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MATHEMATICAL MODELLING OF SOLUTE TRANSPORT IN
GROUNDWATER FROM A POINT SOURCE OF POLLUTION

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PREFACE

The development of a mathematical model begins with a conceptual understanding of the physical system. Once these concepts are formulated they can be translated into a mathematical framework resulting in equations that describe the process. A variety of analytical and numerical techniques can be applied to solve the equations, resulting in practical tools such as type curves or finite difference and finite element computer programmes.

Considering the large number and variety of pollutants that may be released to the subsurface and the wide range of environmental situations that may be encountered, it is apparent that a highly systematic approach must be followed in developing a capability for predicting sub-surface transport sufficient to meet the goals of ground water pollution control. In the present note, a review of the existing methodologies of solute transport phenomena has been made, keeping in view the ultimate aim to provide methodologies which will permit accurate prediction of the effect from a point source pollutant activity on the quality of ground water at points of withdrawal or discharge. The basic concepts of the transport phenomenon have been described in detail and various mathematical models to solve the advection-dispersion equation have been critically reviewed.

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ABSTRACT

Considering the large number and variety of pollutants that may be released to the subsurface and the wide range of environmental situations (geological, hydrological, chemical, and biological) that may encounter, it is apparent that a highly systematic approach must be followed in developing a capability for predicting subsurface transport sufficient to meet the goals of groundwater pollution control. Accordingly, the major thrust of transport research should be directed towards the development of mathematical models that integrate physical process descriptions with pollutant properties and environmental characteristics to yield quantitative estimates of subsurface transport.

In the present note, a review of the existing methodologies of solute transport phenomena has been made, keeping in view the ultimate aim that is to provide methodologies which will permit accurate prediction of the effect from a point source pollutant activity will have on the quality of groundwater at points of withdrawal or discharge.

The basic concepts of the transport phenomenon have been described in detail and various mathematical models to solve the advection-dispersion equation have been critically reviewed.

1.0 INTRODUCTION

The future will see a growing dependence on groundwater supplies to satisfy the needs of agriculture, industry and our increasing population. Consequently, it is our duty to become familiar with this resource - how and where it occurs, and how various activities can affect its quality. We do not know the current extent of groundwater pollution, but from available information, we know that the threat is substantial. Many activities can lead to the deterioration of groundwater quality. In fact, groundwater may get polluted solely because of nature's input.

For centuries, man has been disposing of his waste products by placing them in streams, or storing them either in or on the ground. Water soluble substances in these wastes may be dissolved and carried into the ground and eventually pollute the underlying groundwater.

Until recently, relatively little attention has been focussed on groundwater pollution in India. The causes of groundwater pollution are numerous and are as diverse as the activities of man. According to Fried (1975), groundwater pollution is traced back to four main origins: industrial, domestic, agricultural and environmental pollution, each family being divided up into continuous and accidental types.

(i) Industrial pollution is carried to the aquifer by:

- used waters which contain chemical compounds and trace elements or which are at a rather high temperature. Radio active pollution from atomic plants can also be brought in in this way,
- rain infiltrating through waste disposals,
- accidents like the breaking of a pipe line.

- (ii) Domestic pollution is carried to the aquifer by
 - rain infiltrating through sanitary land fills,
 - accidents like the breaking of septic tanks.
- (iii) Agricultural pollution is due to irrigation water or rain carrying away fertilizers, minerals, salts, herbicides and pesticides.
- (iv) Environmental pollution is mainly due to sea water intrusion in coastal aquifers.

1.1 Factors Controlling Pollution

The process of pollution of groundwater is controlled by several factors like nature and concentration of effluents, soil and subsoil characteristics, time factor, porosity, permeability, hydraulic gradient, storage capacity of aquifers etc. The following considerations are significant during pollution of groundwater from effluents:

- (i) Reactions in the top soil and vadose zone: Some of the processes like biological degradation, filtration, sorption, oxidation and reduction, precipitation, buffering etc. take place in the top soil and vadose zone. These reactions are affected by micro-stratigraphy, pore velocities, hydrodynamic dispersion and hydrochemical factors. As a result of these reactions, several trace elements may be removed or added depending on the characteristics of effluents and nature of strata through which infiltration takes place.
- (ii) Effect of soil moisture deficiency: storage capacity and moisture characteristics of vadose zone are important factors in controlling percolation of polluted waters. In areas where moisture deficiency is there due to lack of recharge, considerable amount of pollutant may remain in the soil and vadose zone.

(iii) Laminar flow of pollutants: unlike nonlaminar and at times turbulent flow of polluted surface waters, the flow of groundwater through strata is laminar. According to Walker (1973), recharged water with pollutants appears to maintain a bulb like mass as it moves downward to the lower part of surficial aquifers, then horizontally through the aquifer material to some nearby discharge point. McKee and Wolf (1963) have observed that a small ribbon of polluted water injected into groundwater flow will move in a well defined streamline with a minimum of lateral or vertical diffusion and in many cases vertical diffusion is inhibited by horizontal clay lenses or extensive aquicludes. These findings indicate that dilution of polluted water by native groundwater during movement of pollutants from recharge to discharge areas can take place only to a limited extent.

(iv) Specific gravity, viscosity effects: the specific gravity and viscosity of effluents are usually different from natural groundwater and difference in these characteristics may play an important role to prevent diffusion of effluents with groundwater.

(v) Slow movement of effluents: the flow of groundwater and polluting constituents that it may contain is very slow as compared with flow on land surface. Underground flow may be a few feet per year through sandstone and other finer grain deposits and a few feet per day through sand and gravel or creviced limestone. As a result of slow movement of effluents, it may take considerable time for polluting materials to move away from the source of pollution and degradation in water quality may remain undetected. However, when pollution effects are evidenced,

rectification cannot be achieved by stopping the pollution from source as process of purification by leaching takes more time than initial period of pollution.

1.2 The Modelling of Groundwater Pollution

Simulation of a groundwater system refers to the construction and operation of a model whose behaviour assumes the appearance of the actual aquifer behaviour. The model can be physical, electrical analog, or mathematical. A mathematical model is simply a set of equations which, subject to certain assumptions, describes the physical processes active in the aquifer. The mathematical modelling of groundwater pollution has actually started, developed and been recognized, during 1950s and 1960s, as a possible and perhaps efficient tool in the description and prediction of pollution behaviour in aquifers. It took advantage of the interest in the study of the fundamental and applied aspects of miscible displacements in porous media. Particularly, it benefited by the introduction of the dispersion-convection equations, the study of the physical meanings of their various parameters, the derivation of numerical solutions (Fried and Combarous, 1971). Simultaneously, as modelling was confronted to real field situations and not only to laboratory work, difficulties and even limitations to its use started to appear related among others to the scale effects and the heterogeneities of natural grounds, to the scarcity of data, and also to the mathematics of the models, which after the quick developments of the late sixties, resulted in slowing down of the applications of modelling to real field situations.

The modelling of groundwater pollution consists in describing

- (i) the convection of the contaminant, i.e. its movement with the mean flow,

- (ii) the dispersion of the contaminant, i.e., its scattering by mixing or spreading around the mean flow,
- (iii) the chemical and physio-chemical reactions of the contaminant with the solid matrix of the porous medium,
- (iv) the biochemical reactions of the contaminant with its environment,
- (v) the reactions within the contaminant,

by means of mathematical tools, like systems of partial differential equations or probabilistic processes, used in well chosen functional or probabilistic spaces representing the porous medium.

1.2.1 Types of models

Generally three types of models have been considered:

- (i) Black box models, which represent the aquifer as a system without any assumed structure and relate the inputs and outputs of contaminant in the system by means of a very general mathematical formulation, like a convolution relationship or a general mass conservation equation, based on a few and simple working assumptions. They are usually characterised by a transfer function which, combined in some way to the input, yields the output, its form and numerical values have to be determined by calibration on existing data.
- (ii) Grey box models, which represent the aquifer as a system equipped with a few structural properties: for instance a sequence of reservoirs with various behaviours. They are also characterized by a transfer function, the form of which is imposed as a consequence of the physical structural assumptions; the value of its parameters are determined by calibration on existing data.

(iii) Complete structural models describing the various aspects of contaminant transport with all possible details and predicting the distribution of pollution in space and time. The most usual models of that category have been derived by considering that the convection and the dispersion of the contaminant are best described by a general diffusion equation, while the other phenomena will be accounting for by adding various functions and their derivatives to this diffusion equation.

1.3 Applications

Ground water pollution models or solute transport models have extensively used in predicting the effects of problems involving hazardous wastes. Some of the applications include: sea water intrusion, underground storage of radioactive wastes, movement of leachate from sanitary land fills, groundwater contamination from holding ponds and waste injection through deep wells.

2.0 REVIEW

Since 1970s, investigations have been carried on fostered by the appearance of various groundwater pollution problems to be accounted for in water resources management and aimed at improving the modelling of groundwater pollution. These investigations mainly concern:

- (i) the changes of scales, involving the possible derivation of a diffusion equation, the spatial variability of the dispersion coefficients, the description of the early stages of the dispersion process;
- (ii) the improvements of the numerical solutions of the general diffusion equation;
- (iii) the derivations of black and grey box models;
- (iv) the experimental research in the laboratory and in the field resulting from new groundwater pollution problems and from improved theoretical approaches to modelling.

2.1 Changes of Scales

Theoretical studies have been recently performed to test the representativity of the general diffusion equation as a model of the dispersion process at field scale and, not surprisingly, have concluded that a diffusive regime does not necessarily govern the dispersion. At least three different papers have treated this problem in 1980:

- (i) Analyzing longitudinal dispersion data in open channel or pipe flows. Chatwin (1980) discusses the assumptions made by Taylor in his approach of dispersion, stressing the consequences on modelling when these conditions are not met i.e. the occurrence of a nondiffusive regime, illustrated by nongaussian

curves. The author does not propose a new equation but a quantitative assessment of the deviations of observed concentration profiles from gaussianity by series of Hermite polynomials depending on various moments of the concentration distribution.

(ii) Studying a bidimensional flow in a horizontally stratified medium, characterized by a constant horizontal velocity per stratum, Matheron (1980) uses a stochastic process to describe the movement of tracer particles in that flow. This movement is the sum of a convective movement with the velocity in the stratum and a dispersive movement assumed to be fickian and isotropic; the expectation of the concentration at a point and at a given time is the probability density function of a particle at that point and at that time. Taking the x-axis along the velocity direction, Matheron computes the variance of the coordinate $x(+)$ of a particle as a function of the vertical variations of the velocities: a gaussian process being classically characterized by a variance linearly proportional to time, Matheron, defines the mathematical conditions on the variance to obtain a diffusive regime. Justifying the derivation of such a regime by authors like Marle (1966) or Gelhar (1979) who make the right assumptions for that, he shows that in many cases there is no reason for a diffusive regime to exist even for very large times: this is particularly the case of stratified flow with horizontal velocities in an infinite bidimensional medium, where no mixing occurs by convection.

(iii) Applying the old concept that dispersion in porous media is due to the variations in the velocity distribution and is therefore

related to the spatial heterogeneity in permeability of the aquifer, Smith and Schwartz (1980) develop a stochastic process consisting of the deterministic motion of tracer particles with the flow velocities in a macroscopically heterogeneous permeability field combined by addition to a random motion of these particles accounting for anisotropic dispersion.

These studies conform to two main ideas: a dispersion process is not necessarily of the diffusive type; the emergence of a diffusive regime is related to a sufficient spatial averaging conditioned by good mixing. Under the assumptions of the emergence of a diffusive regime, studies have been performed to describe the early stages of a dispersion process and to evaluate the asymptotic time i.e. the time necessary for a diffusion regime to take place. The knowledge of this time is essential for a correct scaling of the field experiments aimed at measuring dispersion coefficients, as the dimensions of the experimental domain should at least be equal to the product of the mean velocity by this time.

Analysing unsteady convective diffusion in two dimensional open channel turbulent flows with a given initial concentration distribution of solute, Lee and Gill (1980) developed a generalized dispersion theory which models the early stage of the dispersion process by an equation relating the time derivative of the concentration to an infinite series composed of the space derivatives of the concentration at all orders with time dependent coefficients. Gelhar et al (1979) used a classical method of turbulence analysis (as did previously by Bear or Fried) in studying a bidimensional flow in a horizontally stratified medium with a horizontal velocity constant in each layer.

It appears that recent theoretical studies concern the change of scale from an already macroscopic continuous medium and not the basic

problem of the derivation of the dispersion equation at macroscopic level from pore size (microscopic) level. It means that the medium is always considered as continuous in the sense that all variables (like concentrations or velocities) are defined everywhere and that, for some authors, the dispersion process is even described by a diffusion equation at the lower scale.

2.2 Numerical Solutions

Although the method of characteristics proved to be free of numerical diffusion, it was seldom used because of the complexity of its programming and authors mostly investigated the possible decreases of the numerical diffusion using dispersion correction terms in the numerical expressions either with finite differences or finite elements with mitigated success (Gray, Pinder, Ehling and Van Genuchten). A simplified adaptation of the method of characteristics was successfully tested by Migault (1979) and could prove quite useful.

Work on overshoot has been simultaneously performed, mainly on Galerkin finite element schemes, essentially based on possible reductions of space or time increments and then limited by problems related to the solution of large size systems of linear equations. Varoglu and Finn(1980) tested a combination of finite elements and method of characteristics for the convective part of the diffusion equation, both for numerical dispersion and overshoot. Sauty (1980) produced easily usable numerical solutions in the form of type curves based on analytical solutions of the diffusion equation with simple boundaries and boundary conditions.

Already discussed by Fried (1975) for a Cauchy problem, the dependence of the uncertainty of the concentration function on the uncertainties of the dispersion equation parameters has been again examined by Tang

and Pinder (1979) showing a relative stability of the solution of the equation.

Finally some attempts have been made to solve the general inverse problem (i.e. the determination of dispersion coefficients from concentration distributions) essentially by an optimization method (Umare et al, 1979), while a new deconvolution method was introduced in a black box modelling of contaminant transport in ground water (Migault, 1979).

2.3 Black or Grey Box Modelling

The limitations in the use of the general diffusion equation for the various reasons (such as inadequacy of the equation related to the dimensions in space and time of the proposed study, unpredictable dispersion coefficients, sparse or unaccurate data) have involved the use of black box models.

Although most of the work concerning deconvolution has been performed for the determination of the hydraulic parameters of the aquifers, the necessities of modelling transport (to describe new laboratory work, for instance concerning motion with physico chemical interactions between the contaminant and solid matrix, or field problems like the transfer of contaminants between a river and its alluvial aquifer) have implied some theoretical work on deconvolution within the frame of groundwater pollution modelling and the development of an original method by Migault (1979).

To operate a black box model, a preliminary study of the consistency of the input and output data must be made, especially to analyse the time sequences, when the modeller does not have complete control of the experimental setting and procedures. Collongues (1979) used statistical methods, especially spectral analysis, with success to take care of possible missing or unadequate data.

Grey box models, either distributed parameter models, or lumped parameter models, have been conceptually developed before 1972. From the extensive review made by Anderson (1979), they appear to have been used with some improvements afterwards.

In brief, it appears that although some progress has been made in the understanding of the modelling of field conditions and the significance of the parameters and their so called variability, which could be of help for setting and scaling field experiments, the practical applicability of the diffusion equation to field problems as a forecasting tool is not insured while other possible models, like stochastic motion models, proposed to simulate the situations when the diffusion equation does not hold, are yet too cumbersome to operate. The classical field methodology correcting the deficiencies of the complete structural models by non numerical considerations on the lithology, geology, morphology of the medium, by the use of black or grey box modelling and by pure kinematic considerations is still very practical.

3.0 TRANSPORT PHENOMENA

Many articles have been written over the past several years reviewing the science and art of groundwater transport modelling. These reviews have generally been written at a fairly well sophisticated level. While a great deal of accessible literature exists for groundwater flow models in standard groundwater hydrology texts, the concepts of transport modelling have been reported in many different sources and at many different levels of difficulty. Very few articles exist to explain transport models at a basic level for hydrologists, hydrogeologists, and groundwater resource managers concerned mainly with the migration of contaminants from various waste sources.

3.1 Basic Concepts

Transport processes of concern in ground waste include advection, dispersion, adsorption, decay and chemical reaction. The incorporation of these transport mechanisms into groundwater model formulation is described in more detail by Bredehoeft and Pinder (1973), Fried (1975), Anderson (1979), and Freeze and Cherry (1979).

3.1.1 The advection-dispersion equation

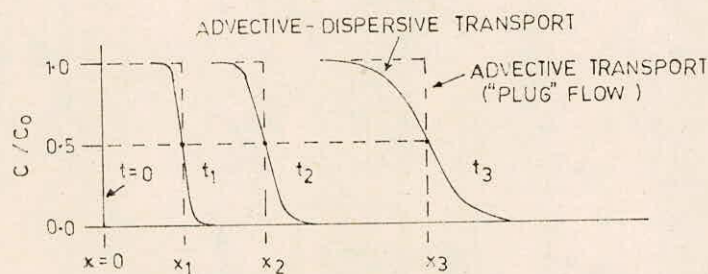
Solute transport is generally viewed as the net effect of two processes, advection and dispersion. Advective transport is attributed to the average motion of the fluid. In processes involving displacement of miscible fluids in one dimension, with advection the only transporting mechanism, a sharp front would be maintained between the initial and displacing fluids, and this front would move at a velocity equal to the average linear pore-water velocity. The average linear pore-water velocity, defined macroscopically at a point in the porous medium is the microscopic solution velocity

vector averaged over a representative elementary volume (REV) about the point, referred to as average solution velocity, \bar{V} . The advective solute flux is given by

$$\bar{J}_a = \bar{q}c \quad (3.1)$$

where \bar{J}_a is the mass of solute crossing a unit area of porous medium oriented normal to the flow direction per unit time $[ML^{-2}T^{-1}]$, \bar{q} is the specific discharge or Darcy flux $[LT^{-1}]$, and c is the solute concentration (mass of solute per unit volume of solution) $[ML^{-3}]$.

Dispersion causes mixing at the interface between two fluids of different composition, and according to Fried (1975), it is the occurrence and evolution of a transition zone between two domains of the fluid phase with different composition. Bear (1972) further describes dispersion as being nonsteady and irreversible. The effects of advection and dispersion are shown schematically in Fig.1 for one dimensional displacement of miscible fluids.



$$x_3 > x_2 > x_1 > x$$

$$t_3 > t_2 > t_1 > t$$

$$x_3/t_3 = x_2/t_2 = x_1/t_1 = \bar{v}$$

FIG. 1 SCHEMATIC REPRESENTATION OF THE ADVECTIVE AND DISPERSIVE SOLUTE TRANSPORT PROCESSES

Dispersion is the result of two processes, molecular diffusion and mechanical mixing. Diffusion is the result of the thermal kinetic energy of the molecules, which, in the presence of a concentration gradient, results in a net flux of solute toward the low-concentration zone. By modifying Fick's first law to account for the presence of the solid phase, the diffusion flux in a porous medium becomes

$$\bar{J}_d = -\eta D_d \text{grad } c \quad (3.2)$$

where \bar{J}_d is the diffusive solute flux (mass of solute per unit area of porous medium per unit time) $[ML^{-2}T^{-1}]$, D_d is the coefficient of molecular diffusion in the porous medium (effective diffusion coefficient) $[L^2T^{-1}]$, η is the porosity of the medium, and c is the solute concentration. The porosity term is introduced because the cross sectional area available for diffusion is reduced by the presence of the solid phase.

The mechanical mixing component of the dispersion process is the result of velocity variations within the porous medium. For homogeneous media, there are three microscopic mechanisms that give rise to velocity variations. These mechanisms, shown schematically in Fig. 2, include

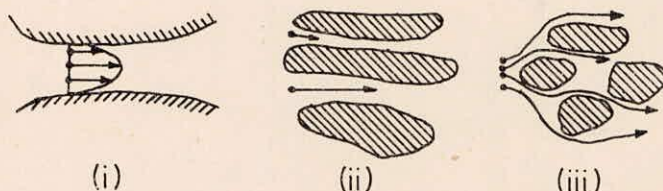


FIG. 2. MICROSCOPIC COMPONENTS OF MECHANICAL MIXING

- (i) the velocity distribution associated with the flow of viscous fluid through a pore,
- (ii) variations in velocity as a result of different pore geometries, and
- (iii) fluctuations in the stream lines with respect to the mean flow direction.

The mechanical-mixing component of dispersion is analogous to diffusion in that spreading of the solute is the result of velocity variations across a concentration gradient. Consequently, on the macroscopic scale, the mechanical mixing component of the solute flux is commonly represented by

$$\bar{J}_m = -n D_m \text{grad } c \quad (3.3)$$

where D_m is the coefficient of hydrodynamic (mechanical) dispersion.

Adding eqns. (3.2) and (3.3) gives the dispersive flux of the solute as

$$\bar{J} = -n D \text{grad } c \quad (3.4)$$

where D is the dispersion coefficient, defined as

$$D = D_d + D_m \quad (3.5)$$

Recognizing the advective and dispersive flux components, and applying the principle of conservation of mass gives

$$\frac{\partial (nc)}{\partial t} = \text{div}(n D \text{grad } c - \bar{q}c) \quad (3.6)$$

The specific discharge \bar{q} in eqn. (3.6) is generally replaced by the average solution velocity according to the relation

$$\bar{V} = (\bar{q}/n)^w \quad (3.7)$$

where \bar{V} is the average solution velocity [LT^{-1}] and w is an empirical

exponent. The work of Eliis and others (1968) indicates that the value of the exponent is very nearly 1 in granular materials. Substituting eqn. (3.7) into eqn.(3.6) and assuming the porosity to be constant and the fluid incompressible gives

$$\frac{\partial c}{\partial t} = \text{div}(D \text{ grad } c) - \bar{V} \text{ grad } c \quad (3.8)$$

This is frequently referred to as the advective dispersion equation, or simply the dispersion equation for solute transport. Although, eqn.(3.8) is in a more general form than is commonly applied to contaminant migration, it is nevertheless subject to several assumptions and limitations:

- (i) The contaminants are soluble in water.
- (ii) The fluid properties (density and viscosity) are independent of solute concentration.
- (iii) The fluid is incompressible.
- (iv) The coefficients of molecular diffusion and mechanical mixing are additive.
- (v) Eqn.(3.7) is applicable.
- (vi) The solute is nonreactive.

3.1.2 Effect of velocity on the dispersion coefficient

Dispersion is due to the combined action of both a purely mechanical phenomenon and a physicochemical phenomenon. It must be stressed that it is not generally possible to distinguish the proper effects of each phenomenon.

Mechanical dispersion

When a fluid flows through a porous medium, its velocity distribution is not uniform, due to boundary effects acting in three different ways:

- (i) the velocity is zero on the solid surface, which creates a velocity gradient in the fluid phase, as in a capillary tube;
- (ii) the variation of pore dimensions cause discrepancies between the maximum velocities along the pore axes; and
- (iii) the streamlines fluctuate with respect to the mean direction of flow.

These three processes combined yield the mechanical dispersion.

The coefficient of mechanical dispersion \bar{D} depends on the flow pattern, e.g. through the velocities, on the Peclet number P_e , which is defined as

$$P_e = \frac{LV}{D_d} \quad (3.9)$$

where L is some characteristic length of the pores, V is average pore velocity and D_d is molecular diffusion coefficient, and on some basic medium characteristics. Many investigators consider the sum $\bar{D} = (\bar{D}_m + \bar{D}_d)$ as the coefficient of dispersion (or rather, of hydrodynamic dispersion) which depends on the velocity, molecular diffusion, and medium characteristics.

Taylor (1953) in his one-dimensional analysis obtains D proportional to \bar{V}^2 . Bear and Todd (1960) in their one-dimensional analysis suggested $D = a_1 \bar{V}$, i.e. D proportional to \bar{V} , with a_1 being some characteristic medium length. In the analysis of variances, the dispersion, or the spread of particles around their average displacement, is described by the matrix of covariances $\overline{x_i(t)x_j(t)}$. There it is shown that these covariances may be related to the coefficient of dispersion D_{ij} for large times in the form $D_{ij} = r_{ij}(0)\bar{V}_i\bar{V}_j t_0$, where t_0 is the time during which velocities are still effectively correlated. If, following Nikolaevskij (1959),

let $r_{ij}(0)t = L/\bar{V}$, where \bar{V} is the absolute value of the average velocity and L is a characteristic medium length (e.g. length of a channel in a porous

$$D_{ij} = (\bar{V}_i \bar{V}_j / \bar{V})L \quad (3.10)$$

i.e. \bar{D} is proportional to the first power of the velocity.

Scheidegger (1957) summarizes his analysis on these two possible relationships between D and \bar{V} according to the role played by molecular diffusion.

- (i) $D \approx a' \bar{V}^2$, where a' is a constant of the porous medium alone (dynamical dispersivity) is derived by a dynamic procedure applicable where there is enough time in each flow channel for applicable mixing by molecular transverse diffusion to take place.
- (ii) $D \approx a'' \bar{V}$, where a'' , another constant of the porous medium (geometrical dispersivity), is derived by a geometric procedure applicable where there is no applicable molecular transverse diffusion from one stream-line to another.

Thus in all models in which the combined effect of a velocity distribution across a channel and transverse molecular diffusion are considered (e.g. Taylor 1953), the coefficient of dispersion is proportional to \bar{V}^2 . Where only the mean motion in a channel is considered while mixing occurs at junctions connecting different channels, disregarding molecular diffusion, one obtains $D \approx \bar{V}$. Of course, intermediate cases where D is proportional to some power of the velocity between 1 and 2, lie between these two extremes.

3.2 Parameters Used in Quantitative Approaches of Dispersion Model

Several concepts are introduced in the quantitative approaches:

densities, concentrations, velocities and coefficients, describing the phenomena.

Three levels are needed in the study of dispersion phenomena: a local level or microscopic level, a fluid volume or pore volume level, and a macroscopic level.

- (i) Local level: It is the usual level encountered in fluid mechanics. The parameters which are defined at this level describe a physical quantity at a point, i.e. in an 'infinitely small' volume element, consistent with molecular physics data.
- (ii) Fluid volume level: The parameters at this level are defined as 'means' of the corresponding local parameters over a finite fluid volume. In a porous medium, this definition is necessary to introduce the concept of 'pore quantities' (such as the pore velocity) and then the average is taken over a set of pores. The way of defining an average is described in each case, especially when nonadditive quantities are involved.
- (iii) Macroscopic level: This level is only used in porous media, when a solid matrix exists, to define an equivalent continuum. The parameters at this level are the averages of the corresponding local parameters taken over a finite volume of porous medium.

3.2.1 Densities

The notation ρ used alone represents the classical density at the pore volume or macroscopic levels. At these levels ρ_i is the specific gravity of constituent i and ρ is the specific gravity of the mixture. Some

times ρ is used at a local level, but in such cases this symbol is always coupled to a symbol of velocity or concentration which defines its scale; for instance, ρu is a local motion quantity. We have

$$\rho = \sum_i C_i \quad (3.11)$$

where C_i is the concentration defined below.

3.2.2 Concentrations

Several definitions of the microscopic concentration of one compound A in a mixture M may be used.

The mass concentration C is the mass m_a of the compound A in a small volume v of mixture, divided by the volume v , or

$$C = m_a / v \quad (3.12)$$

Such a definition is useful when mixing occurs without volume changes, i.e., the total volume of a mixture of two chemical species of small volumes v_1 and v_2 is $v_1 + v_2$.

The mass fraction C^* is the mass m_a of A divided by the mass m_m of M contained in the same volume, or

$$C^* = m_a / m_m \quad (3.13)$$

where C^* is an intrinsic quantity which does not depend upon the physico-chemical ways of mixing C and C^* are related by

$$C = \rho C^* \quad (3.14)$$

where ρ is the density of the mixture.

The molecular concentration C_M is the number n_a of molecules of

A divided by the volume of mixture v which contains the molecules or

$$C_M = n_a / v \quad (3.15)$$

The molecular fraction C_M^* is the number n_a of molecules of A in a volume of mixture divided by the total number n_m of mixture molecules in the same volume.

$$C_M^* = n_a / n_m \quad (3.16)$$

At the fluid volume level, the same definitions may be used, the reference fluid volume being large. Hence the mass concentration is C , the mass fraction C^* , the molecular concentration C_M , and the molecular fraction C_M^* .

3.2.3 Local velocities

The various compounds (i) of the mixture move with different velocities u_i . Two definitions of the average local velocity of the mixture are mainly used.

The mass average velocity u

$$u = \frac{\sum_i C_i u_i}{\sum_i C_i} = \frac{\sum_i C_i u_i}{\rho} \quad (3.17)$$

where C_i is the mass concentration of compound (i)

The molecular average velocity u_M

$$u_M = \frac{\sum_i C_{Mi} u_i}{\sum_i C_{Mi}} \quad (3.18)$$

C_{Mi} being the molecular concentration of compound (i).

These velocities are referred to stationary coordinate axes. But diffusion and dispersion are mainly relative phenomena and it may be interesting to introduce relative velocity concepts, indicating the motion of one compound relative to the motion of the mixture $u_i - u$ is the diffusion or dispersion velocity of compound(i) with respect to u , and $u_i - u_M$ is the diffusion or dispersion velocity of compound(i) with respect to u_M .

These velocities u_i, u and u_M are the usual local or microscopic velocities in fluid mechanics.

3.2.4 Mean velocities in the fluid phase and at the macroscopic level

In a fluid volume B of any kind (for instance, the volume of a stream tube or the volume of several pores), the mean velocities are defined as follows:

The mass average velocity V of the mixture is defined by

$$V = \left[\int_{\beta} \rho u \, dx \right] / \left[\int_{\beta} \rho \, dx \right] \quad (3.19)$$

The mass average velocity V_i of one compound is defined by

$$V_i = \left[\int_{\beta} C_i u_i \, dx \right] / \left[\int_{\beta} C_i \, dx \right] \quad (3.20)$$

Evidently V may also be defined by

$$V = \left[\sum_i C V_i \right] / \rho \quad (3.21)$$

At the macroscopic level, the velocity is the usual Darcy velocity V_D . When V is defined for a large number of pores, it is linked to V_D by the relationship:

$$V = V_D / \phi \quad (3.22)$$

where ϕ is the porosity of the medium.

4.0 SOLUTION METHODOLOGY

Numerous analytical solutions to advective dispersion equation are available, most of which represent one-dimensional cases for steady flow in homogeneous semi-infinite or, finite porous media. Most of the solutions of interest to hydrogeologists are included in Ogata and Banks (1961), Brenner (1962), Biggar and Nielsen (1976), and Ogata (1970). Solutions for homogeneous media with uniform steady flow and three-dimensional dispersion are described by Baetsle (1967,1969) for contaminants entering the systems as point sources, and by Codell and Schreiber (1979) for point source, line source and planar source inputs. Analytical methods and solutions are described in the texts by Bear (1972) and Fried (1975).

For analysis of contaminant migration in heterogeneous hydrogeological systems with complex flow patterns and time-dependent boundary conditions typical of many field situations, numerical solution procedure have been developed. These include finite difference methods, finite element methods and method of characteristics. The finite element method is described in detail by Pinder and Gray (1977). Each solution procedure has limitations when applied to practical field problems. These can include restrictive boundary conditions, numerical dispersion, convergence and stability problems, and excessive computer storage or time requirements.

4.1 Analytical Models

To solve the dispersion scheme, both analytical and numerical methods can be applied. Analytical solutions of the dispersion equation exist only in very few cases, extensively discussed by Bear (1972). Analytical solutions to this equation have been developed either by neglecting adsorption (Lapidus and Amundson, 1952) or by assuming the adsorption isotherm to be linear (Lapidus and Amundson, 1952, Lindstrom et al,1967,

Cleary and Adrian, 1973).

Analytical methods that handle solute transport in porous media are relatively easy to use. Various mathematical techniques can be applied to the finding of analytical solutions, such as Green functions, Laplace transforms or Fourier transforms. Here we present two basic examples (Fried, 1975) that can be used to derive pollution type-curves for mono- or bi-dimensional flow.

4.1.1 Laplace transform approach

Let us consider a one dimensional case. Assuming longitudinal dispersion, at a constant velocity V in a semi-infinite medium, with a step initial function. The dispersion coefficient D is constant.

The mathematical problem is defined by the set of equations:

$$D\left(\frac{\partial^2 C}{\partial x^2}\right) - V\left(\frac{\partial C}{\partial x}\right) = \frac{\partial C}{\partial t} \quad (4.1)$$

$$C(x=0, t > 0) = C_0, \quad C(x=\infty, t \geq 0) = 0,$$

$$C(x \geq 0, t=0) = 0.$$

The problem is solved by Laplace transformation, which is defined as under.

Let f be a function of the variable x , defined for all x and equal to zero for $x < 0$. The Laplace transform of f is the function:

$$L(f) = \bar{f}(p) = \int_0^{\infty} e^{-px} f(x) dx \quad (4.2)$$

provided that this integral exist. p is a complex number, equal to $\eta + i\xi$. If η is zero, $\bar{f}(p)$ is the Fourier transform of f .

The properties of the Laplace transform used here are the

following:

$$L(f') = p\bar{f}(p) - f(0)$$

$$L(f'') = p^2\bar{f}(p) - pf(0) - f'(0)$$

easily proved by applying Eqn.(4.2) to the functions $f'(x)$ and $f''(x)$, first and second derivative of $f(x)$, respectively. Setting

$$\bar{C}(x,p) = \int_0^{\infty} e^{-pt} C(x,t)dt, \text{ Eqn.(4.1) yields:}$$

$$D\left(\frac{d^2\bar{C}}{dx^2}\right) - V\left(\frac{d\bar{C}}{dx}\right) = p\bar{C}$$

$$\bar{C}(x=0) = C_0/p, \quad \bar{C}(x=\infty) = 0 \quad (4.3)$$

and eqn.(4.3) has solution:

$$\begin{aligned} \bar{C} &= \frac{C_0}{p} \exp \left[-\frac{V-(V^2+4pD)^{\frac{1}{2}}}{2D} x \right] \\ &= C_0 \exp \left(\frac{Vx}{2D} \right) \cdot \frac{1}{p} \exp \left[-\frac{x}{D^{\frac{1}{2}}} \left(\frac{V^2}{4D} + p \right)^{\frac{1}{2}} \right] \end{aligned} \quad (4.4)$$

From a table of Laplace transforms, we obtain:

$$C = \frac{C_0}{2} \operatorname{erfc} \left[\frac{x-Vt}{2(Dt)^{\frac{1}{2}}} \right] + \frac{C_0}{2} \exp \left(\frac{Vx}{D} \right) \operatorname{erfc} \left[\frac{x+Vt}{2(Dt)^{\frac{1}{2}}} \right] \quad (4.5)$$

Fig.(3) provides the solution of this equation as type-curves.

4.1.2 Green function approach

We now consider a bidimensional horizontal model. The aquifer is horizontal, monolayered and homogeneous. The water velocity v is constant and parallel to $0x$. The dispersion coefficients are constant,

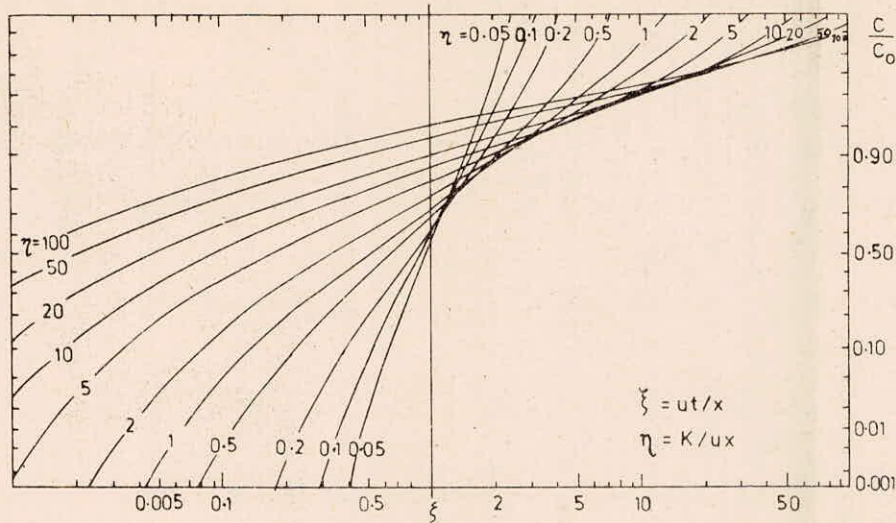


FIG. 3 TYPE CURVES FOR MONODIMENSIONAL DISPERSION CONSTANT VELOCITY (OGATA AND BANKS, 1961).

proportional to the velocity (dynamic dispersion regime). At the origin, pollution is injected at concentration C_0 , and at the rate Q , during period dt , the mass of the injected pollution is $C_0 Q dt$. The initial concentration is zero. The domain is infinite and the concentrations are equal to zero at infinity. The mathematical model is the equation:

$$\alpha_L v \frac{\partial^2 C}{\partial x^2} + \alpha_T v \frac{\partial^2 C}{\partial y^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (4.6)$$

The Green function, i.e. the solution of this equation for the injection of a unit amount of pollution at the origin, instantaneously at $t=0$ is:

$$G(x, y, t) = \frac{1}{4\pi vt (\alpha_L \alpha_T)^{\frac{1}{2}}} \exp \left[-\frac{(x-vt)^2}{4\alpha_L vt} - \frac{y^2}{4\alpha_T vt} \right] \quad (4.7)$$

and the solution of the problem is then:

$$C(x, y, t) = \frac{C_0 Q}{4\pi v t (\alpha_L \alpha_T)^{\frac{1}{2}}} \exp \left[-\frac{(x-vt)^2}{4\alpha_L vt} - \frac{y^2}{4\alpha_T vt} \right] \quad (4.8)$$

For a continuous injection at rate Q , the solution at time t is:

$$C(x, y, t) = \frac{C_0 Q}{4\pi v (\alpha_L \alpha_T)^{\frac{1}{2}}} \int_0^t \exp \left[-\frac{(x-v\theta)^2}{4\alpha_L v\theta} - \frac{y^2}{4\alpha_T v\theta} \right] \frac{d\theta}{\theta} \quad (4.9)$$

The steady-state regime is obtained for $t=\infty$:

$$C(x, y) = \frac{C_0 Q}{2\pi v (\alpha_L \alpha_T)^{\frac{1}{2}}} \exp \left(\frac{x}{2\alpha_L} \right) K_0 \left(\frac{x^2}{4\alpha_L^2} + \frac{y^2}{4\alpha_L \alpha_T} \right) \quad (4.10)$$

where K_0 is the modified Bessel function of the second kind and zero order. It should be noticed that on the x -axis ($y=0$) when α_T tends to zero the concentration tends to infinity, which has no physical meaning: one should revert to the monodimensional case. If the velocity v increases, the concentration decreases everywhere: pollution is quickly washed out. If Q and v are constant, c tends to 0 when α_L tends to infinity: when dispersion increases, the concentration at a point decreases.

An interesting computation of eqn.(4.9) is due to Emsellem (Arlab, 1974) and leads to practical type-curves by the introduction of the tabulated Hantush function $W(v, b)$:

$$W(v, b) = \int_v^\infty \exp \left(-y - \frac{b^2}{4y} \right) \frac{dy}{y}$$

Eqn.(4.9) can be written:

$$C(x, y, t) = \frac{C_0 Q}{4\pi v (\alpha_L \alpha_T)^{\frac{1}{2}}} \exp \left(\frac{x}{2\alpha_L} \right) \int_0^t \exp \left[-\frac{v\theta}{4\alpha_L} - \left(\frac{x^2}{4\alpha_L v} + \frac{y^2}{4\alpha_T v} \right) \frac{1}{\theta} \right] \frac{d\theta}{\theta} \quad (4.11)$$

Setting $y = v\theta/4\alpha_L$, we have:

$$C(x, y, t) = \frac{C_o Q}{4\pi v(\alpha_L \alpha_T)^{\frac{1}{2}}} \exp\left(\frac{x}{2\alpha_L}\right) \int_0^t \exp\left(-y - \frac{b^2}{4y}\right) \frac{dy}{y} \quad (4.12)$$

with
$$b^2 = \frac{x^2}{4\alpha_L^2} + \frac{y^2}{4\alpha_L \alpha_T}$$

and eventually:

$$C(x, y, t) = \frac{C_o Q}{4\pi v(\alpha_L \alpha_T)^{\frac{1}{2}}} \exp\left(\frac{x}{2\alpha_L}\right) [W(0, b) - W(t, b)] \quad (4.13)$$

The values of $W(t, b)$ can be found in Hantush tables (Walton, 1962).

4.2 Numerical Methods

An analytical solution is interesting because it does not introduce errors due to the approximations by the finite differences. But the analytical solutions are only found for very simple cases or for research purposes. The numerical solutions, which take full advantage of the digital computer's capacity are of more practical interest to regional groundwater modelling. The numerical methods, which exist in practice are Finite difference methods, Finite element methods, and Method of characteristics.

4.2.1 Finite-difference approximations

The finite difference scheme is derived by replacing the differential equation by finite difference approximations. In these approximations, the domain (space-time) is discretized and the solution is computed at the centers of the elementary domains of the grid. The equations are then discretized, for instance, at each center of the grid, with Taylor's expansion

theorem. In a unidimensional space, for instance, with Δx the increment on the x axis, Δt the time increment, and $C_{i,n}$ the concentration at time $n\Delta t$ and abscissa $i\Delta x$, Taylor's theorem yields

$$C_{i+1,n} = C_{i,n} + \Delta x \left(\frac{\partial C}{\partial x}\right)_{i,n} + \frac{1}{2}(\Delta x)^2 \left(\frac{\partial^2 C}{\partial x^2}\right)_{i,n} + \dots \quad (4.14)$$

$$C_{i-1,n} = C_{i,n} - \Delta x \left(\frac{\partial C}{\partial x}\right)_{i,n} + \frac{1}{2}(\Delta x)^2 \left(\frac{\partial^2 C}{\partial x^2}\right)_{i,n} - \dots \quad (4.15)$$

Thus $(\partial C/\partial x)_{i,n}$ and $(\partial^2 C/\partial x^2)_{i,n}$ can be approximated by

$$\left(\frac{\partial C}{\partial x}\right)_{i,n} = \frac{(C_{i+1,n} - C_{i-1,n})}{2\Delta x} \quad (4.16)$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_{i,n} = \frac{(C_{i+1,n} - 2C_{i,n} + C_{i-1,n})}{(\Delta x)^2} \quad (4.17)$$

Similarly

$$\left(\frac{\partial C}{\partial t}\right)_{i,n} = \frac{C_{i,n+1} - C_{i,n-1}}{2\Delta t} \quad (4.18)$$

Other possible ways of writing the first-order partial derivatives are:

$$\left(\frac{\partial C}{\partial x}\right)_{i,n} = \frac{(C_{i+1,n} - C_{i,n})}{\Delta x} \quad \text{forward derivative}$$

or
$$\left(\frac{\partial C}{\partial x}\right)_{i,n} = \frac{(C_{i,n} - C_{i-1,n})}{\Delta x} \quad \text{backward derivative}$$

or
$$\left(\frac{\partial C}{\partial x}\right)_{i,n} = \lambda \frac{(C_{i+1,n} - C_{i,n})}{\Delta x} + (1-\lambda) \left[\frac{(C_{i,n} - C_{i-1,n})}{\Delta x} \right] \quad \text{Crank Nicolson approximation when } \lambda = 0.5$$

$$\lambda \in [0,1]$$

Though Δx and Δt are often assumed constant, they may be varied. Δx can be reduced to create a higher density of grid points in zones where C changes rapidly with x . Δt may be varied to increase computational efficiency.

The quality of the finite differences numerical schemes can be checked on the basis of the following criteria:

Suppose we call $C(x,t)$ the computed solution and $\gamma(x,t)$ the exact solution of the dispersion equation.

- i) Consistency: A finite difference scheme is consistent if the finite differences operator has as limit the original differential operator when the discretisation step, Δx on the dimension x for example tends to zero.
- ii) Convergence: A finite difference approximation is convergent if the difference between $\gamma(x,t)$ and $C(x,t)$ tends to zero when Δx and Δt tends to zero, at given x and t .
- iii) Stability: When time varies, we compute $C(x,t+\Delta t)$ from $C(x,t)$. This is an iterative process, which is valid if the difference between $\gamma(x,t)$ and $C(x,t)$ is bounded in some sense, when $t \rightarrow \infty$, for given Δx and Δt . If such a condition is verified, the approximation is stable.

4.2.1.1 Explicit scheme

The dispersion equation is approximated by the finite-difference scheme: This equation is written between time t_n and time t_{n+1} , taking a square grid of space $(\Delta x, 2\Delta x, \dots, i\Delta x, \dots, I\Delta x)$ and backward difference of the convective term:

$$D \frac{C_{i+1,n} - 2C_{i,n} + C_{i-1,n}}{(\Delta x)^2} - V \frac{C_{i,n} - C_{i-1,n}}{\Delta x} = \frac{C_{i,n+1} - C_{i,n}}{\Delta t} \quad (4.19)$$

or

$$C_{i,n+1} = C_{i-1,n} \left[\frac{D\Delta t}{(\Delta x)^2} + \frac{V\Delta t}{\Delta x} \right] + C_{i,n} \left[1 - \frac{V\Delta t}{\Delta x} - 2 \frac{D\Delta t}{(\Delta x)^2} \right] + C_{i+1,n} \frac{D\Delta t}{(\Delta x)^2} \quad (4.20)$$

This system of equations may be written under the matrix form:

$$C(t_{n+1}) = MC(t_n) \quad (4.21)$$

$$M = \begin{bmatrix} 0 & 0 & 0 \\ a_1 & a_2 & a_3 \\ 0 & 0 & 0 \end{bmatrix}$$

with:

$$a_1 = \frac{D\Delta t}{\Delta x^2} + \frac{V\Delta t}{\Delta x} ; a_2 = 1 - \frac{V\Delta t}{\Delta x} - 2\frac{D\Delta t}{\Delta x^2} ; a_3 = \frac{D\Delta t}{(\Delta x)^2}$$

$C(t_n)$ is a vector of components $C_{i,n}$.

From Gerschgorin theorem, the eigen values of M lie in the interval $[1 - 2(V\Delta t/\Delta x) - 4(D\Delta t/\Delta x^2), 1]$. From the general convergence theorem, the iterative process defined by eqn.(4.20) does not converge if the eigen values of the iteration matrix are greater than 1 in absolute value. Thus, the explicit approximation is stable if:

$$1 - 2\frac{V\Delta t}{\Delta x} - 4\frac{D\Delta t}{(\Delta x)^2} > -1$$

or

$$\Delta t < \Delta t_c \quad (4.22)$$

with

$$\Delta t_c = \frac{\Delta x}{2\frac{D}{\Delta x} + V}$$

Δt_c is called the critical time step, and the approximation is said to be stable, conditionally to eqn.(4.22).

With central or forward differences, Δt_c is different of course.

Computation of Δt_c is obvious in all cases.

In general the use of an explicit scheme for the integration of dispersion equation requires the simultaneous satisfaction of two stability criteria,

$$\begin{aligned} C \frac{\Delta t}{\Delta x} &\leq 1 \\ D \frac{\Delta t}{\Delta x^2} &\leq \frac{1}{2} \end{aligned} \quad (4.23)$$

4.2.1.2 Implicit scheme

Discretizing in the same manner, we obtain:

$$C_{i-1,n+1} \left(-\frac{D\Delta t}{\Delta x^2} - \frac{V\Delta t}{\Delta x} \right) + C_{i,n+1} \left(1 + \frac{V\Delta t}{\Delta x} + 2\frac{D\Delta t}{\Delta x^2} \right) + C_{i+1,n+1} \left(-D\frac{\Delta t}{\Delta x^2} \right) = C_{i,n} \quad (4.24)$$

or, under matrix form:

$$N C(t_{n+1}) = C(t_n) \quad (4.25)$$

N being the triangular matrix:

$$N = \begin{pmatrix} & & & 0 \\ a_1 & a_2 & a_3 & \\ & & & \\ 0 & & & \end{pmatrix} \quad (4.26)$$

with

$$a_1 = \frac{D\Delta t}{\Delta x^2} - \frac{V\Delta t}{\Delta x}; \quad a_2 = 1 + \frac{V\Delta t}{\Delta x} + 2\frac{D\Delta t}{\Delta x^2}; \quad a_3 = -\frac{D\Delta t}{\Delta x^2}$$

The iteration matrix is then N^{-1} . From Gerschgorin theorem, the eigenvalue of N lie in the interval $[1, 1 + 2(V\Delta t/\Delta x) + 4(D\Delta t/\Delta x^2)]$ which implies that they are greater than 1. Thus eigen values of N^{-1} have

their absolute values smaller than 1. From the general convergence theorem, the iterative process converges.

We say that the implicit scheme is unconditionally stable, which does not imply that the solution given by numerical computation fits the true solution. For given mesh size and time-step, the accuracy of the numerical solution depends on the 'smoothness' of the boundary and initial functions. The solution depends continuously on these functions; if they vary slowly, the discretization will not introduce a large error.

4.2.1.3 Crank-Nicolson scheme

It is also possible to use values at both time levels, with a general form for the second derivative

$$\lambda \frac{C_{i-1,n+1} - 2C_{i,n+1} + C_{i+1,n+1}}{(\Delta x)^2} + (1-\lambda) \frac{C_{i-1,n} - 2C_{i,n} + C_{i+1,n}}{(\Delta x)^2} \quad (4.27)$$

where $\lambda \in [0,1]$. If λ is $\frac{1}{2}$, the derivative is centered in time: it is the Crank-Nicolson approximation of the second derivative. For the first derivative

$$\lambda \frac{C_{i,n+1} - C_{i-1,n+1}}{\Delta x} + (1-\lambda) \frac{C_{i,n} - C_{i-1,n}}{\Delta x} \quad (4.28)$$

So using the same discretization as previously we have:

$$D \left[\lambda \frac{C_{i-1,n+1} - 2C_{i,n+1} + C_{i+1,n+1}}{\Delta x^2} + (1-\lambda) \frac{C_{i-1,n} - 2C_{i,n} + C_{i+1,n}}{\Delta x^2} \right] - V \left[\lambda \frac{C_{i,n+1} - C_{i-1,n+1}}{\Delta x} + (1-\lambda) \frac{C_{i,n} - C_{i-1,n}}{\Delta x} \right] = \frac{C_{i,n+1} - C_{i,n}}{\Delta t} \quad (4.29)$$

or

$$\begin{aligned}
 & C_{i-1,n+1} \left[-\frac{1}{2} \left(\frac{D\Delta t}{\Delta x^2} + \frac{V\Delta t}{\Delta x} \right) \right] + C_{i,n+1} \left[1 + \frac{1}{2} \left(\frac{V\Delta t}{\Delta x} + 2 \frac{D\Delta t}{\Delta x^2} \right) \right] + C_{i+1,n+1} \left[-\frac{1}{2} \frac{D\Delta t}{\Delta x^2} \right] \\
 & = C_{i-1,n} \left[\frac{1}{2} \left(\frac{D\Delta t}{\Delta x^2} + \frac{V\Delta t}{\Delta x} \right) \right] + C_{i,n} \left[1 - \frac{1}{2} \left(\frac{V\Delta t}{\Delta x} + 2 \frac{D\Delta t}{\Delta x^2} \right) \right] + C_{i+1,n} \left[\frac{1}{2} \frac{D\Delta t}{\Delta x^2} \right] \quad (4.30)
 \end{aligned}$$

written under matrix form as

$$MC(t_{n+1}) = NC(t_n) \quad (4.31)$$

where M and N are tridiagonal matrixes, the coefficients on a line being the coefficients, respectively, of C_{i-1}, C_i, C_{i+1} .

Calling P the tridiagonal matrix a line of which is made up of the coefficients:

$$\frac{D\Delta t}{\Delta x^2} + \frac{V\Delta t}{\Delta x}, \quad -\frac{V\Delta t}{\Delta x} - 2 \frac{D\Delta t}{\Delta x^2}, \quad \frac{D\Delta t}{\Delta x^2}$$

We notice that P, $M = 1 - \frac{1}{2}P$ and $N = 1 + \frac{1}{2}P$ have the same eigen vectors, which implies that $(1 - P/2)^{-1}$ and $M^{-1}N$ have the same eigen vectors as P.

p being the corresponding eigen value of P, $1 - p/2$ and $1 + p/2$ are the corresponding eigen values, respectively, of M and N. Thus the corresponding eigen value a of the iteration matrix $M^{-1}N$ is

$$a = \frac{1 + p/2}{1 - p/2}$$

According to Gerschgorin's theorem, the eigen values of P lie in the interval $[-2 \{ (V\Delta t/\Delta x) + 2(D\Delta t/\Delta x^2) \}, 0]$ and are negative, which shows that a is smaller than 1.

The Crank-Nicolson approximation is unconditionally stable.

4.2.1.4 The alternating direction implicit procedure (ADIP)

This method has been developed for the bidimensional and generalized cases. Two equations are solved per time-step in the bidimensional case, one of the derivatives appears in the implicit form, whereas the other appears in the explicit form in each equation. This method has a great advantage: instead of computing the inverse of a general matrix, one computes the inverses of two tridiagonal matrices. This is done by the simplified Gaussian elimination method and is very quick in terms of computer time. There are many alternating direction methods. We present the Peaceman and Rachford scheme in the case of the dispersion equation without convection.

Consider the dispersion equation

$$D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (4.32)$$

An approximation of this equation during one time-step consists in dividing up this time-step into two and expressing the derivatives with respect to x implicitly and the derivative respect to y explicitly during the first half time step. During the second half time step the derivatives with respect to x are expressed explicitly and the derivative with respect to y implicitly.

$$D_L \frac{C^+(i+1,j) - 2C^+(i,j) + C^+(i-1,j)}{\Delta x^2} - v \frac{C^+(i,j) - C^+(i-1,j)}{\Delta x} = \frac{C^+(i,j) - C_1(i,j)}{\Delta t/2} - D_T \frac{C_1(i,j+1) - 2C_1(i,j) + C_1(i,j-1)}{\Delta y^2} \quad (4.33)$$

$$D_T \frac{C_2(i,j+1) - 2C_2(i,j) + C_2(i,j-1)}{\Delta y^2} = \frac{C_2(i,j) - C^+(i,j)}{\Delta t/2} - D_L \frac{C^+(i+1,j) - 2C^+(i,j) + C^+(i-1,j)}{\Delta x^2} + v \frac{C^+(i,j) - C^+(i-1,j)}{\Delta x} \quad (4.34)$$

$C_1(i,j)$ and $C_2(i,j)$ are the concentrations at time t_1 and t_2 ($t_1 - t_2 = \Delta t$), at points (i,j) and $C^+(i,j)$ is an intermediate value which has no physical meaning. The solution progresses by computing C^+ for all lines i by tridiagonal Gaussian elimination, assuming C_1 is known, and then by computing C_2 for all columns j by tridiagonal Gaussian elimination. The ADIP is convergent and unconditionally stable.

4.2.2 Some difficulties of the finite-difference approximations

Finite-difference methods are easy to handle, sometimes fast and usually fairly well known. But in the case of dispersion models, two difficulties arise, which are not completely solved upto now: overshoot and numerical diffusion.

4.2.2.1 Overshoot

Consider the injection of a unit concentration step-input function in a one-dimensional flow governed by the dispersion equation

$$D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}$$

Comparison of the analytical solution and the computed solution at time t is given in Fig.4.

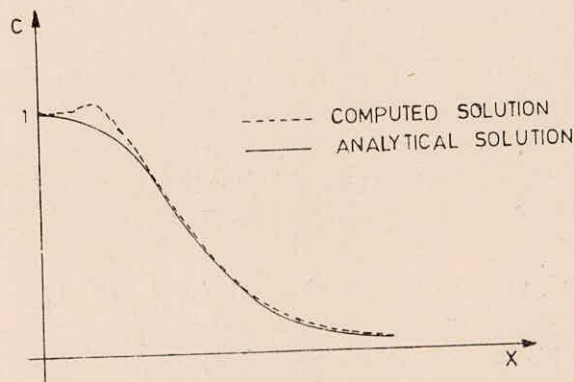


FIG.4 OVERSHOOT

It very often appears that computed concentration exceeds one near the C-axis. This discrepancy is known as 'overshoot'. It may be explained as follows. Time-steps and spatial dimensions are not well adjusted and the aquifer cannot 'adsorb' numerically the injected mass of pollutant. The time-steps should be chosen carefully and adapted to the problem. Often the choice of the time increment as the general term of the geometrical series ($\Delta t_n = a\Delta t_{n-1}$, with $1 < a < 2$) is found to erase the overshoot. For instance, Shamir and Harleman (1967) have used $a = 1.3$ in some of their problems.

We recommend testing any model with a unit-concentration step-input function to adjust time-steps and grid spacing before using it for general boundary conditions.

4.2.2.2 Numerical diffusion

Consider the injection of a unit concentration step-input function in a one-dimensional flow, governed by the dispersion equation

$$D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}$$

Take $D=0$. Analytical and computed solutions at time t are given in Fig.5

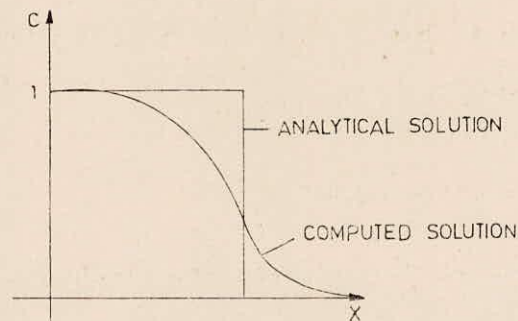


FIG.5 NUMERICAL DIFFUSION

The shape of the computed curve explains why the name 'numerical diffusion' has been given to the phenomenon: it behaves as if the finite difference approximation of the convection equation

$V(\partial C/\partial x) = \partial C/\partial t$ was some diffusion equation

$$D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}$$

the coefficient D having no physical meaning. Some explanations have been given by Lantz (1969,1970): numerical diffusion is a truncation error, the finite difference approximation to the first-order derivatives (both time and space) give rise to error terms proportional to second-order derivatives, the proportionality constants depending both on space and time increments.

Take our simple example, the space first derivative being approximated by a backward difference

$$V \frac{\partial C}{\partial x} \approx V \frac{C(x) - C(x - \Delta x)}{\Delta x} - V \frac{\Delta x}{2} \frac{\partial^2 C}{\partial x^2}$$

A numerical dispersion coefficient $-V\Delta x/2$ is thus introduced, which may be of the order of the physical-dispersion coefficient D . This artificial dispersion is a matter of concern in the domain of dynamic dispersion (when $D = \alpha V$) for values of the order of $\Delta x/2$. No real solution has yet been found for this anomaly, except by testing a mean longitudinal dispersion coefficient of the form $(\alpha V - V\Delta x/2)$ allowing some erasing of the numerical dispersion.

4.2.3 The method of characteristics

In order to reduce or suppress the above-mentioned difficulties Garder et al (1964) have introduced a tentative improvement of the classical finite-difference resolution schemes which they call the method of

characteristics. The problem is still approached by finite differences but physical considerations on the evolution of dispersion lead to establishing a first-order partial differential equation equivalent to the dispersion equation and to determining its characteristics lines.

The problem is defined by the dispersion equation

$$D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} - V_x \frac{\partial C}{\partial x} - V_y \frac{\partial C}{\partial y} = \frac{\partial C}{\partial t} \quad (4.35)$$

where

$$V_x = -\frac{k}{\phi\mu} \left(\frac{\partial p}{\partial x} + \rho g \frac{\partial h}{\partial x} \right), \quad V_y = -\frac{k}{\phi\mu} \left(\frac{\partial p}{\partial y} + \rho g \frac{\partial h}{\partial y} \right) \quad (4.36)$$

k is the intrinsic permeability coefficient. μ is the dynamic viscosity, ϕ is the porosity, p is the pressure, h is head, ρ is density and g is gravity.

Considering that dispersion may be neglected with respect to convection, they assimilate the equation to a first-order partial-differential equation and look for its characteristics, solving the usual system

$$dx/dt = V_x, \quad dy/dt = V_y \quad (4.37)$$

$$\frac{dC}{dt} = D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} \quad (4.36)$$

The characteristics (Garabedian, 1964) span the solution. A moving point (x_p, y_p) is associated with each characteristics p , which is given by its parametric equation $x_p(t)$, $y_p(t)$ where t is time.

The experimental domain, which is assumed to be rectangular, is divided by a conventional stationary grid into rectangles of dimensions Δx and Δy . Each point (i, j) is made the center of the rectangle $R_{i,j}$. Initially the moving points per grid interval being sufficient (a greater number

does not really improve the accuracy of the method), with initial coordinates $x_p(0)$ $y_p(0)$ and an initial concentration $C_p(0)$.

$C_{i,j,n}$ being known at the grid points, the viscosity and density at each point are known, and the pressure is determined from the equation (ϕ is taken as constant)

$$\text{div}[(k/\mu)(\text{grad } p + \rho g \text{ grad } (h))] = 0 \quad (4.39)$$

using the Peaceman and Rachford method. From the set (4.37) the velocity components are determined at the centers of the grid intervals and everywhere by bilinear interpolation. The new positions of point (x_p, y_p) are obtained from (4.35) as

$$\begin{aligned} x_{p,n+1} &= x_{p,n} + \Delta t_n V_x(x_{p,n}, y_{p,n}) \\ y_{p,n+1} &= y_{p,n} + \Delta t_n V_y(x_{p,n}, y_{p,n}) \end{aligned} \quad (4.40)$$

All points are then examined to determine which rectangle $R_{i,j}$ they lie in. Each rectangle $R_{i,j}$ is assigned a concentration $C_{i,j,n}^+$ equal to the average of the concentration $C_{p,n}$ of all the points in their new positions in $R_{i,j}$. The change in concentration due to dispersion in each rectangle is derived from Eqn. (4.36) as

$$\Delta C_{i,j,n}^+ = (\Delta t / \phi) (D_L \Delta x^2 C_{i,j,n}^+ + D_T \Delta y^2 C_{i,j,n}^+) \quad (4.41)$$

where Δx^2 and Δy^2 are the approximations of $\partial^2 C / \partial x^2$ and $\partial^2 C / \partial y^2$.

Each moving point is then assigned a new concentration

$$C_{p,n+1} = C_{p,n} + \Delta C_{i,j,n}^+ \quad (4.42)$$

The change in concentration due to dispersion is the same for all moving points falling in the same rectangle.

The concentrations at the stationary grid points at the new time-step are then given by

$$C_{i,j,n+1} = C_{i,j,n}^+ \quad C_{i,j,n}^+ \quad (4.43)$$

This procedure is then repeated for each subsequent time-step. This method prevents numerical dispersion: if dispersion is zero ($D_L = D_T = 0$) there is no change in concentrations $C_{p,n}$: thus any discontinuity in concentration is preserved and translated.

Although numerical dispersion does not appear, overshoot is not easily overcome (Reddell and Sunada, 1970). This method may be of interest for very particular problems (Robertson, 1974) but is hard to generalize, its uses being very tedious computer-time requirements are high.

4.2.4 Finite element methods (FEM)

There are two fundamental problems in calculus: (i) examining the area under a curve, i.e., integration and (ii) examining the tangent of a curve at a point, i.e., differentiation. Both of these concepts were fairly well understood by the 17th century. In 1667 Isaac Barrow, the teacher of Newton, discovered that integration and differentiation are essentially inverse to one another, which is the fundamental theorem of calculus. Whereas FDM approximates differential equations by a differential approach, FEM approximates differential equations by an integral approach.

The FEM actually refers to the numerical method whereby a region is subdivided into subregions called elements, whose shapes are determined by a set of points called nodes. The flexibility of elements

enables consideration of regions with complex geometry. For transient problems, the time domain may also be approximated using finite elements. In general, however, most studies use finite difference approximations for the time derivatives.

The unknown function C is approximated by a trial solution \hat{C} of linear form

$$\hat{C} = \sum_{i=1}^n a_i u_i \quad (4.44)$$

where the u_i are linearly independent selected functions, which exist over the domain and its boundaries and a_i are unknown parameters to be determined subsequently. In the subdivided domain n nodes are chosen, usually at element vertices and at particular geometric locations. The trial solution is represented in a piecemeal fashion across the domain, element by element, in terms of the space variables and the nodal values of the solution and its derivatives.

There are mainly two type of methods, namely residual and variational methods, using trial functions like \hat{C} .

- i) If C verifies some equation $L(C)=0$, the trial solution \hat{C} verifies some equation $L(\hat{C})=R$, where R is the residual. The problem is to minimize R in some way, usually by minimizing a weight function of R in a well chosen vector space. The minimizing conditions yield a set of algebraic equations that can be solved classical linear system methods.
- ii) In a variation method, the solution C gives an extremum value to some functional $F(C)$. The technique is then to substitute \hat{C} in F and to minimize $F(\hat{C})$ which yield a set of algebraic equations and the solution of this set, by classical linear system

methods, yields the coefficient a_i (Norrie and DeVries, 1973).

A possible application of the residual method, called Galerkin's method, has been proposed by Pinder (1973) to solve the dispersion scheme and applied to a chromium pollution of an aquifer.

The dispersion scheme is defined by the equations

$$L_c(C) = \text{div}(D \text{ grad } C) - \text{div}(vC) - \frac{\partial C}{\partial t} + QC' = 0 \quad (4.45)$$

$$L_h(h) = \text{div}(T \text{ grad } h) - \frac{\partial h}{\partial t} + Q = 0 \quad (4.46)$$

with the usual notations. Q is a sink function incorporating well discharge and leakage into a confining layer and C' is the pollution concentration in the source fluid. Trial solutions are

$$\hat{C} = \sum_{i=1}^n C_i(t) u_i(x) \quad \hat{h} = \sum_{i=1}^n H_i(t) w_i(x) \quad (4.47)$$

where x means (x, y, z, \dots) , u_i and w_i ($i=1, 2, \dots, n$) are basic functions satisfying the boundary conditions for each equation. These basic functions are linearly independent and represent first n functions of complete systems in the domain. The objective is to determine the coefficient functions $C_i(t)$ and $H_i(t)$ that minimize the linear forms $L_c(C)$ and $L_h(h)$. The minimization of $L_c(C)$ is obtained by setting n integrals of the weighted residual $L_c(\hat{C})$ equal to zero.

$$\int_A L_c(\hat{C}) u_i dA = 0 \quad i = 1, 2, \dots, n \quad (4.48)$$

The weighting functions are the basic functions u_i . In the same way we have

$$\int_A L_h(\hat{h}) w_i dA = 0 \quad i = 1, 2, \dots, n \quad (4.49)$$

The suitability of the Galerkin technique for computer application

depends upon the choice of basic functions and elements. Pinder uses the curved isoparametric quadrilateral (Fig.6) linear, quadratic, cubic polynomial basis functions may be defined along the edges of the elements

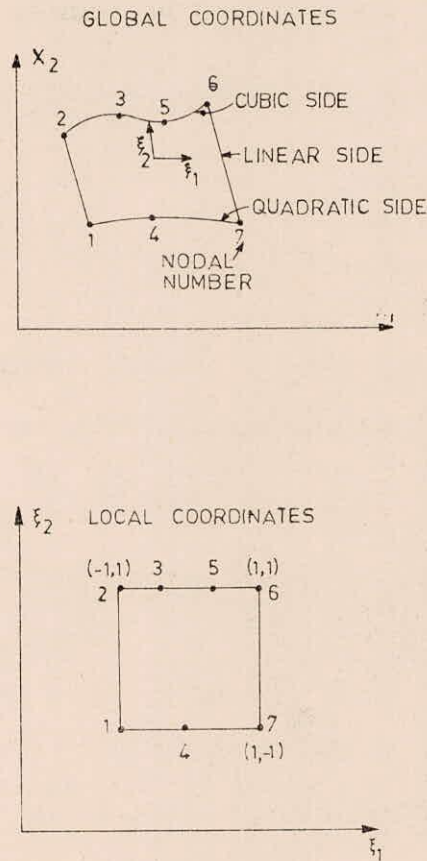


FIG. 6 DEFORMED MIXED ISOPARAMETRIC QUADRILATERAL ELEMENTS ON GLOBAL x AND ξ COORDINATES (PINDER, 1973).

and different order functions may be used along each side to accommodate the geometry of the boundaries or the anticipated form of the unknown solution. To facilitate integration; a dimensionless and curvilinear local (ξ) coordinate system is introduced in which the elements appear as a square with the side nodes located at mid points (quadratic side) or one third point (cubic side). The functions $u_i(x)$ and $w_i(x)$ are written in terms of ξ and are selected such that they fulfill the basic requirements of a basis function and relate the global and local coordinate systems.

From the dispersion scheme and Eqns.(4.48 & 4.49) two sets of algebraic equations can be obtained

$$[N] \{C\} + [M] \{dc/dt\} + \{F\} = 0 \quad (4.50)$$

$$[P] \{H\} + [R] \{dH/dt\} + \{U\} = 0 \quad (5.51)$$

where N,M,P,R are (n-m)x(n-m) matrices(m being the number of passive nodes due to Dirichlet boundary conditions), and C,H,dC/dt and dH/dt are vectors containing the undermined coefficients and their time derivatives. The coefficients of the coefficient matrices are expressed in terms of integrals over the domain of the basis functions and their derivations. The computation of these integrals are performed in the local rather than the global coordinate system, with limits of integration of -1 and +1 and Gaussian quadrature is used. According to experience, exact solutions must be obtained from these integrals. The coefficients depend on the boundary conditions.

Systems (4.50) and (4.51) are solved by approximating the time derivatives of concentration and hydraulic head by a finite difference scheme with a backward difference in the dispersion equation

$$[N] \{C\}_{t+\Delta t} + [M] \frac{\{C\}_{t+\Delta t} - \{C\}_t}{\Delta t} + \{F\} = 0 \quad (4.52)$$

$$[P] \{H\}_{t+\Delta t} + [R] \frac{\{H\}_{t+\Delta t} - \{H\}_t}{\Delta t} + \{U\} = 0 \quad (4.53)$$

These equations are solved sequentially for each time step, for given initial and boundary conditions.

The method of finite elements is more difficult to understand and program than finite differences. It also requires, in general, more computer storage and is more time consuming. Its main advantage is the flexibility of the shape of the elements. This is particularly so when a

moving interface has to be modelled. Another advantage of FEM is the ease of handling anisotropy of model parameters. The method suffers from numerical dispersion and overshoot in the same way as the finite difference method.

4.3 Boundary and Initial Conditions

In order to obtain a unique solution of a partial differential equation corresponding to a given physical process (as solute transport), additional information about the physical state of the process is required. This information is described by boundary and initial conditions. For steady state problems only boundary conditions are required, whereas for unsteady state problems both boundary and initial conditions are required. Mathematically, the boundary conditions include the geometry of the boundary and the values of the dependent variable or its derivative normal to the boundary. The boundary conditions are generally of three types:

- i) Dirichlet type, where the value of the dependent variable, i.e. concentration, is specified along the boundary.
- ii) Neumann type, where the flux or the gradient of concentration is specified normal to the boundary.
- iii) Mixed type, where the flow rate of concentration is related to both the normal derivative and the value at the boundary.

The initial conditions are simply the values of the dependent variable specified everywhere inside the boundary, at some specified time before the beginning of actual operation.

4.4 Data Requirement and Model Verification

The data requirements for transport models are prodigious. Lack of data is perhaps the severest limitation on the type of model which can

be used and its capabilities. Two classes of data are required.

Firstly, data associated with boundary conditions, such as aquifer geometry, fluxes, heads concentrations, abstractions etc. In regional scale studies, fluxes associated with water transfers, and land use can involve large amounts of data, especially if several solutes are involved. Two types of boundary conditions may be identified. Internal boundary conditions require the specification of contaminant concentrations in water entering the aquifer. Such inputs may be localized, as from landfills, surface water bodies, septic tanks and chemical spills. The input concentrations of the contaminant will often not be known with any certainty though the total mass input may be known. The equation of solute transport is usually linear, however, so that sensible adjustments to the model inputs to achieve an acceptable match between the computed results and observations are straight forward. External boundary conditions require the specification of contaminant concentrations or fluxes at the model perimeter. If the model boundary is a ground water divide, then the contaminant flux may be set to zero. In all other cases, the type of boundary conditions selected will depend on local constraints.

A constant ground water potential, due to contact between the aquifer and a river or lake will usually result in a constant concentration boundary condition to the transport model. It may be possible to locate the model boundaries far from the areas of interest in which case the boundary conditions can be of minor importance.

The second class of data consists of parameters characterising the aquifer and the various processes which are occurring. These include storage coefficients, hydraulic conductivities, dispersivities, porosity and reaction -, adsorption - and diffusion - rate constants. These parameters

are usually defined from field and laboratory experiments and model calibration. In particular, transport models are found to be very sensitive to aquifer porosity and hydraulic conductivity because of their importance in defining the pore water velocity. Also, dispersivities are found to be scale dependent because of the influence of averaging. For example, values measured on core samples in the laboratory are several orders of magnitude smaller than values appropriate to region scale. This problem does not arise in lumped models.

Verification of a model usually consists of comparison of computed results with historical observations. It is desirable during the stage to test the model for parameter sensitivity. This, of course, is easier to accomplish on the simpler models.

The development of a mathematical model begins with a conceptual understanding of the physical system. Once these concepts are formulated they can be translated in to a mathematical framework resulting in equations that describe the process. A variety of analytical and numerical techniques can be applied to solve the equations, resulting in practical tools such as type curves or finite difference and finite element computer programs.

The solute transport equation is used with the ground water flow equation to address pollution problems. These problems are not as well understood, especially the characterisation of source terms and dispersion. One may choose a solute transport model according to need and convenience. In selecting a model for a particular application, it is obviously sensible to keep the model as simple as possible and in any case not to have a more sophisticated model than is warranted by the available data and knowledge of the system. Lumped models are probably most appropriate to large scale problems, particularly where the solute originate from a distributed source. Two and three dimensional model are probably most appropriate to small scale problems where a detailed description of solute movement is needed.

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