CHAPTER-2

SUBSURFACE WATER MODELING – FLOW AND CONTAMINANT TRANSPORT

2.1 Introduction

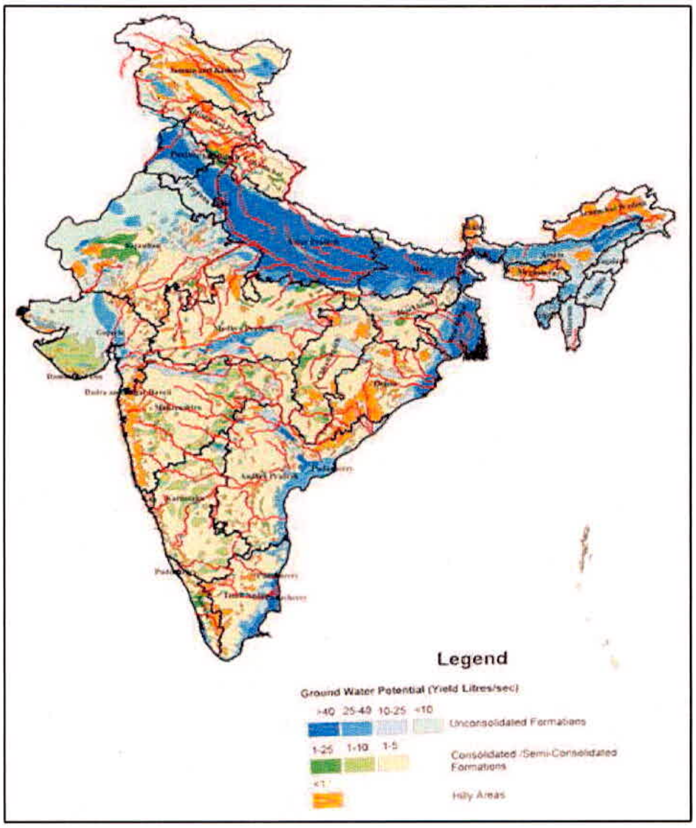
2.1.1 General

Groundwater is an integral part of a complex hydrological cycle that involves the continuous movement of water on earth (Alley et al., 2005). From occurrence as rainfall on earth until it moves out from the land masses, water available on earth as surface water, soil moisture and groundwater, interacts with one other and shapes the space-time distribution of groundwater.

Groundwater as it occurs in various aquifers (defined by their geometry and relationship to topography and the subsurface geology) namely, unconfined, confined, and perched aquifer are under continuous depressurization and expansion of water because of natural processes of recharge, discharge and movement, and extraction (pumping) by human interventions (Winter et al., 2013). The natural processes of groundwater movement that are governed by formational heterogeneity, permeability and potential gradient of flow, is generally slow; while the human interventions to the natural systems not only accelerate the processes but may also mismatch recharge and discharge component as well as geochemical/geo-environmental conditions. Groundwater levels depletion and quality deterioration, in many parts of the world including India, are examples of changing groundwater scenarios. Impact of climate change on groundwater is another emerging issue that poses a new challenge to the supply and demand management of groundwater resources. Groundwater potential plays a supplementary source of water to mitigate drought. Rising demands of, and increasing pressure on, groundwater driven by booming population growth and their allied demands for food and drinking water security pose other challenges on management of space-time availability and demand. These eventually call for the need of scientific tools and techniques, which are process based, robust, less complex, easy to handle, satisfy the hydrogeological settings, capable to simulate responses both local and regional scale with reasonable certainty, and can be used for policy evaluation, drought mitigation and for management of groundwater quality.

2.1.2 Hydrogeological settings of India

India with its varied hydro-geological settings (Fig.2.1) comprising; 12.5% as Himalayan highland province, 15.27% as Ganges-Brahmaputra alluvium province, 14.25% as Alluvium Sandstone composition and Precambrian sedimentary formation, 44.45%as Precambrian Crystalline province, 12.13% as Deccan trap province (Basalt), and 1.4% as Gondwana sedimentary province, of contiguous land areas of 3,188,111 sq. km. (CGWB,2006) supports 85% of rural domestic needs, 50% of urban and industrial needs and about 65% of irrigation water requirements (CGWB, 2011a; Planning Commission, 2011).



Source: CGWB, 2006

Figure 2.1: Hydrogeological map of India with superimposed major river networks

Usages of groundwater in India have increased at a very rapid pace by the advent of tube wells as the groundwater extraction structures. The data of the Minor Irrigation Census conducted in 2001 together with the data compiled by Singh and Singh (2002) showed enormous growth of groundwater structures, about 18.5 million in 2001. Many people predicted (Shah, 2009) that by 2009, the number of groundwater structures might have gone up to 27 million. There is no reason to believe that the growth of groundwater structures and uses of groundwater in India are going to slow down in future, unless otherwise controlled by enforcing legislation, rather will continue to rise because of growing concern on water quality, socio-economic improvement and socio-cultural dimensions of the rural sector. With such huge number of groundwater abstraction structures and nearly 62% status of groundwater development (CGWB, 2014), India is placed now the largest groundwater user in the World (Shah, 2009). These intervening characteristics have put India's groundwater systems into a number of challenges, which include: (i) depletion of aquifer storage and groundwater levels, and their effects on availability, terrestrial and aquatic ecosystems, (ii) drying up of shallow wells, intensification of deep tube wells, and failure of tube wells in hard and fractured rock areas, (iii) deteriorating groundwater quality due to contaminants of geogenic origin (Arsenic, Fluoride, Iron, etc.) and intrinsic salinity, (iv) leaching of contaminants from anthropogenic activities (both organic and inorganic constituents),(v) groundwater salinization arising from various different processes of induced hydraulic disturbance and soil fractionation,(vi) changes of geochemical properties due to geological minerals mining and mineralization, (vi) threat of saline water ingress in coastal aquifers, etc.

Climate change impact on groundwater is an added complexity. Many areas in India are prone to hydro-meteorological drought. In the context of climate change, the severity of drought may increase. Groundwater planning and management in those areas would play a vital role for drought mitigation. Groundwater management in the hard and fractured rock areas possess a lot of uncertainty and has emerged as a big challenge to the stakeholders and policy makers.

2.1.3 Rainfall and groundwater resources of India

Alike varied hydrogeological provinces, India has wide variability of climatic conditions and hydrometeorology. The country has uneven spatial and temporal distribution of rainfall. The annual spatial variation of rainfall [based on data of 193 years (1813-2005)] showed variation ranged from less than 100 mm over parts of Ladakh (Jammu & Kashmir State) and Jaisalmer district (Rajasthan State) to less than 400 mm over central peninsula, between 1000 mm and 1788.4 mm over central highlands and eastern plateau, between 1000 mm and 11405.8 mm over northeast, and between 1000 mm and 7445.7 mm over Sahyadri range (Ranade et al., 2007). The temporal distribution has characteristics of both seasonal and annual variation. The annual variation of rainfall (1813-2005) ranged between 730.14 mm and 1487.05 mm with the mean annual for the whole country as 1165.9 mm, whose seasonality varied: 0.7% during winter, 9% during summer, 77.4% during monsoon, and 12.9% during post-monsoon (Guhathakurta and Rajeevan, 2006; Ranade et al., 2007).

India's groundwater resources are primarily rainfall recharge driven. The annual dynamic (replenish annually) groundwater resources, as per the estimate of 2011 (CGWB, 2014), was 433 BCM (billion cubic meter or km^3), of which net available groundwater was 398 BCM, and annual draft for irrigation, domestic and industrial uses was 245 BCM that indicated an average stage of development as 62%. The availability and draft of groundwater are highly uneven; while availability is primarily characterized by rainfall, hydrology, hydrogeology, and surface and sub-surface interaction of water; on the other hand, groundwater draft is governed by availability and demands for various sectoral uses. Uses of groundwater conversely depend on usage and groundwater withdrawal infrastructural facilities available to the users.

2.1.4 Groundwater related issues in India

India is primarily an agro-economic based country and currently, 90.73% of groundwater usages are done for irrigation purposes (CGWB, 2014). Projection showed (Kumar et al., 2005) that by 2025 and 2050, groundwater based irrigation requirements may increase, respectively, by 11% and 38.5% over the withdrawal of 222 km^3 (BCM) in year 2010; while the total groundwater requirements for different sectoral uses may increase by 17% and 50%over the total withdrawal of 245 km^3 in year 2010. It means, there could be a possibility of equalizing groundwater demands with net availability, if no other impinging issues like climate change, impact the groundwater resources. The situation of groundwater resource prospects pronounces more challenging, when risk emerging from groundwater quality deterioration due to anthropogenic (leaching of both organic and inorganic contaminants from surface activities) and geogenic (Arsenic, Fluoride, Iron, Salinity, etc.) sources of contaminants is linked to the quantity of fresh water available. Over exploitation beyond the safe limit of withdrawal (70 % of annual replenishable quantity) together with the quality deterioration of groundwater is given/giving rise to a number of conflicting issues amongst the groundwater stakeholders, which include; increasing energy cost for withdrawal of groundwater, base flow reduction, abandoning of wells due to influence of contaminants, influences of multiple wells in close proximity of freshwater zones, livelihood problem of small farmers due to scarcity of groundwater, etc. On the other hand, in areas or a region likely to face hydro-meteorological drought, how groundwater particularly the static sources, can sustainably support demands of domestic and agricultural sector, is another issue that needs to be addressed by management strategy derived from mathematical modeling.

India has a long coastline of about 7500 km, of which about 5400 km belongs to peninsular India and the remaining to the Andaman, Nicobar and Lakshadweep Islands. The Country houses more than 63 million people living in low elevation coastal areas (land area 82,000 km^2 that constitutes about 3% of India's land area) and nearly 250 million people living within 50 km of the coastline (NIH, 2014). The coastal zones also provide sites for productive agriculture, export-processing zones, industries, harbours, airports, land ports, and tourism. Coastal aquifers are vital strategic resources that provide and supplement the demand for freshwater. Due to excessive groundwater withdrawals, a number of coastal stretches, viz. Minjur coast in Tamilnadu, a long stretch in Odisha, Saurashtra region in Gujarat, Sunderbans in West Bengal are under threat of ingress of sea water intrusion.

According to many experts (Tuinhof and Heederik, 2003; Zektser and Everett, 2004; Planning Commission, 2007; Siebertet al., 2010; Vijay Shankar et al., 2011; Gardunu et al., 2011) groundwater scarcity, depletion of water table and contamination of groundwater problems worldwide, including India, are not only because of limiting availability of groundwater resource but due to unscientific and haphazard extractions, lack of understanding of aquifer characteristics and management of groundwater, which got triggered by a number of unresolved cross-cutting issues.

As a step towards revival of depleted groundwater table, augmentation of groundwater resource in water scarce areas and dilution of contaminated aquifers, Government of India (CGWB, 2002; 2011b; 2013) together with State governments, as a countrywide program, is promoting artificial groundwater recharge by rainwater harvesting and conservation of monsoon surface runoffs. Artificial recharge basically addresses groundwater supply augmentation by recharge management. However, the groundwater problem resolving issue seems to remain unresolved, unless and until the demand-side (groundwater discharge) management is also taken up simultaneously.

Supply-side and demand-side management together with groundwater quality can effectively be managed when a sufficient understanding about groundwater systems, aquifers geometry and hydraulic properties are adequately known. The concept, based on which the groundwater availability and movement has been developed, is the 'Elementary Representative Volume (ERV)' (Bear, 1972). The application of idealized concept of groundwater theory to aquifers having heterogeneity and antistrophic properties/characteristics of materials, which a real-life groundwater system generally possesses, poses the primary challenges in defining a groundwater system. The tasks become further challenging when the aquifer databases are inadequate and a regional groundwater management plan is derived based on those scarce databases.

2.1.5 How modeling can help groundwater management?

To meet the goal of increasing demand of groundwater, modeling and management should go side by side. Groundwater Modeling is an efficient scientific tool, for management of resource that provides the framework to decide and predict the fate of decision variables, which are expected from a hydrogeological system (Ghosh and Sharma, 2006). Groundwater models are developed based on conceptual descriptions or approximations of physical systems or processes, which are translated into well-posed mathematical equations. The mathematical representation converts the physical system into the conceptual framework of computation through mathematical variables that helps perform the job of simulation and scenarios development for imposed stresses and/or strains without physically intervening into the system (Bear, 1972; 1979; Bear et al., 1992). In other words, a groundwater model is a simplified version of a groundwater system that approximately simulates the relevant excitation-response relations of a system. The simplification is introduced by a set of assumptions, which expresses the nature of the system, their features, and behaviors, which are relevant to the problem under investigation. Therefore, no model can be said to be unique for all hydrogeological setups and conditions.

2.1.6 Issues related to modeling

Numerous numerical groundwater models have been developed in the past and applied for groundwater modeling with different degrees of success. Some of those, viz. MODFLOW coupled with MT3D, or its various forms of development, have wide acceptability amongst groundwater professionals. In India, groundwater modeling, using either MODFLOW or its various forms or by using self developed source codes, has also gained popularity. However, a lot of uncertainty in model setups and predictions has been reported owing to scale effects in regionalization of hydraulic properties derived from scarce data. These uncertainties, many a times, have posed questions about efficacy of using available numerical models and modeling tools. Whether the existing widely accepted numerical models are adequate to apply in India's complex hydrogeological setups with the available databases or there is a need to modify components of the existing models by integrating site-specific hydrological modules, or there is a necessity to develop altogether a separate model code to satisfy the hydrogeological conditions and requirements of India's groundwater professionals. The subsequent sections bring out a critical appraisal on existing groundwater models, their capabilities, scope of using in India's hydrogeological contexts, modification/improvement needed to reduce uncertainty in predictions, etc.

2.1.7 Modeling as the management tool

Use of groundwater models should not remain in the framework of model building, calibration and validation based on historical data; it should go beyond, as a tool for decision support system, for policy evaluation based on different management scenarios, and depicting the results in such a way that field professionals could interpret those as the decision variables. This is possible by coupling Simulation-Optimization models together with an interfaced platform based on demand driven decision support system for depicting results in different modes viz. graphs, thematic maps and tabular forms. These eventually call for development of a comprehensive integrated modeling tool, which is user friendly; process based and can navigate with advanced tools.

2.2 Subsurface Modeling

2.2.1 General

The sub-surface water system comprises two zones; the zone above the groundwater table called unsaturated zone or vadose zone, and the zone below the groundwater table called saturated zone (Fig. 2.2). In the vadose zone, the inter-granular space is partly filled with water; the remaining space is occupied by air. The zone of saturation is saturated by water. The unconfined aquifer represents the upper surface of the zone of saturation, which varies depending on recharge and discharge. The zone of aeration is further sub-divided into three categories from top to bottom; i.e., soil water zone, intermediate vadose zone and capillary zone (Fig. 2.2). There is no sharp boundary between these zones.

Unlike the saturated zone, the unsaturated zone is a source of readily available water for human consumption. It is of great importance in providing water, nutrients and contaminants to the saturated zone. Hydrologically, the unsaturated zone is often the main factor that controls water movement from land surface to aquifer. Thus, it strongly affects the rate of recharge and the transport of nutrients and contaminants to the saturated zone. It is often regarded as a filter that removes undesirable substances. To some extent this is true, but a more general fact is that flow rates and chemical reactions in the unsaturated zone control the fate of contaminants enter into the aquifer. Understanding of unsaturated-zone processes is crucial in determining the amount and quality of groundwater that is available for human use.

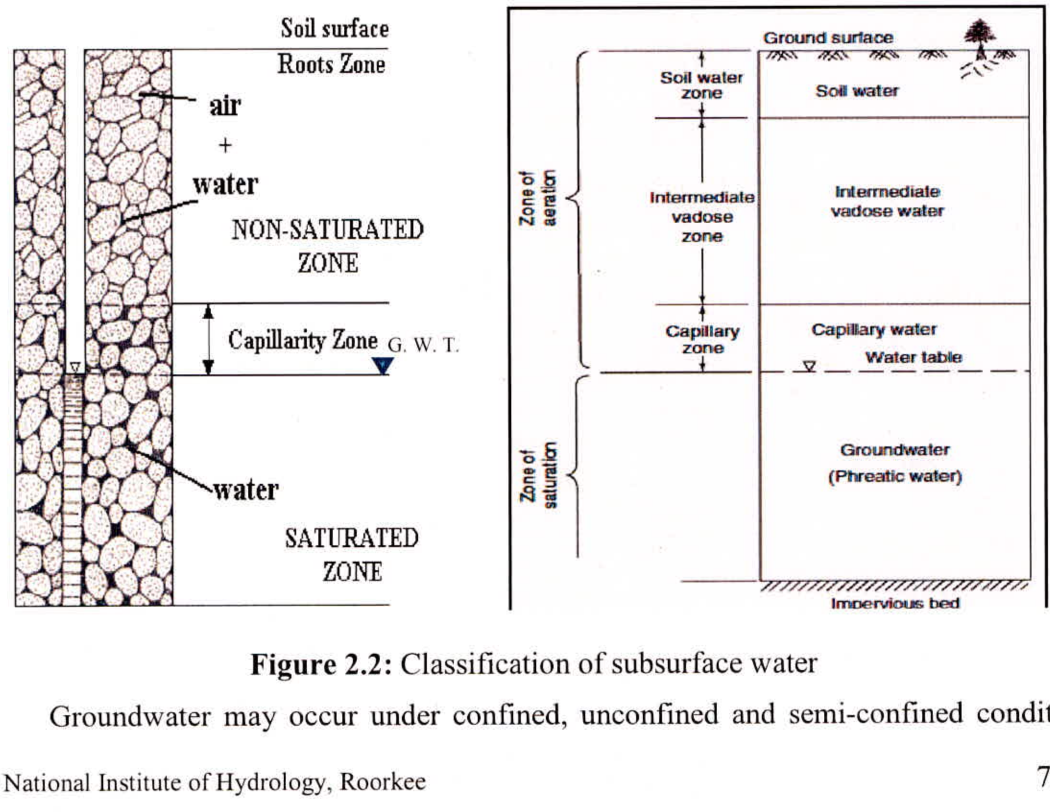


Figure 2.2: Classification of subsurface water

Groundwater may occur under confined, unconfined and semi-confined conditions.

The top aquifer that receives direct recharge from rainfall is the unconfined aquifer. In alluvial areas, confined and unconfined aquifers may be separated by clay or silty clay layers. Such clay layers may vary from few meters to several kilometres. Sometimes the confined and unconfined aquifers may be separated by clayey sand, silty sand or sandy loam that forms semi-confined conditions. The confined or semi-confined aquifers may be under unconfined conditions in some upper reaches. In hard rock areas, unconfined aquifers are formed from the weathering or deposition of rock materials. In these areas, groundwater occurs in fractures and fissured conditions, and under confined conditions depending on the type of formations.

2.2.2 Issues Related to sub-surface zone Modeling

The occurrence and movement of groundwater, both in terms of quantity and quality, in different aquifer systems (coastal, hard-rock, arid, semi-arid, etc.) are controlled by the local or regional physiographic, hydrology and subsurface geology and the forcing interventions onto the aquifers. Numerous spatiotemporal variables such as; aquifer parameters, recharge and discharge govern the flow and transport processes of sub-surface system.

The occurrence and movement of groundwater is not local. The localized or point scale estimation of groundwater system's response may cause erroneous results. A complete water balance approach, by following the governing laws of groundwater flow with initial and boundary conditions, is necessary to accurately estimate the responses of aquifer system. Analysis of groundwater systems is necessary to supplement the decision variables. Groundwater modeling provides a framework to decide and predict the fate of decision variables. Groundwater model tools help simulate current groundwater behaviour and predict future groundwater scenarios. Models analyze and predict the behaviour of aquifer systems representing varying hydro-geological settings on local and regional scale. Mathematical modeling tools provide a quantitative framework for visualization, analyzing data and quantitative assessment of system's response subjected to various internal and external forcing functions. The sub-surface water modeling is required to address the following main purposes:

- For evaluation of groundwater quantity and quality based on present and future developmental activities;
- Impact of proposed waste-disposal activities;
- Planning, design and evaluation of remediation strategies for both quantity and quality of groundwater;
- Assessment of transport of pollutants;
- Assessing and control of sea water intrusion in coastal aquifers;
- Reclaiming water logging and salinity problem by providing the subsurface drainage system;
- Optimization of existing and future groundwater monitoring system;
- Controlling groundwater level depletion and managed aquifer recharge;
- Studying river-aquifer interaction and enhancing base flow contribution to rivers and streams;

- Studying effect of channel on groundwater flow and chemical quality;
- For long-term risk assessment and management;
- Assessment of overall environmental impacts.

Water resource evaluation often involves an integrated analysis of groundwater and surface water conditions. Examples of questions generating a need for a modeling evaluation of surface water and groundwater interactions include (Varda et al., 2002):

- How will a transfer or new use of groundwater affect existing water uses on a stream system? (or, how will transfer of surface water uses impact present groundwater conditions?)
- How re-engineering of stream hydrograph impact groundwater elevations in the riparian zone?
- How will channel restoration activities change stream gains/losses and resulting shallow groundwater conditions?
- How will scheduling of groundwater use under a drought management plan impact base flows in a stream at present, and into future years, as lagged impacts?

The perfect analysis of an aquifer environment and its processes depend on one of the following four aspects and the method of modeling (Balasubramanian, 2001):

- Analysis pertaining to groundwater occurrence and flow, sources of recharge - discharge and their impacts (single phase or multi-phase; steady or transient groundwater flow models).
- Analysis of dispersal, mobility and distribution of solutes (contaminants) in groundwater systems (chemical mass or solute; steady or transient transport models).
- Analysis of the mechanisms of rock-water geochemical interactions controlling the distribution of solute species (aqueous geochemical models).
- Analysis of salinity intrusions in the complex coastal ecosystems (saltwater intrusion; steady or transient; sharp or dispersed interface models).

Each one of these, require careful application of unique numerical principles, typical databases and complicated solution strategies. Despite these challenges, attempts have been made so far by several eminent workers in using the mathematical models for various field problems and laboratory applications.

2.2.3 What Groundwater models can do?

A groundwater model can have two distinct components: (i) flow component, and (ii) contaminant transport and reactive reactions component. Groundwater flow and contaminant transport modeling together play an important role in characterization of groundwater bodies and management of groundwater. A groundwater flow modeling is a pre-requisite for developing a contaminant transport model of an area of interest, but *vice-versa* is not true. A groundwater flow model can provide a quantitative assessment of resources along with the following components: (i) estimating groundwater recharge, discharge, and storage at spatial scale; (ii) assessing the cumulative effects on existing and proposed water resources uses and developments; and (iii) evaluating the cumulative impacts on water resources due to various water management options. A groundwater contaminant transport model, however, assists in predicting the transportation or movement of dissolved constituents including their chemical reactions in groundwater and soil matrices.

For management of a groundwater system, a thorough understanding of the physical, chemical and biological processes in integrated environment is vital and modeling is a very effective tool to answer the system's response. Groundwater flow models provide valuable information on the occurrence, movement and flow of groundwater by integrating various inputs, outputs and storage parameters for a local or regional scale by solving specific problems like:

- Estimation of groundwater balance components, regional inflow and outflow patterns of groundwater, interaction with neighbouring water bodies;
- Changes in aquifer recharge pattern due to urbanization; changes resulting from irrigation return flow and canal seepage; long-term climatologically changes in piezometric levels and impacts of anthropogenic changes;
- Regional parameter estimation using inverse modeling;
- Estimation of groundwater withdrawal patterns and impacts on base flow contribution of rivers and streams;
- Prediction and movement of saline water interface;
- Estimation of seepage velocities for control of transport of pollutants;
- Management of groundwater resources and future development;
- Assessment of feasibility of conjunctive use.

Earlier models were concentrated on the analysis of flow behaviour in groundwater systems, whereas the recent attempts aim at addressing the water quality problems and simulate the transport contaminants in groundwater. Even though, there has been significant development in modeling tools and techniques, however, scientific challenges exist, as the credibility of field level application of the models have to be ascertained due to the existence of uncertainty in the conceptualization of boundary conditions, aquifer heterogeneity, natural recharge and others (Mohan, 2001).

2.3 Unsaturated/Vadose Zone Modeling

2.3.1 General

Various processes occurring within the unsaturated zone play a major role in determining the quality and quantity of water recharge to the groundwater. A quantitative analysis of water flow and contaminant transport in the unsaturated zone is a key factor in the improvement and protection of the quality of groundwater supplies.

2.3.2 Governing equations of water and transport in unsaturated soils

Analytical, semi-analytical, and numerical models are used for unsaturated zone modeling. These are usually based on the following three governing equations for water flow, solute transport, and heat movement, respectively:

$$\frac{\partial\theta(h)}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} + 1\right)\right] - S \qquad \text{... (2.1)}$$

$$\frac{\partial\theta Rc}{\partial t} = \frac{\partial}{\partial z}\left[\theta D\left(\frac{\partial c}{\partial z}\right) - qc\right] - \emptyset \qquad \text{... (2.2)}$$

$$\frac{\partial C(\theta)T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda(\theta)\left(\frac{\partial T}{\partial z}\right) - C_w qT\right] \qquad \text{... (2.3)}$$

Suitable simplifications (mostly for analytical approaches) or extensions thereof (e.g. for two- and three-dimensional systems) are also employed. In equation (2.1), often referred to as the Richards equation, z is the vertical coordinate positive upwards, t is time, h is the pressure head, θ is the water content, S is a sink term representing root water uptake or some other sources or sinks, and $K(h)$ is the unsaturated hydraulic conductivity function, often given as the product of the relative hydraulic conductivity, K_r, and the saturated hydraulic conductivity, K_s. In equation (2.2), known as the *convection-dispersion equation* (CDE), c is the solution concentration, R is the retardation factor that accounts for adsorption, D is the dispersion coefficient accounting for both molecular diffusion and hydrodynamic dispersion, q is the volumetric fluid flux density, and Φ is a sink/source term that accounts for various zero- and first order or other reactions. In equation (2.3), T is temperature, λ is the apparent thermal conductivity, and C and C_w are the volumetric heat capacities of the soil and the liquid phase, respectively.

Solutions of the Richards equation (2.1) require knowledge of the unsaturated soil hydraulic functions, that is, the soil water retention curve, $\theta(h)$, describing the relationship between the water content θ and the pressure head h, and the unsaturated hydraulic conductivity function, $K(h)$, defining the hydraulic conductivity K as a function of h or θ. While under certain conditions (i.e. for linear sorption, a concentration-independent sink term Φ, and a steady flow field) equations (2.2) & (2.3) are linear equations; equation (2.1) is generally highly nonlinear because of the nonlinearity of the soil hydraulic properties. Consequently, many analytical solutions have been derived in the past for equations (2.2) and (2.3) and these analytical solutions are now widely used for analyzing solute and heat transport under steady-state conditions. Although a large number of analytical solutions of (2.1) exist, they can generally be applied only to drastically simplified problems. The majority of applications for water flow in the vadose zone require a numerical solution of the Richards equation.

2.3.3 Input data for unsaturated zone modeling

Simulation of water dynamics in the unsaturated zones requires input data concerning the model parameters, the geometry of the system, the boundary conditions and, when simulating transient flow, initial conditions. With geometry parameters, the dimensions of the problem domain are defined. With the physical parameters, the physical properties of the system under consideration are described. With respect to the unsaturated zone, it concerns the soil water characteristic, $h(\theta)$ and the hydraulic conductivity, $K(\theta)$.

To model the retention, movement of water and chemicals in the unsaturated zone, it is necessary to know the relationships between soil water pressure, water content and hydraulic conductivity. It is often convenient to represent these functions by means of relatively simple parametric expressions. The problem of characterizing the soil hydraulic properties then reduces to estimating parameters of the appropriate constitutive model. The measurements of $\theta(h)$ from soil cores (obtained through pressure plate apparatus) can be fitted to the desired soil water retention model. Once the retention function is estimated, the hydraulic conductivity relation, $K(h)$, can be evaluated if the saturated hydraulic conductivity, K_s, is known. A number of models for water retention function and unsaturated hydraulic conductivity are well reported in literature, one of the most popular being van Genuchten model. For the van Genuchten (1980) model, the water retention function is given by

$$S_e = (\theta - \theta_r)/(\theta_s - \theta_r) = [\,1 + (\alpha_v |h|\,)^n\,]^{-m} \quad \text{for } h < 0$$

$$= 1 \qquad \text{for } h \geq 0 \qquad \ldots \qquad (2.4)$$

and the hydraulic conductivity function is described by

$$K = K_s\, S_e^{1/2}\, [1 - (1 - S_e^{1/m})^m]^2 \qquad \ldots \qquad (2.5)$$

where α_v and n are van Genuchten model parameters, $m = 1 - 1/n$, subscript s refers to saturation, i.e. the value of θ for which $h = 0$, and the subscript r to residual water content.

The number and type of parameters required for modeling flow and transport processes in soils depend on the type of model chosen. These parameters can be categorized as control parameters (controlling the operation of the computer code), discretization data (grid and time stepping), and material parameters. The material parameters can be grouped in seven sets (Jury and Valentine, 1986) – static soil properties, water transport and retention functions, time-dependent parameters, basic chemical properties, contaminant source characteristics, soil adsorption parameters, and tortuosity functions. Table 2.1 lists many of the relevant material model parameters.

Table 2.1 Selected Material Parameters for Flow and Transport Modeling

Model Parameters		
Static Soil Properties **Porosity** Bulk Density Particle Size Specific Surface Area Organic Carbon Content Cation Exchange Capacity pH Soil Temperature	***Flow and Transport Variables and Properties*** Saturated Hydraulic Conductivity Saturated Water Content Moisture Retention Function Hydraulic Conductivity Function Dispersion Coefficient	***Basic Chemical Properties*** Molecular Weight Vapour Pressure Water Solubility Henry's Constant Vapour Diffusion Coeff.in air Liquid Diffusion Coeff.in water Half-life or decay Rate Hydrolysis Rate (s)
Time Dependent Parameters Water Content Water Flux Infiltration Rate Evaporation Rate Solute Concentration Solute Flux Solute velocity Air Entry Pressure Head Volatization Flux	***Contaminant Source Characteristics*** Solute Concentration of Source Solute Flux of Source Source Decay Rate	
	Soil Adsorption Parameters Distribution Coefficient Isotherm Parameters Organic Carbon Partition Coefficient	
	Tortuosity Functions Vapour Diffusion Tortuosity Liquid Diffusion Tortuosity	

2.3.4 Modeling of unsaturated Flow

Analytical solutions to the Richards equation for unsaturated flow under various boundary and initial conditions are difficult to obtain because of the nonlinearity in soil hydraulic parameters as well as governing equation. This difficulty is exaggerated when soil is heterogeneous. Generally, one has to rely on numerical approaches for predicting moisture movement in unsaturated soils, even for homogeneous soils. However, numerical approaches often suffer from convergence and mass balance problems. The nonlinearity of Richards equation is usually solved using an iterative procedure such as Newton or Picard methods. Perhaps the most important advantage of finite element techniques over standard finite difference methods is the ability to describe irregular system boundaries in simulations more accurately, as well as easily including non-homogeneous medium properties.

To numerically solve coupled systems of equations, the solution process requires some manipulation at each time step so that the dependence of one equation on the solution of the other is dealt with accurately. One way to overcome this is to use a fully implicit approach to solve the equations simultaneously. Any nonlinearity of the generated system can be handled by Newton's method. The implicit nature of this scheme allows for larger time steps in simulation to find stable solutions compared to the time steps for explicit schemes. An alternative to the fully implicit scheme is to use the mixed implicit-explicit scheme. However, the explicit part of the scheme means that the algorithm is subject to a stability constraint which severely restricts the time step size and introduces numerical artefacts.

Initial and Boundary Conditions

Initial conditions must be defined when transient soil water flow is modeled. Usually values of matric head or soil water content at each nodal point within the soil profile are required. When these data are not available, water contents at field capacity or those in equilibrium with the ground water table might be considered as the initial ones.

While the potential evapotranspiration rate from a soil depends on crop and atmospheric conditions, the actual flux through the soil surface and the plants is limited by the ability of the soil matrix to transport water. Similarly, if the potential rate of infiltration exceeds the infiltration capacity of the soil, part of the water runs off, since the actual flux through the top layer is limited by moisture conditions in the soil. Consequently, the exact boundary conditions at the soil surface cannot be estimated a priori and solutions must be found by maximizing the absolute flux. The minimum allowed pressure head at the soil surface, h^{lim} (time dependent) can be determined from equilibrium conditions between soil water and atmospheric vapour. The possible effect of ponding has been neglected so far. In case of ponding, usually the height of the ponded water as a function of time is given. However, when the soil surface is at saturation then the problem is to define the depth in the soil profile where the transition from saturation to partial saturation occurs.

In most of the dynamic transient models, the surface nodal point is treated during the first iteration as a prescribed flux boundary and matric head h is computed. If $h^{lim} \leq h \leq 0$, the upper boundary condition remains a flux boundary during the whole iteration. If not, the surface nodal point is treated as a prescribed pressure head in the following iteration. Then in case of infiltration, $h = 0$ and in case of evaporation $h = h^{lim}$. The actual flux is then calculated explicitly and is subject to the condition that actual upward flux through the soil-air interface is less than or equal to potential evapotranspiration(time dependent).

At the lower boundary, one can define three different types of conditions: (a) Dirichlet condition, the pressure head is specified; (b) Neumann condition, the flux is specified; and (c) Cauchy condition, the flux is a function of a dependent variable. The phreatic surface (place, where matric head is atmospheric) is usually taken as lower boundary of the unsaturated zone in the case where recorded water table fluctuations are known a priori. Then the flux through the bottom of the system can be calculated. In regions with a very deep ground water table, a Neumann type of boundary condition is used.

Evapotranspiration (water extraction by roots)

In the field, steady-state conditions hardly exist. The living root system is dynamic (dying roots are constantly replaced by new ones), geometry is time dependent, water permeability varies with position along the root and with time. Root water uptake is most effective in young root material, but the length of young roots is not directly related to total root length. In addition, experimental evaluation of root properties is hardly practical, and often impossible. Thus, instead of considering water flow to single roots, a more suitable approach might be the macroscopic one, in which a sink term S representing water extraction by a homogeneous and isotropic element of the root system (volume of water per volume of soil per unit of time) is added to the conservation of mass equation. As it seems to be impossible and unpractical to look for a complete physical description of water extraction by roots, Feddes et al. (1988) described S semi-empirically by:

$$S(h_m) = \alpha(h_m)\, S_{max} \qquad \text{... (2.6)}$$

where $\alpha(h_m)$ is a dimensionless prescribed function of pressure head and S_{max} is the maximal possible water extraction by roots. In the interest of practicality, a homogeneous root distribution can be assumed over the soil profile and define S_{max} according to

$$S_{max} = \frac{T_p}{|Z_r|} \qquad \text{... (2.7)}$$

where T_p is the potential transpiration rate and $|Z_r|$ is the depth of the root zone.

Groundwater Recharge

There are two types of unsaturated zone (or soil-water) models which can be used for groundwater recharge estimation.

1. Water-balance models
2. Numerical models based on the Richards equation

The literature about practical applications of various types of models for assessing groundwater recharge is limited and does not contain straightforward recommendations about which type of model should be used under different conditions. It is commonly considered that Richards equation-based models are the most theoretically proven and allow to represent flow processes in the porous medium more realistically than water-balance models.

However, large-scale applications of Richards equation-based models to highly heterogeneous soils with variable hydraulic properties can be difficult and expensive.

A number of studies have used numerical models to solve Richards' equation for assessing groundwater recharge. A review of previous studies indicates that unit-gradient and fixed water table lower boundary conditions have been applied to models of both constant and variable vertical grid spacing (discretization). It is also reported that whenever the unsaturated flow modeling approach is used to estimate groundwater recharge, a fixed-head lower boundary condition should be selected because it also allows upward flux from the water table during dry periods, a situation that prevails on both sub-humid and semi-arid areas, where accurate groundwater recharge estimates are needed the most. The use of a fixed water table is a simple representation of the regional water table, which in reality interacts with the regional groundwater flow and surface water bodies (e.g., lakes and wetlands).

The use of a variable discretization at the points where both the wetting and drying fronts fluctuate (i.e., top and bottom of soil columns) improve simulation efficiency for the nonlinear unsaturated flow regime. The adequate selection of discretization and boundary conditions, which affect the simulation time, is of utmost importance when a large number of simulations is required (e.g., analysis of climate change scenarios).

2.3.5 Modeling of solute transport through unsaturated zone

Transport of dissolved solutes in soils is commonly described by the advection-dispersion equation. Prediction of solute migration under field conditions requires the simultaneous solution of the unsaturated flow and solute transport equations. First approximations involve or assume steady flow and constant water contents. Because of the natural complexity of unsaturated flow, methods of predicting solute transport have relied largely on finite difference or finite element approximations of the governing equations.

One of the distinctive features of the porous media on the field scale is the spatial heterogeneity of transport properties. These features have a distinct effect on the spatial distribution of contaminant concentration, as has been observed in field experiments and demonstrated by simulation of contaminant transport in unsaturated, heterogeneous soil. Description of the mixing process due to spatial variability of the unsaturated hydraulic conductivity has been advanced with the development of numerical solutions, which assume spatially variable soil properties; stochastic models; and stochastic stream tube models, which decompose the field into a set of independent vertical soil columns.

2.3.6 Unsaturated zone modeling software

Most of the early models developed for studying processes in the near-surface environment mainly focused on variably saturated water flow. They were used primarily in agricultural research for optimizing moisture conditions to increase crop production. This focus has gradually shifted to environmental research, with the primary concern now being the subsurface fate and transport of various agricultural and other contaminants. While the earlier models solved the governing equations (1) through (3) for relatively simplified system-independent boundary conditions (i.e. specified pressure heads or fluxes, and free drainage), models developed recently can cope with much more complex system-dependent boundary conditions evaluating surface flow and energy balances and accounting for the simultaneous movement of water, vapor, and heat. There are also composite models which simulate the processes both in unsaturated and saturated zones and other components of hydrological cycle. A few widely used unsaturated flow and composite models have been listed in Table 2.2.

Table 2.2 Numerical Models for Simulating Unsaturated Flow and Solute Transport

S.No.	Modeling Software	Salient Features
Unsaturated Flow Models		
1.	HYDRUS-1D	Public domain Modeling environment for analysis of water flow and solute transport; includes the one-dimensional finite element model HYDRUS for simulating the movement of water, heat, and multiple solutes in variably saturated media; supported by an interactive graphics-based interface for data-preprocessing, discretization of the soil profile, and graphic presentation of the results.
2.	HYDRUS 2D/3D	Software package for simulating water, heat, and solute movement in two- and three-dimensional variably saturated media; consists of a computational computer program and an interactive graphics-based user interface.
3.	R-UNSAT	USGS computer model for the simulation of reactive, multispecies transport in a heterogeneous, variably-saturated porous media; designed for simulating transport of volatile organic compounds in the unsaturated zone from point and nonpoint sources; can also be applied to other unsaturated-zone transport problems involving gas diffusion, such as radon migration and the deposition of compounds from the atmosphere to shallow groundwater.
4.	SWIM	A mechanistically-based model designed to address soil water and solute balance issues in unsaturated zone.
5.	UNSAT SUITE	Handle one-dimensional groundwater flow and contaminant transport in the unsaturated zone; simulates the downward vertical flow of groundwater and migration of dissolved contaminants in the groundwater through a thin column of soil.
6.	VS2DI	USGS graphical software package for simulating fluid flow and solute or energy transport in variably saturated porous media.
Composite Models		
7.	FEFLOW	Commercial software based on the finite element method for simulation of saturated and unsaturated flow, transport of mass (multiple solutes) and heat, with integrated GUI.
8.	HydroGeoSphere	Commercial three-dimensional control-volume finite element simulator designed to simulate the entire terrestrial portion of the hydrologic cycle; uses a globally-implicit approach to simultaneously solve the 2D diffusive-wave equation and the 3D form of Richards' equation.
9.	MIKE SHE	Commercial software for integrated catchment Modeling, with integrated GUI; uses the finite difference method for saturated groundwater flow, several representations of unsaturated flow, including the 1D Richards equation, MIKE 11 for flow in river and stream networks and the 2D diffusive-wave approach for overland flow.

S.No.	Modeling Software	Salient Features
10.	MODFLOW-SURFACT	Commercial software for simulation of saturated and unsaturated flow and solute transport: developed to overcome specific limitations in open source versions of MODFLOW and MT3D: also available in an extended form called MODHMS, which includes 2D diffusive wave simulation of overland flow and 1D simulation of flow in river and stream networks.
11.	SUTRA	Open source USGS software based on the finite element method for simulation of saturated and unsaturated flow, transport of mass and heat. It has been designed for density-coupled flow and transport.

2.3.7 Concluding remarks

Predicting water flow and contaminant transport on a field-scale based on the current monitoring and modeling techniques is a challenging task. There are large uncertainties in predictions mainly due to our inability to depict detailed spatial distributions of soil hydraulic properties on the field-scale. Due to the high costs of data acquisition, few field measurements are usually available for characterization of flow and contaminant transport, even though the spatial distribution of a contaminant plume may be highly irregular. Also, more research associated with water flow and contaminant transport in the unsaturated zone of aquifers containing fractures and karstic conduits is needed for future investigations.

2.4 Groundwater Modeling Process

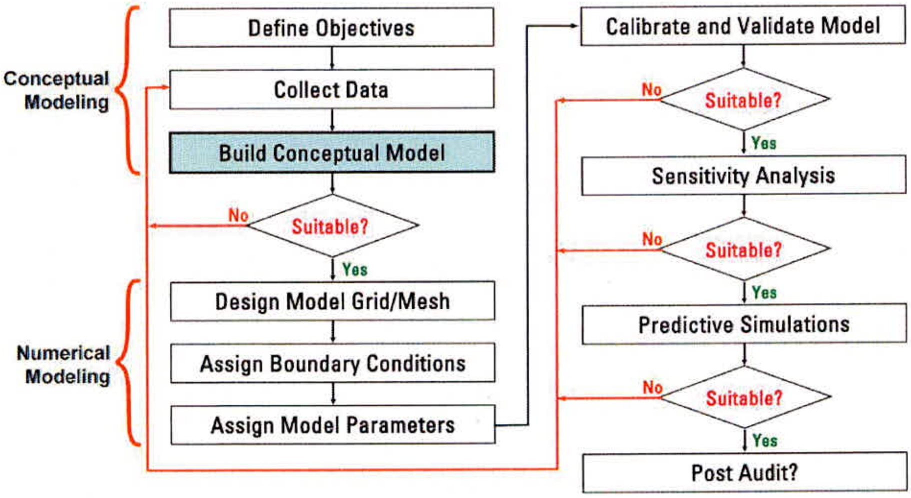
2.4.1 General

Groundwater modeling is an integrative process. Therefore, the modeling team should possess a range of skills and broad knowledge of hydrogeology, groundwater flow processes, mathematical equations describing groundwater flow and solute movement, numerical and analytical methods for solving the governing equations, geo-statistics, and parameter estimation. For many modeling projects, expertise in bio- and geochemical reactions, subsidence, geologic modeling, and optimization may also be required.

2.4.2 Steps associated in modeling

Groundwater modeling studies (with the use of groundwater models) are very effective in understanding the nature and extent of groundwater regimes, and to arrive at feasible solutions to complex problems involving groundwater resource development, aquifer contamination, aquifer management as well as sustainability of aquifer systems. Here, we refer to groundwater models as mathematical models based on governing equations of groundwater flow (saturated / unsaturated flow as well as constant density / variable density), contaminant transport (non-reactive/ reactive and miscible/ immiscible), heat transport, as well as multiphase flows. Various advanced numerical techniques are being utilized to facilitate solving the model equations (which are differential equations that can be solved only by approximate methods using a numerical analysis) at various nodes in the domain. Since the computations in mathematical groundwater models are based on numerical techniques, these models are often called numerical or computational groundwater models.

Fig.2.3 presents the flow chart of any modeling endeavour. Here, the first stage is planning that involves identifying the intended use of the model, modeling objectives, and the type of model needed to meet the project objectives. The next stage focuses on conceptualization or formulation of the conceptual model that describes the known physical features and groundwater flow processes within the area of interest. Under the design stage, it is decided how to best represent the conceptual model using a mathematical model. Model construction is the implementation of model design by defining the inputs for the selected model including the boundary conditions. The calibration and sensitivity analysis of the model occurs through a process of matching model outputs to a historical record of observed data. In some cases, model calibration is not necessary, e.g. when using a model to test a conceptual model. Model validation is the process of testing the calibrated model by demonstrating that it can successfully predict a set of observations not used previously for model calibration. Field data collection that occurs during model development may require updates to both the conceptual and mathematical models. If significant effort has been expended on mathematical modeling, additional data may require re-calibration and re-validation. Model application or predictions comprise those model simulations that provide the outputs to address the questions defined in the modeling objectives. The predictive analysis is followed by an analysis of the implications of the uncertainty associated with the modeling outputs.



After Anderson & Woessner (1982)

Figure 2.3: Flow chart of modeling endeavour

Most groundwater models in use today are deterministic mathematical models. Deterministic models are based on conservation of mass, momentum, and energy and describe cause and effect relations. Deterministic groundwater models generally require the solution of partial differential equations. Exact solutions can often be obtained analytically, but analytical models require that the parameters and boundaries be highly idealised. Some deterministic models treat the properties of porous media as lumped parameters, but this precludes the representation of heterogeneous hydraulic properties in the model.

Heterogeneity, or variability in aquifer properties, is characteristic of all geologic systems and is recognised as playing a key role in influencing groundwater flow and solute transport. It is, therefore, often preferable to apply distributed-parameter models, which allow the representation of more realistic distributions of system properties. Numerical methods yield approximate solutions to the governing equation (or equations) through discretization of space and time. The space and time are divided into discrete intervals where for each model grid cell, parameter values are defined including hydraulic conductivity, porosity, aquifer thickness, initial contaminant concentration, etc. Thus, within the discretized problem domain, the variable internal properties, boundaries, and stresses of the system are approximated. Instead of the rigid idealised conditions of analytical models or lumped-parameter models, usage of deterministic, distributed-parameter, numerical models permit a flexible approach for simulating field conditions and provides a more realistic solution for the field problem under consideration.

The number and types of equations to be solved are determined by the concepts of the dominant governing processes. The coefficients of the equations are the parameters that are measures of the properties, boundaries, and stresses of the system; the dependent variables of the equations are the measures of the state of the system and are mathematically determined by the solution of the equations. Groundwater models are broadly divided into two categories: groundwater flow models, which solve for the distribution of head in a domain, and solute transport models, which solve for the concentration of solute as affected by advection, dispersion, and chemical reactions.

2.4.3 Flow and transport processes

The process of groundwater flow is generally assumed to be governed by the relations expressed by Darcy's law and the conservation of mass. The purpose of a model that simulates solute transport in groundwater is to compute the concentration of dissolved chemical species in an aquifer at any specified time and place. Changes in chemical concentration occur within a dynamic groundwater system primarily due to four distinct processes (Bear, 1979; Domenico and Schwartz, 1998):

1. Advective transport, in which dissolved chemicals are moving with the flowing groundwater;
2. Hydrodynamic dispersion, in which molecular and ionic diffusion and small-scale variations in the flow velocity through the porous media cause the paths of dissolved molecules and ions to diverge or spread from the average groundwater flow direction;
3. Fluid sources, where water of one composition is introduced into and mixed with water of a different composition;
4. Reactions, in which some amount of a particular dissolved chemical species may be added to or removed from the groundwater as a result of chemical, biological, and physical reactions in the water or between the water and the solid aquifer materials or other separate liquid phases.

2.4.4 Governing equations

2.4.4.1 Groundwater flow equation

A general form of the equation describing the transient flow of a compressible fluid in a non-homogeneous anisotropic aquifer may be derived by combining Darcy's law with the continuity equation. A general groundwater flow equation may be written in Cartesian tensor notation as (Bear, 1979):

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial h}{\partial x_i}\right) = S_S\frac{\partial h}{\partial t} + W^* \quad \text{... (2.8)}$$

where K_{ij} is the hydraulic conductivity of the porous media (a second-order tensor), $[LT^{-1}]$;h is the hydraulic head, [L]; S_S is the specific storage, $[L^{-1]}$; t is time, [T]; W* is the volumetric flux per unit volume (positive for outflow and negative for inflow), $[T^{-1}]$; and x_i are the Cartesian co-ordinates, [L].

Equation (2.8) can generally be applied if isothermal conditions prevail, the porous medium only deforms vertically, the volume of individual grains remains constant during deformation, Darcy's law applies (and gradients of hydraulic head are the only driving force), and fluid properties (density and viscosity) are homogeneous and constant. Aquifer properties can vary spatially, and fluid stresses (W*) can vary in space and time.

In some field situations (e.g. coastal aquifers), fluid properties such as density and viscosity may vary significantly in space or time. This may occur due to significant changes in water temperature or total dissolved solids concentration. In such cases, the flow equation is written and solved in terms of fluid pressures, fluid densities, and the intrinsic permeability of the porous media (Konikow and Grove, 1977; Bear, 1979).

2.4.4.2 Solute transport equation

A generalized form of the solute-transport equation in which terms are incorporated to represent chemical reactions and solute concentration both in the pore fluid and on the solid surface is (Grove, 1976; Bear, 1972):

$$\frac{\partial(\varepsilon C)}{\partial t} = \frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(\varepsilon C V_i) - C' W^* + \text{CHEM} \quad \text{... (2.9)}$$

where CHEM equals:

$-\rho_b\frac{\partial \overline{C}}{\partial t}$ for linear equilibrium controlled sorption or ion-exchange reactions,

$\sum_{k=1}^{s} R_k$ for ‘s’ chemical rate-controlled reactions, and (or)

$-\lambda(\epsilon C + \rho_b\overline{C})$ for decay,

and, where D_{ij} is the coefficient of hydrodynamic dispersion (a second-order tensor), $[L^2T^1]$; C is the concentration of solute (single dissolved chemical species) in flowing groundwater $[ML^{-3}]$; C' is the concentration of the solute in the source or sink fluid, $[ML^{-3}]$; $\overline{C}$is the concentration of the species adsorbed on the solid (mass of solute/mass of solid); ρb is the bulk density of the solid, $[ML^{-3}]$; R_k is the rate of production of the solute in reaction k, $[ML^3T^{-1}]$; and λ is the decay constant, $[T^{-1}]$.

The first term on the right side of equation (2.9) represents the change in concentration due to hydrodynamic dispersion. This expression is analogous to Fick's Law describing diffusive flux. This Fickian model assumes that the driving force is the concentration gradient and that the dispersive flux occurs in a direction from higher concentrations towards lower concentrations. The second term represents advective transport and describes the movement of solutes at the average seepage velocity of the flowing groundwater. The third term represents the effects of mixing with a source fluid that has a different concentration than the groundwater at the location of the recharge or injection. The fourth term lumps all of the chemical, geochemical, and biological reactions that cause transfer of mass between the liquid and solid phases or conversion of dissolved chemical species from one form to another. The chemical attenuation of inorganic chemicals can occur by sorption/desorption, precipitation/dissolution, or oxidation/reduction; organic chemical can adsorb or degrade by microbiological processes.

2.4.5 Classification of groundwater models

Groundwater models can broadly be grouped into three categories: Analytical Models; Numerical Models; and Analytic Element Models.

2.4.5.1 Analytical models

Analytical models use exact solutions to the equations that describe groundwater flow or contaminant transport. In order to produce these exact solutions, the flow/transport equations have to be considerably simplified such that they are typically applicable only to simple flow and contaminant transport systems. Analytical models can be simple formulae, spreadsheets, or sequences of calculations packaged in a piece of software. The main advantage of analytical models is the ease of use and transparency of such models which will facilitate sensitivity analyses. Their main disadvantage is that they can only be applied to relatively simple flow (or transport) problems. The main uses of analytical models are to assist in conceptual modeling, simulate flow and/or transport in simple physical settings (or where there are only one or two simple objectives), and check results of the numerical model.

2.4.5.2 Numerical models

A numerical model uses numerical methods to solve the governing equations of groundwater flow and/or contaminant transport. In distributed numerical models, space and time are divided into discrete intervals where for each model grid cell, parameter values are defined including hydraulic conductivity, porosity, aquifer thickness, initial contaminant concentration, etc. Numerical models enable more complex systems to be represented than can be represented by analytical models. Furthermore, numerical models may allow for multiple modeling objectives to be addressed in parallel. Numerical models still require simplifications to be made about system behaviour.

The main advantage of numerical models is that different parameter values can be assigned to each cell, so that lateral and vertical variations in property values can be taken into account. The geometry of the model can be designed to reflect the geometry of the system. In addition, models can be constructed that include more than one layer; this enables multi-layered aquifers to be represented. For time variant models, model inflows (e.g. recharge and its contaminant concentration) and outflows (e.g. ground water abstractions) can be specified for each model time step. The main disadvantage of numerical models is that they can be costly and time-consuming. Another potential disadvantage is that the model complexity reduces the transparency of the model calculations and/or can mask the model uncertainty. Numerical models will generally be applicable where:

- Previous modeling studies using simple analytical models have shown that a more sophisticated approach, such as incorporating spatial variability, is required.
- Groundwater regime is too complex to be robustly represented by an analytical model.
- Required model accuracy (as defined by the model objectives) requires the use of a numerical model.
- Processes affecting contaminant transport cannot be adequately represented by simple transport equations.
- An analytical model is inadequate for the design of mitigation measures, e.g., in determining the optimal location and pumping rate for boreholes in a pump and treat scheme.

Numerical models should be considered where the scale and importance of the problem warrant the use of a more sophisticated approach. For such sites, the scale of the problem should demand detailed site investigations which should provide sufficient information to allow the construction of a numerical model.

2.4.5.3 Analytic element models

An analytic element model uses superposition of closed-form (analytical) solutions to the governing differential equation of groundwater flow to approximate both local and (near-field) and regional (far-field) flow. Hence, analytic element models do not require grid discretization or specifications of boundary conditions on the grid perimeter (Hunt et al., 1998). These characteristics allow for representation of large domains that include many hydrogeologic features outside the immediate area of interest (i.e., far-field) and easy modification of the regional flow field by adding analytic elements representing regional hydrologic features (Wels, 2012).

Analytic element models are well-suited for use as screening models (Hunt et al., 1998). Analytic element models can be used to develop conditions on the grid perimeter for a smaller numerical model, similar to the process of telescopic mesh refinement (TMR). The advantage over traditional TMR using finite difference models is that this method: (i) allows easy addition of far-field elements until the far field is correctly simulated; and (ii) avoids discretization problems that can occur in large-scale models with large cell/element sizes. A major limitation of analytic element models is that the method is computationally efficient only for steady-state flow in large aquifers where the vertical flow component can be ignored.

2.4.6 Numerical methods to solve flow and transport equations

Two major classes of numerical methods are well accepted for solving the governing flow equations, namely the finite-difference (FD) methods and the finite-element (FE) methods. Each of these two major classes of numerical methods includes a variety of subclasses and implementation alternatives. Although FD and FE models are commonly applied to flow and transport problems, other types of numerical methods applied to transport problems include method of characteristics (MOC), particle tracking, random walk, Eulerian-

Lagrangian methods, and adaptive grid methods. All of these have the ability to track sharp fronts accurately with a minimum of numerical dispersion.

The widely used MODFLOW is the USGS's open source three-dimensional (3D) FD based groundwater model. Originally developed and released solely as a groundwater-flow simulation code in 1984, MODFLOW's modular structure has provided a robust framework for integration of additional simulation capabilities that build on and enhance its original scope. The family of MODFLOW-related programs now includes capabilities to simulate coupled groundwater/surface-water systems, solute transport, variable-density flow (including saltwater), aquifer-system compaction and land subsidence, parameter estimation, and groundwater management.

FEFLOW (Finite Element subsurface FLOW system) is a computer program for simulating groundwater flow, solute and heat transfer in porous media and fractured media. The program uses FE based analysis to solve the groundwater flow equation of both saturated and unsaturated conditions as well as solute and heat transport, including fluid density effects and chemical kinetics for multi-component reaction systems.

In addition, many other simulation codes have been developed over the years for groundwater modeling applications. Appropriate model codes may be selected depending upon associated complexities in groundwater flows.

Flow through fractures and conduits. In case of uniformly distributed and well connected fracture system, an equivalent porous medium (EPM) approach may be adopted to simulate the system. The EPM approach may adequately represent the behavior of a system at regional scale, but local groundwater flows are poorly represented. Flow through discrete fractures within a porous matrix can be simulated using available codes such as FEFLOW, conduit flow processes in MODFLOW, and specialty codes such as Fracman (www.fracman.com). Presence of conduits and fractures in carbonate rocks offers additional challenges owing to changes in secondary permeability resulting from dissolution and precipitation.

Variable density flow: Examples of variable density flows (i.e., fluids that mix with groundwater) are seawater intrusion into coastal aquifers, mixing of highly concentrated dissolved contaminants in groundwater, freshwater storage in saline aquifers etc. Modeling variable density flow requires coupling of a density dependent flow model to a solute transport model. Codes such as SEAWAT (derived from MODFLOW and MT3DMS), SUTRA, FEFLOW can be used to simulate variable density flows.

Multiphase flow: Immiscible fluids move as separate phases within subsurface. Examples of multiphase flow include air and water in unsaturated zone; oil, gas and water in a petroleum reservoir; water and steam in a geothermal reservoir. The most common type of multiphase flow involves non-aqueous phase liquids or NAPLs that may be either lighter (LNAPL) or denser (DNAPL) than groundwater. Models simulating NAPLs movement in groundwater are complex and require a separate set of flow and transport equations for groundwater and each NAPL.

Linked and Coupled Models. On linking a flow model to a solute transport or rainfall-runoff model, the flow model is solved first and the results are input to the other model which is solved within the same time step as the flow model. However, when results from one model significantly affect parameters in another model within a time step, coupling of the models becomes necessary. Here, the models are solved iteratively within the time step and input to each model is updated to reflect output from the other.

2.4.7 Concluding remarks

Development of both simulation and management models for alluvial and hard rock regions (including coastal regions) supported by advanced numerical modeling and optimization tools as well as remote sensing technology is essentially needed. At the same time, usage of better field instrumentation, data acquisition and integration into models (as more data becomes available under the National Aquifer Mapping Program) will enormously help the modeling activities in developing reliable groundwater models for the water resources problems of the future.

2.5 An Overview of Groundwater Models

2.5.1General

Depending upon the flow domain, groundwater models can be one-dimensional, two-dimensional and three-dimensional. Two and three-dimensional models can account for the anisotropy of the aquifer system wherein the hydraulic properties may vary with respect to the principal directions. Again, based upon the objectives, groundwater models may be grouped into prediction/simulation models; identification or evaluation models; and management 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, as well as hydrological responses.

A numerical simulation model may be developed 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, adjusting the value of parameters and/or boundary conditions to reproduce the observed aquifer response to known stresses.

Three dimensional groundwater simulation models applied to complex, heterogeneous aquifer systems have often been utilized to explore groundwater management alternatives. For this purpose, the groundwater model may be executed repeatedly under various scenarios designed to achieve a particular objective, such as obtaining a sustainable water-supply, preventing saline water encroachment or controlling a contaminant plume. Further, groundwater management models are being developed by 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.

2.5.2 Groundwater simulation models

Depending upon the flow domain, different approaches are employed to simulate groundwater flow and solute transport in natural aquifer systems:

- Equivalent porous medium
- Discrete fracture network
- Dual porosity medium

The equivalent porous medium (EPM) approach assumes that the aquifer system can be represented by an equivalent porous medium, i.e. the aquifer system behaves like a porous medium and standard flow and transport equations apply. EPM approach is commonly used for unconsolidated materials such as overburden soils (colluviums), fluvial, alluvial and glacio-fluvial sediments, and highly weathered bedrock with high primary porosity.

EPM approach is commonly used to describe groundwater flow through fractured bedrock in which the primary porosity is very low and the effective permeability is controlled by fractures, fissures and bedding planes (i.e. secondary permeability). This approach is based on the assumption that at a sufficiently large scale (i.e. the representative elementary volume (REV)), the bedrock mass will behave like a porous medium and can be described by "effective" hydraulic properties. The majority of groundwater modeling codes uses the EPM approach to model groundwater flow.

In the discrete fracture network (DFN) approach, it is assumed that flow through the bedrock matrix is negligible and all groundwater flow occurs through an interconnected network of fractures. Such a discrete fracture network may either be described explicitly (with known geometry) or generated randomly using fracture network statistics (e.g. Dershowitz et al., 2004; Parker and Cherry, 2011). Sophisticated Modeling codes are available to generate DFNs and to simulate groundwater flow and solute transport in such a medium, including FracMan (available from http://www.fracman.com/) and Fractran.

Flow and transport in fractured bedrock and structured porous media (e.g. fractured sandstone) can be described using dual porosity models (DPM). This approach assumes that the medium consists of two regions, one associated with the macro pore or fracture network and the other with a less permeable pore system of soil aggregates or rock matrix blocks (Gerke and van Genuchten, 1993). Different models exist to describe the nature of flow and transport in these two domains and the extent of their interaction. In its simplest form, groundwater flow and advective transport is assumed to only occur in the highly permeable ("active") domain. Groundwater flow in the low-permeable ("inactive") domain is assumed to be negligible but this stagnant zone influences solute transport by diffusion.

At present, DFN and dual porosity models are predominantly used in research and/or in assessment of contaminated sites with very high risk and/or consequence (e.g., storage of radio-nuclides, large contaminated sites impacting drinking water supplies, etc.). The primary challenge with DFN and DPM models is model parameterization. A characterization of the fracture network and/or the dual porosity regime requires extensive field studies and/or detailed model calibration usually not available for natural resource projects.

In certain hydrogeological situations, fluid density variations occur because of changes in the solute or colloidal concentration, temperature, and pressure of the groundwater. These include seawater intrusion in coastal aquifers, high-level radioactive waste disposal, groundwater contamination, and geothermal energy production. When the density of the invading fluid is greater than that of the ambient one, density-driven free convection can lead to transport of heat and solutes over larger spatial scales and significantly shorter time scales than compared with diffusion alone. In such cases, variable density models are employed to simulate groundwater flow.

2.5.3 Groundwater management models

Distributed-parameter numerical models are important tools for assessment of groundwater flow systems and groundwater development strategies. Commonly, these models are used to test specific water resource management plans, or, in a trial-and-error approach, to select a single plan from a few alternative plans that best meets management goals and constraints. Because of the complex nature of groundwater systems, however, and the large number of engineering, legal, and economic factors that often affect groundwater development and management, the process of selecting a best operating procedure or policy can be quite difficult. To address this difficulty, groundwater simulation models have been linked with optimization-modeling techniques to determine best (or optimal) management strategies from among many possible strategies. Optimization models explicitly account for water resource management objectives and constraints, and have been referred to as management models (Ahlfeld and Mulligan, 2000).

Groundwater management models may be divided into three categories (Gorelick, 1990):

- Groundwater hydraulic management,
- Groundwater quality management, and
- Groundwater policy evaluation and allocation.

Simulation-optimization groundwater management models have been developed for a variety of applications, such as restoration of contaminated groundwater, control of aquifer hydraulics, allocation of groundwater and surface water resources, and evaluation of groundwater policies (Yeh, 1992).In some cases, however, the model may determine that none of the possible strategies are able to meet the specific set of management goals and constraints. Such outcomes, though often not desirable, can provide useful information for identifying the hydrologic, hydrogeologic, and management variables that limit water resource development and management options.

2.5.4Transport processes

While simulating solute transport in highly heterogeneous and fractured media, the advection-dispersion equation is a poor predictor of solute transport processes. The dual porosity approach is utilized to describe exchange of solute/heat between fractures or highly preferential flow paths and the surrounding porous medium. The dual porosity option is present in both MT3DMS (Zheng, 2009) and FEFLOW. To simulate reaction between two or more chemical species, geochemical reaction modules are interfaced with the transport code, such as MT3DMS interfaces with RT3D or PHT3D.

2.5.5 Surface water - groundwater interactions

Exchange of water from surface water bodies such as, rivers, lakes, wetlands and oceans are an integral component of groundwater modeling. In all groundwater models, simple surface water exchanges with groundwater system are adequately simulated via boundary conditions. Advanced options for representing surface water processes in groundwater models include stream flow routing in channels via Manning's equation, representation of lakes etc. using suitable packages in MODFLOW. The simplified representations of surface water processes in groundwater models may be appropriate for many situations but in some cases coupling of rainfall-runoff model to a groundwater model is required.

2.5.6 Stochastic groundwater modeling

Using stochastic modeling, probabilities and multiple realizations can capture inherent uncertainties of the hidden subsurface. Multiple realizations may be generated using geostatistical methods, geologic process models and multiple-point geostatistics. In geostatistical methods, uncertain parameters are represented by random variables with assigned statistics. Stochastic modeling is computationally intensive, however, with advances in computer hardware and computational capabilities, the ability to evaluate multiple stochastic realizations in groundwater modeling will improve.

2.5.7 Optimization and decision making

Increasingly, groundwater applications are driven by regulatory requirements of water management planning. Optimization techniques can be used in conjunction with groundwater models to find an optimal solution for a given set of constraints (Ahlfeld and Mulligan, 2000; Anderson et al., 2015). With the perceived need for groundwater modelers to engage and include stakeholders, it is important that groundwater models are updated and maintained as ongoing management tools. Groundwater models are also being incorporated in Decision Support Systems (DSS). As part of DSS, the runtime of a groundwater model becomes important, because a DSS has to supply answers to 'what if?' queries quickly. If the runtime of a groundwater model is too long, then it will not prove to be useful in a DSS. However, simple groundwater models with short runtimes may not adequately simulate processes important for decision-making. Research is continuing for extracting fast-running simple models from long running complex models.

2.6 Data Requirements for Saturated Zone Modeling

2.6.1General

The first phase of any groundwater study consists of collecting all existing geological and hydrological data on the groundwater basin in question. This will include information on surface and subsurface geology, water tables, precipitation, evapotranspiration, pumped abstractions, stream flows, soils, land use, vegetation, irrigation, aquifer characteristics and boundaries, and groundwater quality. If such data do not exist or are very scanty, a program of field work must first be undertaken, for no model whatsoever makes any hydrological sense if it is not based on a rational hydrogeological conception of the basin. All the old and newly-found information is then used to develop a conceptual model of the basin, with its various inflow and outflow components.

A conceptual model is based on a number of assumptions that must be verified in a later phase of the study. In an early phase, however, it should provide an answer to the important question: does the groundwater basin consist of one single aquifer (or any lateral combination of aquifers) bounded below by an impermeable base? If the answer is yes, one can then proceed to the next phase: developing the numerical model. This model is first used to synthesize the various data and then to test the assumptions made in the conceptual model.

2.6.2 Data requirement

The data needed in general for a groundwater flow modeling study can be grouped into two categories: (a) Physical framework and (b) Hydrogeologic framework. The data required under physical framework are:

- Geologic map and cross section or fence diagram showing the areal and vertical extent and boundaries of the system.
- Topographic map at a suitable scale showing all surface water bodies and divides. Details of surface drainage system, springs, wetlands and swamps should also be available on map.
- Land use maps showing agricultural areas, recreational areas etc.
- Contour maps showing the elevation of the base of the aquifers and confining beds.
- Isopach maps showing the thickness of aquifers and confining beds.
- Maps showing the extent and thickness of stream and lake sediments.

These data are used for defining the geometry of the groundwater domain under investigation, including the thickness and areal extent of each hydrostratigraphic unit.

Under the hydrogeologic framework, the data requirements are:

- Water table and potentiometric maps for all aquifers.
- Hydrographs of groundwater head and surface water levels and discharge rates.
- Maps and cross sections showing the hydraulic conductivity and/or transmissivity distribution.
- Maps and cross sections showing the storage properties of the aquifers and confining beds.
- Hydraulic conductivity values and their distribution for stream and lake sediments.
- Spatial and temporal distribution of rates of evaporation, groundwater recharge, surface water - groundwater interaction, groundwater pumping, and natural groundwater discharge.

Some of the compiled information will be used not only during the conceptualisation, but also during the design and calibration of the model. This includes the data about the model layers and hydraulic parameters as well as observations of hydraulic head, watertable elevation, and fluxes. The conceptualisation stage may involve the development of maps that show the hydraulic heads in each of the aquifers within the study area. These maps help illustrate the direction of groundwater flow within the aquifers, and may infer the direction of vertical flow between aquifers.

The data used to produce maps of groundwater head is ideally obtained from water levels measured in dedicated observation wells that have their screens installed in the aquifers of interest. More often than not, however, such data is scarce or unavailable and the data is sourced from, or complemented by, water levels from production bores. These may have long well screens that intersect multiple aquifers, and be influenced by preceding or coincident pumping. The accuracy of this data is much less than that obtained from dedicated observation wells. The data can be further supplemented by information about surface expressions of groundwater such as springs, wetlands and groundwater-connected streams. It provides only an indication of the minimum elevation of the watertable (i.e. the land surface) in areas where a stream is gaining and local maximum elevation in areas where a stream is losing. As such, this data has a low accuracy, but can be very valuable nonetheless.

2.6.2.1 Hydrogeological domain

The hydrogeological domain involves:

- Describing the components of the system with regard to their relevance to the problem at hand, such as the hydrostratigraphy and the aquifer properties
- Describing the relationships between the components within the system, and between the system components and the broader environment outside of the hydrogeological domain
- Defining the specific processes that cause the water to move from recharge areas to discharge areas through the aquifer materials
- Defining the spatial scale (local or regional) and time scale (steady-state or transient on a daily, seasonal or annual basis) of the various processes that are thought to influence the water balance of the specificarea of interest
- In the specific case of solute transport models, defining the distribution of solute concentration in the hydrogeological materials (both permeable and less permeable) and the processes that control the presence and movement of that solute
- Making simplifying assumptions that reduce the complexity of the system to the appropriate level so that the system can be simulated quantitatively. These assumptions will need to be presented in a report of the conceptualisation process, with their justifications.

2.6.2.2 Hydrostratigraphy

A hydrostratigraphic description of a system consist of:

- Stratigraphy, structural and geomorphologic discontinuities (e.g. faults, fractures, karst areas)
- The lateral extent and thickness of hydrostratigraphic units
- Classification of the hydrostratigraphic units as aquifers (confined or unconfined) or as aquitards
- Maps of aquifer/aquitard extent and thickness (including structure contours of the elevation of the top and bottom of each layer)

2.6.2.3 Aquifer properties

The aquifer and aquitard properties control water flow, storage and the transport of solutes, including salt, through the hydrogeological domain. Quantified aquifer properties are critical to the success of the model calibration. It is also well understood that aquifer properties vary spatially and are almost unknowable at the detailed scale. As such, quantification of aquifer properties is one area where simplification is often applied, unless probabilistic parameterisation methods are applied for uncertainty assessment. Hydraulic properties that should be characterised include hydraulic conductivity (or transmissivity), specific storage (or storativity) and specific yield.

2.6.2.4 Conceptual boundaries

The conceptualisation process establishes where the boundaries to the groundwater flow system exist based on an understanding of groundwater flow processes. The conceptualisation should also consider the boundaries to the groundwater flow system in the light of future stresses being imposed (whether real or via simulations). These boundaries include the impermeable base to the model, which may be based on known or inferred geological contacts that define a thick aquitard or impermeable rock. Assumptions relative to the boundary conditions of the studied area should consider:

- Where groundwater and solutes enter and leave the groundwater system
- The geometry of the boundary; that is, its spatial extent
- What process(es) is(are) taking place at the boundary, that is, recharge or discharge
- The magnitude and temporal variability of the processes taking place at the boundary. Are the processes cyclic and, if so, what is the frequency of the cycle?

2.6.2.5 Stresses

The most obvious anthropogenic stress is groundwater extraction via pumping. Stresses can also be imposed by climate through changes in processes such as recharge and evapotranspiration. Description and quantification of the stresses applied to the groundwater system in the conceptual domain, whether already existing or future, should consider:

- If the stresses are constant or changing in time; are they cyclic across the hydrogeological domain?
- What are their volumetric flow rates and mass loadings?
- If they are localised or widespread (i.e., point-based or areally distributed).

2.6.2.6 Solute transport data

All available solute concentration data should be used during conceptualisation to determine the spatial distribution of solutes, identify source zones and migration pathways, and to determine appropriate boundary conditions. Solute transport models require input parameters that describe the combined effect of advection, dispersion and diffusion. This typically involves quantification of the following parameters:

- Effective porosity
- Longitudinal and transverse dispersivity
- Diffusion coefficient
- An equation(s) of state (for variable density problems).

An assessment of the relative importance of advection, diffusion and dispersion should be made during the conceptualisation stage, and a decision should be made on which processes are to be included in the solute transport model. The importance of variable-density flow should be assessed with a quantitative analysis using all available head and concentration data.

2.7 Applicability, Limitations and Future Trends of Groundwater Modeling

2.7.1 General

A good groundwater management strategy should aim at: (i) sustainable use of groundwater and preservation of its quality; (ii) incorporation of groundwater protection plans into environmental protection planning; and (iii) protection measures towards prevention of groundwater pollution and over-use. Thus, the sustainable management of groundwater resources implies equilibrium between groundwater development and groundwater protection, and should be based on scientific understanding of the processes involved, scientific assessment of present and prognostic scenarios, robust planning and judicious management strategies culminating in effective action.

Although groundwater 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 groundwater. There are point sources and dispersed sources of pollution contributing to groundwater contamination. Therefore, groundwater regimes can be stressed by contamination, over-exploitation, or a combination of these two. In order to formulate technically-sound, robust and environmentally sustainable groundwater resources management policies, one has to ponder over 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?
- How long a pollutant may take to reach the supply source?
- 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 systems and also the ability to predict system responses to various stresses as far as the aquifer system is concerned. Groundwater models are the best tools available to help groundwater hydrologists to meet these kinds of challenges and to come out with effective solutions as groundwater models are capable of simulating and predicting aquifer conditions.

2.7.2 Applicability of groundwater models

The development of groundwater simulation models provided groundwater managers with quantitative techniques for analyzing alternative management strategies. Mathematical modeling techniques have demonstrated their value in furthering the understanding of groundwater systems and, thereby improving evaluation, development, and management of groundwater resources. Groundwater modeling can be applied to issues like water supply management of regional aquifers, planning of groundwater development, optimisation of pumping rates, planning of cropping pattern for given groundwater withdrawals or given canal supplies supplemented by groundwater irrigation, optimal locations of wells, all kinds of groundwater quality/contamination problems including pollution source identification using contaminant transport models, aquifer depletion problems as wells as conjunctive use of groundwater and surface water for agriculture applications.

As per GEC norms, groundwater resources are estimated based on an assessment unit, i.e. block, taluka, etc. which is lumped within that assessment unit. However, distributed models have the beauty of resource estimation at the defined grid size; even further refinement of any grid is possible. Therefore, groundwater resource estimation based on distributed models (even in a very small grid) is more realistic as it is based on scientific principles.

There are situations, wherein it is not possible to monitor all aspects of groundwater flow and solute distribution just by investigations only. Information pertaining to the future and between monitoring locations is required for making meaningful and scientific decisions. Groundwater models can replicate the processes of interest at the respective sites and may be used to facilitate in evaluating and forecasting groundwater flow as well as transport.

Groundwater optimisation models can provide optimal groundwater planning or design alternatives in the context of each system's objectives and constraints. Such 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.

Conventionally, linked simulation-optimization models are employed to arrive at the optimal groundwater development plans. The plans may relate to well operation (Katsifarakis, 2007) or regional groundwater development (Kashyap and Chandra, 1982; Werner et al., 2006). The planning problem is posed as an optimization problem with the simulation model computing the state variables of the groundwater system appearing in the objective function and constraints. Optimization invariably involves sequential computation of the objective function and the constraints; therefore, the linked simulation-optimization approach restricts the scope of the planning because of the usually huge computational cost of repeatedly running a simulation model (Safavi et al., 2009). The problem of excessive computational cost may be overcome by replacing the traditional simulation models by approximate models such as regression (Alley, 1986) and Artificial Neural Networks (ANN) (Coppola et al., 2003). Other alternative strategies that do not compromise upon the rigor of the simulation are embedded technique (Gorelick and Remson, 1982; Gorelick, 1983) and the kernel function approach (Morel-Seytoux and Daly, 1975). Embedded technique treats the discrete heads as additional decision variables and embeds the simulator into the optimizer by treating the finite difference equations as additional constraints. The other strategy viz. the kernel function approach, is mostly applied to linear systems. It is based upon the concept of kernel function that describes the system response to a unit impulse/pulse of the input such as pumpage. Ghosh and Kashyap (2012a, b) have reported applications of computationally inexpensive simulators employing kernel model functions and ANN for planning of optimalgroundwater development for irrigation.

2.7.3 Uncertainty and limitations of groundwater models

Numerical groundwater flow 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 modeled. As such, accurate field data is a pre-requisite for model reliability. Thus, predictive results of groundwater simulations may vary from true values, which can be attributed to the uncertainty in model formulation, structure, processes, parameters, as well as data inputs. Besides, there can be scenario uncertainty, an uncertainty caused by boundary conditions. For this purpose, the modeler has to ensure and be careful about the selection of proper boundary condition types. The selected boundary conditions must be nearly true representative of the real field conditions. Similarly, the forcing functions like recharge, evapotranspiration, withdrawals as well as system parameters must be precisely estimated and verified alternatively before assigning into the model. Otherwise, inherent errors in these forcing functions and parameters will ultimately lead to model uncertainties. The uncertainty in regionalization of aquifer parameters and assigning parameters particularly in hard rock areas should be realistic enough, scientifically based and must be clearly defined. Therefore, in the application of groundwater models, especially of groundwater quality models, scientific judgement tempered with wide experience of field observation is desirable to produce sound interpretations.

It may be noted that solution procedures of all numerical groundwater models have certain inherent shortcomings. First of all, the solution is sought for the numerical values of state variables only at specified points in space and time domains defined for the problem, and not their continuous variations in the domain. Secondly, as analytical solutions of the partial differential equations that represent balances of the considered extensive quantities are not feasible, those 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. Further, 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. Lastly, computerized numerical solution techniques, which are employed to solve the set of simultaneous equations, have inherent instability issues. Thus, certain degree of inaccuracy may be expected in the state variables computed at discrete points (discontinuity).

Different levels of uncertainty are associated with modeling of aquifer systems. The degree of uncertainty varies with type of issues and complexity of the aquifer systems as well as the architecture of the model itself (e.g. inadequacies in mathematical representation of processes, numerical instabilities etc.). Uncertainties exist in the transport mechanisms; various sink/source phenomena for the considered extensive quantity; values of model coefficients, and their spatial/ sometimes temporal variation; initial conditions; domain boundaries and the conditions prevailing on them; data employed in model calibration; and the robustness of the model to cope with heterogeneity of varying scales. To estimate the uncertainty, methods are basically statistical and probabilistic. Some of the commonly used methods include Monte Carlo method, probabilistic method, joint aggregation method and method of moments.

When groundwater models are used as predictive tools, field monitoring must be incorporated to verify model predictions as predictive simulations are estimates that depend upon the quality and uncertainty of the input data. If the basic principles of groundwater flow/ contaminant transport and the underlying assumptions of Modeling are lost sight of, there is serious danger of gross mis-interpretation of model outputs. This is more likely to occur when models are automated, and commercially packed. Therefore, a groundwater 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.

In an aquifer system, management decisions are to be taken with respect to flow/ pumping rates, location of pumping, artificial recharge, water quality, contamination chances, well-interferences, well head protection/ capture zone management etc. Often, management goals are linked with minimization of cost while maximizing benefits. The management objective function may depend on the decision variables, like pumping and the consequent response of the aquifer system. Constraints are expressed in terms of future values of state variables of the considered groundwater system. Only by comparing predicted values with specified constraints can decision makers conclude whether or not a specific constraint has been violated. In the management of a groundwater system in which decisions must be made with respect to both water quality and water quantity, a tool is needed to provide the decision maker with information about the future response of the system to the effects of management decisions.

Three-dimensional groundwater simulation models applied to complex, heterogeneous aquifer systems have often been utilized to explore groundwater management alternatives. For this purpose, the groundwater model may be executed repeatedly under various scenarios designed to achieve a particular objective, such as obtaining a sustainable water-supply, 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. In such cases, the groundwater model needs to be linked with an optimizer as discussed in section 7.2.

In the case of contaminant transport modeling, 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 Modeling 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 behaviour of those pollutants involved in more complex chemistry cannot yet be predicted reliably.

In general, the underlying mathematical equations have been adequately verified, and the physical meaning of the parameters involved is clearly understood in the case of groundwater flow models. However, in the case of contaminant transport, more insight is needed on the mathematical characterisation and measurement of hydrodynamic dispersion, and about the best way to identify, measure, and 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 greater care.

2.7.4 Emerging issues and future trends in groundwater modeling

Groundwater Modeling is a key component in a wide variety of projects including water supply, agriculture, environmental, mining, chemical, and energy industries. Since it is difficult for a groundwater modeller to keep pace both with advances in groundwater Modeling as well as advances in these related fields, a team approach would be a more viable option in future where groundwater modellers work closely with computer professionals, atmospheric scientists, surface water hydrologists, and geochemists.

Need for efficient utilization of water resources will increase interaction of groundwater professionals with communities and stakeholders with different self-interests. With the fast pace of changes in the 21st century, interdisciplinary approaches would be required to address the complex flow mechanisms occurring within the hydrologic cycle as well as the water availability issues within the broader framework of societal, ecological, and environmental policy issues (Refsgaard et al., 2010; Langevin and Panday, 2012). For example, climate change and its impact on water availability through changes in precipitation patterns, air temperature, and sea level are complex issues wherein groundwater modeling would play a vital role as part of a larger inter disciplinary effort. With the ongoing aquifer mapping program in India, as the knowledgebase increases about various hydrogeologic units in alluvial and hard rock terrains in India, the groundwater quantity and quality issues present today will continue to be addressed with a more rigorous approach in future.

For groundwater models to be used effectively for the multidisciplinary problems of tomorrow, several technical components will require technological advances, i.e., multi-scale simulation, coupling with other processes, improvements in computational efficiency, and better data integration.

2.7.4.1 Multi-scale issues

Many groundwater problems are complicated due to scale related issues. Often, our interests lie in phenomenon occurring at a large scale, but the physical processes controlling the outcome operate at a much finer scale. To improve the accuracy of groundwater models, research in simultaneous solution of groundwater processes at multiple scales, using flexible gridding methods is needed. Efforts have been made to combine the strengths of numerical and analytic element methods to address scale issues (e.g., Haitjema et al. 2010), and to add the flexibility of unstructured, control volume finite difference (CVFD) methods to MODFLOW (Langevin et al. 2011).

2.7.4.2 Process coupling and alternative modeling frameworks

The best way to support multiple hydrologic processes in a modeling framework, either by linking/coupling using one-way sequential methods or by using a standard protocol is a debatable issue in the hydrologic Modeling community. Combining separate models, either directly as is done in GSFLOW (Markstrom et al., 2008), or through a coupling protocol, allows individual fields to develop and progress independently as has been done in the past. Conversely, a new modeling framework is a much larger endeavor, but it could be designed to use the latest advances in numerical methods, programming, and parallel computing. A common modeling framework would likely be easier to use than learning two or more separate codes. The trend now and in the near future is likely to be a need to couple MODFLOW with more complicated processes. More customized versions of MODFLOW (e.g., MODFLOW-FMP, MODFLOW-CFP, SEAWAT, MODFLOW-VSF) are expected if a process model does not fit cleanly into the MODFLOW structure.

It should be noted that scripting languages, such as Python, contain extensive library collections for linear and nonlinear systems of equations, performing spatial manipulations, and visualizing results in 3D. Usage of scripting languages, containing these libraries, frees the groundwater modeler from having to learn the details of these other fields and allows them to focus on applying the power of these tools to groundwater simulation.

Another new development in groundwater simulation is the emergence of general-purpose multi-physics computer programs that can be instructed, because of their flexibility, to solve one or more governing partial differential equations, such as saturated or unsaturated groundwater flow and solute or heat transport. As continental-scale models, including 3D hydrostratigraphic and geologic models, continue to advance and become more reliable, an increase in application of methods for rapidly developing in set models is expected using the best available hydrologic and geologic information.

2.7.4.3 Advances in computational efficiency

Advances in computer science and powerful new hardware technologies that offer much higher computational capabilities will be harnessed for future modeling problems. Recently, there seems to be a growing trend toward retail cloud computing, where computing resources appear almost endless. For tasks that require numerous independent forward simulations, it is relatively straightforward to use these computational resources, including the cloud-based resources. Splitting individual forward runs across multiple processors, however, has been a challenge for most modeling approaches. Parallelization methods for forward runs will continue to improve for shared memory systems, such as multiple-core processors, and for distributed memory systems, such as networks of desktop computers and cloud resources. These computational advances are also expected to be used to improve visualization and presentation of data and model results. These new and enhanced capabilities will help identify and correct deficiencies in models and more effectively communicate results to a wide variety of technical and non-technical audiences.

2.7.4.4 Uncertainty and optimization

In future, groundwater models will need to make more rigorous predictions and reveal the uncertainty of modeled estimates. Recent advances in sophisticated methods for quantifying uncertainty and increased availability of parallel computing will help such techniques to be incorporated into the pre- and post-processing toolkits, and create more reliable models, for assessing how estimated parameter values and distributions are affected by measurement and structural errors, and for evaluating the resulting uncertainty in predictions.

In many groundwater modeling contexts, the purpose of the modeling effort is to help identify effective management strategies, whether it be for optimizing a data collection network, maximizing effectiveness of a remediation system, or identifying groundwater extraction patterns that minimize harmful impacts to a wetland or stream. Application of formalized optimization techniques for these types of problems has been steadily increasing. The development and use of optimization techniques is expected to grow and become more widely used in practice. Usage of Artificial Intelligence (AI) techniques, such as artificial neural network, genetic algorithm and simulated annealing etc. has gained popularity over the years to deal with uncertainty and speed up optimization process in groundwater models.

2.7.4.5 Data acquisition and integration

Advanced modeling programs, faster computers, and better calibration strategies, would not be of much use without better quality data. Better future groundwater flow and transport models will require extensive real-time monitoring networks, remotely sensed data, progress in field instrumentation, and advances in related fields such as geochemistry and geophysics. Fast assimilation of new data as soon as they become available will be an important component of groundwater modeling. There are promising efforts toward improved data acquisition, storage, processing, and distribution tools. Work will be needed to address logistical problems inherent to groundwater models that require so many different types of data; each one typically in a different form, with different levels of uncertainty and availability.

The future of data for groundwater modeling will likely include a central repository, perhaps by state offices that store and provide raw data. Modern data encoding rules, such as the Extensible Markup Language (XML), are well suited for handling complex datasets. Having this type of information in an accessible and standardized database would lead to better and more reliable groundwater models. As detailed climatic data, using remote sensing technology, become available, better recharge estimates can be made at the local and regional scales using precipitation records, energy budget data, and soil characteristics.

2.7.5 Common errors in groundwater modeling

The accuracy of model predictions depends upon the degree of successful calibration and verification of the model and the applicability of groundwater flow and solute transport equations to the problem being simulated. Errors in the predictive model, even though small, can result in gross errors in solutions projected forward in time. The common errors in any groundwater modeling study may include the following.

Model Conceptualization Errors

- Inappropriate model selection
- Selection of inappropriate boundary conditions
- Excessive discretization
- Lack of far-field data
- Oversimplification of problem (2-D model when obviously 3-D flow)
- Placing model boundaries too close to area of interest, which may include pumping centre
- Lack of understanding of site hydrogeological processes

Data Input Errors

- Inconsistent parameter units
- Incorrect sign for pumping or recharge
- Well not specified correctly
- Aquifer stresses (pumping, recharge, evapotranspiration, etc.) not specified over entire transient simulation period
- Using interpolated input data
- Forcing questionable data to fit

Calibration Errors

- Forcing a fit either by using unrealistic data values or over-discretizing a aquifer or aquitard layer
- Target wells clustered in a small portion of the model - i.e. lack of far field calibration data
- Target wells too close to, or within, specified head boundaries
- Using interpolated data distribution rather than point data
- Misinterpreting mass balance information

Simulation Results Errors

- Omitting results inconsistent with preconceptions
- Not incorporating data variability or uncertainty into the analysis
- Blind acceptance of model output

One may refer to Kumar (2001) for further details about the above errors. Predictive simulations must be viewed as estimates, dependent upon the quality and uncertainty of the input data. Models may be used as predictive tools; however field monitoring must be incorporated to verify model predictions. The best method of eliminating or reducing modeling errors is to apply good hydrogeological judgement and to question the model simulation results. If the results do not make physical sense, find out why.

2.8 Groundwater Modeling Softwares

2.8.1 General

The development of (numerical) groundwater models in the seventies provided groundwater hydrologists with quantitative techniques for analyzing alternative planning/management strategies. It is well known that the equations describing groundwater flow in porous media are mathematically analogous to those governing the flow of electric current. Hence, electric analogue models were designed and used to study groundwater flow systems in 1950s. However, all analogue models have been superseded by numerical simulation models later, following the development of advanced digital computers.

Our interest here pertains only to numerical groundwater models that are physically founded mathematical models, based on certain simplifying assumptions, derived from equations of flow in porous media (like Darcy's law in saturated soil/ flow in unsaturated porous media etc.) and basic laws of conservation of mass/ solute transport / chemical laws etc. 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, chemical properties and reactions. By mathematically representing a simplified version of a hydrogeological system, reasonable alternative scenarios can be predicted, tested, and compared.

Groundwater flow and contaminant transport models are being applied for arriving at solutions to many aquifer development/ management issues as well as environmentally related problems around the world. The applicability of these models in groundwater pollution investigations are of varying levels of success. These models are of use in all stages of site investigation and remediation processes. Nevertheless, the usefulness of a model depends on how closely the mathematical formulation approximates the physical system being modeled.

2.8.2 Categorization of groundwater modeling software

The evolution of groundwater models in the study of groundwater problems has been in perfect line with the advancement of technology. Therefore, groundwater modeling software may be classified in various manners depending upon their evolution, functionalities, dimensionalities, use of numerical techniques, and applicability.

On the basis of their formulation, we can classify them into Analytical Models, Porous Media Models, Viscous Fluid Models, Membrane Models, Electrical Analogue Models, Empirical Models, Mass Balance Models, and Numerical models. Further, according to their functionalities, one may classify them into aquifer parameter estimation models, flow models, contaminant transport models, and coupled models. Again a model may be classified depending upon the domain where it is applicable, like unsaturated flow model, saturated flow model, fractured aquifer model etc. It may be noted that even though fractured rocks and fractured porous media may behave like an equivalent porous media with regard to certain flow conditions and contaminant transport phenomena, they deserve separate treatment as they are governed by different processes. Likewise, flow and contaminant transport issues in unsaturated zones are also governed by nonlinear processes different from that of Darcy's law. Also, groundwater models may be subdivided according to their objectives, as: Prediction models; Identification or evaluation models; Management models. Flow domain (determined by the hydrogeological setup) also classifies models into one dimensional, two-dimensional or three-dimensional model.

Depending on the numerical technique employed in solving the mathematical model, there exist several types of numerical models: finite-difference models, finite-element models, boundary-element models, particle tracking models (method of characteristics, random walk models), and integrated finite-difference models.

2.8.2.1 Analytical modeling software

Analytical models offer straightforward answers towards evaluation of the physical characteristics of an aquifer system. These models enable one to carry out a preliminary analysis of the groundwater system/ flow aspects and contamination. Even though a number of simplifying assumptions with respect to flow/ transport are necessary to get an analytical solution in an analytical model, its utility in real life situations is valuable as an initiating tool, particularly where few data are available. Because of, complex numerical models are of limited use when there is scanty data. Nonetheless, application of analytical models to field situations demands good professional judgment and experience. Analytical models may be considered complementary to numerical models. Once sufficient data is available, numerical models can be used for evaluation/ simulation or decision making.

2.8.2.2 Numerical modeling software

In most of the practical cases, analytical solutions of the mathematical models are not feasible. Therefore, mathematical models are transformed into numerical models, which in turn are solved by specially designed computer codes. These codes account for physical aspects, Modeling aspects, and optimal management. As a first step towards numerical groundwater modeling, the natural system is to be conceptualized into an idealized system to be amenable to physical laws/ mathematical representations. Once the conceptual model is translated into a mathematical model in the form of governing equations, with associated boundary and initial conditions, a solution can be obtained by transforming it into a numerical model and writing a computer program for solving it using a digital computer.

Different numerical techniques may be employed in solving the set of algebraic equations representing the partial difference governing equations of the mathematical model. In a numerical model, the solution is sought for the numerical values of state variables only at specified points in space and time domains defined for the problem. The input data for a numerical groundwater model include natural and artificial stresses, parameters, dimensions, and physico-chemical properties of all aquifers considered in the model. A finer level of detail of the numerical approximation (solution) greatly increases the data requirements. Input data for aquifers are common values such as transmissivities, aquitard resistances, abstraction rates, groundwater recharges, surface water levels etc. The most common output data are groundwater levels, fluxes, velocities and changes in these parameters due to stresses put into the model.

2.8.3 Available groundwater models

Since 1970s, numerous groundwater models have been formulated in public domain as well as on commercial basis. The earlier attempts of development of groundwater software were towards analytical models with simplified assumptions and confined to one or two dimensional flow domains. With the advancement in digital computing technology, later part of twentieth century and recent years saw development of more sophisticated groundwater models that can be interfaced with GIS environment or coupled with other models for input and even to form decision support systems. It may be clearly discernible that in the evolution process of these models, the capabilities and precision have also been steadily improving with improved technology and more refined knowledge of governing aquifer processes.

The *groundwater modeling software* is generic name, and it includes models pertaining to groundwater flow, solute transport in groundwater flow, geochemical reactions in groundwater flow, groundwater/ surface water interaction, variably-saturated flow and solute transport, streamflow-based programs, and analysis of various aquifer tests.

Enlisting all relevant milestones in the history of groundwater model development may be beyond the scope of the article. Nonetheless, an application-wise listing of some of the popular/ important groundwater related software is given below (year of release of latest version is given in bracket) in Table 2.3.

Table 2.3 Groundwater models and their brief description

Model (Year of release)	**Description of the model**
Groundwater (Saturated) Flow	
GFLOW (2015) (License based)	Developed by Haitjema Software Group. It is an efficient stepwise groundwater flow modeling system based on the analytic element method. It models steady state flow in a single heterogeneous aquifer using the Dupuit-Forchheimer assumption. It is particularly suitable for modeling regional horizontal flow and also facilitates detailed local flow modeling. GFLOW supports a MODFLOW-extract option to automatically generate MODFLOW files in a user-defined area with aquifer properties and boundary conditions provided by the GFLOW analytic element model. GFLOW also supports conjunctive surface water and groundwater modeling using stream networks with calculated base flow.
GMS (2013) (License based)	GMS (Groundwater Modeling System) was developed by Environmental Modeling Research Laboratory or EMRL, USA.A comprehensive package which provides tools for every phase of a groundwater simulation including site characterization, model development, post-processing, calibration, and visualization. It features 2D and 3D geostatics, stratigraphic modeling and a conceptual modeling approach. It supports MODFLOW, MODPATH, MT3DMS, RT3D, FEMWATER, SEEP2D and UTEXAS.
HYDROTHERM (2008)	*Developed by the USGS for simulation of Two-Phase groundwater flow and heat transport in the temperature range of 0 to 1200 °C.It is*

Model (Year of release)	**Description of the model**
(Available in Public domain)	*a three-dimensional finite-difference model with graphical user interface to define simulation, running the HYDROTHERM simulator interactively, and display of results.*
MODFE (1998) (Available in Public domain)	Developed by the USGS. It is a modular finite-element model for areal and axi-symmetric groundwater flow problems and it is based on governing equations that describe two-dimensional and axisymmetric-radial flow in porous media. It is written in FORTRAN 77.
MODFLOW (MODFLOW-96, MODFLOW-2000, MODFLOW-2005) (Available in Public domain)	Developed by the USGS. It is a block-centered finite difference code for steady-state and transient simulation of two-dimensional, quasi-three-dimensional, and fully three-dimensional saturated, constant density flow problems in combinations of confined and unconfined aquifer-aquitard systems above an impermeable base. MODFLOW-2005 versionis the most stable version of MODFLOW series The family of MODFLOW-related programs now includes groundwater/surface water systems, solute transport, variable density flow (including saltwater), aquifer-system compaction and land subsidence, parameter estimation, and groundwater management. It is written in FORTRAN 77.
MODFLOW (MODFLOW-96, MODFLOW-2000, MODFLOW-2005): MODPATH (2012) (License based)	USGS particle-tracking post processing model for MODFLOW that was developed to compute three-dimensional flow paths using output from steady state or transient groundwater flow simulations by MODFLOW.
MODFLOW-NWT (2014)	The USGS MODFLOW-NWT is a Newton-Raphson formulation for MODFLOW-2005 to improve solution of unconfined groundwater-flow problems. MODFLOW-NWT is a standalone program that is intended for solving problems involving drying and rewetting nonlinearities of the unconfined groundwater-flow equation. The Surface-Water Routing (SWR1) and Seawater Intrusion (SWI2) Packages are also included in the MODFLOW-NWT.
MODFLOW-OWHM (2014) (Available on request)	MODFLOW-based integrated hydrologic flow model for the analysis of human and natural water movement within a supply-and-demand framework developed by USGS. It allows the simulation, analysis, and management of human and natural water movement within a physically-based supply-and-demand framework.
MODFLOW-USG (2015) (Available on request)	Unstructured grid version of MODFLOW for simulating groundwater flow and tightly coupled processes. Developed by USGS to support a wide variety of structured and unstructured grid types, including nested grids and grids based on prismatic triangles, rectangles, hexagons, and other cell shapes.
MODOPTIM (2005) (Available on request)	Developed by the USGS. A general optimization program for groundwater flow model calibration and groundwater management in MODFLOW tool that simulates flow with MODFLOW-96 as a subroutine. Water levels, discharges, water quality, subsidence, and pumping-lift costs are the five direct observation types that can be compared in MODOPTIM.

Model (Year of release)	Description of the model
Visual MODFLOW Flex.(License based)	It is promoted by Waterloo Hydrogeologic. The Visual MODFLOW Flex is a graphical user interface for MODFLOW groundwater simulations. It brings together industry-standard codes for groundwater flow and contaminant transport, essential analysis and calibration tools, and stunning 3D visualization capabilities in a single. With Visual MODFLOW Flex, groundwater modelers have all the tools required for addressing local to regional-scale water quality, groundwater supply, and source water protection issues.
FEFLOW (2013) (License based)	Developed by DHI with user interface supports. It is a 2D/3D finite element subsurface flow system - model for density dependent groundwater flow, heat flow and contaminant transport with GIS interface. The program uses finite element analysis to solve groundwater flow equation of both saturated and unsaturated conditions as well as mass and heat transport, including fluid density effects and chemical kinetics for multi-component reaction systems.
Solute Transport (Saturated Flow)	
SUTRA (2014) (Available in Public domain)	Developed by the USGS. SUTRA is a finite-element simulation model for 2D or 3D saturated-unsaturated, fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport model. 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 ground-water flow, and either (2) transport of a solute in the ground water, and (3) transport of thermal energy in the ground water and solid matrix of the aquifer.
HST3D (2005) (Available in Public domain)	Developed by the USGS. It simulates groundwater flow and associated heat and solute transport in three dimensions. The HST3D program may be used for analysis of problems such as those related to sub-surface-waste injection, landfill leaching, saltwater intrusion, freshwater recharge and recovery, radioactive-waste disposal, hot-water geothermal systems, and subsurface-energy storage. The three governing equations are coupled through the interstitial pore velocity, the dependence of the fluid density on pressure, temperature, and solute-mass fraction, and the dependence of the fluid viscosity on temperature and solute-mass fraction. The solute-transport equation is for only a single, solute species with possible linear-equilibrium sorption and linear decay. Finite-difference techniques are used to discretize the governing equations using a point-distributed grid.
MT3D (2010) (Available in Public domain)	Developed by the USGS. It is a modular 3-D multi-species transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems coupled with MODFLOW.
HYDRUS (2014) (License based)	A software package developed by PC-Progress Engineering Software Developer of Czech Republic for simulating water, heat, and solute movement in two- and three-dimensional variably saturated media. The software package consists of a computational

Model (Year of release)	Description of the model
	computer program and an interactive graphics-based user interface.
MOC3D (2004) (Available in Public domain)	USGS three-dimensional method-of-characteristics groundwater flow and transport model. The model computes changes in concentration of a single dissolved chemical constituent over time that are caused by advective transport, hydrodynamic dispersion including both mechanical dispersion and diffusion), mixing (or dilution) from fluid sources, and mathematically simple chemical reactions (including linear sorption, which is represented by a retardation factor, and decay).The model can also simulate ground-water age transport and the effects of double porosity and zero-order growth/loss.
SEAWAT (2012) (Available in Public domain)	SEAWAT developed by the USGS is a generic MODFLOW/MT3DMS-based computer program designed to simulate three-dimensional variable-density groundwater flow coupled with multi-species solute and heat transport. SEAWAT uses the familiar structure of MODFLOW and MT3DMS. It also allows to work with many of the MODFLOW-related software programs, such as MODPATH, ZONEBUDGET, and parameter estimation programs.
SHARP (2004) (Available in Public domain)	It was developed by the USGS. It is a quasi-three-dimensional finite-difference model to simulate freshwater and saltwater flow in layered coastal aquifer systems.
Unsaturated Flow and Transport	
MF2K-VSF (2006) (Available in Public domain)	USGS developed a three-dimensional finite-difference groundwater model (MODFLOW) 2000 version with variably saturated flow.
R-UNSAT (2006) (Available in Public domain)	Reactive, multispecies transport in a heterogeneous, variably-saturated porous media.
SUTRA (2014) (Available in Public domain)	2D and 3D, variable-density, variably-saturated flow, solute or energy transport.
VS2DH (2004) (Available in Public domain)	A graphical software package for simulating for simulation of water and energy transport developed by USGS.
VS2DI (2004) (Available in Public domain)	A graphical software package for simulating fluid flow and solute or energy transport in variably saturated porous media. It allows gravity driven vertical flow out of the domain assuming a unit vertical hydraulic gradient but does not allow flow into the domain. The VS2DI software package includes three applications: VS2DTIfor simulation of water and solute transport, VS2DHI for simulation of water and energy transport, and VS2POST a standalone postprocessor for viewing results saved from previous simulation runs.
VLEACH (2007) (Available in Public	Developed by the US -EPA. It is a one-dimensional, finite difference model for making preliminary assessments of the effects on

Model (Year of release)	Description of the model
domain)	groundwater from the leaching of volatile, sorbed contaminants through the vadose zone. The program models four main processes: liquid-phase advection, solid-phase sorption, vapor-phase diffusion, and three-phase equilibrium.
HELP (1994) (Available in Public domain)	HELP (Hydrologic Evaluation of Landfill Performance) is a hydrologic numerical model developed by the US-EPA for landfill. The model uses a water-balance approach to model evapotranspiration and drainage through soil layers. It is a quasi-two-dimensional, deterministic, water-routing model for determining water balances.
Groundwater Flow & Transport with Geochemical Reactions	
PHAST (2014) (Available in Public domain)	Developed by the USGS. It simulates groundwater flow, solute transport, and multi-component geochemical reactions.
PHREEQC (2012) (Available in Public domain)	Developed by the USGS. It is a computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations. It is a 1-D advective reaction-transport model.
Groundwater/ Surface-Water Interactions	
GSFLOW (2015) (Available in Public domain)	Developed by the USGS. It is a coupled groundwater and surface water flow model based on the USGS Precipitation-Runoff Modeling System (PRMS) and modular groundwater flow model (MODFLOW-2005). It simulates groundwater/surface-water flow in one or more watersheds by simultaneously simulating flow across the land surface, within subsurface saturated and unsaturated materials, and within streams and lakes. It considers climate data consisting of measured or estimated precipitation, air temperature, and solar radiation, as well as groundwater stresses and boundary conditions.
Groundwater Management	
GWM (2015) (Available in Public domain)	Developed by the USGS. Groundwater Management process for MODFLOW using optimization. Current Versions include GWM-2005 and GWM-VI. It uses a response-matrix approach to solve several types of linear, nonlinear, and mixed-binary linear groundwater management formulations. Each management formulation consists of a set of decision variables, an objective function, and a set of constraints.
Stream flow Based Groundwater Models	
PART (2012) (Available in Public domain)	Developed by the USGS. A computer program for base-flow-record estimation.
PULSE (2007) (Available in Public domain)	Developed by the USGS. Model-estimated groundwater recharge and hydrograph of groundwater discharge to a stream. It also allows for a gradual hydrologic gain or loss term in addition to the instantaneous pulse, to simulate the effects of gradual recharge to water table, groundwater evapotranspiration, or downward leakage to a deeper aquifer.
RECESS (2012) (License based)	Developed by the Scientific Software Group. RECESS comprises a group of six programs (RECESS, RORA, PART, TRANS, CURV

Model (Year of release)	Description of the model
	and STREAM) for describing the recession of groundwater discharge and for estimating mean groundwater recharge and discharge from streamflow records.
RORA (2012) (Available in Public domain)	The recession-curve-displacement method for estimating recharge is used for the analysis of streamflow records using data in a particular format developed by the USGS
Aquifer Test Analysis Models	
AIRSLUG (1996) (Available in Public domain)	Developed by the USGS. It is a Fortran program to generate type curves to interpret the recovery data from prematurely terminated air-pressurized slug tests. Air-pressurized slug tests offer an efficient means of estimating the transmissivity (T) and storativity (S) of aquifers.
Analyze HOLE (2009) (Available in Public domain)	An integrated well bore flow analysis tool developed by the USGS.
AQTESTSS (2004) (Available in Public domain)	Developed by the USGS. Several spreadsheets for the analysis of aquifer-test and slug-test data. Each spreadsheet incorporates analytical solution(s) of the partial differential equation for groundwater flow to a well for a specific type of condition or aquifer.
BAT3 Analyzer (2008) (Available in Public domain)	Developed by the USGS. It provides real-time display and interpretation of fluid pressure responses and flow rates measured during geochemical sampling, hydraulic testing, or tracer testing conducted with the Multifunction Bedrock-Aquifer Transportable Testing Tool (BAT3).
FLASH (2011) (Available in Public domain)	Developed by the USGS. FLASH (Flow-Log Analysis of Single Holes) is a computer program for the analysis of borehole vertical flow logs. It is based on an analytical solution for steady-state multilayer radial flow to a borehole. The code includes options for (1) discrete fractures and (2) multi-layer aquifers. Given vertical flow profiles collected under both ambient and stressed (pumping or injection) conditions, the user can estimate fracture (or layer) transmissivities and far-field hydraulic heads.
WTAQ (2012) (Available in Public domain)	Developed by the USGS for calculating drawdowns and estimating hydraulic properties for confined and water-table aquifers. It is based on an analytical model of axial-symmetric ground-water flow in a homogeneous and anisotropic aquifer. The program allows for well-bore storage and well-bore skin at the pumped well and for delayed drawdown response at an observation well.
AQTESOLV (2014) (License based)	Developed by HydroSOLVE Inc. It is a software for slug test analysis including methods for single and multi-well tests, over-damped and under-damped conditions, wells screened across the water table, and for all type of aquifers.
Groundwater Flow and Transport Models in Fractured Mediat	
BIOF&T (1995) (License based)	Developed by Scientific Software Group. It simulates biodegradation and bioremediation, flow and transport in the saturated/unsaturated zones in 2 or 3 dimensions in heterogeneous, anisotropic porous

Model (Year of release)	Description of the model
	media or fractured media. It considers convection, dispersion, diffusion, adsorption and microbial processes based on oxygen limited anaerobic first order or Monod-type biodegradation kineticsas well as anaerobic or first-order sequential degradation involving multiple daughter species.
HYDRO-GEO-SPHERE (2013) (Licensebased)	HydroGeoSphere(HGS) developed by Aquanty Inc., Canadais a 3D control-volume finite element groundwater model based on a rigorous conceptualization of the hydrologic system consisting of surface and subsurface flow regimes in fractured or unfractured porous media. For each time step, the model solves surface and subsurface flow, solute and energy transport equations simultaneously, and provides a complete water and solute balance. Originally, it was known as FRAC3DVS. It uses a globally-implicit approach to simultaneously solve 2D diffusive-wave equation and 3D form of Richards' equation.
SWIFT (1998) (License based)	Developed by Integrated Groundwater Modeling Centre, Colorado. It is athree-dimensional transient flow in fractured or unfractured, anisotropic, heterogeneous porous media. Viscosity dependency as a function of temperature and brine concentrations.
Analytical Groundwater Models	
MPNE1D (Available in Public domain)	Developed by S.S. Papadopulos & Associates, Inc. It is a general analytical solution for one-dimensional solute transport is based on FORTRAN90 code that implements the general analytical solution for one-dimensional solute transport.
3DADE (Available in Public domain)	Developed by the USDA. It is a Fortran computer program for evaluating a series of analytical solutions of the 3-dimensional advection-dispersion equation. The analytical solutions pertain to three-dimensional solute transport during steady unidirectional water flow in porous media with uniform transport and flow properties. The transport equation contains terms accounting for solute movement by advection and dispersion, as well as for solute retardation, first-order decay, and zero-order production.
AGU-10 (Available in Public domain)	A collection of screening level analytical flow and transport programs for homogeneous, isotropic flow fields, based on the American Geophysical Union's Water Resources Monograph 10. Developed by Integrated Groundwater Modeling Center (IGWMC). It consists of five simulation programs in FORTRAN and two pre-/postprocessors in Microsoft BASIC.
AT123D (License based)	Developed by Scientific Software Group. It is based on an analytical solution for transient one-, two-, or three-dimensional transport of a dissolved chemical or radionuclide or heat in a homogeneous aquifer with uniform, stationary regional flow. It models for long-term pollutant fate and migration in groundwater -advection, dispersion, adsorption and decay.
CAPZONE (Available in Public domain)	Developed by Integrated Groundwater Modeling Centre, Colorado. An analytical flow model that can be used to construct groundwater flow models of two-dimensional flow systems characterized by isotropic and homogeneous confined, leaky-confined, or unconfined

Model (Year of release)	Description of the model
	flow conditions.
ONE-D (Available in Public domain)	Developed by the USDA. It is a package of five analytical models of the one-dimensional convective-dispersive transport equation with linear adsorption, zero-order production, and first-order decay.

2.8.4 Selection of modeling software

Some of the frequently used groundwater models (software packages), under various categories and applications, have been listed in Table 3. Many of those models are multi-functional (like simulation of flow/ surface water-groundwater interaction/ solute transport etc.). As such, it may not be possible to confine these groundwater models to a particular category, and then to enlist strictly under that category. Their functionality spreads over a few different categories.

The important aspects to be reckoned with in a groundwater model study are, therefore, model applicability to specific problem, ease of its use, transparency, accuracy of results, closeness in emulating natural aquifer processes in the model, portability, adaptability as well as input data requirements. In recent years, groundwater models as software packages have been developed for almost all classes of problems encountered in the management of groundwater. Some models are very comprehensive and can handle a variety of specific problems as special cases, while others are tailor-made for particular problems. Therefore, in order to make a wise choice of the right model for a given investigation, a modeler need to have prior knowledge of the factors mentioned earlier.

Another significant issue is with regard to freedom in the assignment of input parameters and data. Coping up with the technological advancements, the groundwater models are also under continuous refinement or modifications. Considering the large variability and quick development of groundwater models, a new and more sophisticated model may often replace a previously applied model. Additionally, the reconsideration of the conceptual model and regeneration of the mesh may need a new allocation of the parameters. Therefore, it is important that model data (information) are stored independently from a given model, with a preference for GIS based databases. This makes the set-up and modification of models easier and time effective (e.g. Visual MODFLOW/ FEFLOW). Such popular groundwater models, with modular structure, incorporate mathematical modeling with GIS based data exchange interfaces.

2.8.5 Review of popular groundwater models

Management of groundwater involves determining the quantity and quality of groundwater movement over time and space as influenced by natural processes and human activities. Unlike surface water conditions, groundwater observations are limited to boreholes and pumping test, and thus understanding the hydrogeological system as well as predicting changes is more difficult due to management activities. Therefore, the ability to characterize groundwater systems and to develop and evaluate resource management strategies for sustainable water allocation is greatly dependent on groundwater model predictions. In India, groundwater models are used by water resources managers for:

- Characterizing aquifer properties
- Evaluating groundwater pumping impacts on groundwater levels
- Quantifying sustainable yield
- Identifying groundwater recharge zones and determining the placement and design of groundwater recharge structures (e.g. check dams, tanks, recharge wells),
- Evaluating proposed policies and projects
- Developing conjunctive management strategies
- Developing aquifer storage systems
- Determining the fate and transport of chemical solutes in groundwater
- Computing the saline intrusion in coastal zones
- Evaluating the economic impact of groundwater conditions
- Communicating groundwater quality and quantity conditions to policy makers and stakeholders.

Often, groundwater models are developed to satisfy multiple uses. Distributed hydrogeological models (DHgMs) are physically-based distributed models that represent groundwater movement using 2-D or 3-D gridded finite difference and finite volume solutions based on Darcy's equations. Simulations include both steady-state and transient simulations. The data requirements for DHgMs include the aquifer thickness, hydrogeological parameters (e.g. hydraulic conductivity, transmissivity), boundary conditions (e.g. constant flow, fixed head, non-flow), groundwater recharge, and pumping rates. Typical output includes groundwater heads, drawdown, flow magnitude and direction, and water budgets throughout the Modeling domain. If simulating water quality is required, capabilities include the fate and transport of chemicals and, for some packages, the temperature and multi-density flow (saline intrusion). DHgMs are applicable for the uses listed above and have been successfully applied to aquifers in India.

Borden (2015) has evaluated six DHgM including GMS, Groundwater Vistas, MODFLOW, iMOD, MIKE SHE, and Visual MODFLOW. General descriptions of each package are listed below:

- **GMS** (Aquveo) is a groundwater modeling system, based on MODFLOW code, which provides tools for every phase of a groundwater simulation including site characterization, model development, post-processing, calibration, and visualization.GMS supports TINs, solids, borehole data, 2-D and 3-D geostatistics, finite element, and finite difference model. Currently supported models include MODFLOW, MODPATH, MT3D, RT3D, FEMWATER, SEEP2-D, SEAM3D, PEST, UCODE and UTCHEM. Due to the modular nature of GMS, a custom version of GMS with desired modules and interfaces can be configured. Detailed information regarding GMS is available at:

  http://www.aquaveo.com/software/gms-groundwater-modeling-system-introduction.

- **Groundwater Vistas** (Rockware) is a Windows Modeling environment for the MODFLOW family of model that allows for the quantification of uncertainty. Groundwater Vistas includes a series of tools for assessing risk using more complex and real-world groundwater model. Detailed information regarding Groundwater Vistas is available at: https://www.rockware.com/product/overview.php?id=147.

- **iMOD** (Deltares) is an open source, easy to use Graphical User Interface + an accelerated Deltares-version of MODFLOW with fast, flexible and consistent sub-domain Modeling techniques. iMOD facilitates very large, high resolution MODFLOW groundwater Modeling and also geo-editing of the subsurface. iMOD also facilitates interaction with SEAWAT (for density-dependent groundwater flow) and MT3D (groundwater quality).See detailed information regarding iMOD at: http://oss.deltares.nl/web/imod/about-imod.
- **MODFLOW** (USGS) is 3-D finite-difference groundwater model first published in 1984.Although originally conceived solely as a groundwater-flow simulation code, MODFLOW's modular structure has provided a robust framework for integration of additional simulation capabilities that build on and enhance its original scope. The family of MODFLOW-related programs now includes capabilities to simulate coupled groundwater/surface-water systems, solute transport, variable-density flow (including saltwater), aquifer-system compaction and land subsidence, parameter estimation, and groundwater management. The MODFLOW program is free, open-source software. The software can be used, copied, modified, and distributed without any fee or cost. For information regarding MODFLOW visit: http://water.usgs.gov/ogw/modflow/.
- **MIKE SHE** (DHI) is an integrated hydrological Modeling system for simulating surface water flow and groundwater flow. MIKE SHE simulates the entire hydrologic cycle and allows components to be used independently and customized to local needs. MIKE SHE can be used for the analysis, planning, and management of a wide range of water resources and environmental problems related to surface water and groundwater, especially surface water impact from groundwater withdrawal; conjunctive use of groundwater and surface water; wetland management and restoration; river basin management and planning; and impact studies for changes in land use and climate. MIKE SHE can be used at multiple scales (local to basin wide) and simulates detailed water management operations. Information regarding MIKE SHE can be found at: http://www.mikepoweredbydhi.com/products/mike-she.
- **Visual MODFLOW** (Waterloo Hydrogeologic Software) simplifies model development by providing a workflow driven GUI to guide construction and use of groundwater flow and contaminant transport model. Model development is broken into model development, simulation, and output modules guiding the modeller through the development. It comes with pre-processing and post-processing tools; MODFLOW-88, MODFLOW-96, MODFLOW 2000, and MODFLOW-2005; MT3D, MT3DMS, RT3D and MOC3D; PMPATH 99; and UCODE and PEST-ASP. For detailed information, visit:http://www.novametrixgm.com/groundwater-modeling-software/visual-modflow-flex.

2.8.5.1 Computational capabilities

All packages support a 3-D gridded finite difference model, allowing for construction of multilayer models with varying hydrogeological parameters throughout the domain that are able to simulate flows in confined and unconfined aquifers. The MODFLOW engine based software enables modellers to vary grid cell sizes within the domain for greater grid resolution in regions of interest (e.g. proposed groundwater pumping area or chemical spill). MODFLOW-USG simulates groundwater flow with finite volume solutions, allowing for unstructured grids. iMOD uses an accelerated version of the MODFLOW engine. MIKE SHE uses a 3-D gridded finite difference model based on the Darcy's equations to simulate groundwater movement. The grid in MIKE SHE is fixed throughout the model domain.

MODFLOW system consists of a core program that couples with a series of highly independent subroutines called packages. Each package simulates a specific feature of the hydrologic system (e.g. unsaturated zone flow, river flow), water quality (e.g. solute transport), or a specific method of solving equations that simulate the flow system. Packages supporting calibration routines in PEST (model-independent parameter estimation and uncertainty analysis) and Monte Carlo analysis for quantifying uncertainty are available. MODFLOW's use of packages allows users the ability to examine specific hydrologic features of the model independently, as well as the facilitation for new packages that can be added without modifying existing programs. A list of the MOFLOW packages can be found at http://water.usgs.gov/ogw/modflow/MODFLOW.html. The foundation code for GMS, Visual MODFLOW, and Groundwater Vistas use the MODFLOW engine.

MIKE SHE's structure includes dynamically linked modules to compute saturated zone flow, evapotranspiration, overland flow, river and lake flow, unsaturated zone flow, and anthropogenic use (e.g. irrigation, groundwater pumping, irrigation drains) to allow for the examination of the full hydrologic cycle. For each module, several numerical methods are available, granting flexibility to adjust given the question being addressed and the data available. MIKE SHE can be coupled with the Auto-calibration module to assist in calibration of groundwater model. Within the Auto-calibration module is the ability to perform uncertainty analysis through several methods.

Water quality applications in India include salinity in irrigation, fate and transport of chemical spills, and the prediction of saline intrusion along coastal zones. MODFLOW, iMOD, and MIKE SHE offer multiple means to compute this water quality. Transport packages associated with MODFLOW includeMT3DMS, MT3D99, SEAWAT, RT3D and PHT3Detc. GMS, Visual MODFLOW, and Groundwater Vistas support the use of many of these packages.

iMOD uses the D-Water Quality module that simulates almost any water quality variable and its related water quality processes. A full description is supplied in the Delft 3D Suite water quality description of flooding models. MIKE SHE addresses water quality with ECO LAB, an open-ended ecological and water quality modeling framework that allows user-defined equations and water quality model to be defined. Templates are available for standard constituents to expedite water quality modeling. In India, MIKE SHE with ECO

LAB was used to evaluate the effects of rainwater harvesting on the leakage from an ash-pond on the site of the Himavat Thermal Power Plant.

2.8.5.2 Overview of GUI

ModelMuse (USGS's GUI for MODFLOW), iMOD, GMS, Visual MODFLOW, and Groundwater Vistas use the MODFLOW engine and modules as the simulation base, but have built-in tools for expediting and enhancing the Modeling process. These include site characterization, model development, post-processing, calibration, and visualization. All applications are developed for operation with Windows, though MODFLOW works on Windows, OSX, Linux, and Unix platforms.

All packages evaluated are well supported with sophisticated GUI interfaces for inputting data and viewing results. USGS has developed ModelMuse to support MODFLOW, an interface that provides the basics in editing and viewing function. Third party software including GMS, Visual MODFLOW, and Groundwater Vistas offer more sophisticated visualization and post-processing wrappers around the MODFLOW engine and modules, providing a workflow driven GUI to guide construction, use, and resulting presentation from the groundwater flow and contaminant transport model. Model development is broken into model development, simulation, and output modules, thus guiding the modeller through the development. A 3-D visualization and animation package, 3-D groundwater explorer, is also included.

2.8.5.3 Licensing and support

ModelMuse and iMOD are open source software packages for use in developing groundwater models. Both are supported with manuals, online tutorials, and user forums. Additional support from Deltares and training courses can be purchased and offered for using iMOD. The USGS does not provide training courses, but third party organizations offer MODFLOW courses for a fee.

GMS, Visual MODFLOW, and Groundwater Vistas require licenses. License fees begin from around Rupees 1 lakh per seat for basic model and increases with added interface functionality (pre-processing, post-processing, visualization) and access to additional MODFLOW packages. All packages have online tutorials and courses to promote faster learning. Vendors provide training courses for a fee.

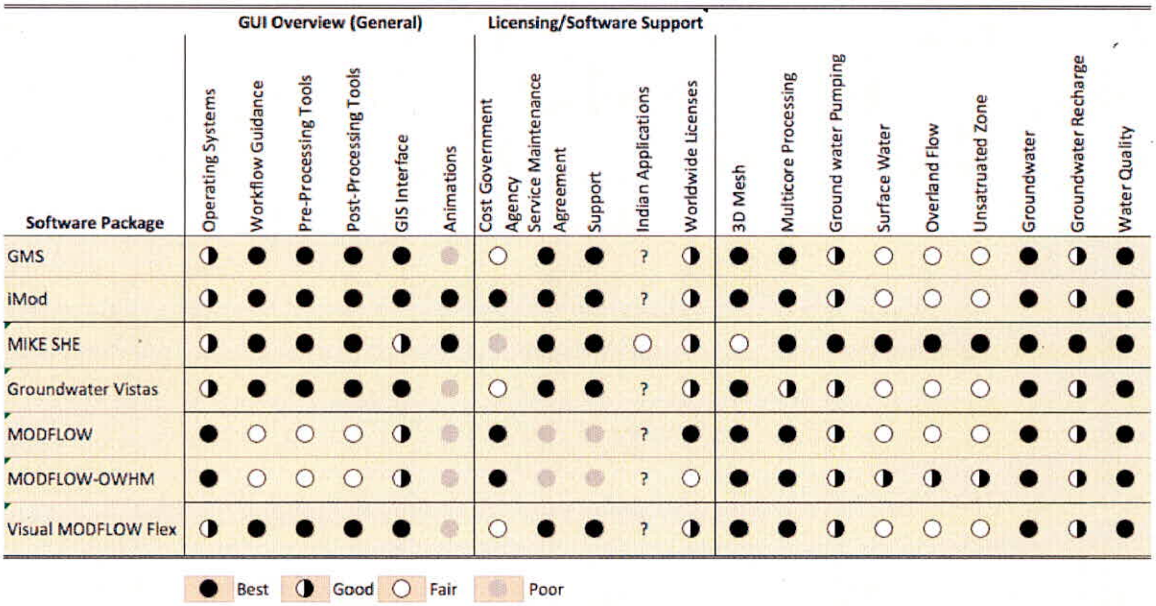
MIKE SHE requires a license that allows access to the core mode functionality listed above, pre- processing and post-processing tools, and limited support during the year. Service maintenance agreements can be purchased annually for additional support, and consulting services are also available. Additional modules for water quality simulations, control structures, and auto-calibration routines are additional cost. The model is supported with manuals, tutorials, training courses, and online materials. Starting at 5.5 lakh INR/seat, MIKE SHE is the most expensive option of the DHgM packages evaluated.

2.8.5.4 Choice of groundwater model

The evaluation matrix for the distributed hydrogeological models has been presented in Table2.4. It provides the evaluation by Borden (2015) for the modeling software packages

- GMS, iMod, MIKE SHE, Groundwater Vistas, MODFLOW, MODFLOW-OWHM and Visual MODFLOW. It presents the evaluation (Best, Good, Fair, Poor) under the categories GUI Overview, Licensing/Software Support, and other Modeling issues (3D Mesh, Multicore Processing, Groundwater Pumping, Surface Water, Overland Flow, Unsaturated Zone, Groundwater, Groundwater Recharge, Water Quality).

Table 2.4 Evaluation Matrix for the Distributed Hydrogeological Models (Borden, 2015)



	GUI Overview (General)						Licensing/Software Support													
Software Package	Operating Systems	Workflow Guidance	Pre-Processing Tools	Post-Processing Tools	GIS Interface	Animations	Cost Government Agency	Service Maintenance Agreement	Support	Indian Applications	Worldwide Licenses	3D Mesh	Multicore Processing	Ground water Pumping	Surface Water	Overland Flow	Unsatruated Zone	Groundwater	Groundwater Recharge	Water Quality
GMS	◑	●	●	●	●	◍	○	●	●	?	◑	●	●	◑	○	○	○	●	◑	●
iMod	◑	●	●	●	●	●	●	●	●	?	◑	●	●	◑	○	○	○	●	◑	●
MIKE SHE	◑	●	●	●	◑	●	◍	●	●	○	◑	○	●	●	●	●	●	●	●	●
Groundwater Vistas	◑	●	●	●	●	◍	○	●	●	?	◑	●	◑	◑	○	○	○	●	◑	●
MODFLOW	●	○	○	○	◑	◍	●	◍	◍	?	●	●	●	◑	○	○	○	●	◑	●
MODFLOW-OWHM	●	○	○	○	◑	◍	●	◍	◍	?	○	●	●	◑	◑	◑	◑	●	◑	●
Visual MODFLOW Flex	◑	●	●	●	●	◍	○	●	●	?	◑	●	●	◑	○	○	○	●	◑	●

● Best ◑ Good ○ Fair ◍ Poor

All packages simulate groundwater quantity and quality using similar algorithms and offer support for users of their software packages. The difference between the evaluated software packages lies in the GUI interface and price of the software. Experienced groundwater modelers familiar with developing MODFLOW model natively or with using GMS, Visual MODFLOW, and Groundwater Vistas will likely want to remain with the software with which they are familiar and can use efficiently.

GMS provides a platform to support the modular nature of MODFLOW while Visual MODFLOW provides GUI that guides groundwater model development through a straightforward workflow. iMOD, with the pre-processing and post-processing, strong visualization abilities, strong support, and open source availability, may also be the strong candidate of the groundwater models evaluated and can be preferred for groundwater Modeling. While MIKE SHE simulates groundwater, its fixed grid system and licensing fee limits adoption for strictly groundwater simulations. MIKE SHE shines in situations where it is important to simulate the interaction between surface water and groundwater.

2.9 Way Forward

Groundwater, one of the India's most important natural resources, is under constant threat of exploitation with increasing population and economic development. Proper understanding and modeling of subsurface water movement has been an enduring challenge for hydrologists and practitioners. Current modeling efforts are plagued by the complex heterogeneity within the subsurface, reconciliation with spatial and temporal scales, and lack of supporting data. Long-term consequences of droughts in aquifers and efficient management of the available resources in arid and semi-arid regions of the country deserve special attention. Assessing the potential impacts of climate change on groundwater is yet another long-term challenge that confounds both researchers and managers. Developing new models that account for uncertainties and provide more realistic assessment of predictive capabilities is needed for devising effective management practices. Current data acquisition techniques need to be improved for reliable modeling and impact studies. Some of the long standing challenges in groundwater are identified as follows:

1. Estimation of recharge is crucial for assessing sustainability of groundwater systems as it is the major replenishing mechanism for most aquifers. However, recharge rates to aquifer are among the most difficult to measure directly. Although these rates are key to conducting water balance studies, they are often treated as calibration quantities. Methods for estimating recharge rates and understanding how they are affected by Climate Changes are needed to assess the fate of groundwater storages and fluxes in the future.
2. Data challenges continue to plague modeling efforts. Complex models have too many parameters that need to be estimated accurately and independently for the models to be used at their full potential. Most efforts rely on calibration and corroboration exercises that are fraught with uncertainty in their own right. Field-scale experiments are time-consuming and costly. There is a need to devise non-expensive and rapid ways to accurately determine hydrogeologic parameters.
3. Heterogeneity is still perhaps the greatest challenge posed to hydrologists, both in terms of characterization and in terms of techniques needed to resolve sub-grid processes. Although some progress has been made in terms of assimilating large remotely-sensed data sets, appropriate algorithms and up-scaling techniques need to be developed.
4. Uncertainties in modeling and in defining climate change scenarios make it difficult to assess the state of future groundwater resources. Future climate scenarios are based on GCMs that do not have a strong groundwater component. Besides, models do not adequately represent the interactions with surface water storage and human intervention. Methods for quantifying and reducing these uncertainties need to be derived using advanced mathematical techniques, and modeling strategies.
5. With increasing threats from competing demands and mounting hydrologic stresses on the groundwater system, there is a pressing need to develop effective management strategies. Aquifer recharge and recovery operations are often met with constraints related to water quality and aquifer integrity. A major task ahead is bridging the gap between researchers and policy makers for successful implementation of conjunctive groundwater management decisions.
6. Fractured and hard rock flow and transport modeling in India have been less explored although the country has more than 70% hard rock areas; some of the reasons are: inadequate and unstructured databases, insufficient understanding of the hardrock

aquifer systems, etc. While the hard rock aquifers in India are under severe groundwater stresses, and failure of wells are very common.

7. India has initiated the task of "Aquifer Mapping" upto a depth of about 400 m and trying to develop groundwater management plan as policy matter.
8. Uptil now, the main focus of groundwater modeling activities in India was towards developing simulation models for groundwater development and formative aquifer responses from various recharge strategies. Discharge (demand) management has got limited attention in the groundwater modeling activities. Managed Aquifer Recharge (MAR) together with demand management in conjunction with surface and ground water under the framework of Integrated Water Resources Development and Management (IWRD&M) can be the most promising way forward towards the futuristic Optimization-Simulation Model.
9. MODFLOW-2005 and its related modules and other software, which are available in public domain and popularly accepted worldwide and have been found formed parts of most commercial software presently used world over, can be an excellent choice to explore further for fitting to Indian conditions. GSFLOW or coupling of SWAT with MODFLOW, both available in public domain, can also be thought as an alternative for IWRD&M. Further, Indian researchers, both in academia and R & D sectors, have developed a number of surface water, groundwater and hydrological models (published in reputed journals) based on knowledgebase and data of Indian conditions, rope in those research models and amalgamation of suitable models to the appropriate components of the MODFLOW framework can also been alternative.
10. Developing/customizing an Indian groundwater model – In view of the above considerations, it would be highly desirable to develop a groundwater model suitable for Indian meteorological, hydrological and hydrogeological conditions commensurate with corresponding availability of relevant data.

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