AN INTRODUCTION TO GROUND WATER MODELLING

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INTRODUCTION

The UN Charter on groundwater management states that: "*Governments should formulate and adopt a long-term policy to protect ground water by preventing pollution and overuse. This policy should be comprehensive and implemented at all appropriate levels. It should be consistent with other water management policies, and should be duly taken into account in other sectorial policies*" (*United Nations, 1989*). Consequently, a groundwater management strategy should aim at:

(i) Sustainable use of ground water and preservation of its quality;
(ii) Incorporation of groundwater protection plans into environmental protection planning,
(iii) Protection measures towards prevention of ground-water pollution and over-use

Such protection measures include, inter alia, monitoring of ground waters, development of aquifer vulnerability maps, regulations for industry and waste disposal sites paying due account to ground-water protection considerations, geo-ecological assessment of the impact of industrial and agricultural activities on ground waters, and zoning of ground-water protection areas.

Thus, the sustainable management of groundwater resources implies a balance between groundwater development and groundwater protection, and is based on a judicious mix of scientific understanding, informed planning and effective action.

Understanding the nature and extent of groundwater regimes, problems, and prioritization forms an important aspect, and groundwater modelling is an effective tool that helps in a great way to achieve these objectives.

Groundwater Problems and Role of Models

Groundwater is one of the major sources of drinking water. With the increasing development of the groundwater resources and the growing impact of human activities on the aquifers, groundwater problems are being noticed in many regions.

Although ground water is a renewable resource, few aquifers can withstand enormous extraction rates (exceeding that of the natural recharge rates) indefinitely. Similarly, all activities carried out on the land surface have a potential to pollute ground water. There are point sources and dispersed sources of pollution contributing to groundwater contamination. Clearly, groundwater problems can be thought of caused by contamination, overexploitation, or a combination of the two.

Therefore, approaches of sustainable development and management must be developed to guarantee the right of use of groundwater, and environmental protection. To formulate technically-sound groundwater resources management polices, decision makers have to ask questions like:

- How long can an aquifer maintain the current rate of groundwater abstraction?
- What is the safety yield that the aquifer can sustain the continuous abstraction?
- What is the capture zone of a water supply well field?
- What is the most likely pathway of contaminants from domestic wastewater and leaches from solid waste disposal sites?
- What are the chances that the pollutants from those sources would arrive at water supply-wells? and how long it takes?
- What should be the size of the protection zone to protect the well fields from pollution?

Providing answers to such questions necessitates good understanding of the groundwater flow systems and the prediction of the system responses to various stresses. The best tool available to help groundwater hydrologists to meet the challenges of prediction is usually a groundwater model.

Realization of groundwater problems in the right perspective is an important aspect of groundwater modelling studies. In fact, a well poised problem is halfway solved.

Evolution of Groundwater Models

The development of groundwater simulation models in the seventies provided groundwater planner with quantitative techniques for analyzing alternative management strategies. The equations describing groundwater flow in porous media are mathematically analogous to those governing the flow of electric current. Subsequently, electric analog models were designed to study groundwater systems. However, all analogue models have been superseded by numerical simulation models, following the development of advanced digital computers.

Basically, numerical groundwater models are physically founded mathematical models, based on certain simplifying assumptions, derived from Darcy's law and the law of conservation of mass. The simplifying assumptions typically involve the direction of flow, geometry of the aquifer, the heterogeneity or anisotropy of sediments or bedrock within the aquifer, the contaminant transport mechanisms and chemical reactions. By mathematically representing a simplified version of a hydrogeological system, reasonable alternative scenarios can be predicted, tested, and compared. The usefulness of a model depends on how closely the mathematical equations approximate the physical system being modelled.

Of late, groundwater optimisation models provide optimal groundwater planning or design alternatives in the context of each system's objectives and constraints. These models aid decision-making in groundwater management by incorporating numerical groundwater flow and/ or transport models into mathematical programming formulations. The advantage of this approach is that the methods allow expression of management goals explicitly in terms of objective functions that are to be optimised. Since the evaluation of groundwater management schemes is inseparable from the decision-makers' judgement, it is necessary to couple groundwater model with a decision support model, which takes into account the preferences expressed as multiple criteria.

REVIEW OF GROUNDWATER MODELS

It can be seen that the evolution of groundwater models in the study of groundwater problems has been in perfect line with the advancement of technology. We shall consider a few mile stones in this stride. Those are: the Analytical Models, Porous Media Models, Viscous Fluid Models, Membrane Models, Electrical Analog Models, Empirical Models, Mass Balance Models, and Numerical models.

Analytical Models

These are analytical solutions to groundwater equations after applying boundary conditions. The use of analytical solutions is restricted due to over simplification of the real situation. Analytical solutions find application in pump test analyses, in steady state flow in homogeneous systems etc. In transport problems analytical solutions are so complex that it becomes unwieldy to take advantage of this approach.

Porous Media Models

Porous media or bench-scale models belong to the group of hydraulic models widely used in hydraulic engineering. The aquifer system can be represented in an appropriate scale in laboratory with its boundaries. Sand models are widely used in studying flow and transport problems in the laboratory. The experiments by Darcy (1856) can be regarded as the first porous media groundwater model!

Viscous Fluid Models

Hele-Shaw or parallel plate models use the analog of a viscous fluid motion between two closely placed parallel plates and groundwater flow. The specific flux in this model is represented by Poiseuille's equation (which is analogous to Darcy's law of groundwater flow).

Membrane Models

A membrane model consists of a mechanism for depressing a membrane covering a frame and a device to measure deformations precisely. For instance, to represent a single well a nail can be applied to depress the membrane. Line or area sources can be represented by depressing the membrane by line or area loads respectively. The measured deformations are directly related to known equations from groundwater hydraulics.

Electrical Analog Models

The analogy between electrical current flow and groundwater flow were well utilised before the evolution of numerical models. Conducting paper, electrolytic tank, resistance-capacitance network etc. were used to study the groundwater flow characteristics. The relation between hydraulic conductivity and electrical conductivity (which is reciprocal of electrical resistance) can be computed using Ohm's law and Darcy's by applying appropriate scaling factors.

Empirical Models

Empirical models, also known as lumped parameter models, are used to represent physical or chemical processes by generalities, simplifications, or at a larger scale compared to the process itself. These models may be placed in between simpler analytical models and complex numerical models in regard to sophistication. Empirical models can be either representing individual processes (*eg.* Darcy's law) or representing an entire groundwater problem by invoking a series of physical laws, and empirical laws (*eg.* landfill process analysis, HELP, model)

Mass Balance Models

Mass balance models are known as black-box or single-cell models. These may be considered as a numerical model in its simplest form with mass fluxes, either of groundwater or of solutes are balanced over large volumes (groundwater basins). Due to simplicity of black box models evaluation of field data is only concerned with fluxes in and out of the system. Thus, only storativity of the groundwater system is considered. Obviously, averaging over the entire area is a crude approximation. Despite its simplicity, the mass balance model is useful in examining the global mass balance, a feature utilized in early stages of computations in numerical modelling.

Numerical models

Due to the dominance of numerical groundwater models, they are generally termed as "groundwater models" these days. All the models discussed earlier have serious limitations in so far as application to field problems is concerned. Other than the analytical solution and electrical conducting paper methods, others are not easily applied. Simulating groundwater flow and transport by numerical models had been initiated since early seventies. Numerical models basically represent an assembly of a number of single-cell models. Advancements in computing technology enable them to be the standard procedure for solution of groundwater problems. Computer programs for most common flow and transport problems are available for the user to investigate a scenario. Numerical model can solve simple and complex problems without restricting boundary types, initial conditions, type of groundwater systems or the characteristics of the solute under investigation. Various scenarios may be visualized upon completion of a numerical model.

OBJECTIVES OF GROUNDWATER MODELLING

In the last two decades mathematical modelling techniques have increasingly proved their value in furthering the understanding of groundwater systems and, hence, in improving the evaluation, development, and management of groundwater resources, and the control of groundwater problems.

Groundwater modelling can be applied to issues like water supply management of regional aquifers, optimisation of pumping and infiltration rates, optimal locations of wells, all kinds of groundwater quality/ contamination problems, aquifer depletion problems as wells as conjunctive use of groundwater and surface water for agriculture applications.

Why model? The answer is that combining the available hydrogeological data with the appropriate physical laws (in the form of equations) in a self-consistent mathematical model is generally the best way to make use of these data, for whatever purpose. Most commonly used are mathematical models, which express the behaviour of groundwater systems in terms of a set of physical equations. In simple cases these partial differential equations can be solved analytically, but they normally require computerized numerical solution because of their complexity. For the most part, we are concerned with numerical simulation models, but increasingly a stochastic or statistical approach to model parameters and input data is being adopted.

There are situations, wherein it is not possible to monitor all aspects of groundwater flow and solute distribution just by investigations only. Information in the future and between monitoring locations are required for making meaningful and scientific decisions. Groundwater models that replicate the processes of interest at the respective site may be used to facilitate in evaluating and forecasting groundwater flow as well as transport. However, accurate field data is a pre requisite for model reliability.

In the design of a groundwater model, a number of components (vide Table: 1) need to be combined viz.:

-Natural system for which the model is designed
-Conceptual model as an idealized representation of the natural system
-Mathematical model representing controlling mechanisms in mathematical terms
-Solution of the mathematical model
-Calibration of the solution by adjusting simulated to observed responses of the natural system
- Validation of the accuracy of the model predictions
-Simulations based on the calibrated solution of the conceptual model

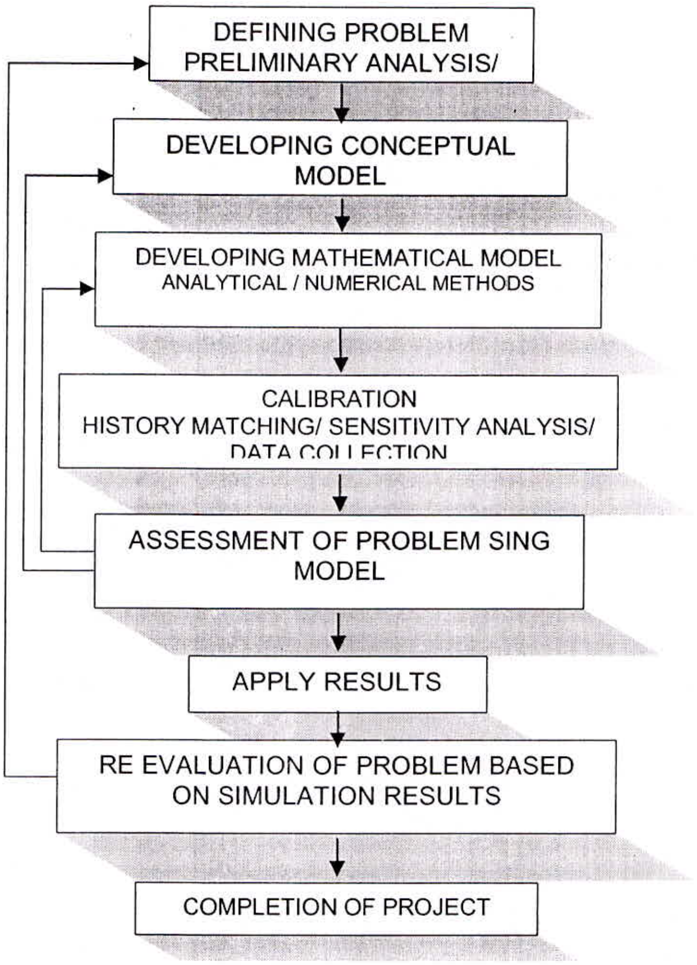

Fig. 1 Flow chart of Groundwater modelling process

Table- 1 Various Components of Groundwater Modelling

Component	Constituent Features	Examples
Natural System	Geometry/ Dimensions/ Hydrogeology/ Material Properties/ Observed responses/ GW Problems	Thickness/ 1D,2D, 3D/ Hydraulic Conductivity/ Porosity / Water level/ Contamination
Conceptual Model	Idealised System Relevant Units Boundary Conditions Controls	- Aquifer, aquitard etc Head-dependent, flow- dependent Flow, transport
Mathematical Model	Physical Laws Differential equations Boundary Conditions Initial Conditions	Conservation of Mass, energy Material relationships Laplace Equation First Kind, second kind, third kind Specified Head/ Concentration
Solution	Analytical Model Porous Media Analog Model Empirical Model Mass balance Model Numerical Model	Analytical Solutions Sand Model Electrical analog model, Membrane model Darcy's law Black box models Finite Difference, FEM, BEM, MOC
Calibration	Solution Vs observation Adjustment of Model Input Data	-
Validation	Testing of Model Prediction Vs Observation	-
Simulations	Parameter sensitivity Predictive Simulation Uncertainty Analysis	-

FORMULATION AND DESIGN OF GROUNDWATER MODELS

When modelling groundwater flow the aim is to predict the groundwater head distribution in the aquifer under different stress conditions. Darcy's law alone cannot describe groundwater flow unless the heads are known everywhere in the aquifer system. Darcy's law gives three equations for flow in three principal directions. However, there are four unknowns viz. the three components of groundwater flux as well as the head. The flow equation yields the fourth equation. The general flow equation can be formulated by applying the law of conservation of mass.

The numerical computer code is a tool for solving the governing equation of flow or transport. The numerical computer code is transformed into a groundwater model by incorporating the site-specific geometry and boundary conditions, by introducing the actual flow and transport parameters, and by calibrating and verifying the model.

Groundwater Flow Model

The three dimensional unsteady groundwater flow through heterogeneous and anisotropic porous earth material is given by the partial differential equation:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) - W = S_s\frac{\partial h}{\partial t}$$

Kxx,Kyy,Kzz : hydraulic conductivities along the major axes
h : potentiometric head
W : volumetric flux per unit volume and represents sources and or sinks
Ss : is the specific storage of the aquifer
t : time

In general, S_s, K_{xx}, K_{yy} and K_{zz} are functions of space, for example: $K_{xx} = K(x,y,z)$, whereas h and W are functions of space and time (*eg*: h = h(x,y,z,t). Thus, the above equation describes groundwater flow under non-equilibrium conditions in a heterogeneous and anisotropic medium. Hence this equation together with specification of flow conditions at the boundaries of an aquifer system and specification of initial head conditions constitutes a mathematical model of ground water flow. Generally analytical solutions of the equation referred above are rarely possible. So, various numerical methods may be used to arrive at approximate solutions.

Solute transport Model

A solute is a substance dissolved in a liquid. For example, chloride is a solute and water is the solvent. Concentrations are measured as mass of the solute per unit volume of solvent (mg/Litre). The major processes of solute migration include *advection, molecular diffusion* and *mechanical dispersion.*

Advection is the process by which the solute moves with the average velocity of the water through the pore spaces. Molecular diffusion is the spread of solute molecules due to thermal motion (expressed by Fick's law). Mechanical dispersion occurs as a contaminated fluid flows through a porous media. It mixes with uncontaminated water causing dilution by dispersion. It is caused by virtue of the differential flow in the porous medium due to pore space distribution, flow path characteristics and heterogeneity in the medium.

In the case of groundwater flow, the processes of molecular diffusion and mechanical dispersion are inseparable. The combined effect of molecular diffusion and mechanical dispersion is expressed by a term called *Hydrodynamic dispersion*. Now, the flux of solute is due to the two major processes, namely, advection (the main process) and dispersion (hydrodynamic dispersion).

When a leachate of initial solute concentration, C_0 is transported along with groundwater flow, its concentration, C at time, t and at a distance, L due to advection-dispersion processes is given by:

$$C = \frac{C_0}{2}\left[erfc\left(\frac{L - v_x t}{2\sqrt{D_L t}}\right) + \exp\left(\frac{v_x L}{D_L}\right) erfc\left(\frac{L + v_x t}{2\sqrt{D_L t}}\right)\right]$$

where,

C = the solute concentration (M/L^3)
C_0 = the initial solute concentration (M/L^3)
L = the distance from the source (L)
v_x = average linear groundwater velocity (L/T)
D_L = coefficient of longitudinal hydrodynamic dispersion (L)
t = time elapsed
erfc = the complementary error function

The above expression is based on the presumption that the centre of the solute mass is moving at the same rate as the average linear groundwater velocity, and hydrodynamic dispersion pattern of the solute follows a normal (Gaussian) distribution.

Boundary Conditions

To obtain solution of the flow equation to a given problem, it is necessary to define additional information that does not appear in the equation itself. This is termed as a *boundary-value problem* in mathematics. As such, it is required to define additional information by defining the area of investigation, finding boundary and initial conditions, and spatially estimating realistic values of aquifer parameters like hydraulic conductivity, storage coefficient etc. In groundwater modelling an important task is in identifying the model area and its boundaries. A model boundary is the interface between the model area and its surrounding environment. Conditions on the boundaries need to be specified. Boundaries occur at the edges of the model area and within the model area where external influences like wells, rivers, lakes etc. exist.

Hydraulic boundary conditions can be selected based on the topography, hydrology, and hydrogeology. Boundary conditions can be different for different locations and can vary with time. There can be various types of boundaries such as potentiometric surfaces controlled by surface water, or recharge/ discharge areas or impermeable strata.

Boundaries can be classified into three major types to facilitate mathematical modelling:

- (i) Boundaries with prescribed hydraulic head,
- (ii) Boundaries of prescribed groundwater flux, and
- (iii) Semi-permeable or Head dependent flux boundary

Boundaries with prescribed hydraulic head

The most common boundary condition is this type where the head (pressure head in case of unsaturated flow) is fixed. This type of boundary condition is mathematically termed as *Dirichlet's condition* (boundary condition of the first kind). In groundwater modelling it is often termed as the constant head boundary. However, the prescribed heads at the boundary may change with time due to water level fluctuation in surface water bodies or draft. This type of boundary condition is encountered when surface water bodies (river, lake, canal, sea, etc) interact freely with the aquifer.

Boundaries of prescribed groundwater flux

Various physical systems exist where groundwater flux at the boundary is known. These boundaries are referred to as prescribed flux boundaries. It is also known as *boundary condition of the second kind, Neumann's condition* in mathematical terms, *or recharge boundaries* in modelling parlance. If the aquifer borders with an impermeable boundary, the flux at that boundary becomes zero. This is a special type, and is considered as a no-flow/ zero-flux/ reflective boundary. Obviously, the groundwater flow will be parallel to the no-flow boundaries, and the no-flow boundaries can be considered identical to streamlines. As such, the models represent the natural groundwater divides or stream lines as no-flow boundaries.

Head dependent flux boundary

Semi-permeable boundaries are generally used to represent leakage from surface water bodies where the exchange of water between aquifer and surface water bodies depend upon the head difference between surface water and groundwater. Such flow conditions exist when the river bed/ lake bed acts as a semi-permeable layer between the water body and the aquifer. This type of boundary condition is also termed as the *mixed boundary, Boundary condition of the third kind, Cauchy's / Fourier's Condition, or Head dependent boundary.* The leakage principle is used to introduce this type of boundary in the model by defining the leakance of the semi-permeable layer of the water body. When the leakance is zero, no interaction can occur and the surface water body is entirely separated from the aquifer.

Initial Conditions

Initial conditions must be specified for the entire model area while modelling transient flow (to accommodate variations with time) problems. In the flow model, the initial conditions can be the measured head distribution at some defined initial time, say t=0. Best estimates may be used where there are no measured heads available. For transport problems, the initial concentrations need to be specifies at each nodes. In steady-state flow problems, an initial steady state head distribution may be provided to assist the iterative numerical computations of the model. Unlike the transient case, here it is only a numerical requirement.

Stages of Model Formulation

In spite of the overall model approach to a given problem remaining the same, alternate numerical theories for solving partial differential equations lead to different types of numerical models. The important phases in model design and construction can be described based on the previous discussion on modelling components:

- Interpretation of field data
- Comprehending the groundwater system
- Conceptualization of the system
- Selection of the model
- Calibration and validation
- Model application
- Presentation of results

Interpretation of field data

Field information is essential to understand the natural system, to specify the problems, to enable model selection, and to prepare model input. The quality of model simulations depends upon the validity of the model physics and on the input data quality ("garbage in, garbage out" rule applies). Model parameters are to be derived from field data (eg. as Transmissivity and Storage Coefficient from pumping test). Time needed to perform a model study will depend significantly on the time required to collect and prepare model input data.

Comprehending the groundwater system

To ensure quality of model results the user should have good appreciation of the natural system. Distribution of parameters and boundary conditions are to be identified. Clarity of the problem at hand is important. This will allow the model user to accomplish the analysis of a complex groundwater system with individual solutions for well defined tasks. Solution to groundwater problems may not always necessarily require the most sophisticated models. The model used should be simple enough to facilitate modelling efforts, but should not be too simple to exclude dominant features of the problem.

Conceptualization of the system

In a model study, the natural system has to be represented by a conceptual model for which an approximate solution is applied. To design an equivalent system with simplified conditions requires extensive information on the natural system. This step is crucial in the whole modelling process as errors crept into the conceptual model can not be corrected during the later stages of model calibration or simulations without major revisions.

Selection of the model

A model gives meaningful results for well defined problems. No single model may be applicable to all types of flow/ transport problems. The user should review various model codes (2D or 3D, flow or transport or both, saturated or unsaturated or combined, finite difference or finite element or BEM or AEM etc.) available to select the most appropriate one useful for the specific problem at hand.

Calibration and validation

Model calibration and validation are required to overcome the lack of input data. They also accommodate the simplification of the natural system in the model. C calibration and validation may fail or yield inadequate results if significant feature of the groundwater system are absent in the conceptual model.

In calibration, simulated values (head or concentration) are compared with field measurements. Model inputs are fine tuned within the permissible ranges until both simulated and observed values agree within the chosen tolerance limits. This process can be done either by trial-and-error adjustment or automatically by means of inverse or parameter estimation models. Model calibration is another crucial stage in the modelling procedure. It demonstrates that the site-specific groundwater model is capable of reproducing observed responses by the natural system.

Model validation is a demonstration on the utility of the developed model in making accurate predictions. A common practice in validation is the comparison of the model with a data set not used in the calibration. If the model does not reproduce accurate results during validation, model data are recalibrated using both data sets.

Model application

Model application is the part of the study in which the numerical model demonstrates its dominance over all other models. The outcome of a numerical model must be reviewed critically. When applying numerical models in the predictive sense, there are limits in model application. Predictions into far future are highly uncertain. Thus, sensitivity analyses become important.

Sensitivity analyses helps to rank the input data in terms of its influence on model predictions and gives answer to "what if?" scenarios. It also allows one to assess unforeseeable groundwater stresses in the future. For instance, future land use practices may change natural groundwater recharge pattern.

Presentation of results

The output of models is numbers representing heads or concentrations at discrete points of the domain at a given times. This output need to undergo post processing to produce outcome that is vivid and more comprehensible. 2D or 3D Plotting/ graphical software packages for pictorial/ graphical viewing, 3D animations for visualizing contaminant movements/ flow underground etc. are useful in presenting modelling results illustratively and informatively. Nevertheless, misuse or misinterpretation of model outcome should be avoided at all costs.

CLASSIFICATION OF NUMERICAL GROUNDWATER MODELS

Groundwater models may be subdivided according to their objective, as follows:

(i) Prediction models;
(ii) Identification or evaluation models;
(iii) Management models.

All three types are closely linked, prediction models forming the basis for the other two types. Each type is discussed below.

Prediction Models

The majority of models in common use are prediction models based on the numerical simulation technique. They predict the response of a groundwater system, in terms of variation of hydraulic heads, to natural and/or artificial hydraulic stresses, especially those associated with pumped groundwater abstractions. Amongst the problems that can be considered with such models are included the prediction of:

- long-term maximum drawdown of a pumped well in an aquifer with seasonal recharge;
- short-term drawdown interference between pumped wells, and thereby associated reduction in yield;
- long-term drawdown trends, and thus the useful life of pumped wells, in overdeveloped aquifers;
- reduced flow in surface water courses in hydraulic connection with aquifers, as a result of groundwater abstraction, through calculation and interpretation of the appropriate draw-downs;
- increased flow in streams and rivers in hydraulic connection with aquifers, as a result of return flows from irrigation areas and leakage from artificial canals;
- groundwater changes resulting from reduced aquifer recharge due to such factors as drought or urbanization;
- groundwater changes resulting from increased aquifer recharge due to such factors as irrigation, leakage from an artificial canal, artificial recharge works, or effects of urbanization;

- movement of the saline-fresh water interface as a result of groundwater abstraction from coastal aquifers;
- pumping rates required to achieve a necessary engineering design;
- design of ditch, tile and other drainage schemes.

In the case of contaminant transport, the concentration distribution associated with a given contaminant loading is also predicted. In view of the current limitations of such models, applications are commonly restricted to prediction of the distribution resulting from a simple, continuous point-source of pollution, with grossly-simplified representation of the processes of contaminant dispersion, sorption and degradation. The modelling of this problem is usually limited to a local site scale. Prediction of contaminant transport at the regional scale, the migration of diffuse-source groundwater pollutants and the behaviour of those pollutants involved in more complex chemistry cannot yet be predicted reliably.

Identification or Evaluation Models

A numerical simulation model may be developed primarily to identify or evaluate the parameters and boundaries of a little known aquifer. This can be undertaken using the simulation model exclusively in calibration mode (Figure 2.1), adjusting the value of parameters and/or boundary conditions to reproduce the observed aquifer response to known stresses.

Management Models

Prediction models employing numerical simulation methods and heterogeneous aquifer parameters have often been utilized to explore groundwater management alternatives. For this purpose the model is executed repeatedly under various scenarios designed to achieve a particular objective, such as obtaining a sustainable water-supply, dewatering an excavation area for construction, preventing saline water encroachment or controlling a contaminant plume. Use of such an approach, however, avoids rigorous formulation of groundwater management goals and may fail to consider important operational restrictions. It is thus unlikely that optimal management solutions will be arrived at using numerical simulation models alone.

More recently, true management models have been developed incorporating rigorous formulation of management objectives and/or policy constraints, through use of decision criteria or linear optimization programming, with numerical simulation of groundwater hydraulic or contaminant behaviour. Such models must be based on decision criteria, such as maximum total water-supply, minimum total project cost or maximum project economic benefit, or on a given policy constraint, such as minimum required water-supply, conforming to some water quality standard or a ceiling for capital and/or running costs. By their nature, management models will only be developed for aquifers, or parts of aquifers, for which a soundly validated prediction model and broad-based reliable field data exist. The idea behind such models is that one often wishes to know where to best locate wells and how much to pump or inject at each location. It is a straightforward matter to formulate aquifer management problems as optimization problems. There, the objective might be to minimize pumping costs or contaminant clean-up costs, for example. In addition, there will be a series of restrictions on hydraulic heads, drawdown values, velocities, and solute concentrations. Economic, logistic, and legal considerations may also be reflected in the constraint set. In such models the groundwater flow and/or contaminant transport equations are included as constraints. Therefore, optimal management solutions simulate the behaviour of the system of interest.

CONCLUDING REMARKS

Mathematical models are tools, which are frequently used in studying groundwater systems. In general, mathematical models are used to simulate groundwater flow and solute and/or heat transport. Model must be regarded as a tool to aid decision-making, but decision should not be based solely on the results generated by the model. Further, groundwater models can be used as predictive tools. However field monitoring must be incorporated to verify model predictions as predictive simulations are estimates that dependent upon the quality and uncertainty of the input data.

If the basic principles of groundwater flow/ contaminant transport and the underlying assumptions of modelling are lost sight of, there is serious danger of gross misinterpretation of model output. This is more likely to occur when models are packaged and automated, as of today. Therefore, in the application of all models, and most especially of groundwater quality models, a high degree of scientific judgement tempered with wide experience of field observation is desirable to produce sound interpretations.

So far as the groundwater flow models are concerned, the underlying mathematical equations have been adequately verified, and the physical meaning of the parameters involved is clearly understood. However, in the case of contaminant transport there need to be more insight on the mathematical characterisation and measurement of hydrodynamic dispersion, and about the best way to identify, to measure and to model the chemical interactions and reactions that can occur in an aquifer. So, application of solute transport models and interpretation of the results thereof should be exercised with great caution.

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