SR—33

GROUNDWATER QUALITY MODELLING

By

P. K. MAJUMDAR
SCIENTIST 'C'

NATIONAL INSTITUTE OF HYDROLOGY
ROORKEE – 247 667

1992–93

PREFACE

Water Resource projects can be better planned and managed to ensure more reliable water availability and efficient water use in the agricultural sector, mitigate flood damage and control water pollution and simultaneously reduce adverse environmental and social impacts such as prevention of development of water logging and salinity, reduction in the spread of water borne diseases and proper resettlement of displaced people. Environmentally sound water management should be able to address and resolve all these issues simultaneously.

In the ecosystem, impacts are usually complex and one impact may lead to another resulting in chain actions and a major may often are to a combination of factors. Various types of water related activities can cause beneficial or adverse impacts on the environment. These activities may include land clearance, construction, water impoundment, water channelization, flood land alterations and changes in land use patterns.

Water Quality is a very important consideration for all water development projects as it affects all aspects of water use with regard to water quality in reservoirs and lakes an understanding of stratification and its effects are essential. Agricultural, industrial and human settlement, development around the new water project area may excerbate the problem of water Quality deterioration. Whilst inspection of the available data can provide a strong insight into a potential pollution hasard, the use of models may provide a more appropriate and rigorous method for

integrating all the available data together and for evaluation of the response of the aquifer system to a contamination event.

This report has been prepared by Shri.P.K. Majumdar, Scientist`C in connection with ongoing UNDP project IND/90/00 entitled "Developing capabilities in Hydrological studies".

Satish Chandra

SATISH CHANDRA

DIRECTOR

CONTENTS

ANNEXURES

1.Ø INTRODUCTION

A model is a simplified representation of a complex system. The purpose of designing a model is to acquire sufficient knowledge of natural processes, that a functioning structure of the process emerges to assist in prediction. It is necessary to learn something of the nature of the process before attempting to predict future behaviour and it is the building of a suitable abstraction of what is probably quite a complex phenomenon that forms the art of modelling.

The knowledge of many physical phenomena gathered over the centuries was deducted solely from experience and often from the comparison of inventions of the intellect with observed behaviour. If we broadly term such inventions as models, then experience has always been the only yardstick of suitability of a particular model. If it works we use it, if not we discard it.

Models can be broadly classified into two categories.

Physical Models

A physical model is a scaled down facsimile of a full scale prototype. It is an alternative to a mathematical model when the problem is too complex that no adequate mathematical model can be formulated. When the experimental results have been obtained there may be self evident relationships between the model behaviour and the behaviour of the full scale prototype. The modeller has to face two problems; the first problem involves the design of the model and experimental procedure and the second

problem involves the correct interpretation of the results.

In physical modelling, it is necessary to identify physical laws that introduce the idea of similarity and dimensional homogeneity. These physical laws apply equally to the behaviour of model and prototype. The ideas of similarity can be formalised mathematically as geometric, kinematic and dynamic similarity.

The idea of dimensional homogeneity expresses the fact that most people intuitively accept the idea of homogeneity or harmony within an equation. Dimensional homogeneity must be true for any equation which purports to describe a set of physical events. From dimensional homogeneity it can be argued that dimensional relationships are arbitrary, since magnitudes depend on the choice of units. For this reason, an equation which is a statement of a physical law is often used in dimensionless form. Dimensionless equations are completely general, and are therefore frequently the basis for the representation of experimental data.

Mathematical Model

In a mathematical model, the system is represented by a set of equations between the variables and parameters, and these equations may be connected by statements. Mathematical models are functions which represent the behaviour of a physical system.

Mathematical models based on simplified concepts of physical processes may be either Deterministic or stochastic. If any of the variables in an equation are regarded as random variables, having a probability distribution, then the model is a stochastic model; stochastic, rather than statistical, to emphasis the time

dependence of the variables related by the model. If all the variables in an equation are regarded as free from random variations so that none is thought of as having a probability distribution, then the model is regarded as deterministic. In the stochastic approach, uncertainty by way of probability laws is woven into the fabric of hydrodynamic and phenomenological relations which define the mean value behaviour of a system with zero mean square error. If the chance of occurrence of the variables involved in such a process is ignored and the model is considered to follow definite laws of certainty but not any law of probability, the process and its model are described as deterministic. On the other hand, if the chance of occurrence of the variables is taken into consideration and the concept of probability is introduced in formulating the model, the process and its model are described as stochastic or probabilistic. Models may be stochastic or deterministic and may be linear or non-linear. The usage of the term linearity has at least two meanings; if the model is linear in the system theory then, the principle of superposition holds. However, linearity has an alternative meaning, the model is linear in the stochastical regression sense, if it is linear in the parameters to be estimated. Deterministic models can further be classified into lumped models and distributed models. A lumped model takes no account of the spatial variations in the parameters. A distributed model describes the spatial variability in the parameters and it takes account of the spatial distribution in the input variables.

Water Quality Modelling

The more developed areas of the world try to achieve regional water quality goals by reducing the discharge of contaminants into natural water, or improving the quality of waste waters, or limiting economic activities and economic development in a particular region or river basin. Those responsible for the formulation and adoption of water quality plans or management policies must have means of estimating and evaluating the temporal and spatial economic environmental ecological impact of these plans and policies. This need has stimulated the development and application of a wide range of mathematical and physical modelling techniques for predicting the impacts of alternative pollution control plans.

It is impossible in a physical model to simulating gradients of growth rate or decay rate of bacteria and biological activities in a water body, or to a model correctly mixing the dispersion. Hence, the general tendency towards the mathematical modelling approach.

2.Ø MODELLING PROCEDURE

2.1 GENERAL

The modelling procedure can be divided into two stages. The first stage is termed the "a priori" stage which derives a set of relationships from the ensemble of general theory for a specific water body. The second stage is called the "a posterior" stage which demonstrates the good or bad approximation of the behaviour of that model to the observed behaviour of reality.

A Priori Stage

The "a priori" stage can be visualised as follows:

(a) Goals and Objectives

The goals and objectives determine the nature of the model. Our attitude is not one of seeking a universal model to solve, in general, all manner of problems. The goals and objectives can be distinguished by two broad categories such as research and management. In a research context a model has to provide indicators for further fruitful directions of investigation. (An awareness of immediate use for the model). An essentially research oriented model may nevertheless be used to make forecasts about the probable future behaviour of the system. In a management context, the immediate application of the model must be known and carefully specified. Management of water quality has traditionally been understood to mean long range planning, the design of treatment facilities or the problem of legislation for discharge

consents and standard setting.

(b) Conceptualisation

For a specific water body and either objective, the first step of the modelling procedure is conceptualisation. At this point, the analyst should be interested in the physical, chemical and biological systems of the water body. A water quality model can be chosen to simulate the properties and interrelationships of any or all of the following external components and processes

Physical : Solar radiation, temperature, pressure, density, external and frictional forces, flow velocity, diffusion flows, heat flows, kinetic and internal energy, entropy, sedimentation, etc.

Chemical : dissolved organic chemicals, particulate organic materials (detritus), inaccessible nutrients, heavy metals, complex synthetic and toxic compounds etc.

Biological : Primary producers (diatoms, green algae, blue green algae, phytobenthos), zooplankton (rapters, selective filters, non selective filters etc) zoobenthos, fish, biota in different life stages etc.

Conceptualisation will involve a choice regarding the possible (spatial) segregation of the water body into a number of discrete segments and layers. Apart from spatial separation of the water body, it may include grouping and differentiation by biotic species according to how their role is visualised in the ecology of the water body. It also includes the partition of the

temporal dimension into ranges of quickly and slowly changing variations.

The formulation of the model also comes under the conceptualisation. The relevant variables for description of the desired water quality characteristics and expressions for their interactions have to be chosen. The most probable variables are as follows:

(1) Measured input disturbances

The measured input disturbances for forcing functions might comprise the recorded day to day variations of total biochemical oxygen demand, suspended solids and ammonia nitrogen concentration etc.

(2) Unmeasured (unknown) input disturbances

A predominant characteristic of the unmeasured inputs is that they will generally be expected to exhibit a random variability.

(3) State variables

The state variables characterise the essential properties and behaviour of a process as a function of space and time.

(4) Measured output variables

The measured output variables are merely measurements of some of the process state variables.

(5) Measurement errors

These variables represent the random and systematic measurement errors that derive from process instrumentation, and laboratory analysis. Such errors are inherent in all measurement of output variables.

(6) Model Parameters

These are coefficients that appear in the system model. The desirable property of these parameters is that they should be invariant with time and space or truly constant. This desirable property will be shown to be an extremely important feature of certain aspects of model development and analysis.

(c) Selection of model type

(1) Research or management models

In the research context, a model has to provide indicators for further fruitful directions of investigations. An awareness of the immediate use for the model is not necessary before the study is undertaken. Rather the concise representation of the "apriori" and measured information that the model offers and the possibility for a gain in comprehension of system behaviour, are of primary importance. Essentially, research oriented models may, nevertheless be used to make forecasts about the probable future behaviour of the system.

In a management context, the immediate application of the model must be known and carefully specified. Management of water quality has traditionally been understood to mean long range planning. The design of the treatment facilities, or the problem of legislation for discharge consents and standard settings.

(2) Distributed or lumped models

A distributed parameter model is one in which variations of all the quantities (measured input disturbances, unmeasured disturbances, state variables, parameters, measured errors and measured outputs) are considered to be continuous functions of time and space. This form of model arises rather naturally in the analysis of water5 bodies. It is probably the most accurate form of model, that one might use to describe the behaviour of quality in a water body, generally accounting for variations in the three orthogonal directions. It is also a difficult form of model to solve. The distributed parameter model is usually defined by partial differential equations.

In a lumped parameter model, parts of the system are lumped together, so that for certain finite volumes of water body or within certain bounded spatial locations, water quality is assumed to be uniform and independent of position within the defined volume. The lumped parameter model is frequently expressed in ordinary differential equation form.

(3) Linear or non-linear models

Generally, distributed parameter models and lumped parameter models are non-linear models. A special case of the general class of non-linear models is the linear model. The tendency of the analyst is to strive to obtain a linear system model, because a linear model obeys the principle of superposition and many powerful techniques are available for the comprehensive analysis of such models.

(4) Stochastic or deterministic models

A deterministic model with input disturbances and random measurement errors will give rise to a stochastic model . The assumption of a deterministic model is tantamount to the assumption that one has perfect knowledge of the behaviour of the system or the future response of the system is completely determined by a knowledge of the present state and future measured input disturbances . Deterministic models are widely used in studying the water quality of lakes,rivers,estuaries and other types of water resources . These models taking into account the physical,chemical and biological processes inside the system as well as the fluxes of matter and energy across its boundaries,are intended to serve as research tools and a basis for water resources management . Deterministic water quality models must be based on the following principles; the conservation of mass,conservation of energy,boundary and initial conditions,and laws governing chemical,biochemical and biological processes and the second law of thermodynamics.

(5) Dynamic or steady state

This is the most significant distinction that can be drawn, since it often furnishes the dividing line in choosing the types of model best suited to a particular problem. A steady state model can be derived by assuming all variables and parameters to be independent of time. Choosing a steady state model has an advantage of simplifying computational effort through the elimination of the independent variables in the model relationships for example, a steady state model may be used to estimate the average spatial variations of the quality of a river system, computed for an average time invariant set of waste water discharges and temperature and stream flow rate conditions.

If all variables but the stream discharge are held constant with time, then the model is called a dynamic model. The time varying discharge implies that water quality at any fixed spatial location is not in a steady state. A typical example of a dynamic model application is that of examining over a period of years, the response of a lake ecological system after installation of nutrient removal treatment at an adjacent waste treatment plant.

(6) Internally descriptive or black box models

The two extremes of the spectrum of models are the internally descriptive model at one end and black box model is closely associated with a "a priori" information and with the deductive reasoning process. The internally descriptive model, characterises how the inputs are connected to the states and how in turn

the states are connected to each other and to the outputs to the system and provides the description of the internal mechanisms. The black box model is much more oriented toward a "a posteriori" information and the inductive reasoning process. It reflects only what changes the input disturbances will effect in the output responses and deals only with what is measurable, that is inputs and outputs.

(d) Computational Representation

It is unfortunate that all water quality models are not sufficiently simple to yield an analytical solution requiring nothing more than pencil and paper. In general, it is found that our analyses are strongly tied to the solution of differential equations and if not equations are employed such that they are readily amenable to the recursive functions of the modern digital computer. Hence, numerical solutions of ordinary differential equation have become so common that the techniques for such solution are a regular feature of standard mathematical texts. The analyst should be prudent enough to check the degree of numerical error in his model solutions. The solution for partial differential equations is not so straight forward. Hence, the differential equations are transformed into an approximate set of difference equations. In this case, the character of a model may depend upon how the differential equations are transformed into difference equation.

A Posteriori Stage

(a) Calibration and Verification

Model calibration is performed using one or more observed data sets of both inputs and outputs. The model parameters and indeed the model itself are adjusted or modified so as to produce an output that is as close to the actual observed water quality as is possible. This is usually a subjective trial and error procedure, again reflecting the art more than the science of modelling.

The main aim of the "a posteriori" phase of the modelling procedure is centered upon the retrieval manipulation and restructuring of measured information. The question is how can we translate information about the external description of the system into information about the internal description of the system, obtaining estimates of parameters and a prediction of state variables.

With restricted computational facilities and very complex models, it is hard to say anything positive about the likelihood of success in the application of technique of calibration and verification.

The most common procedures already applied to water quality model calibration, may be classified as essentially trial and error simulation and least square estimation. The trial and error method is an informal procedure whereby the analyst starts with some model structure and set of associated parameter values, so that the simulated performance of the model is compared with

the observed behaviour of the system under study. If the model is found to be inadequate in its characterisation of reality, the analyst may decide simply to adjust some of the parameter values an ad hoc basis until the desired performance is obtained. On the other hand, the model may be so much in error that the analyst is required to alter the structure of the relationship between the variables accounted for in the model. The least squares deviations between actual measurements and the output of the model. Methods such as maximum likelihood and Markov and Kalman filters are also used to estimate parameters.

Verification is associated with the "a posteriori" phase of the modelling procedure. Model verification requires and independent set of input and output data to test the calibrated model. The verification data must be independent of that used to calibrate the model. A model is verified if the model prediction for a range of conditions, compares favourably with observed field data. Here, again the criterial for deciding whether or not model output and field data are essentially the same for the same output conditions are largely subjective. Satisfactory comparison depends on the nature of the problem, the type of model developed and its purpose, and the extent and the reliability of available input and output data.

(b) Validation

Validation stands at the point of transition between model development and the application of the model to problem solving.

Irrespective of the benefits of model development in terms of acquiring, understanding or as a framework for organising and interpreting experimental data, the ultimate test of a model is whether it can be believed as a mechanism for prediction of conditions expected in the future that would be substantially different from those observed in the past. The validation is the testing of the adequacy of the model against a second independent set of field data and thus entails the design and implementation of new experiments. usually, a model cannot be completely validated; the validity of the model can be determined by the use of statistical hypothesis testing (Schwepps, 1988).

2.2 Groundwater Modelling

Most groundwater models express nothing but a balance of a considered extensive quantity e.g. mass of water, mass of a solute and heat.

The first step in the procedure of modeling is the construction of a conceptual of the problem and the relevant aquifer domain. The conceptual model consists of a set of assumptions that reduce the real problem and the real domain is simplified versions that are acceptable in view of the objectives of the modeling and of the associated management problem. The assumptions should relate to such item as:

the geometry of the investigated aquifer domain,

the kind of material comprising the aquifer (with reference to its homogeneity, isotropy etc)

the mode of flow in the aquifer (three-dimensional, or two-dimensional horizontal)

the flow regime (laminar, or non-laminar)

the properties of the water (with reference to its homogeneity, compressibility),

effect of dissolved solids and/or temperature on density and viscosity,

the presence of assumed sharp fluid fluid boundaries, such as a phreatic surface or a freshwater - saltwater interface

the relevant state variables and the area or volume over which the averages of such variables are taken.

sources and sinks of water of relevant pollutants, within the domain and on its boundaries (with reference to their approximation as point sinks and sources or distributed ones), and

the conditions on the boundaries of the considered domain, that express the way the latter interacts with its surrounding.

Usually, the conceptual model is expressed in words as a set of assumptions. Actually, this set of assumptions constitutes the 'label' of the model being developed. In principle we should not use a ready-made model for a given problem, unless we have examined the former's label and decided that indeed out problem can be described by the same conceptual model.

In the second step, we express the conceptual model in the form of a mathematical model. The latter consists of (i) a definition of the geometry of the considered domain and its boundaries, (ii) an equation (or equations) that express the balance of the considered extensive quantity (or quantities), (iii) flux equations, that relate the flux(es) of the considered extensive quantity(ies) to the relevant state variables of the problem, (iv) constitutive equations that define the behavior of the particular materials-fluids and solids-involved (v) initial conditions that describe the known state of the considered system at some initial time, and (vi) boundary conditions that describe the interaction of the considered domain with its environment, across the boundaries of the former.

In the continue approach the balance equation, takes the form of a partial differential equation written in terms of macroscopic state variables, each of which is an average taken over the representative elementary volume of the domain considered. In other cases, balances of extensive quantities are stated for various forms and sizes of aquifer cells. In such models the stated variables are averages over the considered model cells. Boundary conditions are also expressed in mathematical forms. The most general boundary condition for any extensive quantity takes the form of equality of the flux of that quantity, normal to the boundary, on both sides of the latter.

A special case is that of the momentum balance. In the continuum approach, subject to certain simplifying assumptions

(included in the conceptual model) as to the solid-fluid interaction negligible internal friction in the fluid, and negligible inertial effects, the averaged momentum balance equation reduces to the linear motion equation known as Darcy's law, used as a flux equation for fluid flow in porous media. With certain modification, it is also applicable to multiphase flows such as air-water in the unsaturated zone.

In the passage from the real system to the conceptual model and then to the mathematical one, various coefficients of transport and storage of the considered extensive quantities are introduced. The permeability of a porous medium aquifer transmissivity , aquifer storativity and porous medium dispersivity are examples of coefficients that express the macroscopic effects of the microscopic configuration of the solid-fluid interfaces of a porous medium. They are introduced in the passage from the microscopic level of description to the macroscopic continuum, one. All these coefficients are coefficients of the models, and therefore, in spite of the similarity in their names in different models, their interpretation and actual values may differ from one model to the next.

Obviously no model can be employed in any particular case of interest in a specified domain, unless we known the numerical values of all the coefficients appearing in it. Estimates of natural replenishment and a priori unknown location and type of boundaries may be included in the list of model coefficients and parameters that have to be identified. We refer to the activity

identifying these model coefficients as the identification problem.

In principle, the only way to obtain the values of these coefficients for a considered model is to start by investigating the real aquifer system in order to find a period in the past for which information is available on (i) initial conditions of the system, (ii) excitations of the system, say in the form of pumping and artificial recharge (quality and quantity), natural replenishment, introduction of pollutants, or changes in boundary conditions, and (iii) observations of the response of the system say in the form of temporal and spatial distributions of state variables e.g. water levels, solute concentrations and land subsidence. If such period (or periods) can be found, we (i) impose the known initial conditions on the model, (ii) excite the model by the known excitations of the real system and (iii) derive the response of the model to these excitations. Obviously, in order to derive the model's response, we have to assume for it some trial values of the sought coefficients. We then compare the response observed in the real system with that predicted by the model. The sought values of the coefficients are those that will make the two sets of values of state variables identical. However, because the model is only an approximation of the real system, we should never expect these two sets of values to be identical. Instead we search for the 'best fit' between them, according to some criterion. Various techniques exist for determining the 'best' or 'optimal' values of these coefficients,

i.e. values that will make the predicted values and the measured ones sufficiently close to each other. Obviously, the values of the coefficients eventually accepted as 'best' for the model, depend on the criterial selected for 'goodness of fit' between the observed and predicted values of the relevant state variables. These, in turn, depend on the objective of the modeling. Some techniques use the basic trial and error method described above while others employ more sophisticated optimization methods. In some methods, a priori estimates of values to be expected for the coefficients as well as information about lower and upper bounds are introduced. In addition to the question of selecting the appropriate criteria, there still remains the question of the conditions under which the identification problem, also called the inverse problem will result in a unique solution.

Once a mathematical model has been constructed in terms of relevant state variables it has to be solved for cases of practical interest for example, for planned pumping, or artificial recharge, or for anticipated spreading of a pollutant from a potential source of pollution in the considered aquifer domain. The preferable method of solution is the analytical one, because once such a solution is derived, it can be employed for a variety of planned, or anticipated situations. However, in most cases of practical interest, this method is not feasible because of the irregular shape of the domain's boundaries, the heterogeneity of the domain, expressed in the form of spatial distributions of its transport and storage coefficients, and the irregular temperatures and spatial distributions of the various excitations, or

sink source, functions. Instead, numerical methods are employed for solving the mathematical model.

2.3 Groundwater Quality Modelling

With the increased demand for water in most parts of the world, and with the intensification of water utilization, the quality problem becomes the limiting factor in the development and use of water resources. Although in some regions, the quality of both surface and groundwater resources deteriorates, special attention should be devoted to the pollution of groundwater in aquifers due to the very slow velocity of the water and to the possibility of an interaction of the pollutants with the solid matrix. Although it may seem that groundwater is more protected than surface water, it is till subject to pollution, and when the latter occurs, the restoration to the original non-polluted state, is usually more difficult and lengthy.

The term 'quality' usually refers either to energy in the form of heat or nuclear radiation or to materials contained in the water. Many materials dissolve in water, whereas others may be carried with the water in suspension. Given the very large number of polluting constituents and new materials are coming onto the market every day groundwater quality can be defined in terms of hundreds of parameter. The relevance of any of these materials depends on the water use that is being considered.

Standards have been issued by national and international health authorities with respect to the various constituents according to the origin of the water and the type of consumer

2.3.1 Groundwater pollution may usually be traced back to four sources;

(i) Environmental. This type of pollution is due to the environment through which the flow of groundwater takes place. For example, in flow through carbonate rocks, water dissolves small, yet sometimes significant, amounts of the rock. Sea water intrusion, or pollution of good quality aquifers by invading brackish groundwater from adjacent aquifers as result of disturbing an equilibrium that existed between the two bodies of water may also serve as examples of environmental pollution.

(ii) Domestic. Domestic pollution may be caused by accidental breaking of sewers, by percolation from septic tanks, by rain infiltrating through sanitary land fills, or by artificial recharge of aquifers by sewage water, after being treated to different levels. Biological contaminants (e.g. bacteria and viruses) are usually related to this source.

(iii) Industrial. In many cases, a single sewage disposal system serves both industrial and residential areas. In this case, one cannot separate between industrial and domestic pollution, although their compositions and, hence the type of treatment they require and the pollution they cause are completely different. Heavy metals, for example, constitute a major problem in industrial waste. Industrial waste may also contain radioactive materials and various non-deteriorating, highly toxic compounds.

(iv) Agricultural This source is due to irrigation water and rain water dissolving and carrying fertilizers, salts, herbicides, pesticides etc., as they infiltrate through the ground surface, travel through the unsaturated zone, and replenish the aquifer. Irrigation with reclaimed sewage water may also serve as a source of pollution for an underlying phreatic aquifer.

2.3.2 Three different levels of complexity and sophistication are used to address the prediction of contaminant transport in groundwater. These levels are as follows.

1. Simple analytical methods based on the solution of applicable differential equations are used making a simplified idealization of the field and giving qualitative estimates of the extent of contaminant transport.

2. Semi analytical methods based on the concept of complex velocity potential are used, providing the streamlines for steady state fluid flow and the corresponding contaminant movement in the presence of an arbitrary number of sources and sinks. An average geological environment is assumed and a schematic chemical retardation factor is considered.

3. Sophistiated numerical models are used, accounting for complex geometry and heterogenous media as well as dispersion, diffusion, and chemical retardation processes (e.g. sorption, precipitaion, radioactive decay, ion exchange, degradation).

Analytical Methods

Analytical methods that handle solute transport in porous media are relatively easy to use. However, because of the complexity of the equations involved, the analytical solutions available are generally restricted to either radial flow problems or to cases where velocity is uniform over the area of interest. Numerous analytical solutions are available for time-dependent solute transport within media having steady and uniform flow.

Some of the advantages of using analytical methods for estimating the extent of contamination in groundwater aquifers are listed below.

1. Analytical methods are probably the most efficient alternative when data necessary for identification of the system are sparse and uncertain.

2. Where applicable, these methods are the most economical approach.

3. They are always the most useful means for an initial estimation of the order of magnitude of contamination extent.

4. Experienced modelers and complex numerical codes are not required.

5. In many cases a rough estimate can be obtained. When application of simple computer codes for evaluation of analytical solutions is needed the input data are usually very simple and do not require a detailed familiarity with the codes.

Some of the important limitations of analytical methods are as follows.

1. The analytical solutions available are limited to certain idealized conditions and may not be applicable to a field problem with complex boundary conditions.

2. Spatial or temporal variation of system properties such as permeability and dispersivity cannot be handled with analytical techniques.

Semianalytical Methods

These are the approximate techniques which in some respects are more powerful than analytical methods. Their application is much simpler than most of the complete numerical methods. These techniques apply a well known concept of fluid mechanics, the complex velocity potential, and extend it by employing numerical tools and computer plotting capabilities.

A major limitation of these techniques is that they are only applicable to the study of steady state two dimensional fluid flow through homogeneous media. Furthermore, the effects of transportation by dispersion and diffusion are not considered; contaminant species either move with the water- "water coincident contaminants" or lag behind it due to adsorption on the rock matrix -"adsorption retarded contaminants" .

In summary execution of the semi-analytical methods to determine contamination extent includes the following steps.

1. Identify simple flow components of the system such as uniform regional flow, point sources representing recharging wells, point sinks representing discharging wells, and finite radius circular sources representing waste storage ponds.

2. Combine the expressions for each of the identified simple flow components to obtain the overall complex velocity potential of the system, satisfying the appropriate boundary conditions.

3. Construct the expressions for the velocity potential and stream function of the system.

4. Calculate the velocity field by taking the derivative of the velocity potential.

5. Construct flow patterns and identify locations of any contaminant fronts for various values of time.

6. Using the stream function of the system, calculate the time variation of the rate at which a contaminant reaches any desired outflow boundary.

The following are some of the advantages of semi-analytical methods

1. In the presence of multiple sources of contamination and discharge features such as pumping wells and effluent streams where flow analytical solutions are not available, semi-

analytical methods can be used to estimate the order of magnitude of contamination extent for particular solute species.

2. For preliminary studies with limited budget and time or limited data available, semi-analytical techniques are invaluable for estimating the travel time of a water coincident or adsorption retarded solute to a discharge well.

3. Application of these methods requires only simple computer input data and does not require the design of a mesh as with fully numerical methods.

4. An initial study using semi-analytical methods can indicate whether or not a more sophisticated study based on a long period of observation and expensive data collection is required.

The following are some of the limitations of semi-analytical methods

1. Semi-analytical methods as discussed in this chapter do not consider mass transport by dispersion and diffusion which in many cases may lead to the prediction of travel times which are longer than actual values and may underestimate the true impact of a contaminant source.

2. Since development of the technique is based on a two dimensional plane theory, field problems that are actually three dimensional in nature must be simplified before semi-analytical methods can be applied.

3. Semi-analytical methods cannot handle media with heterogeneous

or anisotropic permeabilities.

4. The methods described in this chapter hold only for steady state problems, although in some cases they could be extended to handle transient problems.

Numerical Methods

Numerical methods are generally required to solve complex equations describing coupled or uncoupled processes in heterogeneous and anisotropic formations under various initial and boundary conditions. In most numerical models the governing equations are approximated by algebraic equations relating unknown variables at discrete nodal points and at different times. The governing equations for fluid flow and solute transport have second order diffusive terms $\nabla\cdot(K\nabla h)$ and $\nabla\cdot(D\nabla c)$, a first order convective term and transient terms $\delta h/\delta t$ and $\delta c/\delta t$. The accuracy and efficiency of a model depend

(1)on the numerical approximations for evaluating the spatial gradient and the time derivative and

(2) on the solution scheme of the algebraic equations.

To calculate fluid pressure and solute concentration, the finite difference, integrated finite difference, and finite element methods are frequently used to approximate first and second order spatial derivative terms. The main distinctions among the different methods are in the numerical approximation of the gradient operator the evaluation of variable dependent coefficients, and the spatial discretization of the region. For the

modeling of complex geological formations, it is important to be able to handle the large number of equations that result from an irregular discretization of multidimensional space.

Finite Difference Method

In most finite difference models, the distribution of nodes is regular, creating a grid with either uniform or nonuniform spacing along orthogonal coordinate systems (Cartesian: x,y,z; cylindrical: r,θ,z etc). Surrounding each nodal point there is a region bounded by interfaces normal to the coordinate axes; this region is called a nodal block, cell, or element, Between two nodes indexed by i and i+1 in the x direction, the interface i+1/2 can intersect the x axis either midway between i and i+1, or at an off center location.

For the evaluation of a spatial gradient the partial differential of a variable is expressed in terms of the difference between two neighbouring nodal values. For example, the x component of the concentration gradient $\delta c/\delta x$ at the interface $i \pm \frac{1}{2}$ is approximated by

$$\frac{C_{i\pm1} - C_i}{x_{i\pm1} - x_i}$$

with the finite difference approximation, the nodal value of C_i is algebraically related to its two neighbouring values for a one dimensional problem, or six neighbours for a three dimensional problem. The components of the second order terms coefficients K and D at the interfaces $i \pm 1/2$ can be evaluated as the arithmetic mean,

$$D_{i \pm 1/2} = \frac{D_{i \pm 1} + D_i}{2}$$

or as the harmonic mean,

$$\left[\frac{1}{D}\right]_{i \pm 1/2} = \frac{(\Delta x/D)_{i \pm 1} + (\Delta x/D)_i}{\Delta x_{i \pm 1} + \Delta x_i}$$

Where

$$\Delta x_i = |x_{i \pm 1/2} - x_i| \qquad \Delta x_{i \pm 1} = |x_{i \pm 1/2} - x_{i \pm 1}|$$

These approximations for interface values can be generalized for an irregular distribution of nodes. For example, the factor 1/2 in the arithmetic mean can be replaced by other fractional weighting factors; the in the Δx_i harmonic mean can be replaced by the normal distance from the nodal point to the interface.

For the first order convective term $v \cdot \nabla C$ in the solute transport equation, $\delta C/\delta x$ may be approximated by the central difference in space, or central weighting.

$$\frac{C_{i+1/2} - C_{i-1/2}}{x_{i+1/2} - x_{i-1/2}}$$

with

$$C_{i \pm 1/2} = 0.5(C_{i \pm 1} + C_i)$$

With this central weighting scheme the space truncation approximation of the convective term is correct to second order. However, there is a tendency for solutions with central weighting to oscillate artificially at high flow velocities. The convective flux associated with the flow velocity carries solute downstream; a nodal point between an upstream and a downstream node will have a concentration closer to the upstream value. Since the central weighting scheme does not take into account this convective effect, other schemes have been devised. In the upstream weighting scheme the interface concentration is set equal to the

upstream value; that is $C_{i+1/2}=C_{i+1}$ if fluid flows from i+1 to i. In other words, a backward difference $C_{i+1} - C_i$, is used for the convective term at node i. The upstream weighting eliminates the oscillation but introduces a space discretization error, called numerical dispersion, which produces the same effect as physical dispersion. The error of numerical dispersion in the upstream weighting scheme and the error of numerical oscillation in the central weighting scheme may be minimized by using the partial upstream weighting $C_{i+1/2} = a C_{i+1} + (1-a) C_i$ with $0.5 \leq a \leq 1$, or discontinuous weighting with central weighting at low flow velocity and upstream weighting at high flow velocity. Other weighting scheme have also been devised.

Integrated Finite Difference Method

The integrated finite difference method (IFDM) is a more flexible version of the finite difference method. In the integrated finite difference method, the distribution of nodal points may form an irregular mesh, and the nodal blocks may be arbitrarily shaped polyhedrons. The numerical equations are formulated from the integral form of the governing equations, as opposed to the simpler finite difference methods that employ the differential form of the governing equations. The IFDM formulation emphasizes the direct representation of the conservation laws in relating the rates of change of fluid mass and solute mass in each nodal block to the fluxes over the interfaces bounding that block (Edwards 1972; Narasimhan and Witherspoon 1976). The evaluation of the rates of change and the fluxes over the boundary surfaces

upstream value; that is $C_{i+1/2}=C_{i+1}$ if fluid flows from i+1 to i. In other words, a backward difference $C_{i+1} - C_i$, is used for the convective term at node i. The upstream weighting eliminates the oscillation but introduces a space discretization error, called numerical dispersion, which produces the same effect as physical dispersion. The error of numerical dispersion in the upstream weighting scheme and the error of numerical oscillation in the central weighting scheme may be minimized by using the partial upstream weighting $C_{i+1/2} = a\,C_{i+1} + (1-a)\,C_i$ with $0.5 \leq a \leq 1$, or discontinuous weighting with central weighting at low flow velocity and upstream weighting at high flow velocity. Other weighting scheme have also been devised.

Integrated Finite Difference Method

The integrated finite difference method (IFDM) is a more flexible version of the finite difference method. In the integrated finite difference method, the distribution of nodal points may form an irregular mesh, and the nodal blocks may be arbitrarily shaped polyhedrons. The numerical equations are formulated from the integral form of the governing equations, as opposed to the simpler finite difference methods that employ the differential form of the governing equations. The IFDM formulation emphasizes the direct representation of the conservation laws in relating the rates of change of fluid mass and solute mass in each nodal block to the fluxes over the interfaces bounding that block (Edwards 1972; Narasimhan and Witherspoon 1976). The equations relate the rates of change and the fluxes over the boundary surfaces

polynomials (linear, quadratic, or cubic) are frequently used as linearly independent basis functions for the interpolation. If both state and space variables in a problem are interpolated with the same function, the element is referred to as an isoparametric element. For linear interpolation the values at the corner nodes are sufficient to define the basis functions for the interpolation. For quadratic or cubic interpolations the basis functions are specified with either the values at additional side nodes or the values of the partial derivatives of the variable at the corner nodes. For example, the three dimensional Hermite interpolation functions are a set of four cubic polynomials defined by the value and its three partial derivates at each corner node.

The finite element numerical equations are usually formulated with either the weighted residual Galerkin scheme or the variational approach. In the Galerkin finite element scheme a trial solution made up of an expansion of basis functions is substituted into the differential equations. The space differential operators operate on the basis functions. The residual of the trial solution is integrated over the element, weighted by the same basis functions. The integration is usually carried out using two or three point Gaussian integration for each dimension. If the trial solution were to be expanded in terms of a complete set of an infinite number of linearly independent basis functions, the trial solution would be exact and the residuals would vanish. In the Galerkin method the number of basis functions is finite and the residuals are forced to be zero by requiring orthogonality of the residuals to the set of basis functions used in the trial solution. For the convective terms the problems

of numerical oscillation and numerical dispersion also exist in the finite element method. Upstream basis functions can be used to minimize these effects.

An equivalent expression of the governing partial differential equations can be given in terms of variation of functionals. A functional is a function of functions such as an integral over space with the integral composed of basis functions. Upon minimization of an appropriate functional the corresponding differential equations emerge. The variational approach for fluid flow or solute transport is based on the same minimum energy principle or Lagrangian formulation as that used to study the equilibrium states in mechanics or stress analysis. In the variational approach to the finite element method, the trial solutions, expansions in basis functions, are substituted into the functional integrals. The differential operators in the functional integrals operate on the basis functions in a manner similar to that in the weighted residual procedure of the Galerkin formulation.

With the use of the Gaussian algorithm for element integration, the coefficients K and D in the second order terms and v in the convection term are evaluated at the Gaussian points within an element. This is different from the finite difference method with the coefficients calculated at the interfaces between blocks. The finite element method with the use of the basis function interpolation over more than two points, can evaluate gradients in both normal and tangential directions and handle censorial quantities more easily.

Flow Path Network Method

Instead of solving the governing differential equation for solute transport, the solute concentration can also be determined by calculating the motion of a large number of discrete solute particles. At each time step he new position of a solute particle is determined by the fluid particle velocity, the retardation factor and the dispersivity. Each particle is also assigned a weight which can be changed at each time step to account for radioactive decay, creation of new daughter nucleides, or chemical reactions. With the position and weight of each particle varying over time, the concentration of each species is calculated for a set of cells by summing the weight of the particles of that species in each cell and dividing by the volume of water in the cell.

Different schemes can be used to account for solute dispersion in determining the position of each particle. One approach is to use random numbers uniformly distributed between -Ø.5 and +Ø.5 to determine the forward or backward net dispersive displacement in each time step (Ahlstrom et. al. 1977n Schwartz and Crowe, 198Ø). With the use of a large number of discrete point particles, the random number approach may adequately represent solute dispersion. Another approach is to consider a given distribution (e.g. Gaussian) for solute particle velocity. Dispersion is treated by dividing the solute in each cell into packets with different velocities which are chosen so as to divide the velocity distribution into intervals of equal area (Campbell et

boundary and each node is surrounded by several elements. Although the transient term can be handled easily in the finite element formulation, the mathematical relationship between the rate of accumulation associated with a block and the fluxes evaluated at the Gaussian points in the surrounding elements is an indirect representation of the conservation law.

Implicit Equations

With either the finite difference or the finite element method the analysis of the transient equation results in a system of equations of the matrix from

$$[A]\left\{\frac{df}{dt}\right\} + [B]\{f\} + \{R\} = 0$$

where the column {f} contains the nodal values of pressure and solute concentrations. The coefficient matrix [A] contains the coefficients of the fluid and solute storage capacity associated with the time derivate $\{df/dt\}$, [B] contains the spatial approximations (finite difference or finite element) of the fluxes, and {R} contains the known information such as source/sink or boundary conditions.

The first order temporal finite difference from time t to $t+\Delta t$ is

$$\left\{\frac{df}{dt}\right\} \approx \frac{\{f\}_{t+\Delta t} - \{f\}_t}{\Delta t}$$

To solve for the unknown $\{f\}_{t+\Delta t}$ from the known solution $\{f\}_t$, the other terms in the governing equations can be interpolated between $t+\Delta t$ & t. With linear interpolation the matrix equation becomes

$$\frac{[A]}{\Delta t}\left(\{f\}_{t+\Delta t} - \{f\}_t\right) + [B]\left(\lambda\{f\}_{t+\Delta t} + (1-\lambda)\{f\}_t\right) + \lambda\{R\}_{t+\Delta t} + (1-\lambda)\{R\}_t = 0$$

For the forward differencing explicit scheme the interpolation factor λ equals zero, and $\{\delta\}_{t+\Delta t}$ can be easily determined by multiplying the matrix equation by $\Delta t[A]^{-1}$. The explicit scheme generally requires a minimum of computational effort. However it is only conditionally stable. Usually, implicit scheme with interpolation factor $0.5 \leq \lambda \leq 1$ are stable. The central differencing Crank-Nicholson scheme ($\lambda = 0.5$) is accurate in t to second order. The backward differencing implicit scheme ($\lambda = 1.0$) is usually unconditionally stable and is correct in time to first order.

Coupling Solution Schemes

The coupled equations of pressure and concentration can be solved either sequentially or simultaneously. The sequential method solves the equations separately and treats the variables as unknowns only when their respective equations are being solved. The fluid flow equation for pressure is solved first. Then the transport equation for concentration is solved using the velocity field calculated from the Darcy's equation based on the new values of pressure. The coupled equations can be solved simultaneously, which involves larger matrices and therefore greater computor time and storage requirements.

The main features of the various numerical methods are:

(a) The solution is sought for the numerical values of state Implicit Equation specified points in the space and time domains defined for the problem (rather than their continuous variations in these domains).

(b) The partial differential equations that represent balances of the considered extensive quantities are replaced by a set of algebraic equations written in terms of the sought, discrete values of the state variables at the discrete points in space and time mentioned in (a).

(c) The solution is obtained for a specified set of numerical values of the various model coefficients (rather than as general relationships in terms of these coefficients).

(d) Because of the very large number of equations that have to be solved simultaneously, a computer code has to be prepared in order to obtain a solution, using a digital computer.

Sometimes, the term numerical model is used, rather than speaking of a 'numerical method of solution' (of the mathematical model). This is justified on the grounds that a number of assumptions are introduced, in addition to those underlying the mathematical model. This makes the numerical model a 'model in its own right. It represents a different approximate version of the real system. It is sometimes possible to pass directly from the conceptual model to the numerical one, without first establishing a mathematical model. The numerical model has its own set of coefficients that have to be identified before the model can be used for any particular problem.

It is of interest to note that even those who consider the numerical model as one in its own right, very often validate it by comparing its predictions with those obtained analytically from a mathematical one (for relatively simple cases for which

such solutions can be derived). One of the main reasons for such a validation is the wish to eliminate errors resulting from the numerical approximations alone.

Another important feature of modeling, closely associated with the problem of parameter identification is that of uncertainty. We are uncertain about whether the selected conceptual model (i.e. our set of assumptions) indeed represents what happens in the real aquifer system, albeit to the accepted degree of approximation. Further more, even when employing some identification technique, we are uncertain about the values of the coefficients to be used in the model. Possible errors in observed data used for parameter identification also contribute to uncertainty in model parameters. As a consequence, we should also expect uncertainty in the values of the state variables predicted by the model. These considerations pave the way to the development of stochastic models. In the latter, the information on coefficients appears in the form of probability distributions of values, rather than as deterministic ones. These probability distributions are derived by appropriate methods of solving the inverse problem, where the input data also appears in probabilistic forms. Probabilistic values of model coefficients, will yield probabilistic predicted values of state variables.

A large number of researchers are currently engaged in developing methods that incorporate the element of uncertainty in both the forecasting and the inverse problems. Hopefully more such methods will be made available to the practicing modeller in the future.

Some of the advantages of applying numerical methods for the study of solute transport in the subsurface are listed below.

1.Spatial and temporal variation of system properties such as hydraulic conductivity,porosity,and dispersivity can be easily managed with numerical methods.

2.Field problems with complex boundary conditions are simple to handle with numerical methods.

3.Three dimensional transient problems can be treated without much difficulty.

Some of the important limitations of numerical methods are listed below.

1.Application of a complex numerical problems requires a certain level of user familiarity with the programme.Achievement of such a familiarity is time consuming and could be prohibitive either when dealing with urgent problems or when funding is limited.

2.Very often errors due to numerical dispersion overshadow the physical dispersion of the solute within the porous medium.

3.Preparation of input data for numerical codes often takes a long time. Even if one wishes to solve a simple problem which is manageable with analytical or semi-analytical methods,far greater time is needed to prepare the input data for a numerical code.

2.3.3 The mechanisms affecting the transport of a pollutant in a porous medium are: advective, dispersive, and diffusive fluxes, solid solute interactions and various chemical reactions and decay phenomena, which may be regarded as source sink phenomena for the solute . In general,we may have a convective mass transport in both a laminar flow regime,where the liquid moves along definite paths that may be averaged to yield streamlines,and a turbulent flow regime,where the turbulence may cause yet an additional mixing . An additional mass transport phenomenon,which occurs simultaneously with mechanical dispersion,is that caused by molecular diffusion resulting from variation in tracer concentration within the liquid phase.

Molecular diffusion produces an additional flux of tracer particles(at the microscopic level) from regions of higher tracer concentrations to those of lower ones . This means,for example,that as the tracer is spread along each microscopic stream tube as a result of mechanical dispersion,and a tracer concentration gradient is produced,molecular diffusion will tend to equalise the concentrations along the stream tube the same time,a tracer concentration gradient will also be produced between adjacent streamlines,causing lateral molecular diffusion across the stream tubes Dispersion term is used to denote the spreading (at the macroscopic level) resulting from both mechanical dispersion and molecular diffusion.

OCCURRENCE OF DISPERSION PHENOMENA

Hydrodynamic dispersion phenomena occur in many problems of groundwater flow, in chemical engineering in oil reservoir engineering etc. In groundwater flow, we encounter it in

(a) The continuous variation of the concentration of some specific polluting constituents, or of total dissolved solids, as flow takes place in an aquifer.

(b) Groundwater pollution from some localized source, such as a faulty sewage installation or waste dump.

(c) Groundwater pollution from a distributed source, such as fertilizers and pesticides applied to the area overlying an aquifer.

(d) Sea water intrusion into a coastal aquifer, producing a transition zone from fresh water to sea water.

(e) Encroachment of saline, or brackish water, into an aquifer as a result of changes in the hydrologic regime.

(f) Seepage of polluted surface water through pervious river beds or lakes.

(g) The movement of pollutants from the ground surface to the underlying water table, under unsaturated flow conditions e.g., the movement of fertilizers or the leaching of salts from the soil in agriculture.

(h) Changes in the quality of water in an aquifer as a result of artificial recharge water spreading in it. Sometimes, reclaimed sewage is used to recharge an aquifer.

In all these cases, we are seeking some tool which should enable us to predict the concentration changes that will occur as a result of planned operations superimposed on the natural flow regime in an aquifer.

COEFFICIENTS OF DISPERSION

A large number of articles have been published in the professional journals mainly in the period 195Ø-197Ø, in which theories on dispersion have been developed. Detailed summaries are given, among others by Bear (1969, [redacted] and 1972 [redacted]) and Fried (1975). The main effort has been to express hydrodynamic dispersion macroscopically through a partial differential equation and to determine the nature of the coefficients which appear in this equation. Of special interest is the relationship between these coefficients and matrix and flow parameters.

Two approaches are commonly employed. In the first one, the porous medium is replaced by a fictitious, greatly simplified, model in which the spreading of a solute that occurs can be analyzed by exact mathematical methods. A single capillary tube, a bundle of capillaries, an array of mixing cells, are examples of such models. The second approach is to construct a statistical (conceptual) model of the microscopic motion of solute particles and to average these motions occupied by a considered phase (water in unsaturated flow) which in turn, is a function of the saturation. Similarly, the components of the tortuous tensor are also a function of the saturation. Hence, when we consider unsat-

urated flow in an isotropic medium, we have to verify that the isotropy of remains for all saturations.

2.3.4 THE FUNDAMENTALS OF BALANCE EQUATION

Five components should be taken into account in the construction of a balance equation for a constituent.

(i) The quantity of the pollutant entering and leaving a control volume around a considered point by advection dispersion and diffusion.

(ii) Pollutant leaving the fluid phase through the water solid interface as a result of chemical or electrical interactions between the pollutant and the solid surface.

(iii) Pollutant added to the water (or leaving it) was a result of chemical interactions among species inside the water or by various decay phenomena.

(iv) Pollutant may be added by injecting polluted water into a porous medium domain, e.g. as part of artificial recharge or waste disposal operations. Pollutant may be removed from a porous medium domain by withdrawing (polluted) water, e.g. by pumping. With $P(x,t)$ and $R(x,t)$ denoting the rates of water withdrawn or added, respectively, per unit volume of porous medium per unit time, and $C(x,t)$ and $Ck(x,t)$ denoting pollutants concentration in the water present in the porous medium and in the water added by injection, respectively,

the total quantity of pollutant added per unit volume of porous medium per unit time is expressed by

$$RC_R - P_c$$

(v) As a result of the above components, the quantity of the pollutant is increased within a control box. With denoting the mass of a pollutant per unit volume of porous medium denotes the rate at which this quantity increases.

2.3.5 GENERAL STATEMENT OF POLLUTION MODEL

The complete model of a pollution problem consists of the following items:

(i) Specification of the geometrical configuration of the closed surface that bounds the problem area, with possible segments at infinity.

(ii) Specification of the dependent variable(s) of the pollution problem i.e. the concentration of the specific constituent or constituents under consideration.

(iii) Statement of a partial differential (balance) equation, for every relevant species. Balance equations, in terms of the various state variables of the problem, as listed in (ii) above, are also required for every extensive quantity that is relevant to the problem.

(iv) Specification of the numerical values of the (transport and storage) coefficients that appear in (ii) Of special inter-

est here is the information on the dispersivity and on the coefficient of molecular diffusion in the porous medium under consideration.

(v) Statement of the numerical values of the various source and sink terms that appear in (ii)

(vi) Statement of initial and boundary conditions that the state variables appearing in (ii) have to satisfy within the considered domain.

A complete numerical scheme for groundwater quality modelling is depicted in the flow chart through Annexure -1

2.3.6 DATA NEEDS

Analytical and Semi-analytical Methods

The data needed for these methods are generally simple. The following is a list of data usually required for analytical methods.

1.Geometry of the system,positions ofvarious significant hydrogeologic features,and means of groundwater discharge.

2.Direction and magnitude of average regional fluid velocity in the vicinity of the study area.

3.Sufficient information about the concentration of different solute species and the rate of leaching and injection,as well as the history of operation at the individual disposal facilities.

4.A representative value of longitudinal dispersivity for one-dimensional problem and both longitudinal and transverse dispersivities for two-dimensional problems.

5.Retardation factor or distribution coefficient for solute which can be adsorbed onto the media and the radioactive decay factor,if appropriate.

Except for the fourth item,the data mentioned above are also required for semi-analytical methods.

Numerical Methods

The following is a list of data needed to predict the extent of contamination in a groundwater system by use of a numerical model.

1.Geometry of the system .

2.Velocity distribution throughout the system.

3.Dispersivity distribution within the system.

4.Present distribution of concentration of various solute species in the system.

5.Complete information about present and future sources of contamination.

6.Location of natural and artificial discharge areas in the system including production wells.

2.3.7 SELECTION OF METHOD

In general ,there are two types of problems which should be solved by employing solute transport theory.

(1) to assess the environmental impact of subsurface waste disposal at a proposed site,and

(2) to assess the long term consequences or the effects of remedial measures at an operating site where a contaminant plume has already been detected.

First problem should be solved in two or three different stages . In the preliminary stage of study ,one needs a very rough estimate of the problem extent of contamination at some point in the future. This can help determine whether the potential site should be eliminated or kept for further extensive studies. There is often little initial data to work with suggesting that analytical methods are the most useful tools in the hand of the investigator. As discussed previously, the amount of data required for these methods is relatively small and application of the techniques is fast and simple, so that the effect of uncertainties in the data can be easily evaluated in a short period of time by simply rerunning a problem with different estimates.

If the site involves several sources of contamination and one or more production wells, one has to resort to semi-analytical methods. These methods are satisfy the limited data

constraints mentioned above.

Once it is established that the site is relatively safe but further study is needed the problem enters the next stage. The next state of study requires a detailed site characterization and further application of the analytical and semi-analytical methods, based on more reliable data. Application of simple numerical methods may also be advisable at this stage.

3.Ø REVIEW OF WORK DONE ON MODELLING ABROAD

The first quantitative study of diffusion was made by Fick in 1855 through an analog between molecular diffusion and heat transfer by conduction . In between 1953 and 1972 the mathematical modélling of solute transport in saturated soil has been started and developed to describe and predict pollution behaviour in aquifer(Fried,1981).

3.1 Analytical Solutions :

The governing partial differential equation describing solute transport is usually written as

$$\frac{\delta}{\delta x_i}\left[D_{ij}\frac{\delta C}{\delta x_j}\right] - \frac{\delta}{\delta x_i}(C v_i) - \frac{C' W^*}{n} + \sum_{K=1}^{N} R_k = \frac{\delta C}{\delta t} \quad \text{——①}$$

Where

$$v_i = \frac{-K_{ij}}{n} \cdot \frac{\delta h}{\delta x_j}$$

and

C => Solute concentration

Vi = Seepage or average pore water velocity in the direction Xi

Dij = Dispersion coefficient tensor

C' = Solute concentration in the source or sink fluid

W* = Volume flow rate per unit volume of the source or sink

n = effective porosity

h = hydraulic head

Kij = hydraulic conductivity tensor

Rk = Rate of solute production in reaction k of n different reactions

Xi = Cartesian coordinate.

In general , Vi is a function of both time and space. Distribution of hydraulic head h at different times should be obtained from the solution of the following equation

$$\frac{\delta}{\delta x_i}\left[K_{ij}\frac{\delta h}{\delta x_j}\right] = S_s\frac{\delta h}{\delta t} + W^*$$

where Ss = specific storage

Grove(1976) gave the equation for Rk for equilibrium controlled ion exchange, as

$$\sum_{k=1}^{N} R_k = -\frac{\rho_b}{n}\cdot\frac{\delta \bar{C}}{\delta t}$$

Where ρ_b is bulk density of the solid

$\bar{C}$ is concentration of species adsorbed on the solid

The relation between adsorbed concentration $\bar{C}$ and the solute concentration C , considering equilibrium transport and assuming that the adsorption isotherm follows a linear and reversible law, is given by

$$\bar{C} = Kd\ C$$

Where Kd is called distribution coefficient

Now equation 1 becomes

$$\frac{\delta}{\delta x_i}\left[D_{ij}\frac{\delta C}{\delta x_j}\right] - \frac{\delta}{\delta x_i}(cv_i) - \frac{c'w^*}{n} = R\frac{\delta c}{\delta t}$$

Where $R = \left[1 + \frac{\rho_b K_d}{n}\right]$ and is called Retardation factor

For one dimensional flow , Davis and Dewiest (1966) shows that,

$$R = V/Vc$$

Where V is the groundwater velocity

and Vc is velocity of contaminants.

Radio-active decay can be incorporated in the term Rk in 1

According to Anderson (1979),

Radioactive decay reaction is given by $-\lambda\left[C + \frac{\rho_b \bar{C}}{n}\right]$

Where λ is the radioactive constant.

Finally ; $$\frac{\delta}{\delta x_i}\left[Dij\ \frac{\delta C}{\delta x_j}\right] - \frac{\delta}{\delta x_i}(C v_i) - \frac{C' W^*}{n} - \lambda C R = R\frac{\delta C}{\delta t}$$

Analytical solution of the equation for anisotropic media is a problem.

For homogeneous and isotropic media under steady state uniform flow without considering recharge and discharge, it becomes

$$\frac{\delta}{\delta x_i}\left[Dij\ \frac{\delta C}{\delta x_j}\right] - v_i \frac{\delta C}{\delta x_i} - \lambda C R = R\frac{\delta C}{\delta t}$$

Where $v_i = -\frac{k}{n}\frac{\delta h}{\delta x_i}$ and $\frac{\delta^2 h}{\delta x_i^2} = 0$

Usually Dij the dispersion coefficient tensor is the result of two processes , molecular diffusion and mechanical mixing. Diffusion is the process whereby ionic or molecular constituents move under the influence of their kinetic activity in the direction of their concentration gradient.

Molecular Diffusion

Fick's first law expressed as,

$$F = -D^* (dC/dx),$$

describes the process of molecular diffusion where F is the mass flux of solute and D* is diffusion coefficient . Values of D* for major ions may be obtained from Robinson and Stokes (1965). In porous media the effective diffusion coefficient is generally smaller if the effective diffusion coefficient is shown by D then

$$D = w D^*$$

Where w is a number less than 1 and should be determined empirically. Perkins and Johnston (1963) suggested that the value of w is approximately Ø.7Ø7 . Bear (1972) suggest that w is equivalent Tortuosity of the granular medium with a value close to Ø.67.

Mechanical Mixing

The physical phenomena considered in solute transport process through constitutive theory was first given by Scheldegger(1961).He identified that the mechanical mixing component of the dispersion process is the result of velocity variations within the porous medium and is dispersion coefficient is directly proportional to seepage velocity.

Hence $D_{ij} = \alpha_{ijlm} \frac{V_l V_m}{V}$

Where α_{ijlm} is the fourth rank tensor

Vi and Vm is the velocity components

V is the magnitude of velocity vector.

Again here the analytical solution is a problem for anisotropic media.

Josselin and Dejong (1972) show the dispersion coefficient is a tensor of infinite rank for anisotropic media.

Bachmat and Bear (1964) have discussed the general form of dispersion coefficient for an isotropic medium in Cartesian coordinate system .That is

$$Dij = aii.\delta ij\, V + (a_i - a_{ii})\frac{V_i V_j}{V}$$

Where Dij is the dispersion coefficient tensor

ai is the longitudinal dispersivity of medium

aii is the transverse dispersivity of the medium

δ_{ij} is Kornecker Delta function = Ø for i = j

Applying Laplace transform technique,Bear,196Ø (Bear,1979) has obtained analytical solution to the partial differential equation for change of concentration with time.

$$\frac{\delta C}{\delta t} = D_h \frac{\delta^2 C}{\delta x^2} - \frac{q}{n}\frac{\delta C}{\delta x}, \quad -\infty < x < \infty$$

Where n = porosity

q = Darcy velocity

$Dh = \frac{\alpha_L |v|}{n} + D_d^*$ = Coefficient of hydrodynamic dispersion

Bear has assumed a steady state uniform flow condition. Initial and boundary conditions are stipulated as below.

$t \leq 0, \quad -\infty < X < 0, \quad C = Co$

$0 \leq x \leq +\infty, \quad C = C_1$

$t > 0, \quad x = \pm\infty \quad \frac{\delta c}{\delta x} = 0$

$x = -\infty, \quad C = C_0$

$x = +\infty, \quad C = C_1$

Ogata and Banks (1961) gave the solution to one-dimensional advective dispersive equation for a step function input of tracer :

$$\frac{C}{C_0} = \frac{1}{2}\left[erfc\left[\frac{x-vt}{2\sqrt{Dt}}\right] + \exp\left(\frac{Vx}{D}\right) erfc\left[\frac{x+vt}{2\sqrt{Dt}}\right]\right]$$

Where erfc(.) = complementary arror function,

x = distance,

t = the time after input,

v = the pore velocity,

D = dispersion coefficient,

Co = concentration of tracer in input, and

C = concentration at a distance x from the input.

This solution is mostly used to predict the amount of pollutant at a distance from the source.

Marino (1974) has solved one-dimensional advection dispersion equation by applying Laplace transform technique. A uni-directional flow field has been assumed in the semi infinite flow medium. The solution has been studied for the following initial

and boundary conditions:

$$C(x,\emptyset) = \emptyset \; ; \; x > \emptyset$$

$$C(\emptyset,t) = Co\, e^{-Yt} \; ; \; t > \emptyset$$

$$C(\infty,t) = \emptyset \; ; \; t > \emptyset$$

Hunt (1978) has shown that many of the solutions for one-dimensional advection dispersion problem, which have been obtained assuming a uniform flow field, are analogous to the solution of heat conduction equation given by Turner, 1972 (Hunt, 1978). Solutions have been given for instantaneous, continuous and steady state point sources of pollution in a uniform flow field. Hunt has determined the effect of a finite aquifer depth upon solution for an aquifer of infinite depth.

Using Laplace transform technique Van Genuchten(1982) has obtained analytical solution for one-dimensional convective-dispersive transport equation considering decay and absorption of a chemical which is injected at one end of an infinitely long homogeneous-isotropic porous medium . Van Genuchten has assumed steady state uniform velocity in the column. The solution has been obtained for the following initial and boundary conditions:

$$C(x,\emptyset) = \emptyset$$

$$\left.\frac{\delta c(x,t)}{\delta x}\right|_{x=\infty} = 0 \quad , \quad \left[-D\frac{\delta c}{\delta x} + v.c\right]_{x=0} = v.f(t)$$

$f(t) = Co \exp(-\alpha t)$, $\emptyset < t \leq to$

$f(t) = \emptyset$, $t > to$, where Co and α are constant and v is the seepage velocity.

Several analytical solutions for two dimensional dispersion problems are available, Ogata (1970) and Cleary and Ungs (1978) have described some of these solutions, however many of them do not represent a realistic field problem.

3.2 Cell Models Developed for Study of Leaching

The theory of leaching developed in drainage engineering basically deals with solute movement through porous media. The various theoretical models which have been proposed in drainage engineering to illustrate the process of solute movement through porous materials are (Vander Molen. 1979)

i) Single reservoir,

ii) Single reservoir with bypass

iii) series of reservoir and

iv) Continuous column.

Of these four models the series of reservoir and continuous column models are of relevance for analysing solute transport in aquifer. In the series of reservoir model, the flow domain is assumed to consists of a series of similar reservoirs, and in each reservoir, the influent is assumed to bet completely mixed with the water previously present in the reservoir before it leaves as effluent. If the concentration of the solute in the influent to the first reservoir is C_0 and C_I is the initial concentration in each reservoir. the solute concentration in the Nth reservoir is given by

$$C_N = C_0 + (C_I - C_0)\, e^{-\frac{t}{t_0}} \sum_{n=0}^{N-1} \left[1 + \frac{t^n}{\lfloor n\, t_0^n} \right]$$

in which to = filling time .Time t is measured since the entry of effluent to the first reservoir.

The continuous column model has been developed by Glueckauf (1949). The soil profile is in fact not made up of several separate reservoirs, but forms a continuous column. Mixing takes place at every depth, but is effective over a limited range. Glueckauf has given the following expression for solute concentration:

$$C = \frac{1}{2} C_I \left[erfc \left[\frac{H - \phi x}{2H} \cdot \frac{\sqrt{H}}{\phi \Delta x} \right] - \exp(x/\Delta x)\, erfc \left[\frac{H + \phi x}{2H} \cdot \frac{\sqrt{H}}{\phi \Delta x} \right] \right]$$

where

$2\Delta x$ = effective mixing length

C_I = original salt concentration in soil moisture

H = depth of water percolated since the beginning of leaching

ϕ = volume fraction of soil filled with water, and

x = depth.

Cell Models Developed for Study of Solute Transport

Wentworth (1948) has suggested perfect mixing model in an array of cells to explain development of transition zone at a moving interface between salt water and freshwater.

Aris and Amundson (1957) have presented an analysis of dispersion as a process of mixing in cells. Comparison of cell

mixing and diffusion mechanism have been made. For (q/v) t = 100, where v= interstitial velocity and q= flow rate, the two mechanism give distribution plots which are indistinguishable.

A simplified model developed by Bear (1972) for the study of one-dimensional dispersion consists of an array of small cells with interconnecting short channels. Bear has assumed that when a liquid with a certain tracer concentration enters a cell occupied by a liquid of different concentration, it displaces part of it, while the liquid remaining in the cell immediately mix to form a new homogeneous liquid. Bear has designated such a cell as a perfect mixer. To obtain perfect mixing. Bear has postulated that the true movement of tracer particles because of molecular diffusion or turbulence must be faster than the average liquid flow. In the analysis suggested by Bear the dispersion phenomenon has been regarded as a combination of two processes (a) a complete mixing in the elementary cell, and (b) translation at average flow velocity from one cell to next through the connecting channels. Designating as the tracer concentration in the liquid entering the jth cell of an array, and C as the concentration in the liquid leaving the jth cell. and performing a tracer balance, the following first order differential equation has been derived by Bear:

$$\frac{\delta C_j^{(0)}(t)}{\delta t} + \frac{C_j^{(0)}(t)}{\tau} = \frac{C_j^{(i)}(t)}{\tau}$$

where τ is the average residence time given by V/Q V is the volume of the cell and Q is the discharge. The solution of the above differential equation given by Bear is

$$C_j^{(0)}(t) = \exp(-t/\tau)\left[\int_0^t \frac{1}{\tau} \exp.(t/\tau).\, C_j^{(i)}(t)\, dt + \text{const}\right]$$

For a constant inflow of concentration C_0 in the first cell and with τ = constant for all cell Bear has derived the following expression:

$$C_j^{(0)} = C_0 \left[1 - \exp(-t/\tau) \sum_{i=1}^{j-1} \frac{1}{i!} \left(\frac{t}{\tau}\right)^i \right]$$

Bear has further proved that if $\Delta l'$ is the length of a mixing cel, and Δl is the distance between centres of cells, a medium property that has been called as the medium's longitudinal dispersivity is found to be equal to $\frac{1}{2} (\Delta l')^2 / \Delta l$.

A simple lumped conceptual model based on a well mixed linear reservoir concept applicable to cases with limited data on aquifer has been developed and applied to simulate the impact of highway deicing salt on ground water quality in Massachusetts (Celhar and Wilson, 1974). The results obtained by digital computer simulation have been found to compare well with observed trends over a 15-year period.

A cell-in-series formulation to simulate riverine transport of dissolved material has been recognised by Stefan and Demetracopoulos (1981) as an alternative way of mass transport modelling in one-dimensional system. The cell in series model has a basic equation that is an ordinary first order differential equation instead of a partial differential equation as used in one dimensional advection dispersion equation.

It has been shown that a cells-in-series model is as good as advection dispersion model. The cells in series model is useful for slowly moving and highly dispersive rivers.

3.3 Computer Codes

With the formulation of governing equations and numerical methods, a specific computer code can be developed by constructing an algorithm, eliminating coding errors, running sample problems, and producing a user"s guide. Many codes are initially developed to model a specific class of problems. When a code is used for other problems, modifications can be added to generalize the code capabilities. The versatility and efficiency of a code can also be improved by adopting better solution schemes and numerical methods. In many cases a code becomes a well established and powerful tool as the result of efforts by both competent developers and experienced users.

With the growing concern over contaminant transport in the environment in the past few years many codes for fluid flow and solute transport have been developed. Organizations such as EPA, NRC, and DOE, among others, have sponsored several surveys to review the capabilities of various codes. The focus of one EPA study (Bachmat et.al. 1978) is on water resource management. As a result of the EPA study, an International Ground Water Modeling Center has been established at Holland Research Institute (Butler University, Indianapolis) to continuously gather information and produce training program for groundwater modeling. In addition to the concern over water quality, the need to predict radionuclide transport from underground repository construction and operation also contributes to the development of transport modeling. DOE and NRC also sponsor surveys on fluid flow and solute transport

(e.g. Science Applications, Inc.1981: Thomas et. al. 1982).Annexure 2,3,& 4 summerizes the main characteristics of a number of finite difference,finite element and flow path network codes,respectively till year 1983.

Traditionally groundwater quality modelling has been based on distributed system representation of the groundwater flow . E.g.,Maddaus and Aaronson (1972) used a computer based finite difference model of two-dimensional aquifer flow to predict quality trends throughout a groundwater basin . Lyons and Stewart (1973) developed a distributed two-dimensional finite difference aquifer model coupled with a storage effect for the unsaturated zone to predict TDS in a basin . Pinder (1973) used the finite element method to predict concentration distribution in an aquifer including the effects of hydrodynamic dispersion.

Konikow and Beredehoeft (1974) have demonstrated the application of a numerical model which includes dispersion to water quality simulation in an irrigated stream-aquifer system,but the model requires extensive field data . Elaborate digital models have been used to evaluate the groundwater quality hazards of the AEC Hanford Project(Cearlock,1971).Lumped parameter models have been used in predicting the salinity of irrigation return flows(e.g.,Hornsby,1973;Thomas,Riley and Isralsen,1972).

3.4 United States Geological Survey has developed number of generalised codes e.g. MOC,SUTRA,and MOD-3D.

SUTRA (Saturated-Unsaturated Transport) is a computer program which simulates fluid movement and transport of either

energy or dissolved substance in a subsurface environment. The model employs a two-dimensionaal hybrid finite element and integrated finite- difference method to approximate the governing equations that describe the two interdependent processes that are simulated:

1) fluid density-dependent saturated or unsaturated groundwater flow and either

(2a) transport of a solute in the ground water, in which the solute may be subject to: equilibrium adsorption on the porous matrix, and both first-order and zero-order production or decay,

2b) transport of thermal energy in the ground water and solid matrix of the aquifer.

SUTRA is primarily intended for two dimensional simulation of flow, and either solute or energy transport in saturated variable density systems. While unsaturated flow and transport processes are included to allow simulation of some unsaturated problems, SUTRA numerical algorithms are not specialized for the non-linearities of unsaturated flow as would be required of a model simulating only unsaturated flow. Lacking these special methods. SUTRA requires fine spatial and temporal discretization for unsaturated flow., and is therefore not an economical tool for extensive unsaturated flow modeling. The general unsaturated capability is implemented in SUTRA because it fits simply in the structure of other non-linear coefficients involved in density dependent flow and transport simulation without requiring special algorithms.

SUTRA Processes

Simulation using SUTRA is in two space dimensions, although a three-dimensional quality is provided in that the thickness of the two-dimensional region in the third direction may vary from point to point. Simulation may be done in either the areal plane or in a cross sectional view. The spatial coordinate system may be either Cartesian (s,y) or radial cylindrical (r,z). Areal simulation is usually physically unrealistic for variable-density fluid problems.

Groundwater flow is simulated through numerical solution of a fluid mass balance equation. The groundwater system may be either saturated, or partly or completely unsaturated. Fluid may be constant, or vary as a function of solute concentrations of fluid temperature.

SUTRA tracks the transport of either solute mass or energy in the flowing groundwater through a unified equation which represents the transport of either solute or energy. Solute transport is simulated through numerical solution of a solute mass balance equation where solute concentration may affect fluid density. The single solute species may be transported conservatively, or it may undergo equilibrium sorption (through linear, Freundlich or Langmuir isotherms). In addition, the solute may be produced or decay through first-or-zero-order processes.

Energy transport is simulated though numerical solution of an energy balance equation. The solid grains of the aquifer

matrix and fluid are locally assumed to have equal temperature, and fluid density and viscosity may be affected by the temperature.

Almost all aquifer material, flow, and transport parameters may vary in value throughout the simulated region. Sources and boundary conditions of fluid, solute and energy may be specified to vary with time or may be constant.

SUTRA dispersion processes include diffusion and two types of fluid velocity-dependent dispersion. The standard dispersion model for isotropic media assumes direction independent values of longitudinal and transverse dispersivity. A velocity dependent dispersion process for anisotropic media is also provided and is introduced in the SUTRA documentation. This process assumes that longitudinal dispersivity varies depending on the angle between the flow direction and the principal axis of aquifer permeability when permeability is anisotropic.

SUTRA simulation is based on hybridization of finite element and integrated finite difference methods employed in the framework of a method of weighted residuals. The method is robust and accurate when employed with proper spatial and temporal discretization. Standard finite element approximations are employed only for terms in the balance equations which describe fluxes of fluid mass, solute mass and energy. All other non flux terms are approximated with a finite element mesh version of the integrated finite difference methods. The hybrid method is the simplest and most economical approach which preserves the mathematical elegance and geometric flexibility of fine element simulation, while

taking advantage of finite difference efficiency.A flow diagram is enclosed vide Annexure -5.

3.5 Review of the papers presented in International conference. On water quality modelling in the inland natural environment, Bournements, Eyland zone rise to following state of art of Atleins Research and Development, Survey, R.W. Raige et. al (1986), presented a computer programme from analysing groundwater flow and pollutant transport for sites where waste is to be buried in the ground at shallow depth. It is shown that ignoring non liner sorption mechanism for pollutant transport, calculations may have a significant effect on the resulted. The model results are compared with other computer programme reports for shallow land waste disposal etc.

H.S. Wheater et. al. (1983) of imperial college, London, identified the parametric relationships for the material properties, primarily the unsaturated hydraulic conductivity function, the soil moisture characteristic and the functional relationship for the coefficient of hydrodynamic dispersion from observed data. Alternate parameter estimates are compared with respect to experimental data for one dimensional flow and solute transport and the numerical model adopted is showing to be robust with respect to parameter variability.

H.C.Ammentorp et al. of Danish Hydraulic Institute Hoersholm and T.H. Christernsen of Dept. of Environmental Engineering, Lyagby (1986) developed a tool for evaluation of irrigation schemes in areas with salinity problems is the form of a numeri-

eal model for solute transport in the unsaturates zone, based on the basic equation for soil water flow is are dimension and the general convection dispersion equation options for solute soil reactions are included in the model comprising immobile water, absorption, in exchange, decay, complexation, precipitation, ionic strength effects on species activity and carbonali system covered PH.

Jems Chritian Refgard et. al. of Danish Hydraulic Institute Hoersholm and T.H. Christensen of Technical University of Denmarll Lyngby (1986) developed sub model to a general numerical model for solute transport is the unsaturated zone, comprising diffusive and convective transport of oxygen in soil air, convective transport and oxygen consumption in free water, and diffusive transport and a constant rate oxygen consumption in the water saturated crumbs. The oxygen model has been developed as a tool for making predictions of the behaviour of surface and waste water infiltration plants in order to optimize the operation of such plants.

G.B. Davis et.al. of CSIRO division of groundwater researchs, western Antrata generated two simple models of methane diffusion through the unsaturated zone at a liquid waste disposal site in Pertt, western Australia. Diffusive flux of methane from ground water at the site was estimated and found to compare with reported diffusive flux from other anoxic environment. Transport through the methane depleted zone by diffusive or dispersive mechanism is postulated as the rate limiting process governing volatilization is to the unsaturated zone at the test

site.

D. Tolikas et. al of Department of Civil Engineering Thessalonite, Greece presented a mathematical model for optimal groundwater quality management. Groundwater contamination is simulated by a two dimensional transport model which requires the numerical solution of the partial differential equation describing solute transport in one dimension only. Although linear programming problems are assumed in the present work, the proposed methodology can also be used in conjunction with other types of management problems.

R. Mockey of Department of Civil engineering New castle upon Type et. al developed a 2-D finite element model incorporating all the major groundwater flow controls. The data assigned to the nodes of the model are generated using a linear interpolation technique known as kriging.

3.6 . Second International conference held in Marrakesh,Morocco,1991 have acknowledged several studies conducted on groundwater and aquifer contamination modelling. H.W. Dargarter et al. from Anchen University of Technology (RWTH),Germany in their paper "Multiphase flow and transport modelling of surface contaminations by immiscible fluids", presents a numerical model for the simulation of coupled three phase flow and transport phenomena, including interface mass transfer processes. L Ait-sei et.al.of INRS,Canada, in their presentation "stochastic Modelling of the transport of pesticides in soils and Groundwater, Application to the Vulnerability of

wells", explains a transport model in saturated zone using finite difference technique to simulate flow, and the discrete parcel random walk method to simulate the solute transport. This model was couples with the unsaturated zone VULPEST model which uses the Monte-Carlo approach to desirable the stochastic process derived from the spatial variability of soil parameters . They conclude through demonstration that this model can be used in control and protection programmes of ground water Quality. K Ratsfelder et. al. from University of Michigan, USA , in their paper "Simulation of Immiscible Phase contaminant Transport on IBM/AT :personal Computers" developed a two dimensional numerical model for simulations of subsurface immiscible phase contaminant transport based on gas, water and organic phase mass balance equation named as VALORE model.

A.R. Bestman of International Center for Theoretical Physics,Italy,in his presentation on "The diffusion of Buried Matter and possible pollution of Aquifer in Presence of Hydrodynamic Dispersion" deals with the problem of diffusion of suried waste in a moist soil. The model is their used to predict the possible contaminants of aquifers situated at a given depth.

"A Vectorized Multicomponent Transport Reaction Models Theory and Application" by M.Vogt of Lahmeyer international GMBH Germany,presents a Vectorcomputer-oriented multicomponent transport reaction model. Through demonstration it has been shown that using this model it is possible to realize even large-scale simulations of coupled chemical and transport processes within a reasonable CPU scale.

C Bicheran et. al. of France in their paper " Comparison of the Behaviours of Two Mercurial compounds during their Transport through a Natural saturated porous medium". presents a study on the ability of an organic and a mineral pollutant to migrate through a saturated porous medium with short column experimental.

G. Genlile et. al from Italy in their paper "Application of FEM to 3D problem of Transport and Diffusion of pollutant into Aquifer" present the 3D Finite Element code SIVAF aimed at solving water flow and non-reactive pollutant transport in saturated/unsaturated porous media, through case study of salt intrusion in aquifer.

3.7 Case Studies

(i) Modelling of An Agricultural Site in Quebec City(1991)

The Site

The studied site is located in the region of Sainte Catherine-de-la-Jacques-Cartier (Portneus region) west of Quebec City. The cultivated lands in this region contain homogeneous soil consisting of marine and fluvial sand with medium to coarse grain sizes, and deposited on the Champlain sea clay with a thickness of about 20 m in some places. Potatoes are intensively grown in this region. In the eighties, a contamination by the pesticide aldicarb was noticed in some wells of this region . The granular form of aldicarb is applied during the sowing period (mid May) at the recommended rate of 2.24 kg/ha. It has a high solubility (60000 mg/t) and is leached by soil humidity. There is a water supply well which pumps water in the aquifer located at the center of the studied field. The depths of the well and the

aquifer are 5 m and 3 m respectively. The thickness of the aquifer affected by pumping is about 2m.

The Model

The developed bidimensional model MSTHP (Modele Stochastique du Transport Horizontal des Pesticides), consists of both flow and transport modules. The model is written in FORTRAN 77 on VAX 780 machine and uses the strongly implicit procedure (SIP; stone (14)) to solve the algebraic equations systems by finite differences. The VULPEST model (Villeneuve et al. (16)) is a stochastic model of pesticides transport in unsaturated zones. It uses the Monte Carlo technique to take into account the spatial variability of different parameters. For the linkage of VULPEST and MSTHP models concentrations reaching the water table and percolated water flux both computed by the VULPEST model form the input data to the MSTHP model . On a regional scale, the water flux infiltrated in the phreatic aquifer does not greatly modify its unsaturated thickness in comparison to its extent. Therefore, the flow has been considered in steady state, whereas the contaminant feeding of the aquifer by the pesticides is in transient regime.

Application

The application of the pesticide aldicarb was done during 1982 and 1983. The stochastic breakthrough curve of the pesticide concentration having reached the water table as calculated by the VULPEST, is shown in Figure 1. The concentration of pesticide in the water reaches its peak 6.5 months after every application. The maximum concentration reaching the water table were found to be about Ø.5 mg/l. This level exceeds largely the water quality

criterion of 9 pg/1 set by Health and Welfare Canada, and the one of 10 pg/1 of the US-EPA. The analysis of the water well at different periods of time, between 1984 and 1988 shows concentrations of the order of few pg/1. The leaching of the contaminant into the well, and its persistence in the soil and groundwater is still present over 4 years after the last application.

The simulated zone has been subdivided into regular grids of 15 m by 15 m with 345 nodes. The values of parameters used are those measured for the hydraulic conductivity(K=7.7*10 m/s) and for the effective porosity (n=0.35) or as reported in the literature for the longitudinal and transverse dispersivity coefficients(=0.2m & =0.01m) . The absence of organic matters in the saturated zone leads to a non adsorption and thus an unit retardation term.

The Sainte-Catherine region does not present major hydrogeological anomalies which may modify hydrodynamic characteristics of the flow. The ground is almost flat and the regional hydraulic gradient is assumed to be 1/1000. However, the boundary conditions are constant head (first type or Dirichlet condition) in the direction of the flow and impervious (second type or Neumann condition) in the transverse direction. With respect to the pesticide concentrations, the extent of the model may be considered large enough to impose null concentrations on boundaries. At the water table level, the concentrations given by VULPEST are imposed on the nodes located directly under the surface of the application of the pesticide.

Results

Figure1 Concentration reaching the water table calculated by VULPEST model

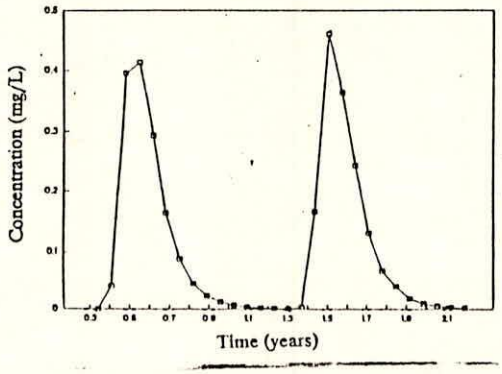
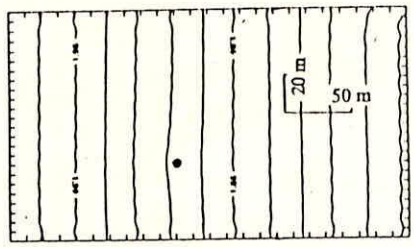


Figure 2.

Hydraulic heads calculated by MSTHP model



igure 3. Pesticide concentrations in well water measured and calculated by MSTHP model

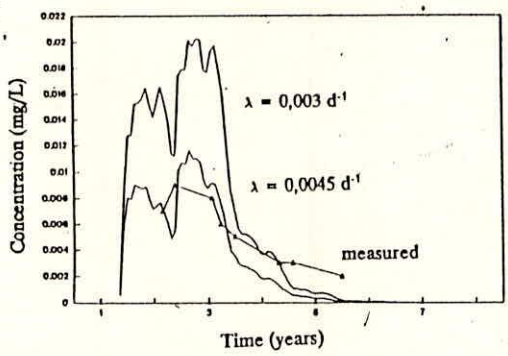
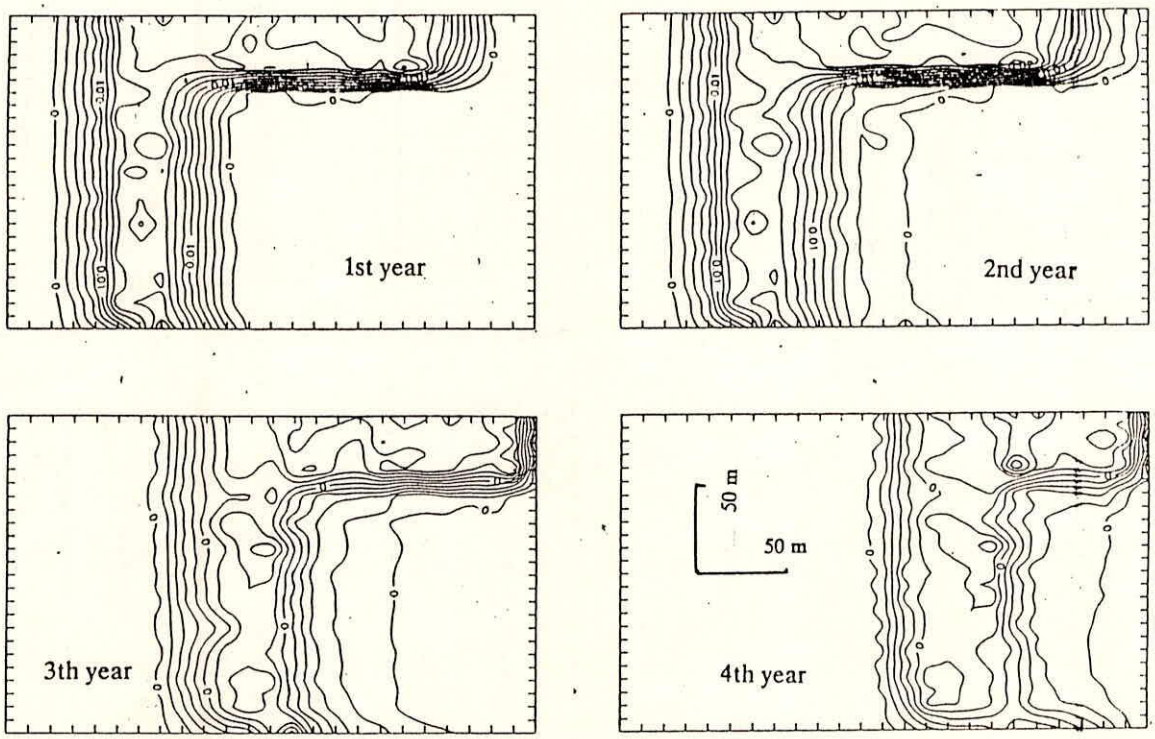


Figure 4. Temporal evolution of concentrations in the aquifer



The hydraulic heads calculated by the model are represented in Figure 2. We note that the pumping influence (rate = 500 m/year, radius of influence = 4 m) on the aquifer is low, as it does not generate any visible depression cone. The well concentrations calculated by taking into account decay are presented in Figure 3. The maximum concentrations obtained are near pg/l and 11 pg/l for decay rats of the pesticide in the aquifer of and respectively. This shows the sensitivity of the model to this chemical parameter which is unfortunately difficult to measure and is rarely documented in the literaature. The decay rate of 0.0045 corresponds to half life of about 5 months of the aldicarb and its toxic residues. This half life is less than the one of 8 months (0.00029) as reported by Jones et al.)

Figure 4 shows the spread of the contamination plume over 4 years. For the purpose of visualising the results, this plume corresponds to the aldicarb application on an area 60 m up stream of the well which is equivalent to a traveling step of about one year. The movement and shape of the plume, as well as the attenuation and dilution of concentrations are very visible with time.

(ii) Modeling of the Pollution Plume at the Villa Farm Lagoon site at Wolvey, Coventry.(1986)

2. The site

Villa Farm has been the subject of extensive investigations since 1975 (Williams). The lagoons, covering an area of about 2500 square metres, originally comprised a group of shallow excava-

tions for sand. The pits were subsequently used between 1945 and 1967 for the disposal of minor quantities of solid domestic refuse and rubble. After this period the site was adopted for the disposal of liquid industrial waste. Records of the type and volume of the dumped waste are not available before the introduction of the Deposit of Poisonous Wastes Act in 1972. However, the character of the wastes disposed of at the site has apparently changed little over the period of the site's usage. Waste disposal ceased in 1982.

The Wolston Sands formation, into which the lagoons penetrate, is the primary aquifer unit of the upper sequence of sediments. These unconsolidated lacustrine sands vary in thickness between 1 and 13 metres over the area of interest, and are interbedded between relatively mpermeable boulder clays. The lower clay is vertically extensive and provides an effective low permeability boundary to the sands. The upper clay is less substantial (1-3 m thick) restricting vertical seepage from surface flow.

The principal direction of groundwater flow is from east to west. To the west and north the hydrogeologicaal boundaries are formed by two streams which cut into the aquifer over most of their length. However, the aquifer has been disturbed in the vicinity of the narrow flood plain of the western preventing accurate analysis of through flow in this region. To the north and west the aquifer thins maarkedly and the elevation of the base of the aquifer effectively controls groundwater flow (in much the same manner as a weir crest in surface flow regulation).

The build up of sludge at the base of the lagoon restricts infiltration to the aquifer since the lagoon level has remained approximately three metres above regional groundwater level subsequent to site closure. However, dredging, undertaken once or twice each year during the operation of the site is known to have disturbed the sealing laver allowing periodic injection of contaminants at relatively high rates for short time periods. The results of its action can be observed by the presence of contaminants far upstream of the lagoons which cannot be explained by uniform discharge.

Model

Although the problem is three dimensional, a two dimensional horizontal flow model gives a valuable initial appraisal of the spatial and temporal groundwater flow patterns. Figure 5 shows a schematic cross section of the aquifer.For the partially confined portion of the aquifer, the two dimensional areal equation of fluid movement takes the form

$$n_e \frac{\delta h}{\delta t} - \frac{\delta}{\delta x_i}\left(K_{ij}(h-b_0)\frac{\delta h}{\delta x_j}\right) - R(x_i,t) - \sum_{K=1}^{P} Q^K(x_i,t)\,\delta(x_i - x_i^K) = 0$$

where h is the hydraulic head of the flud, n_e is the effective porosity, k_{ij} is the vertically averaged hydraulic conductivity tensor. b_0 is the elevation of the base of the aaquifer, R is the rate of recharge to the aquifer and Q^K are the point sources of fluid injection at the points x_j^K iδ the Dirac delta function.

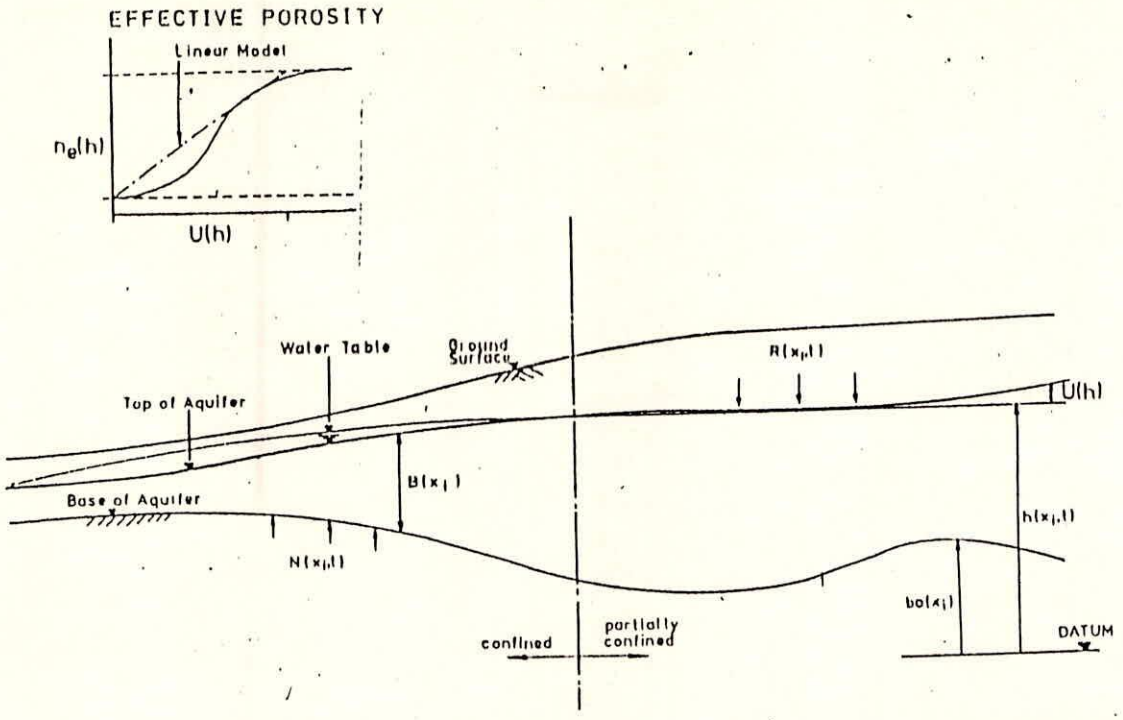


FIGURE 5 SCHEMATIC CROSS-SECTION: WOLSTON SAND AQUIFER

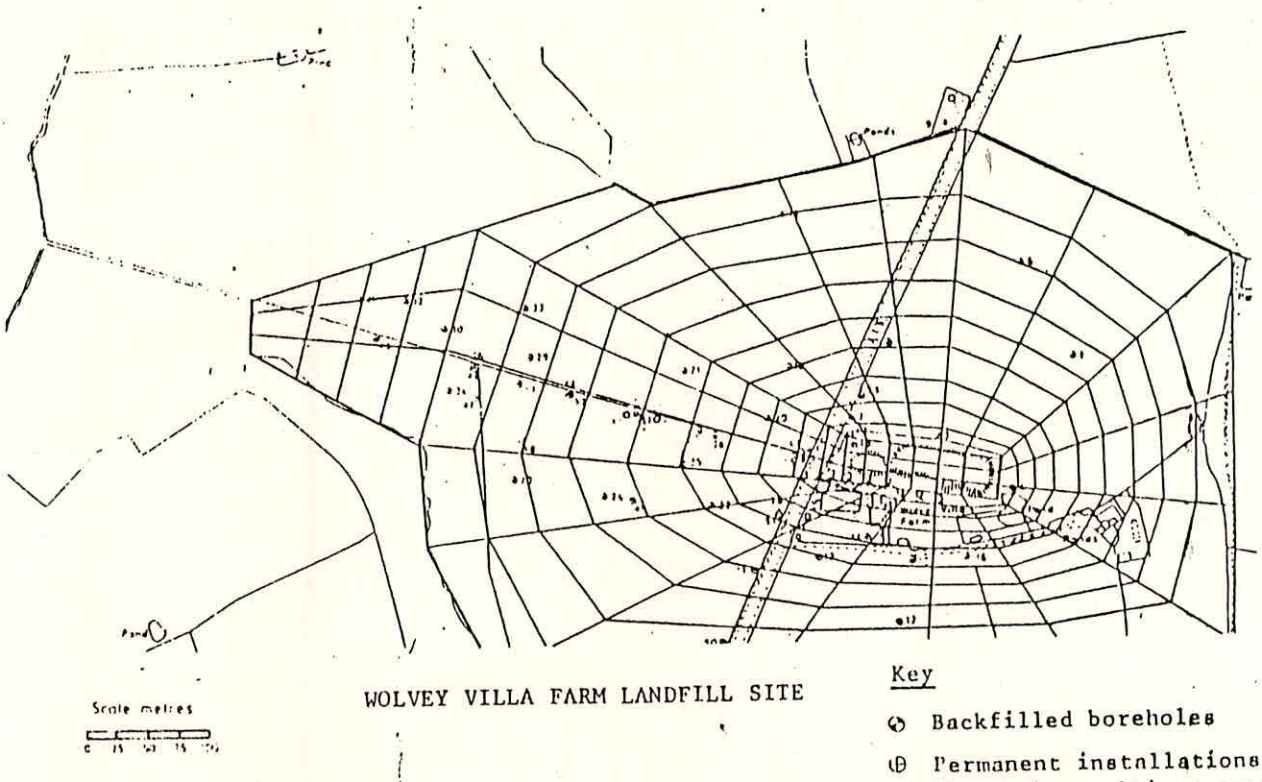


FIGURE 6 FINITE ELEMENT NETWORK

Under the partially confined conditions observed at Villa Farm where the overlying clays lie within the capilary zone above the unconfined surface the storage term is a function of the unsaturated thickness. A linear variation in the phreatic storativity was adopted between the limits defined by fully confined and fully unconfined conditions.

For the case of a fully confined aquifer, the equation of fluid movement is

$$B S_o \frac{\delta \phi}{\delta t} - \frac{\delta}{\delta x_i} \left(K_{ij} B \frac{\delta \phi}{\delta x_j} \right) - R(x_i, t) - \sum_{k=1}^{P} Q^k(x_i, t)\, \delta (x_i - x_i^k) = 0$$

where S_o is the porous medium storativity B is the aquifer thickness and o is the vertically averaged fluid potential.

Following assumptions are considered

(i) fluid density is essentially constant throughout the aquifer.
(ii) the interfaces between the aquifer and the confining strata are non deformable.

The hydrographic records at the site. available for the years 1982-1983, show a seasonal variation of water level about an apparent static mean. In order to establish a satisfactory initial condition for transient calibration the average water levels were used in the steady state analysis of the flow regime. The steady state heads produced are then used as the initial conditions for transient runs. Compatible starting dates for transient runs are estimated from the hydrographic record.

Across the base of the aquifer zero vertical flow is assumed. Recharge through the upper confining clay was estimated from vertical permeability and varied in response to the available meteorological data for the area. An average recharge value of 3 x 10 metres per day has been calculated. The recharge is applied uniformly over the entire model area.

For the numerical solution scheme a Galerkin finite element formulation was considered to be the most suitable (see Huyakorn, P.S. and Pinder, G.F.). The particular finite element code employed used quadrilateral elements with linear sides for mesh construction. The mesh for the Villa Farm site is shown in Fig 6. The size and orientaion of the mesh elements were varied in respone to the spatial distribution of the data and to the more complex conditions in the vicinicity of the lagoons. A bilinear interpolation function is used to describe the heads within each elements. The values of heads at the nodal positions being the parameters to be determined.

Boundary conditions are incorported directly into the finite element formulation. For boundary nodes of prescribed head, the finite element equation at these nodes is replace by for example.

$$\Phi_j = \Phi_0$$

Where Φ_0 is the prescribed value of Φ at the boundary node j. Boundaries where the potential is not prescribed are treated as no flow boundaries. The formulation of the finite element equations made provision for time stepping by explicit or implicit schems. For this application an implicit formultion was adopted.

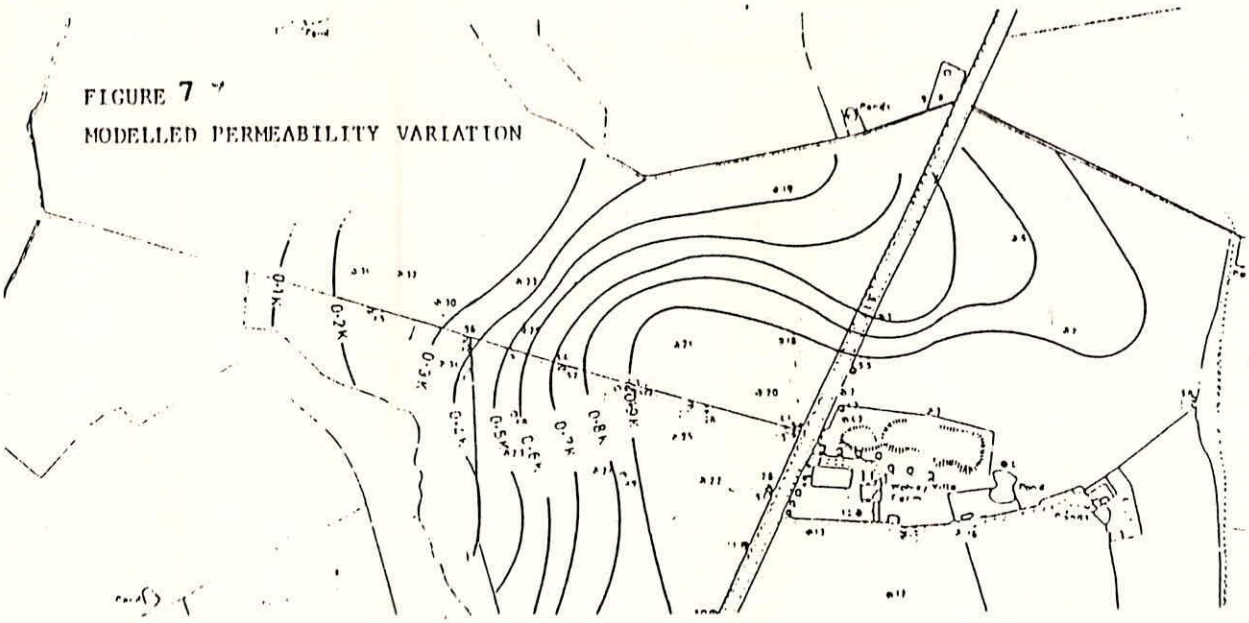
A direct iteration approach was adopted and was found to converge satisfactorily for all cases considered.

Modelling Results

Using the Kriged estimates of the various surfaces defined at the grid points of the finite element mesh, the numerical model has been calibrated. An iterative procedure for the calibration was adopted. The permeability estimates fed into the model were successively adjusted in response to the derived head distribution for a number of plausible boundary condtions whilst maintaining the same aquifer geometry. Throughout the modelling it has been necessary to re-evaluate the total flow pattern to ensure at each stage a conceptually valid system (i.e. no extraneous sources and sinks). For all calibration runs performed, the permeability distribution showed higher values in the central porion of the area with rapidly reducing values close to the boundaries of the system. This aspect of the model results support the evidence derived from the field investigations which showed increasing permebility with aquifer thickness and an increased median grain size in the thicker units. Ths coupled with a higher percentage of clays mixed in the aquifer near the edges of the model area governs the changing permeability pattern.Figure 7 shows a typical smoothed representation of the permeability,averaged over the model area,used to simulate the water level patterns.

It is estimated from the modelling of the site that the total lateral inflow in the region is of the order of 10,000 cum per

FIGURE 7
MODELLED PERMEABILITY VARIATION



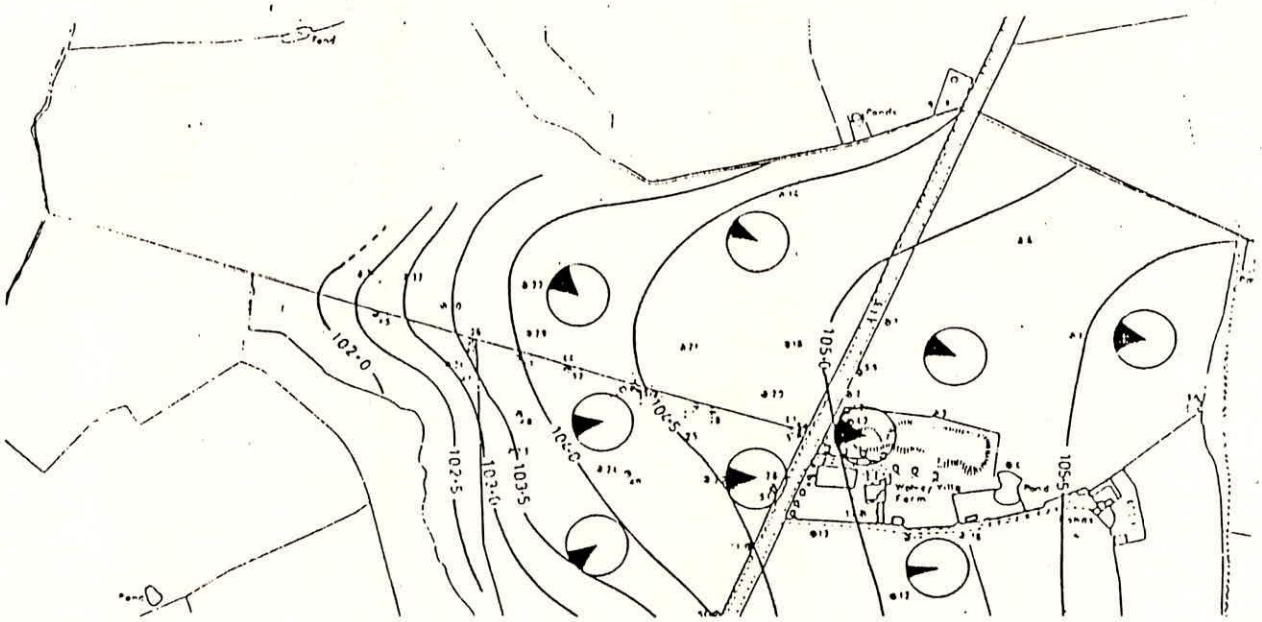
Scale metres

WOLVEY VILLA FARM LANDFILL SITE

0·1K — Percentage of max. permeability - K

Key

- Backfilled boreholes
- Permanent installations (boreholes multiprezometers, etc)



Scale metres

WOLVELY VILLA FARM LANDFILL SITE

Variation in Calibrated Flow Directions

102 — Typical Steady State Water Levels

Key

- Backfilled boreholes
- Permanent installations (boreholes multiprezometers, etc)

FIGURE 8 RANGE OF MODELLED FLOW DIRECTIONS

annum. With this low level of flux the stresses induced by even small changes in the levels of recharge are sufficient to change the head distribution coniderably: It is apparent therefore that knowledge of the temporal distribution of recharge needs to be improved before extending the studies to the transient case and to include three dimensional flow components. Figure 8 shows the range of possible flow directions determined from the calibration runs for a number of points over the model area.

The present studies of Villa Farm Lagoons have so far attempted to analyse the range and availability of data needed from field investigations for input to a staandard flow model. Therefore a number of areas which have been shown to be of importance in the development of a numerical modelling capability for extension to mass transport studies at landfill sites. These can be summarised as follows.

1. The determination of the processes of infiltration of the leachate into the saturated zone.
2. The analysis of the boundary conditions controlling the flow pattern, and the requirements for collection of field data suitable for analysing the response of the boundary conditions in time.
3. The development of clear procedures for quantifying the uncertainty in model predictions based on the errors in the estimation and interpolation procedures adopted.
4. The evaluation of the vertical components of the groundwater flow pattern.

The model studies of the Villa Farm site have so far been

successful in demonstrating the feasibility of formulating a two dimensional model describing the macroscopic processes of groundwater flow. However, the modelling has shown that even for a simple aquifer system, the level of data required to provide confident predictions.

4.Ø REVIEW OF WORK ON MODELLING IN INDIA

Groundwater quality modelling is comparatively a new field and as such there is not much research work has been acknowledged in India.

Anand Prakash (1982) developed simple analytical models to simulate groundwater contamination due to point,line, plane or parallelopiped sources in a confined or unconfined aquifer. The effects of the upper and lower confining boundaries is an artesian aquifer and those of the bedrock and water table to an unconfined aquifer are accounted for by the method of images. The same technique is used to model the contribution of a constant concentration boundary in the flow field like the one provided by a full penetrating perennial stream the number of images at which accuracy of the results is indicated. Uniform flow velocity has been assumed in the analysis.

Third symposium on Hydrology at CWPRS,Pune noticed the work of ,Pawar et.al.on Effect of Vibration in the Quality of Ground water in Bhairoba Basin,Pune and Patil et.al.on Geochemistry of Ground water and its Implications on the Precipitation of Carbonates in the Saswad-Nira Area,Western Maharashtra.

5.ØREFFERED PROBLEM TO NIH

Pollution Studies In Vaniyambadi-Ambur Area of Palar River Basin.

LOCATION

Palar river basin is located in North Arcot Ambedkar district in Tamil Nadu and also in parts of Andhra Pradesh. The total area of the basin within Tamil Nadu is about 10656 sq. km. (N. Latitude 12 2'30" - 13 05'"and E. Longitude 78 28'ØØ" - 80 50'ØØ") The area Vaniyambadi and Walajapet lies between the coordinate N. Latitude 12 35'ØØ" to 13 ØØ'ØØ" and E. Longitude 78 30"ØØ" to 79 25'ØØ". (Location map appended)

GEOLOGY

The major portion of the area studies is covered by granites and charnockites of Archaean age which is in turn covered by Alluvium comprising of sand clay and gravel. Thickness varies from 20-40 metrs.

LOCATION OF INDUSTRIES

Number of industries are located in Vaniyambadi-Walajapet area, of which Tanneries Constitute 90% and the rest are chemicals, sugar, soaps, leather goods and paper industries.

BACKGROUND AND JUSTIFICATION

The surface water and also groundwater are getting contaminated and rendering it unuseable for drinking or for irrigation in several parts of the river basins. Pollution may be one of the causes for the reported occurrences of various water borne

diseases confronted by human population and poor production capability of Agricultural land. Industrial effluents which are untreated for partially treated are letout into river and extensive application of fertilisers in the agricultural areas are the main source of pollution which needs special study, monitoring and control.

Monitoring of the rate of pollution in already affected areas will be the most handy test with which, control could be effected either by reducing or by eliminating such areas, as source of water supply. Further by such studies areas of good quality and bad quality waters can be delineated, earmarking for future groundwater development on the basis of users demands. Preliminary data collection, processing and analysis of various details give rise to following conclusions.

Total dissoved solids are much more in the locations like Ambur, Minnur, Vengili, Kailasagiri, Gudiyattam and Pernampet. Breakeup details shows that sodium and chloride concentration are more in all the above said locations and with an increasing temporal trend. Bicarbonate is found more in Vaniyambadi, Vengili, Kailasagiri and Gudiyattam. In Ambur, Minnur, it is more in some years but reduced subsequently with good amount of rainfall.

IS 10600-1983 depicts that for drinking purpose desirable limit for TDS is 500 mg/1 and tolerance level is 1500 mg/1. Therefore locations like Vaniyambadi, Ambur, Minnur, Vengili, Pernampet has already corssed the tolerance limit. Gudiyattam and

Kallasagiri has also corssed the desirable limit but yet to reach the tolerance limit as far as drinking purpose is concerned. Water for some of the wells may well be used for irrigation but overall picture is grim as bicarbonate content is more in most of the locations.

In general contaminant level of the ground water system has been on the increasing trend. Most effected areas are Ambur and Minnur.

The preliminary study reveals that contanminants are more when groundwater recharge is less that is when rainfall is less. Therefore it may be concluded that if proper flushing arrangement of the surface and sub-surface contaminants can be made during dry periods, the contaminant levels may be controlled.

Overall picture of the deteriorating phenomenon reveals tht source of pollution may be largely due to the disposal of untreated affluence from tanneries and other small scale industries. This may be joined hands by some non point source created through excess use of fertilizers in the command area. In crease of the numbers of tanneries are manifold in the Vaniyambadi Ambur region. Effluent tanneries should be treated before disposal to the river which is the only way to protect further deterioration.

6.Ø WHAT THE SCIENTIST PROPOSES UNDER UNDP TRAINING AND HOW IT WILL BE UTILISED SUBSEQUENTLY.

Over the last two decades there was been a substantial more towards a more complete understanding of groundwater contamination and how the impacts of contamination can be mitigated by appropriate management actions and technological developments.

Ground water quality modelling is a relatively new area and as such there is still much research to be undertake before an optimal approach to environmentally sound water management can be defined.

Models only yield information with the level of confidence dependant on the availability and quality of field data and the skillful interrelation of the results by an experienced modeller with a strong background in ground water analysis.

Therefore under the UNDP training author would like to gain knowledge of latest modelling techniques and its implications in the ground water quality modelling studies. Development of a model is an exercise in conceptualizing the true nature of the ground water regime from the available data and not simply of the generation of numbers by a computer code. Outcome of the training will meet the requirement of exercise in groundwater polluted areas like upper Palar zone in palar river basin, near Trichy in

Cauvery river basin, salt water intrusion in Madras, and Kuttur coastal area etc. all in Tamilnadu State of India and also to deal the pollution problems in Mundargi taluk of Dharwad, Sidhner in Bellary, Pavagada and Tiptur in Tumkur, Sirguppa in Bellary, Navalgund and Gadag in Dharwad all in Karnataka state of India.

7.Ø CONCLUDING REMARKS

Given present stresses on groundwater resources in most countries of the world, it is important that resource managers begin to come to terms with very real. Complex or multidisciplinary problems of quality management. Advancement of knowledge in this field cannot have second idea in the national context.

Due to the complexity of most groundwater systems the solutions, the solution to the flow and transport problem is generally derived by numerical treatment of the equation. A variety of numerical scheme have been applied to the groundwater flow and transport problems using computers and a number of generalized computer codes are now available which can be used for the simulation of most aquifer systems. However, although simulation models can be very complex in their formulation, it must be remembered that they remain highly simplified representation of the true aquifer system.

The literature contains a wide range of studies demonstrating the use of simulation models to both groundwater flow and contaminant migration studies. However, it must be pointed out that by far the majority of studies presented in the literature have been related to research programs and less to real management applications. It is unfortunate that most real applications undertaken by consultants are not presented in open literature. Moreover while consultants are frequently employed to develop and use a groundwater for analysing particular problem it is more for

the client to take over these models and use then for continuous monitoring and appraisal of the groundwater resources of the region.

Given the limitations of the models, it must be stressed that models require experienced personnel who have knowledge of both simulation methods and groundwater system in order to maximise the benefit of a modelling exercise . Extensive training is therefore of primary importance in this field.

REFERENCES

(1) Ammentorp H.C., Jenson R.H., Christensen T.H. and Refsguard J.C., 1986," solute transport and chemical processes: The present state of the unsaturated Zone component of the SHE modelling system", Proc. of Int. Conf. on Water Quality Modelling in the Inland Natural Environment, Paper E3.

(2) Bear Jacob 1979, Hydraulics of Groundwater, McGrow Hill, New York.

(3) Bear Jecob and Verruijit Arnold, 1987, Modelling Groundwater flow and pollution, D. Peidel Publishing Company, Holland.

(4) Bestman A.R., 1991, "The Diffusion of Burried matter and possible Pollution of Aquifers in Presence of Hydrodynamic Dispersion", Vol.1, PP.163, Proc.of the second Int.Conf.in Computor methods and Water Resources.

(5) Davis G.B. and Barber C., 1986, "Modelling the Volatilization of Methane from Contaminated Groundwaters" Proc. of Int. Conf. on Water Quality Modelling in the Inland Natural Environment, Paper F1.

(6) Borgarten H.W., Braxbin A, Rouveg G., 1991, "Multiphase flor and Transport Modelling of subsurface contaminaton by Immiscible fluids", Vol.1, PP.129, Proc. of the second Int. Conf. in Computer methods and Water Resources.

(7) Gelharb L.W. and Wilson J.L. 1974 "Groundwater Quality Modelling ", Vol12 No.6 -Groundwater .

(8) Gentile G., A. Maffio., P. Molinaro, R. Rangogni, 1991 "Application of FEM to 3D Problem of Transport and Diffusion of Pollutant into Aquifer", Vol.1, PP.197 , Proc.of the second Int. Conf. in Computor methods and Water Resources.

(9)Iamandi C. Manescu M., Bica I., 1986," Experimental Studies on the migration of Petrochemical Pollution into unsaturated Aquifere", Proc. of Int. Conf. on Water Quality Modelling in the Inaland Natural Environment, Paper F2.

(10) Javandel I., Doughty C. and Tsang C.F , 1984, Groundwater Transport: Handbook of methametical models, American Geophysical Union, Washington) D.C.

(11) Mackay R., Porter J.C., Williams G.M., Rose C.A.M. and Noy D., 1986, "Modelling Mass Transport is the Saturater zone. A case study" Proc. of Int. Conf. on Water Quality Modelling in the Inland Natural Environment Paper G3.

(12) Raige R.W., Broyd T.W., Stephens J.L., 1986, "The Prediction of Pollutant transport from shallow disposal sites in low permeability media", Proc. of Int. conference on Water Quality Modelling in the Inland Natural Environment, Paper E1.

(13) Rathfelder K., Abriola L.M., Yadav S., Maiza M., 1991, "Simulation of Immiscible Phase contaminant Transport on IBM/At Personal Computers " Vol.1,PP.153, Proc, of the second Int. Conf. in Computor methods and Water Resources.

(14) Reddell D.L. and Sunada D.K., 1970,Simulation of Dispersion in Ground Water Aquifer, Hydrological Papers, Colorado state University, Fort Collins, Calarado.

(15) Refsgaard J.C., Christensen T.H. and Ammentorp H.C., 1986 "Aproposal for an Unsaturated Zone Oxygen Transport and Consumption Model". Proc. of Int. Conf. on Water Quality modelling in the Inland Natural Environment, Paper E4.

(16) Ssi L. A., Banton O., Nilleneuve J.P., 1994," Stochastic Modelling of the Trnasport of Pesticides in Soils and Groundwaters, Applications to the vulnerability", Vol.1, PP. 141,Proc.of the second Int. Conf. in Computor methods and Water Resources.

(17) Thanh N.C. and Biswas A.K., 1980, Environmentally sound water management, Oxford University press, New Delhi.

(18) Tolikas D. Latinopoulos P. and Mylopoulos Y., 1986 ,"A Model for Water Quality management of Aquifers", Proc. of Int. Conf. on Water Quality Modelling in the Inland Natural Environment Paper G2.

(19) Turkeman A., 1986, "Groundwater Pollution Problems of Eornova Plain in Turkey". Proc. of Int. Conf. on Water Quality Modelling in the Inland Natural Environment, Paper G1.

(20) Vogt M.,1991 "Avectorized Multi component Trnasport Reacton Model: Theory and Application " Vol.1,PP.173, Proc.of the second Int.Conf. in Computor methods and Water Resources.

(21) Voss, Clifford I., 1984, SUTRA, U.S. Geological survey water Resources Investigations Report 84-4369.

(22) Wang H.F., Anderson M.P. , 1982, Introduction to Groundwater modelling, W.H. Freeman and Company USA.

(23) Wheater H.S., Abeliule R. and Perry R., 1986, "Parameter Identification In models of Unsaturated solute Transports". Proc. Of Int. Conf. on Water quality modelling in the Inland Natural Environment ,Paper E2.

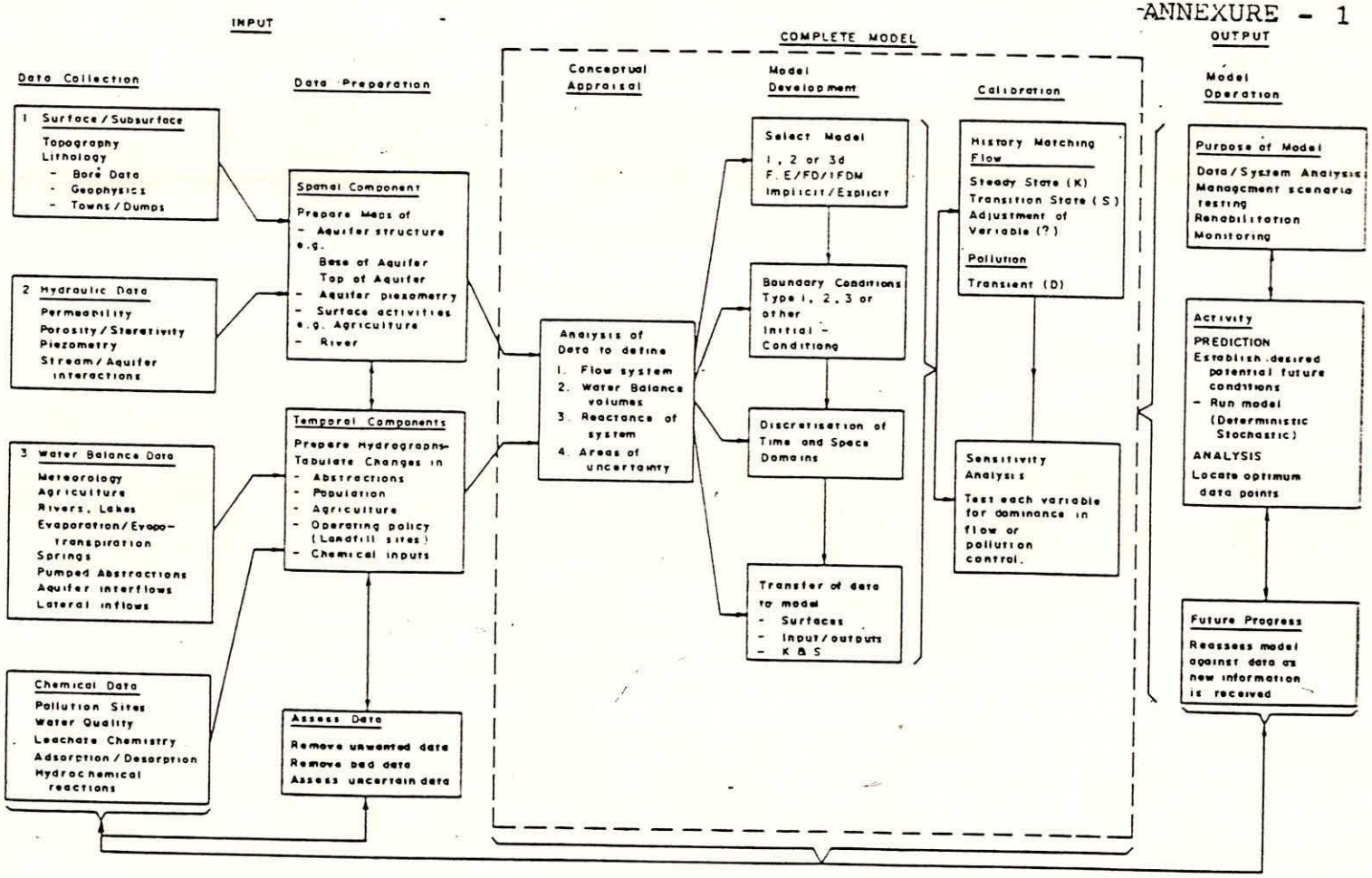
A C K N O W L E D G E M E N T

Deep sense of gratitude is expressed for the unremitting encouragement and perfect guidance given by Dr. P.V.Seethpathi, Scientist'F' and Shri K.S.Ramasastri,Scientist'F' , National Institute of Hydrology,Roorkee(U.P.),India.

The author also wishes to express his deep sense of gratitude to Dr. G.C.Mishra,Scientist 'F',National Institute Of Hydrology, Roorkee(U.P.),India , for extending literature support.

The author is thankful to Dr.J.S.Rawat,Head, Ch.A.V.Shetty,Scientist'B,Dr.B.K.Purandara,SRA, and Shri S.Gavane, Typist ,Regional Centre,Belgaum ,for their support in the respective area.

ANNEXURE - 1



Numerical modelling schemes

Finite difference solute transport codes

Authors (Institute)	Code Name (Reference Date) Simulation Examples	Numerical Characteristics	Fluid Flow Processes	Solute Transport Processes
R. J. Dillon P. B. Lantz S. B. Pahwa (Sandia Natl. Lab.)	*SWIFT* (1978) Radionuclide transport	Three-dimensional Two line SOR iterative or direct ordered Gaussian elimination	Transient Well-bore Nonisothermal Convection	Advection Dispersion Diffusion Adsorption
G. R. Dutt M. J. Shaffer W. J. Moore (Bureau of Reclamation)	*Salt Transport in Irrigated Soils* (1972) Predict quality of irrigation return flow	One-dimensional vertical coupled with chemistry model	Transient Unsaturated Homogeneous, isotropic media	Ion exchange
Intera Environmental Consultants, Inc.	*HCTM* (1975) Tritium transport Mine dewatering needs	Three-dimensional Method of characteristics for advection	Saturated/ unsaturated	Advection Dispersion Diffusion Sorption; Decay
L. F. Konikow (Texas Dept. of Water Research)	*GWSIM II* (1981)	Two-dimensional areal	Transient Confined/unconfined aquifer	Advection Dispersion Diffusion
L. E. Konikow J. D. Bredehoeft J. V. Tracy (U.S. Geological Survey)	*KONBRED*[a] *USGS-2D-Transport/MOC*[a] (1978; *Tracy*, 1982) Chloride movement, Rocky Mountain Arsenal, CO and stream-aquifer system Radionuclide transport INEL, ID	Two dimensional areal ADI for flow equation Method of characteristics for solute transport equation	Transient Confined, semi-confined, water table aquifer Diffuse leakage Injection/withdrawal	Advection Dispersion Adsorption Decay
A. Kerrer Intera Livermore Lab	*OGRE* (1970) Radionuclide transport around underground openings	Two-dimensional axisymmetric Three dimensional[b] ADI	Transient Saturated/ unsaturated	Advection Dispersion[b] Adsorption[b]
J. Ledoux (Ecole des Mines de Paris)	*NEWSAM* (1976) Salt transport	Two-dimensional areal Heirarchical grid	Transient	Advection Adsorption
T. N. Narasimhan A. E. Reisenauer C. L. Key R. W. Nelson (Lawrence Berkeley Lab., Pacific Northwest Lab.)	*TRUST* *FLUX/MULTL* (*Reisenauer*, 1982) Soil columns Field consolidation	IFDM; Three-dimensional Complex geometry Pathline solutions	Saturated/ unsaturated Deformable porous medium	Advection
R. Pickerson (Science Appl. Inc.)	*MIGRAIN* (*Claborne et al.*, 1980) Migration of brine inclusions in salt	Two dimensional, Three-dimensional Upstream weighting	Heat-induced migration	
J. B. Robertson (U.S. Geological Survey)	*Robertson I* (1974) Radioisotope migration, National Reactor Testing Station	Two-dimensional areal ADI Method of characteristics for transport	Transient Bounded aquifer	Advection Dispersion Sorption; Decay Ion exchange
A. Runchal D. Inger G. Segal (Dames & Moore)	*GWTHERM* (1979) Repository studies	Two-dimensional vertical IFDM; ADI Particle tracking option	Transient Nonisothermal Convection	Advection Diffusion Adsorption Decay

[a] Alternate names for the same code

[b] Features added after 1980

Finite element solute transport codes

Authors (Institute)	*Code Name* (Reference Date) Simulation Examples	Numerical Characteristics	Fluid Flow Processes	Solute Transport Processes
R. G. Baca R. C. Arnett I. P. King (Rockwell Hanford Operations)	*MAGNUM2D*[a]*-CHAINT*[b] (1981) Multicomponent nuclide transport, basalt repository	Two-dimensional isoparametric elements for porous matrix One-dimensional elements for discrete fractures Galerkin Solute transport in fractures	Nonisothermal Convection-diffusion Double porosity	Advection Dispersion Sorption Decay chains Mass release
J. O. Duguid M. Reeves (Oak Ridge Natl. Lab.)	*Dissolved Constituent Transport Code* (1976) Seepage pond	Two-dimensional vertical Galerkin Linear basis functions L-U decomposition	Given saturated or unsaturated flow	Advection Dispersion Diffusion Adsorption Decay
D. B. Grove (U. S. Geological Survey, Denver)	*Grove/Galerkin* (1977) Chloride, Tritium, and ^{90}Sr transport	Two-dimensional areal Galerkin Linear and Hermite cubic basis functions SOR iterative	Finite difference for flow	Advection Dispersion Decay Ion exchange
S. K. Gupta C. R. Cole C. T. Kincaid F. E. Kaszeta (Pacific Northwest Lab.)	*FE3DGW, CFEST*[c] (1980) Hypothetical salt and hard rock repositories	Three-dimensional Galerkin *FE3DGW*-mixed order isoparametric elements *CFEST*-linear elements Sequential solution	Transient Multi-aquifer Nonisothermal Convection	Advection Dispersion Diffusion
P. S. Huyakorn B. H. Lester J. W. Mercer (GeoTrans, Inc.)	*FTRANS*[d] (1983) Transport of ^{237}Np from a waste repository in a uniform flow field	Two-dimensional for flow and transport in fractures One-dimensional for the matrix Upstream weighting for fractures	Transient Flow through fractured porous media	Advection[e] Dispersion[e] Diffusion[f] Adsorption[f] Decay
Intera Environmental Consultants, Inc.	*VCHFLD* Multi-species chemical transport	Two-dimensional areal or cross-section Galerkin Bilinear basis functions Gaussian elimination or SOR	Confined aquifer Injection/production	Advection Sorption Multi-species reactions
J. Marlon-Lambert I. Miller (Golder Assoc.)	*Groundwater computer package* (1978)	Two-dimensional areal or axisymmetric Galerkin L-U decomposition, Doolittle method	Transient Layered aquifer Confined or unconfined aquifer	Advection Dispersion Diffusion Adsorption Decay Ion exchange

ANNEXURE - 3

(continued)

Authors (Institute)	*Code Name* (Reference Date) Simulation Examples	Numerical Characteristics	Fluid Flow Processes	Solute Transport Processes
J. Noorishad M. Mehran (Lawrence Berkeley Lab.)	*Flows* (1982)	Two-dimensional areal or cross-section Galerkin Upstream weighting Quadrilateral isoparametric elements	Transient Discrete fractures	Advection Dispersion Adsorption Decay
J. F. Pickens G. E. Grisak (Environment Canada)	*SHALT* (1979) Well testing, Chalk River	Two-dimensional areal or cross-section Triangular elements Sequential solution	Transient Nonisothermal Convection	Advection Dispersion Sorption; Decay
L. Picking (Stone and Webster Engineering)	*SALTRP* (*Frind and Trudeau*, 1980) Salt transport and dissolution	Two-dimensional vertical cross-section Galerkin	Transient Confined aquifer	Advection Dispersion Diffusion Dissolution
G. F. Pinder (Princeton Univ.)	*ISOQUAD* (1973) Chromium contamination, Long Island, N. Y.	Two-dimensional areal Galerkin	Transient Confined aquifer	Advection Dispersion Diffusion
G. Segol E. O. Frind (Univ. Waterloo)	*3D Saturated/ Unsaturated Transport Model* (1976) Flow from ponds	Three-dimensional Galerkin Isoparametric elements	Transient Saturated/ unsaturated Free surface	Advection Dispersion Diffusion Adsorption Decay
J. W. Warner (Colorado State Univ.)	*RESTOR* (1981) Two solute transport	Two-dimensional areal Triangular elements Gauss-Seidel or point SOR Leap frog solution	Transient Confined or leaky aquifer	Advection Dispersion Diffusion Ion exchange
G. T. Yeh D. S. Ward (Oak Ridge Natl. Lab.)	*FEMWATER*[a]-*FEMWASTE*[b] (1981) Seepage pond	Two-dimensional areal or cross-section Upstream weighting Quadrilateral bilinear elements	Saturated/ unsaturated Density as function of moisture content	Advection Dispersion Sorption; Decay

[a]Calculates fluid flow

[b]Calculates solute transport using fluid flow calculated by (a)

[c]CHEST is an extension of FE3DGW to include energy and solute transport

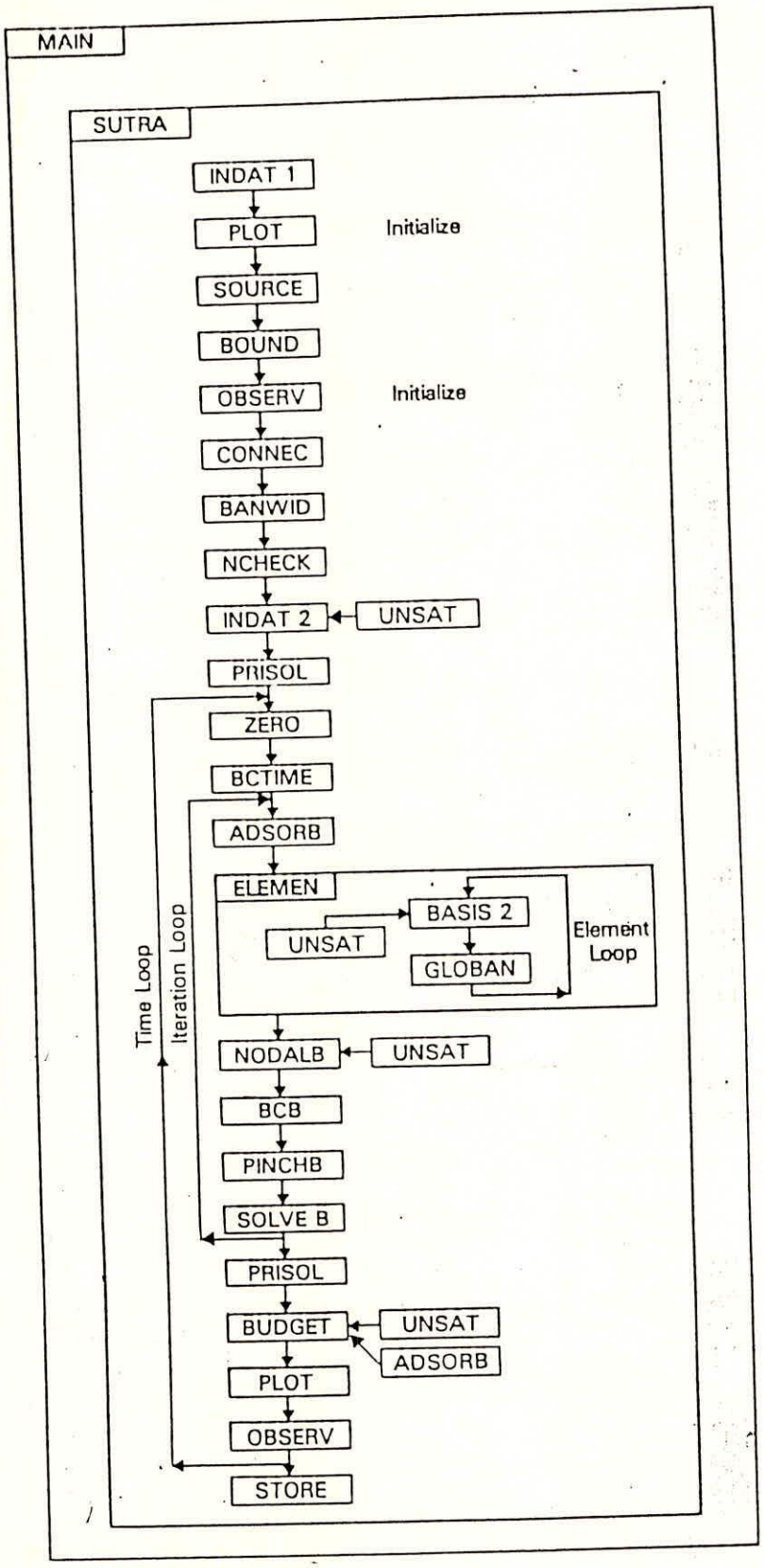
[d]One member of a family of codes, other members consider variably-saturated flow, solute and energy transport, and nuclide decay chain transport [*International Ground Water Modeling Center*, 1983]

[e]In fractures

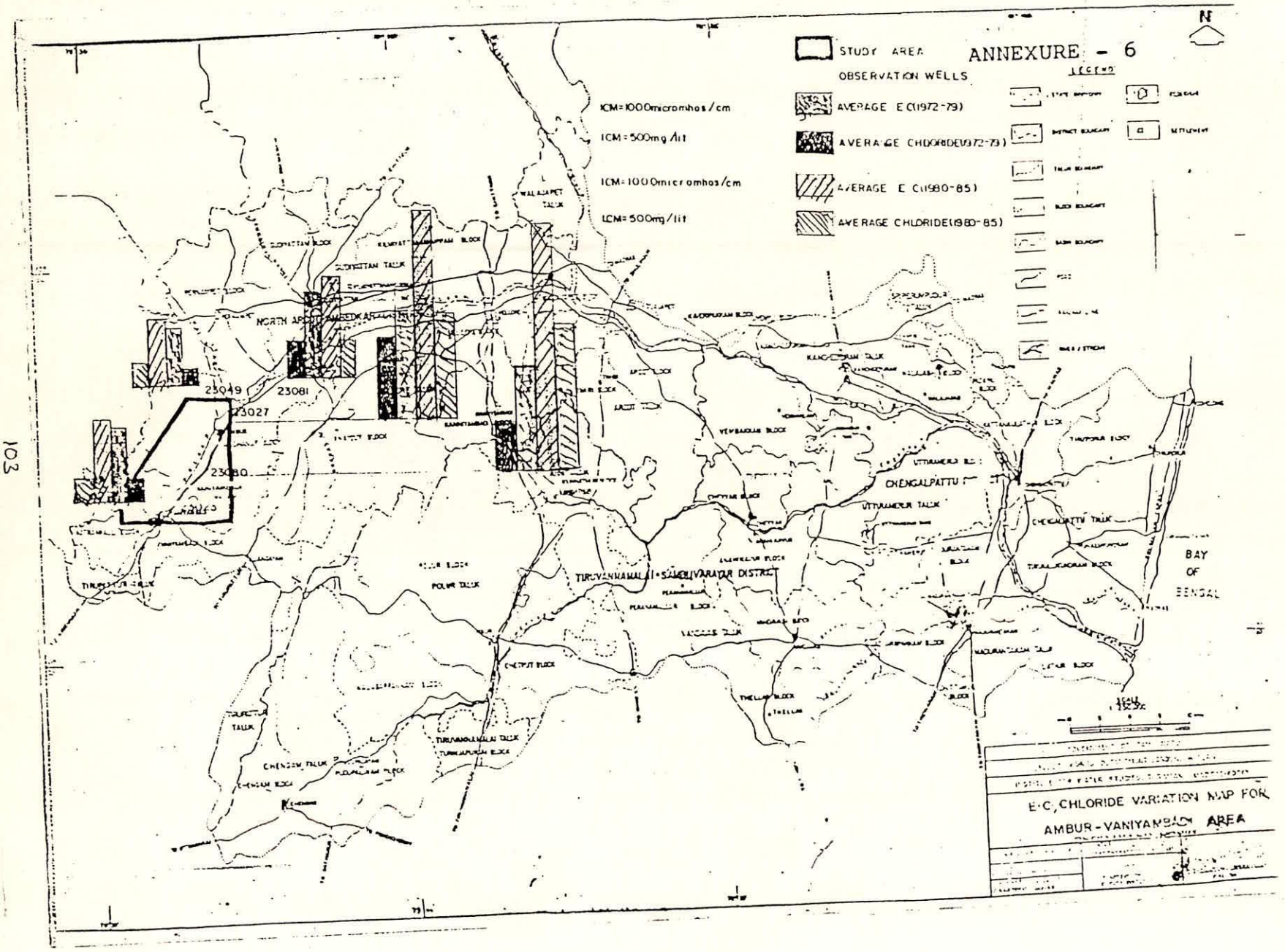
[f]In matrix

Flow path network solute transport codes

Authors (Institute)	*Code Name* (Reference Date) Simulation Examples	Numerical Characteristics	Fluid Flow Processes	Solute Transport Processes
S. W. Ahlstrom H. P. Foote R. C. Arnett C. R. Cole R. J. Serne (Pacific Northwest Lab.)	*MMT* (1977) Radionuclide contamination, Hanford, WA.	Two-dimensional Monte Carlo for dispersion (discrete-parcel-random walk approach)	Given saturated or unsaturated flow	Advection Dispersion Adsorption Decay Ion exchange Precipitation Dissolution
J. E. Campbell D. E. Longsine R. W. Cranwell (Sandia Natl. Lab.)	*NWFT/DVM* (1981) Radionuclide transport with chain decays	Flow in network of one-dimensional path segments Dispersion by distributed velocity method with Gaussian distribution for contaminant packets	Steady state Stratified sedimentary rocks Density varies with salt concentration	Advection Dispersion Sorption Decay chains Equilibrium solubility Kinetic leaching
R. W. Nelson J. A. Schur (Pacific Northwest Lab.)	*PATHS* *(1980)* Accidental contaminant release evaluation, S.C., WA. Copper tailing seepage	Two-dimensional areal Analytical flow potential Numerical pathline	Steady/transient Uniform confined aquifer Line-source wells Constant head pond	Advection Adsorption Ion exchange
T. A. Prickett J. G. Naymik C. G. Lonnquist (Illinois State Water Survey)	*Random-Walk* (1981)	Two-dimensional areal Particle-in-a-cell for advection Random-walk for dispersion	Transient Confined, semi-confined, or unconfined aquifer	Advection Dispersion Diffusion Adsorption Decay
B. Ross C. M. Koplik M. S. Giuffre S. P. Hodgin J. J. Duffy (Analytic Sciences Co.)	*NUTRAN* (1979) Long-term hazard from waste repositories	Flow in network of one-dimensional paths Green's function for transport	Resaturation of repository Withdrawal through wells	Advection Dispersion Sorption Decay chains Leaching Dissolution Diffusion through barriers
F. W. Schwartz A. Crowe (Univ. Alberta)	*DPCT* (1980) Long-term effects of waste repositories	Two-dimensional vertical cross-section Particle tracking with random number for longitudinal and transverse dispersion	Steady state Describe water table Finite element for flow	Advection Dispersion Sorption Decay



SUTRA logic flow.


ANNEXURE - 6
STUDY AREA
OBSERVATION WELLS
AVERAGE E C(1972-79)
AVERAGE CHLORIDE(1972-79)
AVERAGE E C(1980-85)
AVERAGE CHLORIDE(1980-85)
1CM=1000micromhos/cm
1CM=500mg/lit
1CM=1000micromhos/cm
1CM=500mg/lit
LEGEND
N
23049
23081
23027
23080
CHENGALPATTU
TIRUVANNAMALAI • VILLUPURAM DISTRICT
BAY OF BENGAL
E.C, CHLORIDE VARIATION MAP FOR
AMBUR - VANIYAMBADI AREA