TRAINING COURSE

ON

SOFTWARE FOR GROUNDWATER DATA MANAGEMENT

UNDER

WORLD BANK FUNDED HYDROLOGY PROJECT

LECTURE NOTES
ON

GROUNDWATER MODELLING SOFTWARES

(UNIT-6)

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GROUNDWATER QUALITY MODELLING

1.0 INTRODUCTION

Groundwater is becoming an important source of water supply in many regions due to rapid growth of the world's population, which is placing an increasing demand upon fresh water supplies. Use of aquifers as operating reservoirs will require an understanding of water quality problems created by sea-water intrusion in to coastal aquifers, recharge of surface water into aquifers, underground waste disposal and infiltration of pollutants from surface sources into aquifers. Since pollutants, wastes, and recharge waters are normally miscible with the native ground water, an understanding of the mechanics of miscible fluid displacement is necessary for the analysis of groundwater quality problems.

Mass transport modelling in the ground, both in the saturated and in the unsaturated zone has attracted the attention of many groundwater and oil scientists and engineers over the last two and half decades. Many of the current posed hydrochemical problems, groundwater and soil pollution studies, analysis of the behaviour of chemical, biological and radioactive substances in the disposal sites and repositories, heat transport to the sub-soil and geothermal fluid behaviour need ground water treatments.

The basic principles for these quantitative treatments, method of solution and data gathering techniques have been the object of intense and successful developments in the last two and half decades, with the improvement of existing mathematical tools and the implementation of powerful new ones over the last twenty years. Progress is still being made as the mathematical tools sometimes present numerical problems, are cumbersome, need parameters that are not readily available, are not appropriate for commonly available computers, or refer to media having properties that have still not been well defined, such as fissured rocks and highly heterogeneous, unconsolidated formations.

Plenty of good publications from scientific and technical community are available which deal with the advances of the groundwater flow modelling which control the transport of substances and pollutants through advection and hydrodynamic dispersion, numerical and as well analytical solution and basic concepts of dispersion or fluid rock interaction. Inverse methods are becoming practical tools for ground water flow problems, but as yet, as far as mass transport is concerned, they are still in the early stages of development.

Pollution is a modification of physical, chemical and biological properties of water, restricting or preventing its use in the various applications where it normally plays a part. In case of groundwater, it is usually traced back five main origins:

i) Industrial pollution through used waters which contain chemical compounds and trace elements, rain infiltrating through waste disposal and accidents like the breaking of a pipe line.

ii) Domestic pollution through, rain infiltrating through sanitary landfills, accidents like the breaking of septic tanks.

iii) Agricultural pollution through irrigation water or rain carrying away fertilizers, minerals, salts, herbicides and pesticides.
iv) Environmental pollution mainly seawater intruding in coastal aquifers.
v) Pollution due to dumping of nuclear wastes (radiological pollution)

1.1 Physical, Chemical and Biological Aspects of Groundwater Contamination

Most potential groundwater contaminations are released at or slightly beneath the land's surface. Here the wastes are subject to the processes of leaching and percolation which may lead to their introduction into the groundwater. As they move through the unsaturated zone above the groundwater table it is tendency of contaminants to attenuate; a process which sometime eliminates potential contamination sources as serious problems, because the contamination simply does not reach the groundwater in sufficient strength. It is attempted to describe the physical, chemical and biological processes that influence the movement of contaminants through the soil of the unsaturated zone and in groundwater aquifers.

1.1.1 Physical aspects

Contaminants which are introduced into the environment as waste solutions are already mobile, but dry solid materials must be leached; that is, they must be dissolved before they can move. The solution of various contaminants is basically a chemical phenomenon. Once available in mobile form the solute is subject to an array of physical properties and characteristics which influence its movement and distribution.

Consider first the movement of s solute through the unsaturated zone, or zone of aeration, to the water table. The movement through this zone is primarily vertically downward from the surface, and the solute is suspended to undergo only a mild degree of horizontal displacement. Since the solute movement depends to a great extent on the movement of water, it must also depend on the same physical factors.

The climate of a region also influences these physical properties and characteristics. The distance that solutes move downward depends on the amount of water entering a given soil. If it is in the upper 30 cm of soil, a solute may travel back toward the surface due to evaporation. If enough rain falls to remove the solute from this zone it will probably enter the groundwater. therefore, in arid regions or during the summer, when evapotranspiration is important, the total rainfall of each storm is just as important as the total precipitation. But when evaporation is negligible, low intensity rainfall is more efficient in moving contaminants.

The climate also influences the hydraulic properties of the soil water, viscosity and surface tension, since they depend on temperature. Consequently soil drain slowly during cold weather and not at all when frozen. As the solution freezes salts are concentrated in the non-frozen liquid. It is not unusual to find brines in partially frozen soils resulting from this concentration process; brines that becomes selectively mobile because of their hydraulic properties.

It may take years for a solute to percolate through the zone of aeration,even in the absence of chemical effects, due to the slow rate of movement of percolating water. On the other hand, it may take a pulse of water only a few weeks or months to move the same distance. The pulse of 'water' is like a flood wave in a river, representing not the actual movement of water particles, but only the movement of a pressure ridge. Even so, under favorable circumstances the solute may reach the water table in a matter of hours, although days or weeks is a more realistic time span. Once the pollution reaches this saturated zone it usually spreads out laterally and moves in the general direction of groundwater flow.

Located along the top of the aquifer at the water table the contaminants must either penetrate into the aquifer or float on top. The latter occurs when the contaminated water is buoyant, say due to a high temperature for a miscible pollutant; or more likely in groundwater systems, this is due to an immiscible fluid of low density as in the case of hydrocarbons like fuel oil or gasoline. After entering the groundwater system the pollutant is convected toward the natural discharge area of the aquifer, which may be a stream, river, lake, spring or wetlands, or toward groundwater extraction activities in the vicinity.

The movement of the polluted water is subject to a number of physical factors identical or similar to those for the zone of aeration. This is, the convective motion of the pollution depends on the groundwater flow field, which in turn depends on the piezometric head distribution (called the water table configuration in an unconfined aquifer), hydraulic conductivity, an the sources and sinks of water influencing the aquifer (boundary conditions). In confined aquifers the flow is primarily horizontal due to the presence of the confining layers, unless there is a significant dip of the formation. In unconfined aquifers the flow is still primarily horizontal, although density effects, additional recharge at the surface and dispersion lead to limited vertical movement.

When dealing with a quantitative analysis of aquifers we often average its properties and characteristics over the vertical. Thus, for example, the hydraulic conductivity (K) is replaced by a factor called the transmissivity ($T=KB$, where B is the aquifer height and K is an average conductivity). A flow field evaluated on this basis assumes horizontal flow and, since this is often the case in practice, it is usually an adequate representation of reality. But the rate of movement of the pollutant depends on the effective porosity (n_e), as well as the flow field, and it, too, is often average over the vertical. The resulting velocity or rate of movement (V) is given by $V_i=(K/n_e)\delta\Psi/\delta x_i$ where x_i is the direction of flow. In a porous media field observations indicate that the natural rate of movement of pollutants varies from 2 m/year to 2 m/day; in fractured or fissured media, because of the low porosity, the rate may approach 300 m/day. Naturally the direction of pollution movement is aligned with the flow field.

As the pollution moves through the aquifer it mixes due to density effects, if any, and due to a phenomenon described by the term "dispersion". The term really represents a hierarchy of effects, each on a different scale. At the smallest scale there is molecular diffusion, due to the "Brownian motion of individual molecules, which results in the mixing of two adjacent miscible liquids even if there is no flow. This phenomenon is generally of

no importance in groundwater situations, but it may be very important in the unsaturated system.

On a slightly higher scale there is mechanical dispersion. This is mixing due to the local velocity field in the porous media. The local velocity varies from point to point, because the media is tortuous and because there is a velocity profile across each individual saturated pore. consequently, two water particles which are initially adjacent will experience different velocity histories in strength and direction as they move through the porous media, and at some time late they will arrive at different locations. Their general movement will have been in the direction of flow as shown by the verage of many particles initially in the same general location; but their final location will differ from the average with respect to longitudinal ((in the direction of flow) and lateral or transverse (in the orthogonal direction) displacements.

Molecular diffusion leads to isotropic mixing with respect to the flow. Mechanical dispersion, which depends on the flow velocity ((V_i), causes a greater degree of mixing in the direction of flow, the longitudinal direction, than in the lateral direction. It can be shown that these dispersive phenomena are represented by a Fickian law, in terms of a concentration gradient and a dispersion coefficient. For molecular diffusion this co-efficient (D^*_d) is the diffusion coefficient (D_d) for the given solute in bulk water at a given temperature and concentration, adjusted for the presence of the porous media ($D^*_d \cong 2/3\ D_d$ for saturated flow). For mechanical dispersion the coefficient is often simplified to linear relationships $D_L = \alpha_L V_i$ for longitudinal dispersion and $D_T = \alpha_T V_i$ for lateral dispersion where α_L and α_T are "dispersivities" representing the effect of the pore structure on the dispersion. Typical laboratory tests indicate α_L is in the range of 0.1 mm to 10 cm, and that is roughly correlated to the grain size of the porous media. In unsaturated flow the relationship is more complicated, and α depends on moisture content.

The two effects as characterized by their coefficients can be added to yield a "hydrodynamic" dispersion coefficient ((e.g. $D'_L = D_L + D^*_d$), and it is this coefficient which is used in most modelling. If the flow velocity is high enough, then $D'_L \cong D_L$ and molecular diffusion is neglected.

There is another higher level of dispersive mixing. Natural aquifer materials are made of stratified layers, or fractures and fissures with a geometrically consistent pattern. Considering only the case of stratified materials, each layer of the material has its own characteristic hydraulic conductivity. Consequently, the rate of flow and pollutant movement through the different layers varies; for example, the more permeable layer is characterized by a high velocity. At the same time, many models, mathematical analyses and field data average properties over the vertical. In the case of field data this is due to the finite vertical length of perforated well casing. Consequently the average velocity in each layer and the mixing about it is not dealt with but an average velocity in the aquifer and the mixing about this new average is dealt with. The degree of mixing at this scale will be characterized by the geometry and conductivity variation of the aquifer materials. It has been shown that the gross mixing in heterogeneous deposits like these can still be assumed to behave as does the mixing due to hydrodynamic dispersion. In this case, however, the dispersivities are much

larger reflecting the field conditions.

The mechanism of pollution introduction also influences the behaviour of the plume. So far, this section has emphasized pollution due to the leaching of soluble materials, percolation through the zone of aeration and introduction to the water table. Pollution can also come from a hydraulic connection with contaminated surface water, direct injection, short-circuiting from one aquifer to another through abandoned well-casings, through leakage via a semi-permeable confining bed, or from salt water intrusion. Each of these either influences the flow field and/or determines the type of contaminant boundary condition on the flow field.

When the source of pollution is widespread, such a non-point agriculture pollution, plumes do not exist or are unimportant on a regional scale. Instead there is a gradual decline in the quality of water as it moves through the aquifer. Users in the up-gradient portions of the aquifer have relatively high quality water. Users at the downstream end of the aquifer receive all of the non-degradable pollution inputs to the aquifer and have a much lower quality of water.

1.1.2 Chemical Aspects

As water moves through the soil in the zone of aeration, or through rock or porous material in a groundwater aquifer, its composition changes. The water is in contact with various soil and rock materials, with the organic and inorganic constituents of soils and with gases in the atmosphere or produced by biological or other processes. The result of these contacts is solution, or chemical reaction followed by solution, and the water accumulates numerous dissolved impurities. This, however, is only the most basic reaction or chemical characteristic that must be considered in an analysis of groundwater pollution. It is this natural leaching process which leads to the background concentration levels of organic, salts, metals, etc. in groundwater.

The basic chemical phenomena that are important in many groundwater pollution problems are : volatility, acids and bases, solubility and precipitation - solution, oxidation-reduction (redox), surface phenomena including ion-exchange and adsorption, and the particular aspects of organic and heavy metals, including hydrolysis.

1.1.3 Biological Aspects

Biological activities have several mechanisms by which they influence groundwater quality. First there is the threat of transmission of pathogenic organisms from organic wastes to the soil, the groundwater and eventually to humans. Second, there is the threat of an increase in concentration of organic material which originates as wastes. These two mechanisms are associated with each other. Third there is the presence of microorganisms which add in oxidation-reduction reactions of organic and inorganic in the subsurface environment. In terms of global nutrient cycling and the threat of increased inorganic contamination of groundwater, this may be the most important.

2.0 SYNTHESIS

The physical, chemical and biological mechanisms influencing the movement and distribution of groundwater pollution can be synthesized and represented conceptually. A mass balance in volume V of a certain chemical species "A" requires:

$$\begin{bmatrix}\text{Rate of Accumulation}\\ \text{of mass of A in the}\\ \text{volume v}\end{bmatrix} = \begin{bmatrix}\text{Net mass flux of}\\ \text{A into V due to}\\ \text{convection}\end{bmatrix} +$$

$$\begin{bmatrix}\text{Net mass flux of}\\ \text{A into V due}\\ \text{to dispersion}\end{bmatrix} + \begin{bmatrix}\text{Source of}\\ \text{sink}\\ \text{of A}\end{bmatrix} \quad \ldots . (1)$$

The term flux refers to the rate at which a mass of A is transported through the boundary of V. This is a rather simplistic model which places all the chemistry and biology into the source or sink term. For example, consider a situation in which adsorption becomes important: term (4) would be negative for adsorption (loss of "A" from liquid) and positive for desorption (gain of "A" of liquid).

Usually this model is presented in mathematical form as a mass transport differential equation. Several authors provide descriptions of the resulting equation, with emphasis on the physical and chemical aspects.

3.0 SIMULATION TECHNIQUES

3.1 Numerical Models of Groundwater Quality

Simulation consists essentially of synthesizing a real or abstract system. The outputs of this system are supposed to approximate the outputs of the prototype within a given degree of accuracy. The simulation model is used to try to reproduce some of the characteristics of the prototype, leading to the evaluation of alternatives or policies That is why they are sometimes called "performance-prediction models".

According to Dooge (1973), ".....the various types of simulation (also called models) could be grouped under the headings of regression models, analog simulation, digital simulation and physical models". All of them are of interest in groundwater hydrology. However, the recent development of high speed digital computers provides the possibility of developing numerical models which reproduce complex prototype systems with increasing accuracy. Since almost all the developed groundwater quality models are numerical, the emphasis will be on them.

A numerical model can be defined as a set of mathematical expressions that is solved numerically and which is supposed to describe the various relations within the system. It can be in the form of differential equations with their auxiliary conditions or of semi-empirical relations, or a combination of both. Two types of information must be available in preparing a numerical model:

(i) laws or relations governing the phenomenon

(ii) auxiliary conditions such as geometry, hydraulic or chemical characteristics, and initial and boundary conditions.

The numerical model, as any other type of simulation reproduces some but not all the characteristics of the prototype. Of course, it is quite legitimate to try to simplify the model by eliminating all characteristics which are unimportant for the purposes of the study. The required accuracy may be fixed and all characteristics discarded which have a negligible contribution to the features one is trying to reproduce. So there should be a tradeoff between sophisticated but costly models and simple but inexpensive ones. However, as usually happens in groundwater quality models, important features may have to be neglected or the model may have to be considerably simplified because of: lack of physical knowledge, very complex quantitative relations between the parameters, lack of proper numerical schematic, very high computer costs or limited capacity of available computers, or limited data (perhaps the most important factor).

It is because of these restrictions that it is important to know what a groundwater quality numerical model can and cannot do. A thorough understanding of the potential of groundwater quality models is necessary to organize data collection and management, to obtain available help for the planning and management process, and for directions for future research.

From the modellers point of view, pollutants move in groundwater by a complex interaction of four processes:

a) Convection is the transfer of pollutants by the moving water with the same velocity and direction. Freeze (1972) suggests that this is the primary mechanism, so that in cases in which the other processes can be ignored, any groundwater flow model can be used for groundwater quality modelling.

b) Mechanical dispersion is the spreading phenomenon caused by velocity variations. This must be included in the model whenever there are strong concentration gradients that may influence the distribution of pollutants as would be observed by a pumping or observation well or other observation technique.

c) Molecular diffusion is usually unimportant compared to dispersion, except if the flow is very slow (e.g. in the unsaturated zone). The molecular diffusion coefficient is often lumped together with the mechanical dispersion coefficient into what is known as the "hydrodynamic dispersion coefficient".

d) Hydrochemical interaction between fluid and soil is sometimes an important process that can change the quality of the groundwater. Basically soil scientists and agricultural engineers have studied some of the complex interactions between dissolved chemical constituents and the soil. Unfortunately, we are only at the beginning of incorporating this body of knowledge into our models.

Most of the work done in groundwater quality modelling is centered on large scale groundwater basins facing salinity problems, or on coastal aquifers with salt-water intrusion. These studies model only conservative pollutants and, although concerned with a very special kind of pollution, are of great practical importance.

By assuming that the quality constituents have conservative properties, the mass transport phenomenon can be described by a set of equations which can be called the dispersion scheme. This scheme can be applied to describe miscible kinds of pollution or immiscible ones, provided that the pollutant behaves like a tracer. It consists of the dispersion equation, the continuity equation, Darcy's law and the state equations of the mixture. A major simplification, which is always included, is to assume that the density and viscosity of the mixture are constant. This implies that the quality constituent behaves like a tracer.

To solve the dispersion scheme, both analytical and numerical methods can be applied. However, the analytical solutions are only found for very simple cases or for research purposes. The numerical solutions, which take full advantage of the digital computer's capacity, are of more practical interest to regional groundwater modelling.

4.0 SUTRA

SUTRA (Saturated-Unsaturated Transport) is a computer program which simulates fluid movement and transport of either energy or dissolved substances in a subsurface environment. The model employs a two-dimensional 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, or

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

SUTRA provides, as the primary calculated result, fluid pressures and either solute concentrations or temperatures, as they vary with time, everywhere in the simulated subsurface system. SUTRA may also be used to simulate simpler subsets of the above processes.

Incorporating the various phenomena as discussed earlier with certain mathematical jugglery the final equation as obtained for the use in the SUTRA model is given below:

$$[\epsilon . S_w . \rho + (1 - \epsilon)\rho_s (x_1 . \rho_0) C] \frac{\partial C}{\partial t} + \epsilon . S_w . \rho . V . \nabla C$$
$$\underline{\nabla} \{ \rho [\epsilon . S_w . D_m . I + D] \} . \underline{\nabla} C$$
$$= \epsilon . S_w . \rho . r_0^w - (1 - \epsilon)\rho_s . r_0^s +$$
$$Q_p (C^* - C) + \epsilon . S_w . \rho . r_0^w . \lambda_1^w . C + (1 - \epsilon)\rho_s . r_0^s . \lambda_1^s . \lambda_1 . \rho_0 . C$$

.....(2)

where

$\underline{V}$ = Velocity vector

$$\underline{\nabla} = \frac{\partial^2 C}{\partial X^2} + \frac{\partial^2 C}{\partial Y^2} + \frac{\partial^2 C}{\partial Z^2} \qquad \text{.....(3)}$$

S_w = saturation content
ϵ = porosity
ρ = fluid density (x,y,t)
ρ_s = density of solid grains in solid matrix.
λ_1 = linear distribution
ρ_o = base fluid density at C-C_o
$\underline{I}$ = identity tensor
D_m = apparent molecular diffusivitry
$\underline{D}$ = dispersion tensor
r_o^w = energy source in fluid
r_o^s = adsorborate mass production rate
Q_p = fluid mass rate (pure + solute mass)
C* solute concentration (x,y,t)

4.1 Physical-Mathematical Basis of SUTRA Simulation

The physical mechanisms which derive thermal energy transport and solute transport in the subsurface environment are described by nearly identical mathematical expressions. SUTRA takes advantages of this similarity, and with a simple program structure provides for simulation of either energy or solute transport. In fact, SUTRA simulation combines two physical models, one to simulate the flow of groundwater, and the second to simulate the movement of either thermal energy or a single solute in the ground water.

The primary variable upon which the flow model is based is fluid pressure. Pressure may vary spatially in the groundwater system as well as with time. Fluid density may vary depending on the local value of fluid temperature or solute concentration. Variation in fluid density, aside from fluid pressure differences, may itself drive flows. The effects of gravity acting on fluids with different density must therefore be accounted for in the flow field.

The flow of groundwater, in turn is a fundamental mechanism upon which the physical models of energy transport and solute transport are based. The primary variable characterizing the thermal energy distribution in a groundwater system is fluid temperature which may vary spatially and with time. The primary variable characterizing the state of slute distribution in a groundwater system is solute mass concentration which may also vary spatially and with time.

SUTRA allows only the transport of either thermal energy or a single solute to the modeled in a given simulation. Thus, when simulating energy transport, a constant value of solute concentration is assumed in the ground water. When simulating solute transport, a constant groundwater temperature is assumed.

SUTRA simulation is carried out in two space dimensions with parameters varying in these two directions. However, the region of space to be simulated may be defined as three dimensional, when the assumption is made that all SUTRA parameters and coefficients have a constant value in the third space direction. A SUTRA simulation may be carried out over a region defined over two space coordinate (x,y) in which the thickness of the region measured in the third coordinate direction (z) varies depending on (x,y) position.

4.2 Fundamentals of Numerical Algorithms

SUTRA methodology is complex because: (1) density-dependent flow and transport requires two interconnected simulation models, (2) fluid properties are dependent on local values of temperature or concentration, (3) geometry of a field area and distributions of hydrogeologic parameters may be complex, and (4) hydrologic stresses on the system may be distributed in space and change with time. Furthermore, a tremendous amount of data must be evaluated by SUTRA with precision. This requires great computational effort, and considerable numerical intricacy is required to minimize this effort. The mathematically elegant finite-element and integrated-finite difference hybrid method employed by SUTRA allows great numerical flexibility in describing processes and characteristics of flow and transport in hydrologic field systems. Unlike simulation models based purely on the method of finite differences, however, the numerical aspects of which allow straight-forward interpretation at an intuitive level, some finite-element aspects of SUTRA methodology require interpretation at a less physical level and from a more mathematical point of view.

4.3 Spatial Discretization by Finite Elements

Although SUTRA is a two-dimensional model, the region of space in which flow and transport is to be simulated may be defined in three space dimensions. The three-dimensional bounded volume of an aquifer which is to be simulated by SUTRA is completely divided up into a single layer of contiguous blocks. These blocks are called 'finite elements'. The subdivision is not done simply in a manner which creates one block (element) for each portion of the aquifer system which has unique hydrogeological characteristics. Each hydrogeologic unit is in fact divided into many elements giving the subdivided aquifer region the appearance of a fine net or mesh. Thus, subdivision of the aquifer region to be simulated into blocks is referred to as 'creating the finite-element mesh ((or finite-element net).

All twelve edges of the two-dimensional quadrilateral element are perfectly straight. Four of these edges are parallel to the z-coordinate direction. The x-y plane (which contains the two coordinate directions of interest) bisects each of the edges parallel to z, so that the top and bottom surfaces of the element are mirror images of each other reflected about the central x-y plane is the element. The mid-point of each z-edge (the point where the x-y plane intersects) is referred to as a nodal point (or node). Thus, the element has a three-dimensional shape, but always has only exactly four nodes, each of which in fact, represents the entire z-edge on which it is located. The nodes mark the fact that, in this type of element, some aquifer parameters may be assigned a different value of each z-edge of the element. The lack of nodes outside of the x-y plane is what makes this element two-dimensional; while some aquifer parameters may vary in value from node to node (i.e. from z-edge to z-edge), no parameters may be assigned varying values in the z-direction.

Within a two-dimensional finite-element mesh there is only a single layer of elements, the nodes of which lie in the x-y plane. Nodal points are always shared by the elements adjoining the node. Only noes at external corners of the mesh are not contained in more than one element. The top and bottom surfaces are at every (x,y) point equidistant from the x-y plane, but the thickness of the mesh, measured in the z-direction, may vary smoothly from point to point.

4.4 Time Discretization

Time is broken up into a series of discrete steps, or time steps. The length of a time step. Δt, is the difference in time between two discrete times, at the beginning and end of a time step:

$$\Delta t_{n+1} = t^{n+1} - t^n$$

where Δt_{n+1} is the length of the $(n+1)^{th}$ time step, t^n is the actual time at the beginning of the $(n+1)^{th}$ time step and t^{n+1} is the actual time at the end of this time step. The time steps are chosen to discretize the time domain before a simulation just as a mesh (or 'spatial steps') is chosen to discretize space. The time length may vary from step to step.

Thee entire spatially integrated governing equation is evaluated at the end of each time step, $t=t^{n+1}$. The time derivative of head is over a time step, divided by the time step length:

$$\frac{dh}{dt}_i \simeq \frac{h_i\left(t^n + \Delta t_{n+1}\right) - h_i\left(t^n\right)}{\Delta t_{n+1}} \qquad \ldots\ldots\ldots(4)$$

4.5 Capabilities and Limitations

SUTRA is based on general physical, mathematical and numerical structure implemented in the computer code in a modular design. This allows straight-forward modifications and additions to the code. Eventual modifications may be, for example, the

addition of non-equilibrium sorption (such as two-site models), equilibrium chemical reactions or chemical kinetics, or addition of over and underburden heat loss functions, a well-bore model, or confining bed leakage.

The SUTRA model stresses general applicability, numerical robustness and accuracy, and clarity in coding. Computational efficiency is somewhat diminished to preserve these qualities. The modular structure of SUTRA, however allows implementation of any eventual changes which may improve efficiency. Such modifications may be in the configuration of the matrix equations, in the solution procedure for these equations, or in the finite-element integration routines. Furthermore, the general nature and flexibility of the input data allows easy adaptability to user-friendly and graphic input-output programming. The modular structure would also ease major changes such as modifications for multi-layer (quasi-three-dimensional) simulations, or for simultaneous energy and solute transport simulations.

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 modelling. 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. The unsaturated flow capability is thus provided as a convenience to the user for occasional analyses rather than as the primary application of this tool.