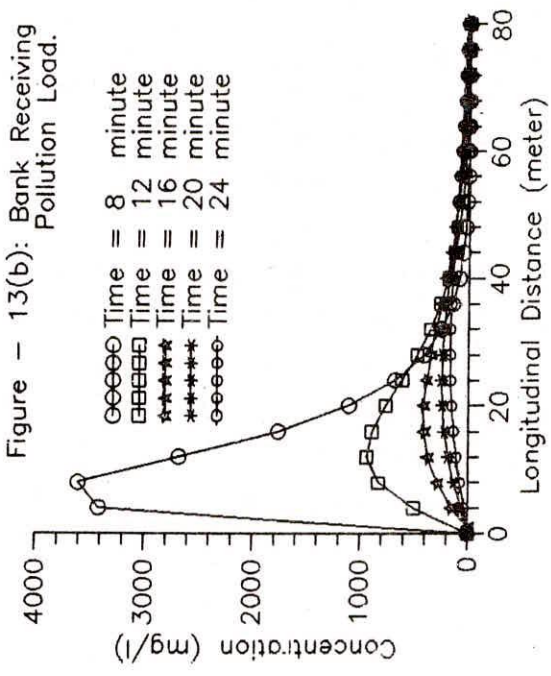


Figure - 13(b): Bank Receiving Pollution Load.

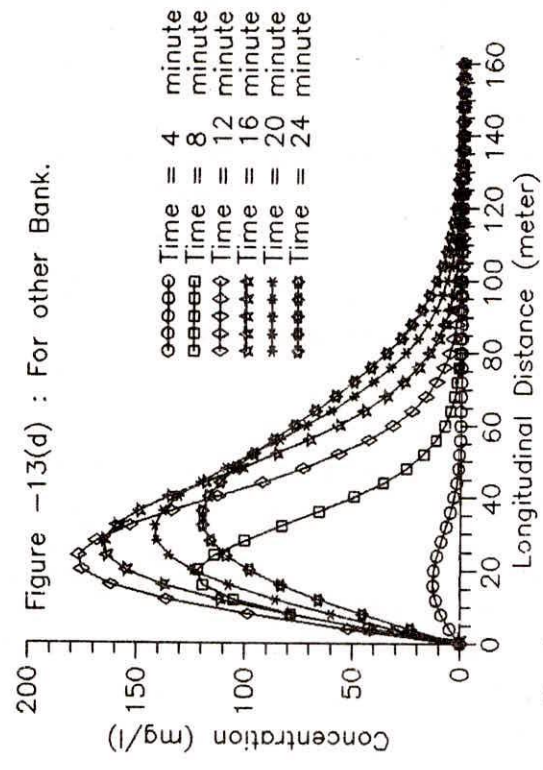


Figure -13(d) : For other Bank.

Figure - 13 : Plots of Longitudinal Concentration Profiles at Different Time after release.

Legends are Same in all Figures.

Figure - 14(a): At Location 25 meter From the Point of Release.

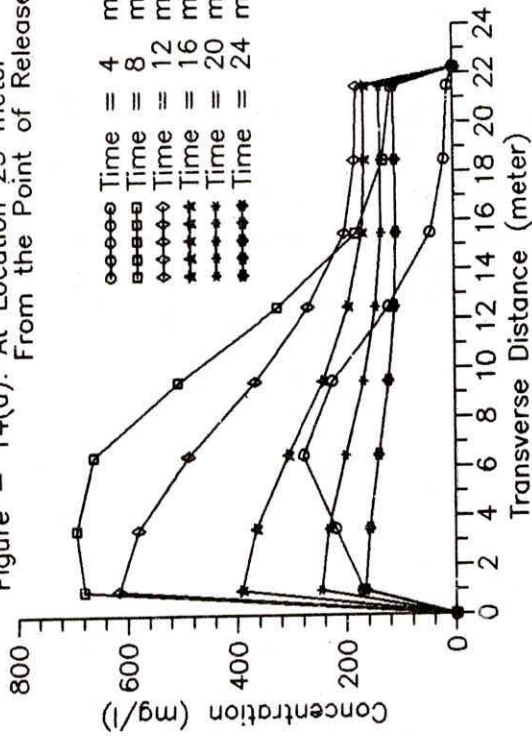


Figure - 14(c) : At Location 100 meter From Release.

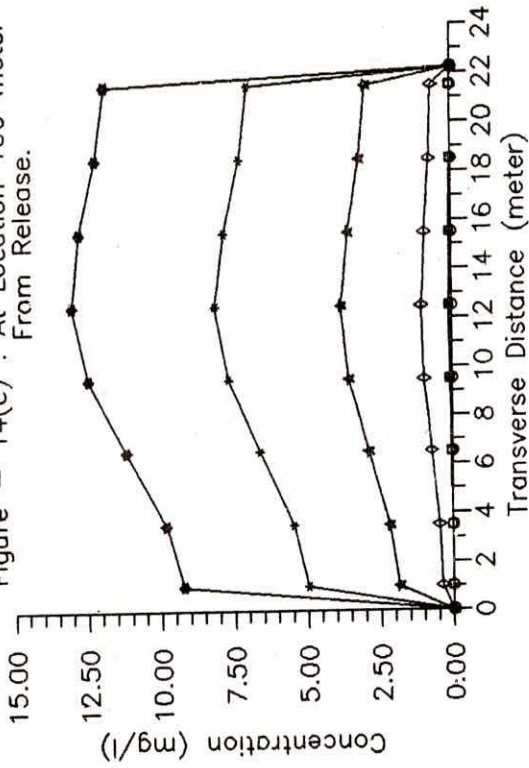


Fig. 14(b) : At Location 50 meter from Release.

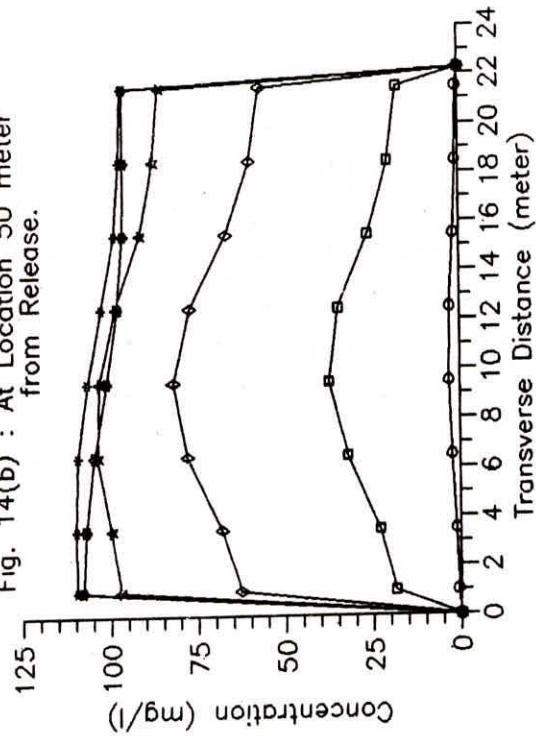


Figure-14(d) : At Location 150 meter From Release.

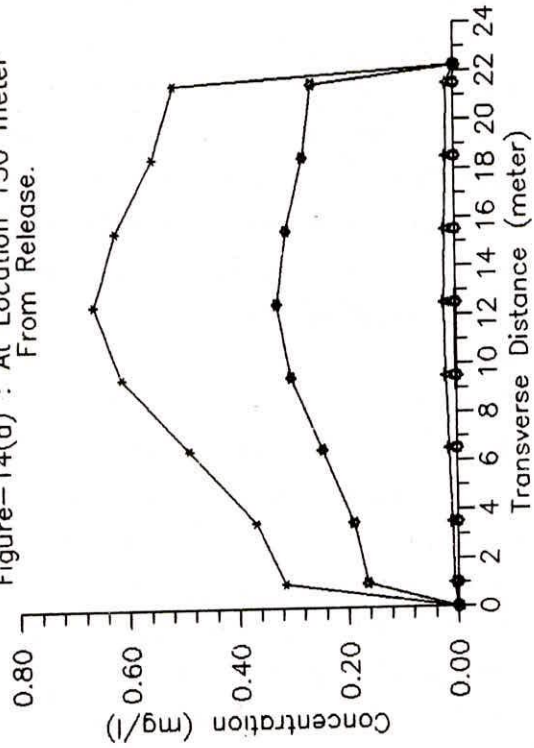


Figure -14 : Plots of Concentration Profiles along the Transverse Direction at Different Time after Release.

7.0 CONCLUSIONS

The effects of advection and dispersion on nonconservative substances have been studied. The assumption of complete mixing just after the point of release of pollutants and ignorance of the effect of longitudinal dispersion coefficient downstream of release which are commonly used in modeling of water quality may lead to a appreciable error in the estimation particularly for a large river. And thus require a due consideration.

Later case i.e., the assumption of neglecting the longitudinal dispersion coefficient could be accepted when pollutants arrive at the stage of complete cross sectional mixing and concentration of pollutants at any time and at any location are accounted for by the first order growth or decay coefficients. In the initial period of mixing, the spreading and concentration of pollutants are governed both by the transverse diffusivity coefficient, and decay or growth rate of substances.

A "Numerical Model" for the initial period of pollutants transport has been developed based on the Finite Difference Scheme, and solved using IADIE (Iterative Alternate Direction Implicit Explicit) technique to determine the spatial distribution of substances. It is noted that before arriving at the stage of complete mixing nonconservative substances undergo some decay equivalent to the exponential of multiple of decay coefficient and travel time of pollutants within the initial period. The model is verified with published data and found the results with reasonable accuracy. The model needs to be tested with different hydraulic and loading conditions.

8.0 REFERENCES

1. Fischer, H.B., (1967), " The Mechanism of Dispersion in Natural Streams", Jour. Hydraulic Div., Proc. ASCE, Vol. 93, pp.187-216.
2. Fischer, H.B., (1968), "Dispersion Predictions in Natural Streams ", Jour. Sanitary Eng. Div., Proc. ASCE, Vol. 94, pp.927-944.
3. Fischer, H.B., E. John List, Robert C. Y. Koh, Jorg Imberger, and Norman H. Brooks, (1979), "Mixing in Inland and Coastal Waters", Academic Press, Inc. New York.
4. Foree, Edward G. and John S. Tapp, (1977), " Utilization of Modeling in Water quality Management Studies", in "Handbook of Water Quality Management Planning", Ed. by Joseph L Pavoni, Van Nostrand Reinhold Company.
5. Ghosh, N.C., (1993), "Dispersion of Pollutants in Streams", NIH Report, 1993-'94, (TN).
6. Ghosh, N.C., (1995), "Prediction of Longitudinal Dispersion Coefficient for Natural Stream", NIH Report No.- TR(BR) 128, 1994-'95.
7. Miller, K.S., (1960), An Introduction to the Calculus of Finite Differences and Difference Equations, Henry Holt, New York.
8. Thomann V. Robert and John A. Mueller, (1987), " Principles of Surface Water Quality Modeling and Control", Harper & Row, Publishers, New York.
9. Young, P.C., and S.G. Walls, (1993), "Solute Transport and Dispersion in Channels", in "Channel Network Hydrology", Ed. by Keith Beven and Michael J. Kirkby, John Wiley & Sons, Ltd., U.K.

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