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ESTIMATION OF DISPERSION COEFFICIENT FROM DATA ON SOIL-COLUMN TEST

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Preface

Dispersion occur in many problems of groundwater flow, such as pollution from concentrated and distributed source, sea water intrusion, seepage of polluted surface water through rivers or lakes, changes in water quality due to artificial recharge. Application of the solution of advection-dispersion equation in soil media for prediction and forecasting of solute concentrations requires the estimate of coefficient of hydrodynamic dispersion (commonly known as 'dispersion coefficient'). One of reliable alternatives for estimation of dispersion coefficient is to conduct a tracer movement test in a soil column and analyze the data for dispersion coefficient. In a tracer movement test, the exit concentration distribution (commonly known as break through curve, BTC) with time is generally observed for known input concentration which often is in the form of step change in concentration input. There is a need to have a simple procedure for quick and reliably accurate estimation of dispersion coefficient making direct use of BTC. In case when peclet number is low, a optimization method is required for accurate determination of dispersion coefficient.

The present report entitled **Estimation of Dispersion Coefficient from Data on Soil Column Test**, deals with the procedures to estimate dispersion coefficient from exit concentration observed due to a step change in the concentration input. Both a simple method and an optimization method have been evolved. The application of the methods on published data sets have been discussed. This report has been prepared by **S.K. Singh, Scientist 'E'**, as per the Work-Plan for the year 1998-99 of Drainage Division.

(S.M. Seth)
Director

Abstract

One of reliable alternatives for estimation of dispersion coefficient is to conduct a tracer movement test in a soil column and analyze the data for dispersion coefficient. In a tracer movement test, the exit concentration distribution (commonly known as break through curve) with time is generally observed for known input concentration which often is in the form of step change in concentration input.

In this report, both a simple method and an optimization method for estimation of dispersion coefficient from data on soil-column test have been evolved. Application of the method have been demonstrated on published data sets. The results indicated that the present methods can estimate dispersion coefficient with reliable accuracy. In the simple method, the calculations are very much simplified using which quick and reliably accurate value of dispersion coefficient can be obtained. Application of the optimization method requires a computer while the calculations for the simple method can easily performed on a simple commercial calculator. A computer program in FORTRAN has been developed for the optimization method.

Contents

1.0 INTRODUCTION

Dispersion is a fundamental physical process to all types of solute transport problems. Besides river and streams, it occurs in many problems of groundwater flow, e.g., pollution from concentrated and distributed source, sea water intrusion, seepage of polluted surface water through rivers or lakes, changes in water quality due to artificial recharge. A widely used approach for mathematical modelling of solute transport is through the solution of advection-dispersion equation(ADE). The solutions of ADE, numerical or analytical requires the coefficient of 'hydrodynamic dispersion' (commonly termed as 'dispersion coefficient') to be known a priori. This gives rise to the problem of estimation of coefficient of hydrodynamic dispersion from field and laboratory tracer experiment data.

One of reliable alternatives for estimation of dispersion coefficient is to conduct a tracer movement test in a soil column and analyze the data for dispersion coefficient. In a tracer movement test, the exit concentration distribution (commonly known as break through curve) with time is generally observed for known input concentration which often is in the form of step change in input concentration.

In this report, both a simple method and an optimization method for estimation of dispersion coefficient from data on soil-column test have been evolved. Application of the method have been demonstrated on published data sets. The results indicated that the present methods can estimate dispersion coefficient with reliable accuracy. In the simple method, the calculations are very much simplified using which quick and reliably accurate value of dispersion coefficient can be obtained. Application of the optimization method requires a computer while the calculations for the simple method can easily performed on a simple commercial calculator. A computer program in FORTRAN has been developed for the optimization method.

2.0 ADE THEORY

The classical approach for dispersion modelling through advection-dispersion equation(ADE) assumes uniform properties at macroscopic level. It also assumes that rate of transport of pollutants due to dispersion in x-direction is directly proportional to the mean concentration gradient $\partial C/\partial x$, which is analogous to the Fickian equation for molecular diffusion. Because of this one dimensional ADE model is commonly referred to as 'one-dimensional Fickian model'. Different approaches of modelling dispersion is summarized and given in the Appendix.

The PDF governing the advection-dispersion process of transport of ideal solute in a homogeneous and isotropic soil medium is given by,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} \tag{2.1}$$

where,

D = coefficient of hydrodynamic dispersion;
C = C(x,t) = concentration of solute;
x = distance w.r.t. a fixed origin;
t = time; and,

$$u = \frac{Q}{n A} \tag{2.2}$$

in which, Q = discharge through the soil matrix, u = pore velocity, n = porosity of sediment, and A = uniform cross-sectional area of porous medium through which flow occurs.

For the movement of a tracer in semi-infinite column, where, initially the tracer concentration is zero everywhere in the column and then the column is connected to a reservoir containing a tracer solution of constant concentration, C_0. The initial and boundary conditions for this case can be expressed as,

$$C(0,t) = C_0 \tag{2.3}$$

$$C(x,0) = 0 \tag{2.4}$$

$$C(\infty,t) = 0 \tag{2.5}$$

The analytical solution of eq.(2.1) under conditions expressed in eqs. (2.3) through (2.5) is obtained by Ogata(1958) and can be written as (Bear, 1972),

$$\frac{C(x,t)}{C_0} = \frac{1}{2}\left[\text{erfc}\left(\frac{x-ut}{2\sqrt{Dt}}\right) + \exp\left(\frac{u\,x}{D}\right)\text{erfc}\left(\frac{x+ut}{2\sqrt{Dt}}\right)\right] \tag{2.6}$$

where

$$\text{erfc}(v) = 1 - \frac{2}{\sqrt{\pi}}\int_0^v e^{-\varepsilon^2} d\varepsilon$$

According to Ogata and Banks(1961), the second term in eq. (2.6) may be neglected when ux/D is sufficiently large. Neglecting the second term of eq.(2.6) for large value of ux/D, we get,

$$\frac{C(x,t)}{C_0} = \frac{1}{2}\,\text{erfc}\left(\frac{x-ut}{2\sqrt{Dt}}\right) \tag{2.7}$$

If exit concentration is observed at the end of the soil specimen, x appearing in eqs. (2.16) and (2.17) becomes the length of the specimen.

2.1 Estimation of Dispersion Coefficient: Past Methods

In a tracer movement test, the exit concentration distribution (commonly known as break through curve) with time is generally observed for known input concentration which often is in the form of step change in concentration input. The methods for

estimation of dispersion coefficient from tracer movement in soil column mostly make use of (2.7)

The method proposed by Bank(1958) makes use of (2.7). Knowing the values of C/C_0 from break through curve (BTC), and using tabulated values of Error-function or inverse error function, $(x-ut)/2\sqrt{Dt}$ can be obtained, which in tern gives value of D for known values of x, u, and t. Thus, each point on BTC gives one value of D, taking the average of these, average value of D can be obtained. They also proposed a graphical method in which when the transformed parameters are plotted, a straight line is obtained. Slope of the line can be used to calculate non dimensional dispersion coefficient. Bear(1972) has described a similar method to estimate dispersion coefficient. The method uses differential of (2.7) w.r.t. $\xi = (x-ut)/(2\sqrt{t})$, which may be written as

$$\frac{\partial}{\partial \xi}\left(\frac{C}{C_0}\right) = \frac{1}{\sqrt{\pi D}} \exp\left[-\frac{(x-ut)^2}{4Dt}\right] \tag{2.8}$$

Eq. (2.8) shows that slope of break through curve at $C/C_0=0.5$ w.r.t. ξ, equals $(\pi D)^{-1/2}$. Hence, knowing the slope, the value of D can be determined.

Fried and Combarnous(1971) proposed the following expression for D utilizing the property of a normal distribution function.

$$D = \frac{1}{8}\left\{\frac{x-ut_{0.16}}{\sqrt{t_{0.16}}} - \frac{x-ut_{0.84}}{\sqrt{t_{0.84}}}\right\} \tag{2.9}$$

Where, $t_{0.16}$ and $t_{0.84}$ are the times for the 16 and 84 percentile concentration respectively.

3.0 STATEMENT OF THE PROBLEM

It is intended to review the different approaches of modelling dispersion and to develop the following methods for estimation of dispersion coefficient from data on soil column test.

1. A simple method for quick and reliably accurate estimation using a commercial calculator.
2. An optimization method for accurate estimation and a Fortran code for the same.

4.0 DEVELOPMENT OF METHODOLOGY

4.1 Simple Method

A bell shaped curve is obtained when $d\bar{C}/dt$(here, $\bar{C}=C/C_0$) is plotted against t on natural graph. Let the coordinates of the peak of this curve be denoted by (t_0,m). Differentiating (2.7) w.r.t. t and applying the conditions at the peak we get the following expression for D.

$$D = \frac{x^2}{4\pi m^2 t_0^3} \tag{4.1}$$

Parameters, t_0 and m can directly be obtained from the BTC resulting from the step change in the input concentration. Time corresponding to $C/C_0 = 0.5$ is given by t_0 and m is the slope of BTC at this time. Knowing the values of t_0 and m from BTC, D can be estimated using eq.(4.1). It is worth mentioning here that the present method is based on the direct use of BTC which is a curve between observed variables C/C_0 and t while in previous such methods transformed variables need to be plotted. Transformed variables are ξ in place of t in Bear's method and ut/x and $(x-ut)/2\sqrt{Dt}$ in Ogata's method(this requires use of the table of Error-function. The present method is free from all these restrictions and labour.

4.2 Optimization Method

The exact analytical solution of (2.1) for a step change in input concentration is expressed by eq. (2.6). This solution does not pose any restriction on Peclet number (ux/D). If response of unit step concentration input is known, the parameters D and u can be estimated making use of (2.6) which can be expressed in functional form as,

$$\hat{C}(x,t) = f(x,t,D,u,C_0) \tag{4.2}$$

Where, $\hat{C}(.)$ is simulated exit concentration. With known values for C(x,t) for different t and C_0, the parameters D and u can be optimized to get the minimum sum of squared error between observed and simulated response at exit. The optimization problem in this case may be formulated as,

$$\text{Minimize } F = \sum_{i=1}^{N} [C(x,t_i)-\hat{C}(x,t_i)]^2 \tag{4.3}$$

Since, the parameters D and u appear in non linear form in (2.6), a non-linear optimization technique can yield the parameters. In the present method, Marquardt(1963) algorithm has been used for the nonlinear optimization. The details of the algorithm may be found in Singh(1988a,1988b). The Gauss-Newton normal equation for (4.3) can be written as,

$$\left[\mathbf{A}^T\mathbf{A}\right].\Delta\mathbf{P} = \mathbf{A}^T\left[\mathbf{c} - \bar{\mathbf{c}}\right] \tag{4.4}$$

where,

$$\mathbf{A} = \begin{bmatrix} \frac{\partial\bar{c}(x,\Delta t)}{\partial V} & \frac{\partial\bar{c}(x,2\Delta t)}{\partial V} & \cdots\cdots & \frac{\partial\bar{c}(x,n\Delta t)}{\partial V} \\ \frac{\partial\bar{c}(x,\Delta t)}{\partial D} & \frac{\partial\bar{c}(x,2\Delta t)}{\partial D} & \cdots\cdots & \frac{\partial\bar{c}(x,n\Delta t)}{\partial D} \end{bmatrix}^T \tag{4.5}$$

and,

$$\Delta\mathbf{P} = \begin{bmatrix} \Delta V \\ \Delta D \end{bmatrix} \tag{4.6}$$

Adding a scalar λ in (4.4) to allow for convergence with relatively poor initial guess for unknown parameters (Marquardt, 1963), we get,

$$\left[\mathbf{A}^T\mathbf{A} + \lambda\mathbf{I}\right].\Delta\mathbf{P} = \mathbf{A}^T\left[\mathbf{c} - \bar{\mathbf{c}}\right] \tag{4.7}$$

Where, I is identity matrix. Initial value of λ are large and decreases towards zero as the convergence is approached. If the convergence is achieved, the final

parameters are calculated using the following equation.

$$P_j = P_j^* + \Delta P_j \tag{4.8}$$

where, j denotes the number of iteration. If convergence is not achieved, P^* is updated by replacing the old values by new values and the process is repeated. ΔP and F approaches zero as convergence is achieved and (4.8) gives the optimized value of the parameter. Marquardt criteria for modifying λ has been used. The derivatives appearing in (4.7) have been computed numerically. Use of analytical expressions for derivatives can further improve the convergence and the location of global minima.

5.0 APPLICATION TO DATA

Both the methods were applied on two sets of data (Ogata 1958) and dispersion coefficient were estimated. The application of the simple method on data set I (u = 0.167 ft/min and x = 3.9 ft) has been illustrated in Fig. 5.1. From the figure t_0=23.2 min. and m=1/4.6 were obtained. Substituting these values in (4.1), we get D=1.852x10^{-3} ft^2/min. Ogata(1958) has reported D=2.116x10^{-3}. This indicates that the present method can estimate dispersion coefficient with reliable accuracy. The results of application of the optimization method on both the data set have been tabulated below.

Data Set	Optimized D (ft^2/min)	Optimized u (ft/min)	Measured u (ft/min)	Integral squared error in relative concentration
I	1.825x10^{-3}	0.1677	0.167	3.78x10^{-4}
II	3.384x10^{-3}	0.2394	0.239	7.59x10^{-4}

The simulated BTCs with optimized values of the parameters have been compared to those observed for data sets I and II in Figs. 5.2 and 5.3 respectively.

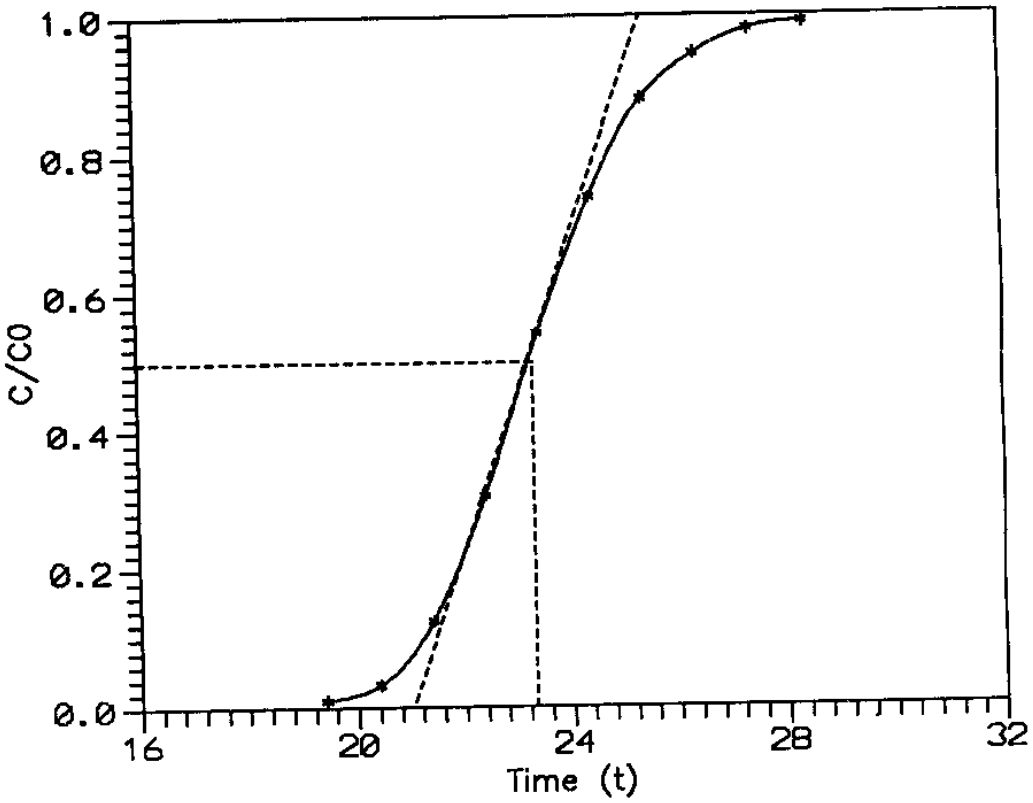

Fig.5.1 Illustration of the Simple Method

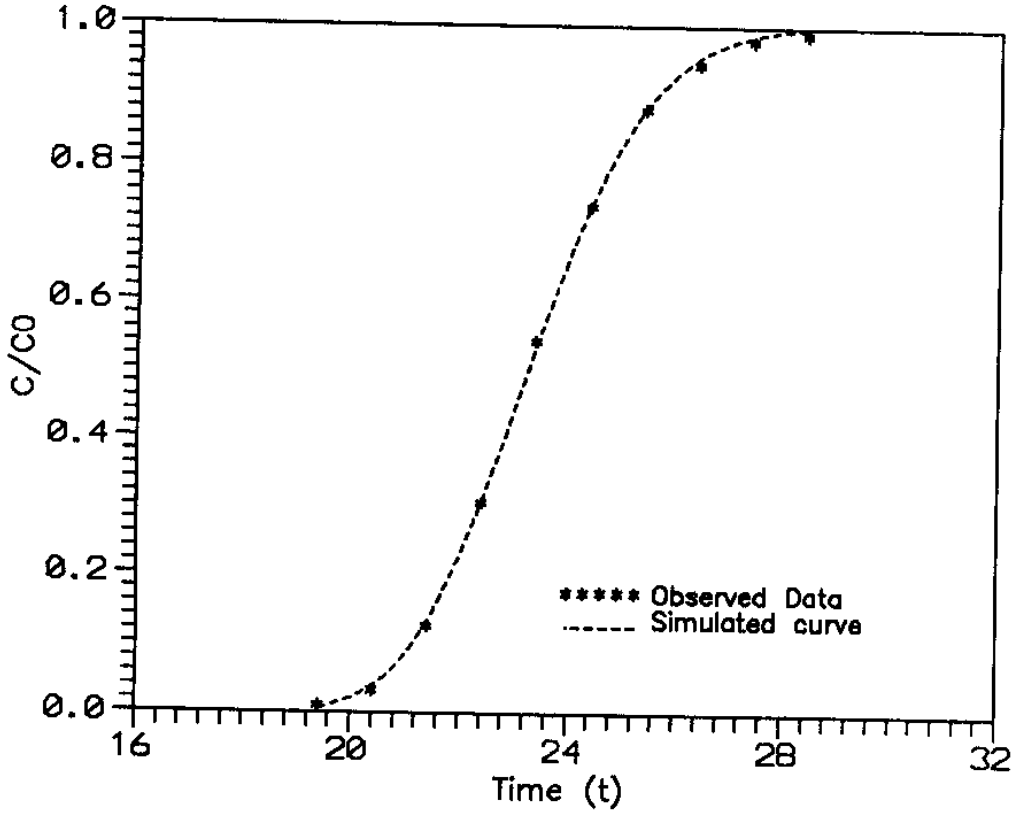

Fig.5.2 Observed and Simulated BTC (Data Set I)

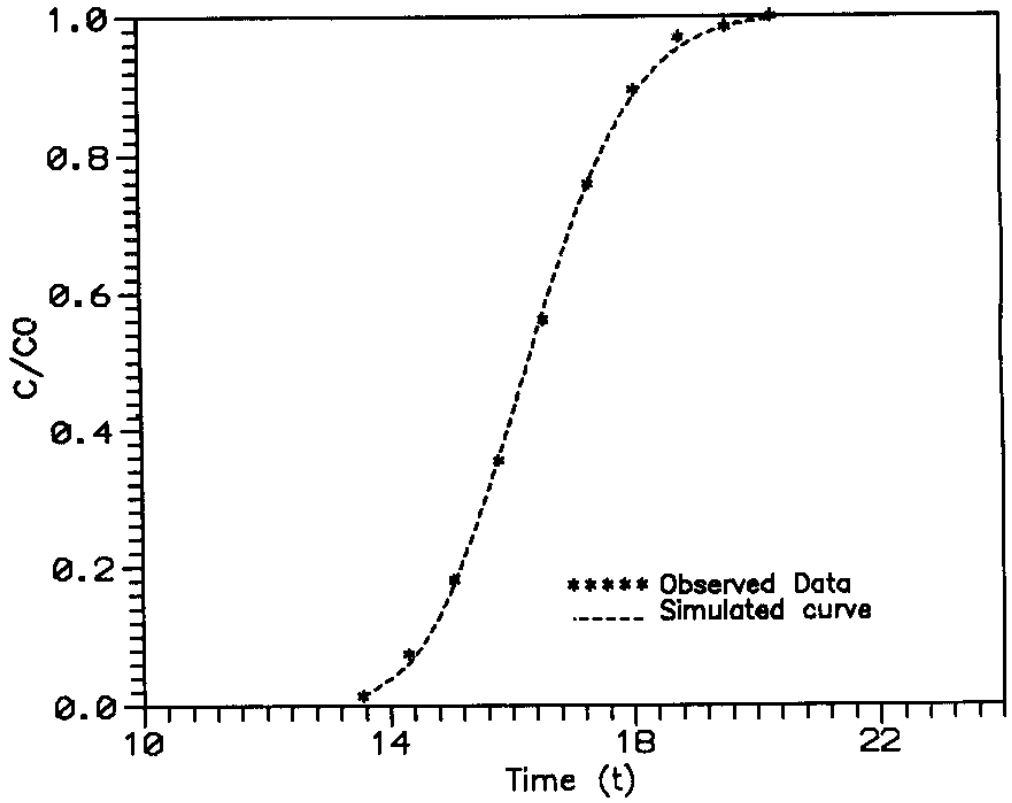

Fig.5.3 Observed and Simulated BTC (Data Set II)

6.0 CONCLUSION

Two methods for estimation of dispersion coefficient have been developed. The first method is very simple and makes direct use of break through curve. It can be used for quick and reliably accurate estimation of parameters. The second method is uses a nonliner optimization technique for accurate estimation of dispersion coefficient. This method is applicable for any value of peclet number and is based on the minimization of integral squared error between observed and computed concentration. A computer code in FORTRAN has been developed for the method.

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APPENDIX

DISPERSION AND ITS MODELLING

In a saturated flow through porous medium, consider a portion of flow domain containing a solute. Let the solute be referred as 'tracer'. According to Bear(1979, p. 227) a 'tracer' is a labelled portion of the same liquid may be identified by its density, colour, electrical conductivity, etc. The tracer gradually spreads and occupies an ever-increasing portion of the flow domain, beyond the region it is expected to occupy according to the average flow alone. The spreading caused by the velocity variation in the direction of average flow and in the direction transverse to it, at microscopic level is termed as 'mechanical dispersion'. Sometimes it is called as 'convective diffusion'. The spreading of tracer from regions of higher tracer concentration to the lower tracer concentration is generally known as 'molecular diffusion'. 'Hydrodynamic dispersion' is a term which denotes the spreading of tracer resulting from both mechanical dispersion and molecular diffusion. The dispersion occur in many problems of groundwater flow, such as pollution from concentrated and distributed source, sea water intrusion, seepage of polluted surface water through rivers or lakes, changes in water quality due to artificial recharge. The earliest observation of dispersion is reported by Einstein(1905) and Slichter(1905).

Different Approaches

The exact modelling of dispersion is possible only when the boundary conditions at the highly irregular boundaries of soil matrix at microscopic level can correctly be defined. Since, it is impossible to define correctly the boundary of pores in the soil matrix in mathematical form, dispersion can not be exactly modelled microscopically. This leads to its modelling by simplified conceptualization at macroscopic level.

The first approach of dispersion-modelling is to replace the actual medium by a fictitious, greatly simplified, model in which mixing can be analyzed by exact mathematical methods. Such models are often applicable for the case of single liquid flow. Capillary tube model and cell-models fall in this group.

In the capillary-tube model, the soil matrix is assumed to be composed of a

bundle of capillaries. Taylor(1954) studied the concentration variation along a capillary due to the injection of a slug of a solute. Bear(1960) presented a simplified cell-model for the study of one-dimensional dispersion. He replaced the medium by a series of small cells with interconnecting short channels. He assumed that a liquid with certain concentration upon entering a cell occupied by a liquid of different concentration, displaces part of it, while the liquid remaining in the cell immediately mix to form a new homogeneous liquid. The model considers the cell as a perfect mixer. For a perfect mixing, movement of tracer particles due to molecular diffusion or turbulence, should be much faster than the average liquid flow. The variation in the tracer concentration in the cell is given by,

$$\frac{\partial C}{\partial t} \alpha \left\{C^i - C\right\} \tag{A1}$$

Where, C^i, C, and C^o are the tracer concentration in the liquid entering the cell, within the cell, and leaving the cell respectively and t is the time. Bear postulated the dispersion phenomenon as a combination of two processes 1) complete mixing in the cell, and 2) translation from one cell to the next through the connecting channels. Mass balance of tracer for the j^{th} cell can be expressed as,

$$\frac{\partial C_j^o(t)}{\partial t} + \frac{C_j^o(t)}{\tau} = \frac{C_j^i(t)}{\tau} \tag{A2}$$

For a constant inflow concentration of C_0 in the first cell and with τ = constant for all cells, we get,

$$C_j^o = C_0\left[1-\exp(-t/\tau) \sum_{i=1}^{j-1} (i!)^{-1}(t/i)^i\right] \tag{A3}$$

Stefan and Demetracopoulos(1981) presented a cell-in-series(CIS) model to simulate riverine transport of dissolved materials. They discussed the advantages and disadvantages of the model vis-a-vis advection-dispersion model. The lumped parameter

in the CIS model is the number of cells into which a river reach is sub-divided. Each cell is well mixed. They observed that a CIS model provides as good a description of riverine transport as a one-dimensional advection dispersion model. The expression for solute-concentration in the n^{th} cell of the river-reach is expressed as,

$$C_n(t) = \frac{(\alpha\ t)^{n-1}}{(n-1)!}\ \frac{M}{V}\ e^{-\alpha t} \qquad (A4)$$

where,

$$\alpha = 1/T\ ,\ \text{and}\ \ T = V/Q \qquad (A5)$$

in which,

T = cell residence time,
V = cell volume,
Q = flow rate within the cell,
M = mass of tracer injected, and;
t = time

Although, the CIS model is widely used in chemical engineering, it has not proved to be of great practical use in modelling longitudinal dispersion in groundwater.

The basic idea behind statistical approach is to apply the rules of probability theory and to predict the spatial distribution of cloud of many tracer particles, which initially were at close proximity and then move under the average condition of flow. Needless to mention that the tracking of individual tracer particle is impossible. This approach considers random motion of tracer particles. The probability distribution of the location of a single tracer particle may be interpreted as the spatial relative-concentration distribution of a cloud of tracer particles originating from the neighbourhood of a certain point at a certain time and moving under the same average conditions. Pioneering work employing this approach for dispersion modelling is by Scheidegger(1954). Other early investigators are Danckwerts(1953) and Aris(1956). A better insight of the dispersion phenomena and relationships between dispersion and the medium characteristics have been provided by Bear and Bachmat(1965,66) while suggesting essentially a statistical approach.

In natural soil matrix, one often encounters regions of varying permeability which give rise to the stagnant water pockets collectively known as 'dead zones' and interconnected bigger pores that allow a part of solute to travel faster than the rest. These invalidates assumption of homogeneity. Thus, the effect of these are not modelled in ADE approach. Aggregated dead zone (ADZ) approach has the scope for the interpretation of dead zones and fast flow of solutes. Bear and Young(1984) introduced ADZ model essentially for dispersion modelling in stream but can also be used for transport modelling in groundwater. ADZ model may be termed as an extension to CIS model. The main difference of ADZ model from the CIS model is that a pure time delay is introduced into the input concentration which allows advection and dispersion to be decoupled.

If n identical cells are placed in series with same cell-time delay for each cell, the differential equation for solute balance can be written as,

$$V \frac{dC(t)}{dt} = Q\, C_u(t-\tau) - Q\, C(t) \qquad \text{(A6)}$$

and, the solute concentration in n^{th} cell is given by,

$$C_n(t) = \frac{(\alpha(t-\tau))^{n-1}}{(n-1)!} \frac{M}{V} e^{-\alpha(t-\tau)} \qquad \text{(A7)}$$

Eq. (A6) can be rewritten in discrete form as,

$$C^m = a\, C^{m-1} + (1-a)\, C_u^{m-\delta-1} \qquad \text{(A8)}$$

where, C and C_u are the d/s concentration and u/s concentration respectively, m denotes time-step, a is a constant, and $\delta=\tau/\Delta t$ denotes number of time-steps for cell-time delay. Precisely, $a=\exp(-\alpha\Delta t)$.

The method outlined above can be generalized in which several first order ADZ elements with different time constants(α), and time delays(τ) or combined in series

and/or parallel. The tracer can also be considered non conservative. The following transfer-Function (TF) representation describe a generalized multi-order model in discrete form.

$$C^{m+1} = a_0C^m + a_1C^{m-1} + a_2C^{m-2} + \ldots + a_iC^{m-i} + b_0C_u^{m-\delta} + b_1C_u^{m-\delta-1} + b_2C_u^{m-\delta-2} + \ldots + b_jC_u^{m-\delta-j} \quad \text{(A9)}$$

Eq. (A8) is the simplified form of (A9). The above equation is a powerful and flexible model. The only difficulty is to determine i, and j, and the coefficients a_i and b_j. These can be estimated using a parameter estimation technique. Recursive estimation of parameters is best suited for this. Eq. (A9) can conveniently be expressed in the form of different TF operators, viz, differential, backward shift or laplacian operator and the parameters of the TF can be estimated suitably. In backward shift operator, this TF takes the following form.

$$C^m = \frac{b_0 + b_1Z^{-1} + \ldots\ldots + b_pz^{-p}}{1 + a_1Z^{-1} + \ldots\ldots + a_qz^{-q}} C_u^{m-\delta} \quad \text{(A10)}$$

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