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Modeling seawater intrusion and groundwater flow pollution

Gaaloul Noureddine [1], Saeid Eslamian[2]

[1] National Institute of Research in Rural Engineering of Water and Forestry, INRGREF, IRESA, University of Carthage, Tunisia;
[2] Department of Water Engineering, Isfahan University of Technology, Iran

Abstract

The objective of this paper is to set the stage for the modeling procedure and methodology presented in subsequent chapters: what is it that we wish to model and why and, especially, how do we model?
We start by presenting some basic definitions related to groundwater and to aquifers, focusing our attention on the flow of water in the saturated zone, noting that due to the heterogeneity of porous material at the pore, or grain size scale, it is practically impossible to predict and observe the flow at that scale. Instead, the continuum approach is proposed as a device for describing and observing flow in porous media, in the absence of information on the microscopic configuration of the solid matrix. As a further simplification, it is proposed to treat the flow in aquifers as approximately two-dimensional in the horizontal plane.
Seawater intrusion in coastal aquifers is a growing concern in mediterranean regions, due to over- population and over-exploitation of coastal groundwater resources. Under these circumstances, it is essential to model the extent of seawater intrusion and to locate the saltwater-freshwater interface taking into account heterogeneity and parameter uncertainty. There are different ways to couple salt transport and freshwater flow in groundwater models

Key Words*:* Integrated Water Resources Management and Climat Change.

Modélisation de l'intrusion d'eau de mer et de la pollution des eaux souterraines

Résumé

L'objectif de cet article est de préparer le terrain pour la procédure et la méthodologie de modélisation présentées dans les chapitres suivants : qu'est-ce que nous souhaitons modéliser et pourquoi et, surtout, comment modéliser ?
Nous commençons par présenter quelques définitions de base liées aux eaux souterraines et aux aquifères, en concentrant notre attention sur l'écoulement de l'eau dans la zone saturée, en notant qu'en raison de l'hétérogénéité du matériau poreux au niveau des pores, ou à l'échelle granulométrique, il est pratiquement impossible de prédire et observer le débit à cette échelle. Au lieu de cela, l'approche continuum est proposée comme un dispositif pour décrire et observer l'écoulement dans des milieux poreux, en l'absence d'informations sur la configuration microscopique de la matrice solide. Pour simplifier davantage, il est proposé de traiter l'écoulement dans les aquifères comme approximativement bidimensionnel dans le plan horizontal.
L'intrusion d'eau de mer dans les aquifères côtiers est une préoccupation croissante dans les régions méditerranéennes, en raison de la surpopulation et de la surexploitation des ressources en eaux souterraines côtières. Dans ces circonstances, il est essentiel de modéliser l'étendue de l'intrusion d'eau de mer et de localiser l'interface eau salée-eau douce en tenant compte de l'hétérogénéité et de l'incertitude des paramètres. Il existe différentes façons de coupler le transport du sel et le débit d'eau douce dans les modèles d'eaux souterraines.

Mots Clés : Gestion intégrée des ressources en eau et changement climatique

INTRODUCTION

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[1] Corresponding author: gaaloul.noureddine@iresa.agrinet.tn

Groundwater modeling is commonly the most important water resource in in arid environments. In areas of high evaporation and limited rainfall, groundwater provides natural storage of water which is protected from surface evaporation, it is spatially distributed, and it can be developed with limited capital expenditure. Groundwater also provides a potential storage that can be managed to increase the useful water resource. Numerical modelling has emerged over the past 40 years as one of the primary tools that hydrologists use to understand groundwater flow and saltwater movement in coastal aquifers. Numerical models that account for the effects of fluid density on ground water flow are being used more frequently to address scientific, engineering, and water resource management problems.

Also being used more frequently are inverse modelling routines based on nonlinear regression methods. As computing power increases and expertise grows, modelling studies will likely use both inverse methods and density-dependent ground water flow simulations to solve complicated water resource or ground water contamination problems. Groundwater models describe the groundwater flow and transport processes using mathematical equations based on certain simplifying assumptions. These 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. Because of the simplifying assumptions embedded in the mathematical equations and the many uncertainties in the values of data required by the model, a model must be viewed as an approximation and not an exact duplication of field conditions. Groundwater models, however, even as approximations are a useful investigation tool that groundwater hydrologists may use for a number of applications.

Numerical models are mathematical representations (or approximations) of groundwater systems in which the important physical processes that occur in the systems are represented by mathematical equations. Application of existing groundwater models include water balance (in terms of water quantity), gaining knowledge about the quantitative aspects of the unsaturated zone, simulated zone, simulating of water flow and chemical migration in the saturated zone including groundwater relations, assessing the impact of changes of the groundwater regime on the environment, setting up/optimising monitoring networks, and setting up groundwater protection zones. The governing equations are solved by mathematical techniques (such as finite-difference or finite-element methods) that are implemented in computer codes. The primary benefit of numerical modelling is that it provides a means to represent, in a simplified way, the key features of what are often complex systems in a form that allows for analysis of past, present, and future groundwater flow and saltwater movement in coastal aquifers. Such analysis is often impractical, or impossible, to do by field studies alone.

Numerical models have been developed to simulate groundwater flow solely or groundwater flows in combination with solute transport (the movement of chemical species through an aquifer). For a number of reasons, numerical models that simulate groundwater flow and solute transport are more difficult to develop and to solve than those that simulate groundwater flow alone. Coastal aquifers are particularly difficult to simulate numerically because the density of the water and the concentrations of chemical species dissolved in the water can vary substantially throughout the modelled area. To address these difficulties, one of two approaches generally is used to simulate freshwater-saltwater interactions. In the first approach, the freshwater and saltwater zones are assumed to be immiscible (that is, they do not mix) and separated by a sharp interface. In the second approach, the freshwater and saltwater are considered being a single fluid having a spatially variable salt concentration that influences the fluid's density; this approach is referred to as density dependent groundwater flow and solute-transport modelling (Reilly, I993).

Mathematical models are tools, which are frequently used in studying groundwater systems. In general, mathematical models are used to simulate (or to predict) the groundwater flow and in some cases the solute and/or heat transport. 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 modelling errors is to apply good hydrogeological judgments and to question the model simulation results. If the results do not make physical sense, find out why. Scientists and groundwater resources managers are involved in numerical modelling studies of environmental problems, such as contaminant migration prediction, aquifer remediation, seawater intrusion, etc.

From a methodological point of view, numerical modelling of such phenomena faces challenges such as characterizing and accounting for complex geological settings. Other challenges are specific to the applications themselves, such as accounting for complex flow and solute transport processes like density effects or reactive solute transport. Those issues affect the accuracy of the forecasts made by numerical models and consequently may affect decisions about groundwater management policies. Numerical models use an approximate form of the governing equation to calculate head at selected locations. In contrast to analytical solutions and the AEM, a numerical solution is not continuous in space or time; head is calculated at discrete points (nodes) in space and for specified values of time.

However, numerical models can solve the full transient, 3D, heterogeneous and anisotropic under complex boundary and initial conditions. The numerical methods most commonly used in groundwater modeling are the finite-difference (FD) method and the finite- element (FE) method. In the FD method, nodes are located in 3D space using indices (i,j,k) to assign relative locations within a rectangular grid.

NUMERICAL MODELS

Finite Differences (FD): The method of finite differences (FD) is generally very intuitive and relatively easy to implement. In the FD method, nodes are designated by i, j, k indices, which here represent the column, row, and layer, respectively, of a node in 3D space (Figure 1). The spacing of nodes along rows is designated by Dx and the spacing along columns by Dy, while the spacing between layers is Dz. The node is situated within an FD cell or block (Figure 1(b) and (c)). Heads are defined only at nodes and the head at a node represents the average head in the FD cell/block (Gaaloul, 1992).

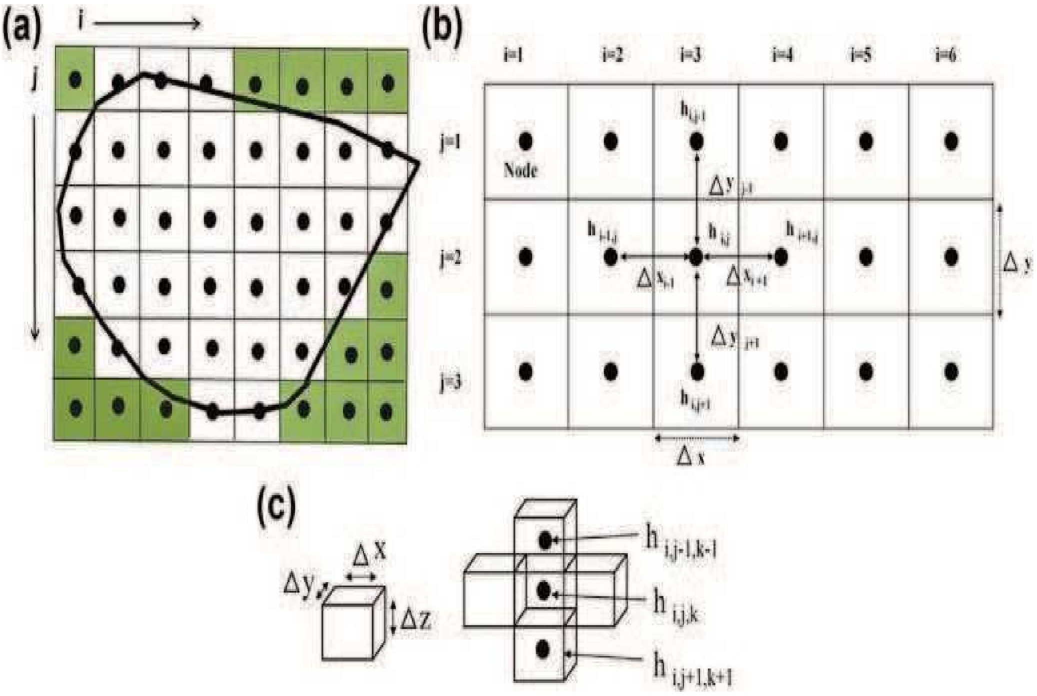


Figure 1. Finite-difference (FD) grid and notation. (a) Two-dimensional (2D) horizontal FD grid with uniform nodal spacing; i ¼ columns and j ¼ rows. Sometimes a different indexing convention is used. For example, in MODFLOW i ¼ rows and j ¼ columns. The cells are block-centered; the heavy dark line represents the problem domain. Inactive cells (those outside the boundary of the problem domain) are shaded. (b) 2D horizontal FD grid with notation for the group of five nodes comprising the FD computational module (star) centered around node (i,j). (c) Three- dimensional notation where Dz represents the vertical distance between nodes and k is the vertical index. The group of blocks at the right is shown in 2D space (the two blocks perpendicular to the page along the y-axis are not shown). The group of seven nodes including node (i,j,k) comprise the FD computational module in three dimensions**.**

Finite Elements (FE): In the FE method, the locations of nodes are designated using spatial coordinates (x,y,z) in a mesh (Figure 2). Numerous texts and reports cover the basic theory of these methods. For example, Remson et al. (1971) discuss finite differences and Diersch (2014), Huyakorn and Pinder (1983), Pinder and Gray (1977), and Istok (1989) discuss finite elements. Wang and Anderson (1982) provide an elementary introduction to both methods. Pinder and Gray (1976) and Wang and Anderson (1977, 1982), among others, have shown that the FD and FE formulations of the Laplace equation yield the same set of algebraic equations. They also demonstrated that both methods yield the same results if nodal spacing is sufficiently small. Thus, while the methods differ in concept, they yield similar results, even for more complex versions of the governing equation than the Laplace equation. The FE solution is piecewise continuous, as individual elements are joined along edges. A large variety of element shapes and nodal locations are possible, although the most common elements are triangular and quadrilateral. Elements are lines in one dimension, planes in two dimensions, and volumetric polygons in three dimensions. The mathematics of the FE method is less straightforward than the FD method. In the FE method, the problem domain is subdivided into elements (Figure 2) that are defined by nodes.

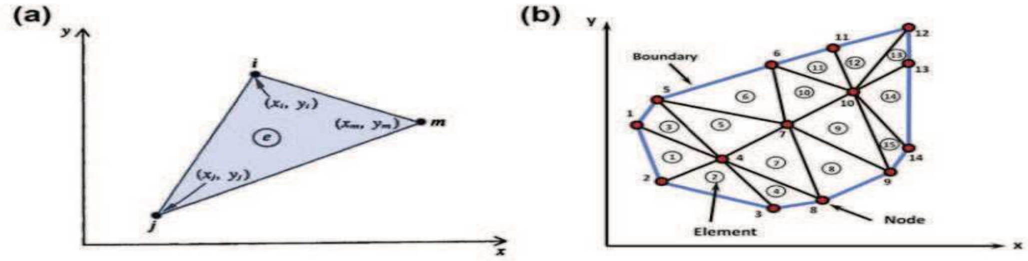


Figure 2. Two-dimensional horizontal finite-element mesh with triangular elements and notation. (a) A representative triangular element with nodes i, j, and m, labeled in counterclockwise order, with spatial coordinates (x,y); (b) Triangular elements, with element numbers inside circles, are defined by numbered nodes. The elements are fitted to the boundary of the problem domain (Wang and Anderson, I982).

The dependent variable (e.g., head) is defined as a continuous solution within elements (Figure 3(a)) in contrast to the FD method where head is defined only at the nodes and is considered piecewise constant between nodes (Figure 3(b)).

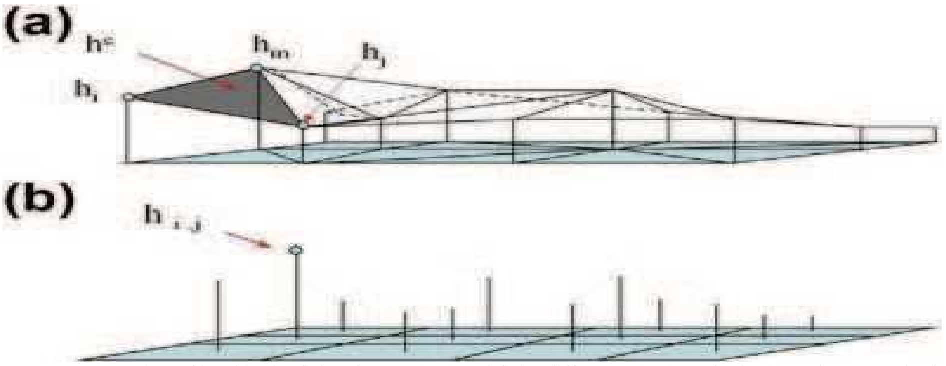


Figure 3 Representation of head in the finite-element (FE) and finite-difference (FD) methods. (a) In the FE method, head (he) is a continuous function within each element. In the FE mesh shown in the figure, the elements are triangular with heads at nodes designated hi, hj, and hm. (b) In the FD method, head (hi,j) is defined only at the node.

Locations of nodes in an FE mesh are designated using x, y, z coordinates. Both nodes and elements are numbered, and the location of each element is defined in terms of the surrounding nodal numbers. The FE method requires more bookkeeping of nodal locations than in FD because not only is the x, y, z location of each node required but the element number and the numbers of the nodes forming the element must be input to the code to generate the mesh. Mesh generation is both tedious and important because the sequence of nodal numbering can have an impact on computer memory during code execution (Wang and Anderson, I982). Hence, FE codes usually include mesh generating software. The FE equations are generated by introducing a trial solution of head within the element. For example, for the triangular element, the trial solution is defined by interpolation functions, usually called basis functions, that relate head at the nodes to head within the element (Figure 4). Typically, a linear interpolation function is chosen, though more complex functions are possible.

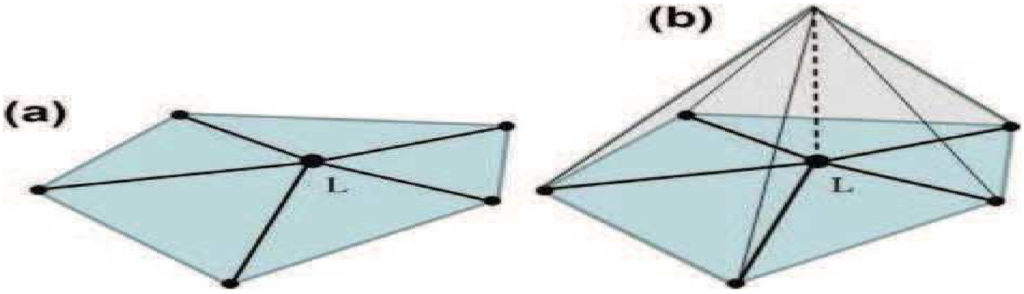


Figure 4 (a) Plan view of a patch of elements around node L in a finite-element mesh. (b) Three- dimensional view of the nodal basis function NL(x,y) (Wang and Anderson, I982 and Cheng, I978).

Control Volume Finite Differences (CVFD): Standard FD methods require rectangular grids and rectangular cells within the grid. Although rectangular grids are simple to code and visualize, they often require inconvenient assumptions about system geometry. Furthermore, rectangular grids have two other drawbacks: they generate cells in areas of the model domain outside the main area of interest and they require that any increased resolution in discretization is extended areally to the edges of the model domain and vertically into all layers of a 3D model. For example, increased resolution (smaller node spacing and smaller FD cells) around surface water features for better representation of groundwater/surface water interaction in layer I of a model requires the same higher level of discretization in all lower layers even though the surface water features are present only in layer I.The control volume finite-difference (CVFD) method was used in one of the first applications of numerical models to a groundwater problem (Tyson and Weber, I964) and was explored in detail by Narasimhan and Witherspoon (1976) in another early application. The method was called integrated finite differences in those early applications.

The CVFD method gives FD methods much of the same flexibility in spatial discretization as the FE method. In a CVFD model, spatial discretization can include a combination of rectangular and square cells as well as hexagons, triangles, and irregular shapes. Moreover, spatial discretization can be different in each vertical layer. Recently, Panday et al. (20I3) used CVFD to develop the code MODFLOW-USG, a version of the FD code MODFLOW with an unstructured grid (USG). As in an FE mesh, nodes in a USG are numbered sequentially, rather than using the i,j,k indexing convention of standard FD methods. Similar to FE, each cell is numbered. Adjacent nodes are said to be connected and the user must input the area of the shared cell face for every cell connection. Given the complexity of assembling the data for a USG, a preprocessor code is recommended to assemble the grid (Panday et al., 20I3). The equations used in the CVFD method are briefly discussed below but the details of the method are beyond the scope of our text. The interested reader should refer to Narasimhan and Witherspoon (I976) and Dehotin et al. (20II) for details of the theory, and to Panday et al. (20I3), who show how to adapt the CVFD approach to the coding used in MODFLOW. We provide an overview of the CVFD method below, following Panday et al. (20I3) and Narasimhan and Witherspoon (I976).

Solution Methods: The set of algebraic equations resulting from applying a numerical approximation to the governing equation using the FD, FE, or CVFD method is solved for head using either direct methods or direct methods combined with iteration. Some general features of solution methods are discussed briefly in this section. Wang and Anderson (I982) discuss basic iterative and matrix solution techniques in more detail. Direct methods solve the global matrix using matrix solvers and give an exact numerical solution of the set of algebraic equations subject to numerical roundoff error. Roundoff errors are generated because the computer stores a finite number of digits to represent each numerical value. Although in principle direct method solutions are desirable, they often require large amounts of computer memory since all entries of the coefficient matrix must be stored in the computer and the number of entries is typically large. Moreover, owing to the large number of calculations required to solve a matrix equation directly, significant numerical roundoff error can occur. In practice, execution time of direct solvers is fastest with small, linear, groundwater problems, but can be unacceptably long if the modeling problem is highly nonlinear. Therefore, convergence problems (Konikow and Reilly, 1998) and computer memory have limited the application of direct solution methods. However, improved solution methods and improved computer power are motivating new developments in direct methods. The FE code FEFLOW (DHI-WASY, 20I3; FEFLOW version 6.2) includes a direct solver that can accommodate up to I million nodes. There is also a direct solver for MODFLOW (Harbaugh, I995, 2005). Nevertheless, direct solutions continue to be more appropriate for steady-state models, which solve for only one set of heads. Transient models, especially models that use variable length time steps (Harbaugh, I995), may be better served by a solver that combines direct methods with iteration.

An iterative solution is the simplest type of numerical solution and point iteration was used routinely to solve FD equations in the early years of groundwater flow modeling. Today, point iterative solutions for the groundwater flow equation are rarely used. Instead, direct (matrix) methods are combined with iteration. With point iteration, the FD equation is solved sequentially for head at each node in the problem domain and then the process is repeated until heads between iterations stop changing (i.e., the solution converges). Methods that combine iteration with a direct solution first simplify the coefficient matrix in the global matrix equation so that more efficient direct matrix solvers can be used. Because the resulting matrix equation has a coefficient matrix that is not exactly correct, the solution is not accurate, and iteration is used to improve the solution. Wang and Anderson (I982) present examples of methods for combining direct and iterative solution methods for 2D groundwater flow problems. McDonald and Harbaugh (I988) discuss direct methods combined with iteration for solving the 3D flow equation. Codes generally include several different solvers from which the user may choose. The solution of large, complex groundwater models may require the modeler to experiment to find the solver that converges most efficiently. Iterative solutions are inexact because the iteration process is stopped when the solution is (subjectively) judged to have converged. Moreover, iteration involves a large number of calculations making the solution prone to roundoff error and associated artifacts. Acceleration parameters and relaxation factors speed up convergence but the modeler has to select values for those parameters. A residual error in head (¼ the difference in heads at the start and end of an iteration) is calculated for each node. The modeler specifies a value for the head closure criterion (also called the head error criterion, error tolerance or convergence criterion) that sets the maximum allowed value of the residual error in head. Many solvers also use a similarly defined second closure criterion for the water balance.).

Multi-component reactive transport models and variable density flow models are important tools for improving the understanding of governing processes in groundwater systems Representatives of multi-component reactive transport models are, for example, PHREEQC-II, PHAST, Hydro Bio Geo Chem and some MODFLOW/MT3DMS based models such as RT3D and PHT3D. Numerous other models were developed for transport of a single solute species in aquifers with variable density, for example

SUTRA, METROPOL, FEMWATER, HST3D, NAMMU, FEFLOW and MOCDENS3D (Gaaloul et al., 20I2). Some of the recently developed simulation models are based on this sharp interface approach. On the other hand, when the transition zone stretches to a considerable extent, the seawater intrusion phenomenon is modelled using the density-dependent miscible flow and transport approach. Coastal aquifers are particularly difficult to simulate numerically because the density of the water and the concentrations of chemical species dissolved in the water can vary substantially throughout the modelled area. A management problem is formulated with two conflicting objectives involving maximization of groundwater development in coastal zones while limiting the head and seawater intrusion to desired levels of salinity by the use of barrier wells. Unlike many earlier models, the proposed model is based on a recently developed 3-D density- dependent seawater intrusion model, SEAWAT. Use of SEAWAT as the simulator is expected to result in a better representation of the flow system, as compared to the sharp interface approach. (Gaaloul et al., 20I2). To simulate the seawater intrusion (SWI), one can either adopt a sharp interface or a density- dependent dispersive model. The freshwater and saltwater are considered immiscible. This simplification allows for treatment of the problem analytically or numerically in a very efficient manner. Reviews of this approach can be found in (Gaaloul et al., 20I2). Despite the fact that assuming a sharp interface allows the development of solutions that are useful for understanding SWI and for solving real-world problems, this approach does not account for hydrodynamic dispersion. However, it is well known that instead of a sharp interface between freshwater and saltwater there is a transition zone since both fluids are miscible. Therefore, several methods have been developed to solve the coupled variable-density flow and advective dispersive solute transport equations. In the case of unstable variable in the case of unstable variable density flow and transport, have shown that heterogeneity can affect transport over many length scales.

Computer models have become an indispensable tool to study aquifers, to understand the interaction of different processes affecting the biogeochemistry and/or the heat distribution, to predict the effect of changes, and to solve practical groundwater problems. Examples are aquifer characterization, capture zone delineation, pumping and recharge well design and management, watershed simulation, groundwater pollution, potential hazards and remediation, acid mine drainage, natural attenuation, geo- and hydrothermics, and saltwater intrusion. The simulation of groundwater flow systems and solute transport using computer codes is standard practices in the field of hydrology. Models are used for a variety of purposes that include education, hydrologic investigation, water resources management, and legal determination of responsibility. The main purpose of the model is to understand the behavior of an aquifer in response to stress conditions or change in the initial conditions. Many studies have focused on the modeling of seawater intrusion, considering it as an important stress condition. The freshwater-seawater relationships in coastal aquifers in open boundaries by a 2-D numerical approach. In spite of diversity of numerical studies treating seawater intrusion problem, some aspects remain unrevealed: relationship of the position and shape of seawater-freshwater interface with pumping rate and other geographical/hydrogeological factors. In particular, occurrence of saltwater up-coning is one of the most interesting phenomena that need to be deepened with 3- D numerical simulations. The provision of adequate data plays an important part in the development of successful models. However, due to practical difficulties and uncertainties of interpretation together with financial constraints, the modeller often considers that insufficient data is available to prepare a reliable model. On the other hand, when detailed data have been collected, the modeller frequently finds that he does not know how to use these data.

GROUND WATER MODELING PROGRAM

To address this issueeffectively, density dependent groundwater model is required to track the movement of the solute in coastal aquifers (Lin et al. 2009). Three-dimensional groundwater flow and solute transport models namely FEFLOW, 3DFEMFAT, HST3D, AQUA3D, FEMWATER, SEAWAT and MOCDENS3D are in useworldwide. SEAWAT is one of the widely used codes to simulate saltwater intrusion (Werner et al., 20I3). There are several ways to classify groundwater flow models. Models can be either transient or steady state, confined or unconfined, and consider one, two, or three spatial dimensions. In setting up the grid of a numerical model, the classification that is most relevant is one based on spatial dimension. We can classify models in terms of spatial dimension as two-dimensional areal, twodimensional profile, quasi three-dimensional, and full three-dimensional. Two-dimensional areal and quasi three-dimensional models assume the aquifer viewpoint, while two-dimensional profile and full three-dimensional models use the flow system viewpoint. Particle tracking codes to simulate the advective transport of contaminants can be used with any of these models. If unsaturated flow, immiscible flow, density effects, dispersion, or flow through fractures is an important feature of the conceptual model, it will be necessary to solve a different governing equation than the general saturated flow equation.

FEFLOW (Finite Element subsurface FLOW and transport system) is an interactive groundwater modeling system for • three-dimensional and two-dimensional • regional and cross- sectional (horizontal, vertical or axisymmetric)• fluid density-coupled, also thermohaline, or uncoupled • variably saturated • transient or steady state • flow, groundwater age, mass and heat transport • reactive multi-species transport in subsurface water environments with or without one or multiple free surfaces. FEFLOW can be efficiently used to describe the spatial and temporal distribution and reactions of groundwater contaminants, to model geothermal processes, to estimate the duration and travel times of chemical species in aquifers, to plan and design remediation strategies and interception techniques, and to assist in designing alternatives and effective monitoring schemes. Sophisticated interfaces to GIS and CAD data as well as simple text formats are provided. The option to use and develop user-specific plug-ins via the programming interface (Interface Manager IFM) allows the addition of external code or even external programs to FEFLOW.

SUTRA (Saturated-Unsaturated TRAansport) simulated using the finite element-based flow and solute transportmodel SUTRA (Saturated-Unsaturated TRAansport) developed by Voss (1984). The model employs hybrid finiteelement and integrated-finite-difference method to solve the governing equations, which describe the variabledensity groundwater flow and transport processes of either solute or energy in aquifer system under saturatedunsaturated conditions. SUTRA uses bi-linear quadrilateral elements in 2D and tri-linear hexahedrons elements in 3D. The implicit finite difference is predominately used for temporal, and thus for nodewise discretization of the non-flux terms (e.g. time derivatives and sources) of these balance equations. The SUTRA code solves the generic equations of Bear (1979), which cover most types of known groundwater flow and transport problems.

SEAWAT 4.0 is a coupled version of MODFLOW and MT3DMS designed to simulate three- dimensional, variable-density, saturated groundwater flow, and transport of dissolved species. The SEAWAT program is a coupled version of MODFLOW and MT3DMS designed to simulate three dimensional, variable-density, saturated ground-water flow. Flexible equations were added to the program to allow fluid density to be calculated as a function of one or more MT3DMS species. Fluid density may also be calculated as a function of fluid pressure. The effect of fluid viscosity variations on ground-water flow was included as an option. Fluid viscosity can be calculated as a function of one or more MT3DMS species, and the program includes additional functions for representing the dependence on temperature. Although MT3DMS and SEAWAT are not explicitly designed to simulate heat transport, temperature can be simulated as one of the species by entering appropriate transport coefficients. For example, the process of heat conduction is mathematically analogous to Fickian diffusion. Heat conduction can be represented in SEAWAT by assigning a thermal diffusivity for the temperature species (instead of a molecular diffusion coefficient for a solute species). Heat exchange with the solid matrix can be treated in a similar manner by using the mathematically equivalent process of solute sorption. By combining flexible equations for fluid density and viscosity with multi-species transport, SEAWAT Version 4 represents variable-density ground-water flow coupled with multi-species solute and heat transport. SEAWAT Version 4 is based on MODFLOW-2000 and MT3DMS and retains all of the functionality of SEAWAT-2000.

SEAWAT Version 4 also supports new simulation options for coupling flow and transport, and for representing constant-head boundaries. In previous versions of SEAWAT, the flow equation was solved for every transport timestep, regardless of whether or not there was a large change in fluid density. A new option was implemented in SEAWAT Version 4 that allows users to control how often the flow field is updated. New options were also implemented for representing constant-head boundaries with the Time-Variant Constant-Head (CHD) Package. These options allow for increased flexibility when using CHD flow boundaries with the zero-dispersive flux solute boundaries implemented by MT3DMS at constant-head cells.

Modflow Flex: Visual MODFLOW (VMOD) Flex is a powerful software package that provides the tools forbuilding three-dimensional groundwater conceptual and numerical models using raw GIS dataobjects. The conceptual model approach to groundwater modeling allows you to: ·Build a conceptual model of the groundwater system, prior to the simulation -Geological formations, property model, and boundary conditions are all designedoutside the model grid or mesh; this allows the flexibility to adjust your interpretation ofthe groundwater system before applying a discretization method and converting to anumerical model.·Build the model with minimal data pre-processing required - Working with grid-independent data allows you to maximize the use of your existing GIS data andincorporate physical geology and geographic conditions before designing a grid ormesh.·Generate and simulate regional and local-scaled models - With support forMODFLOW-LGR, you can design local grids around areas of interest, directly within theconceptual model environment. Calculated heads from a regional model can also beused as boundary conditions for local-scaled models.·Design the correct model faster - The grid- independent raw data is left intact and is notconstricted by grid cells or mesh elements when modifying the data and projectobjective. This allows you to generate multiple numerical models from the sameconceptual model.·Make changes to the model data and immediately see results - The conceptual modelenvironment provides simultaneous 2D and 3D views which are updated wheneverchanges to the data are made.

Visual MODFLOW: MODFLOW is a computer program that numerically solves the three- dimensional ground-water flow equation for a porous medium by using a finite-difference method. Although MODFLOW was designed to be easily enhanced, the design was oriented toward additions to the ground-water flow equation. Frequently there is a need to solve additional equations; for example, transport equations and equations for estimating parameter values that produce the closest match between model-calculated heads and flows and measured values. MODFLOW is a computer program that simulates three-dimensional ground-water flow through a porous medium by using a finite-difference method.

Modflow: MODFLOW is the name that has been given the USGS Modular Three-Dimensional Groundwater Flow Model. Because of its ability to simulate a wide variety of systems, its extensive publicly available documentation, and its rigorous USGS peer review, MODFLOW has become the worldwide standard groundwater flow model. MODFLOW is used to simulate systems for water supply, containment remediation and mine dewatering. When properly applied, MODFLOW is the recognized standard model used by courts, regulatory agencies, universities, consultants and industry. MODFLOW is a block-centered finite difference code that can simulate of the aquifer types discussed in Section 3.2. The sophistication present in MODFLOW means that the input assembly is complex, and readers are referred to the user's manual (McDonald and Harbaugh, 1988) for details. Preprocessors are available to help with data assemble and post-processors can assist in viewing the output. “MODFLOW is developed by the U.S. Geological Survey (USGS); it is a three- dimensional (3D) finite-difference groundwater model. MODFLOW is considered an international standard for simulating and predicting groundwater conditions and groundwater/surface-water interactions”. MODFLOW has been used for more than 30 years, and is widely accepted for its easy of use and flexibility in working with other programs. The code is developed in FORTRAN and runs in a DOS window taking a variety of text files as inputs, and generated both text and binary output files. The main objectives in designing MODFLOW were to produce a program that can be readily modified, is simple to use and maintain, can be executed on a variety of computers with minimal changes, and has the ability to manage the large data sets required when running large problems. The MODFLOW report includes detailed explanations of physical and mathematical concepts on which the model is based and an explanation of how those concepts were incorporated in the modular structure of the computer program. The modular structure of MODFLOW consists of a Main Program and a series of highly-independent subroutines called modules. The modules are grouped in packages. Each package deals with a specific feature of the hydrologic system which is to be simulated such as flow from rivers or flow into drains or with a specific method of solving linear equations which describe the flow system such as the Strongly Implicit Procedure or Preconditioned Conjugate Gradient. The division of MODFLOW into modules permits the user to examine specific hydrologic features of the model independently. This also facilitates development of additional capabilities because new modules or packages can be added to the program without modifying the existing ones. The input/output system of MODFLOW was designed for optimal flexibility.

MT3D: MT3D is a comprehensive three-dimensional numerical model for simulating solute transport in complex hydrogeological settings. MT3D has a modular design that permits simulation of transport processes independently or jointly. MT3D is capable of modeling advection in complex steady-state and transient flow fields, anisotropic dispersion, first-order decay and production reactions, and linear and nonlinear sorption. The new MT3D99 can also handle bio plume-type reactions, monad reactions, and daughter products. This enables MT3D99 to do multi-species reactions and simulate or assess natural attenuation within a contaminant plume. MT3D99 is linked with the USGS groundwater flow simulator, MODFLOW, and is designed specifically to handle advectively-dominated transport problems without the need to construct refined models specifically for solute transport.

MODPATH: MODPATH Is a particle tracking post-processing package that was developed to compute three-dimensional flow paths using output from steady-state or transient ground-water flow simulations by MODFLOW. MODPATH uses a semi-analytic particle tracking scheme that allows an analytical expression of the particle's flow to be obtained within each finite-difference grid cell. Particle paths are computed in MODPATH by tracking particles from one cell to the next until the particle reaches a boundary, an internal sink/source, or satisfies some other termination criterion. Data input for MODPATH is a combination of data files and interactive keyboard input. Output from steady-state or transient MODFLOW simulations is used in MODPATH to compute paths for imaginary "particles" of water moving through the simulated ground-water system. In addition to computing particle paths, MODPATH keeps track of the time of travel for particles moving through the system. By carefully defining the starting locations of particles, it is possible to perform a wide range of analyses such as delineating capture and recharge areas or drawing flow.

MODELING SEAWATER INTRUSION

Seawater intrusion and saline groundwater

What is Saltwater Intrusion? :Saltwater intrusion is the movement of saline water into freshwater aquifers. Most often, it is caused by ground-water pumping from coastal wells, or from construction of navigation channels or oil field canals. When fresh water is withdrawn at a faster rate than it can be replenished, the water table is drawn down as a result.

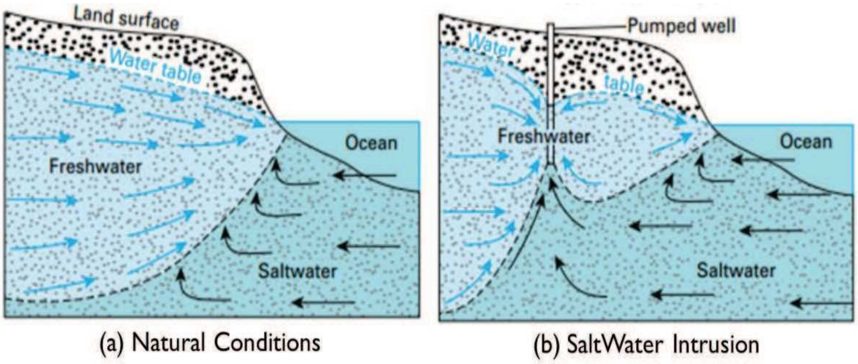
In an unconfined aquifer that contacts the sea at the shoreline or seaward, the freshwater, which is less dense than seawater, floats as a lens-shaped layer on top of seawater, and the weight of the overlying freshwater depresses the seawater below sea level. Generally, freshwater recharge in these aquifers moves downgradient and eventually discharges to low-lying coastal areas and into the sea. But pumping out fresh ground water reduces the weight of the overlying freshwater, which in turn can decrease or even reverse the seaward flow so that seawater moves landward into the freshwater aquifer. This migration of seawater into the freshwater aquifer is known as SeaWater Intrusion (SWI).

Seawater intrusion or called “saltwater intrusion” is a specific process of groundwater contamination. This phenomenon draws special attention in the management of the coastal aquifers. As seawater intrusion progresses, a part of the aquifer close to the saline water. In such case, pumping wells operated there have to be controlled. Seawater intrusion (SWI) is a principal cause of fresh groundwater salinization in many regions of the world (Bear et al., I999). Fresh groundwater in arid and semi-arid regions, like the Mediterranean basin, is even more threatened by this type of contamination. Indeed, such regions are characterized by a constant increase of water demand, especially for agricultural purposes, contrasting with the limited possibility of natural recharge and the high rates of evapotranspiration.

In general, hydraulic gradient from inland toward the sea exists in a coastal aquifer, because the sea serves as main outlet of freshwater from the aquifer. The seawater occupies the void space in the aquifer formation beneath the sea. This seawater zone in the aquifer extends to some distance landward from the coast below freshwater zone. Consequently, a zone of transition between freshwater and saltwater exists and it is referred as “interface zone” or more simply “interface”.

Seawater intrusion associated with groundwater overdraft and lowering of groundwater levels has occurred in many of the coastal aquifers of the world. The extent of seawater intrusion varies widely among localities and hydrogeological settings. Quantifying the extent and rate of seawater intrusion is key to sustainable management and use of groundwater resources. This involves understanding the aquifer-ocean interconnection, and distinguishing among multiple sources of saline water. The Process of Saltwater Intrusion: The figure 5 above illustrates how the process of saltwater intrusion into an aquifer system can occur. The boundary between fresh groundwater and saline groundwater is referred to as the freshwater/saltwater interface. Fresh groundwater discharging to the coast prevents the landward encroachment of saline groundwater. If this balance is upset by too much water being removed from the aquifer system from pumping, then saline groundwater can migrate landward by a process referred to as "saltwater intrusion". If a pumping well is close to the landward migrating freshwater/saltwater interface, the potential exists for saltwater contamination in the well.

Under natural conditions (Figure 5a), the seaward movement of freshwater prevents saltwater from encroaching on freshwater coastal aquifers. This interface between freshwater and saltwater is maintained near the coast or far below the land surface. The interface actually is a diffuse zone where freshwater and saltwater mix. This zone is referred to as the zone of dispersion or the zone of transition. Groundwater pumping (Figure 5b) can reduce freshwater flow toward coastal areas and cause saltwater to be drawn toward the freshwater zones of the aquifer. Saltwater intrusion decreases freshwater storage in the aquifers, and, in extreme cases, can result in the abandonment of wells. Saltwater intrusion occurs by many ways, including lateral encroachment from coastal waters and vertical movement of saltwater near discharging wells. The intrusion of saltwater caused by withdrawals of freshwater from the groundwater system can make the resource unsuitable for use. Thus, groundwater management plans should take into account potential changes in water quality that might occur because of saltwater intrusion.



(a) Natural Conditions (b) SaltWater Intrusion

Figure 5. The Process of Saltwater Intrusion

Coastal aquifers constitute important sources of fresh water in many parts of the world, especially in arid and semiarid zones. Often, coastal areas are also heavily urbanized, a fact that makes the need for fresh water in such areas even more acute. However, the proximity and contact with the sea require special attention when planning the management of such aquifers. In fact, in many coastal aquifers, the intrusion of sea water has become one of the major constraints on groundwater management. As sea water intrusion progresses, the part of the aquifer close to the sea becomes saline, and pumping wells close to the coast start pumping saline water and have to be abandoned. Also, the area above the intruding sea water wedge is, usually, lost as a source of fresh water (by natural replenishment).

Since the famous works of Badon-Ghyben (I888) and Herzberg (I90I), and the less known work of Du Commun (I828) (Konikow and Reilly, I999), extensive research has been carried out, leading to the understanding of the mechanisms that govern sea water intrusion. The dominant factors are (I) the flow regime in the aquifer above the intruding sea water wedge, (2) the variable density, and (3) hydrodynamic dispersion. Reviews of the phenomenon of sea water intrusion, and of the research that has been carried out on this subject, both theoretical work and field and laboratory investigations, may be found in many books and publications, and will not be repeated here (Bear, I972, I979; Reilly and Goodman, I985; Bear and Verruijt, I987; Bear et al., I999; Cheng and Ouazar, 2004). Briefly, under normal conditions in a coastal aquifer, excess fresh water (i.e., natural and artificial recharge minus pumping) is discharged into the sea. This means that close to the coast; a seaward hydraulic gradient exists in the aquifer. Due to the presence of sea water in the aquifer under the sea, a zone of contact is formed between the lighter fresh water flowing towards the sea, and the heavier sea water in the aquifer. A typical cross section, with natural replenishment, pumping, and a transition zone, is shown in Figure 6. The detailed shape of the transition zone, from fresh water to sea water, depends also on whether this zone is advancing inland or retreating. In all cases, the domain in the aquifer that is occupied by sea water has, usually, the form of an advancing or receding wedge. One should note that, like all figures that describe aquifers, these are also highly distorted figures, not drawn to scale.

Sea water and fresh water are often referred to as "miscible liquids," although, actually, both constitute a single liquid phase—water, H2O—with different concentrations of total dissolved matter (salt, TDM). For the sake of simplicity, we shall continue to refer to them as two liquids — fresh water and sea water. Hence, the passage from the portion of the aquifer that is occupied by the former to that occupied by the latter takes the form of a transition zone, rather than a sharp interface. Under certain circumstances, depending on the extent of sea water intrusion and on certain aquifer properties, this transition zone, which is primarily a result of hydrodynamic dispersion of the dissolved matter, may be rather wide. Under other conditions, it may be rather narrow, relative to the aquifer's thickness, and the passage fromthe zone occupied by fresh water to that occupied by sea water may be approximated as a sharp interface. Often, the term "interface" is used for the iso-density surface that is midway between fresh water and sea water. In this article, the term "interface" will, sometimes, be used interchangeably with "transition zone."Under natural undisturbed conditions in a coastal aquifer, a state of equilibrium is maintained, with a steady-state sea water zone and a zone of flowing fresh water above it. The transition zone is also fed from below by sea water (Figure 6). When the discharge to the sea is reduced as a result of pumping fresh water from a coastal aquifer, water levels (or thepiezometric heads in a confined aquifer) close to the seaare lowered and the transition zone rises. The sea water wedge and the transition zone advance landward, until a new equilibrium is reached. Wells that operate within the sea water wedge and the transition zone pump saline water and have to be abandoned. When pumping takes place in a well located above the transition zone, the latter upcones towards the well. Unless the well is at a sufficient distance above this zone and the rate of pumping is sufficiently small, the well will eventually pump saline water.

We should emphasize here that the geological structure and configuration of a coastal aquifer are usually much more complex than the schematic one shown in Figure 6. Often, especially close to the sea, the coastal aquifer is divided into a number of sub-aquifers by impervious or semi-pervious layers, with leakage taking place through the latter. The flow in such multilayered aquifers and the shape of the transition zone(s) are often much more complex than shown in Figure 6. As emphasized so far, a transition zone always exists between fresh water and sea water. Moreover, nowadays, we also have enough tools to handle three-dimensional (3D) transition zone models. Nevertheless, it is useful to use the "sharp interface approximation" of this zone to discuss certain basic features of sea water intrusion. Here, we shall present the concept of a sharp interface to introduce the relation ship between seaward flow of fresh water and the extent of sea water intrusion. We shall do so by a simple steady-state analysis. We start by introducing the famous Ghyben–Herzberg rule that describes the relationship between the freshwater flow to the sea and the extent of sea water intrusion, say, as expressed in terms of the length of the sea water wedge.

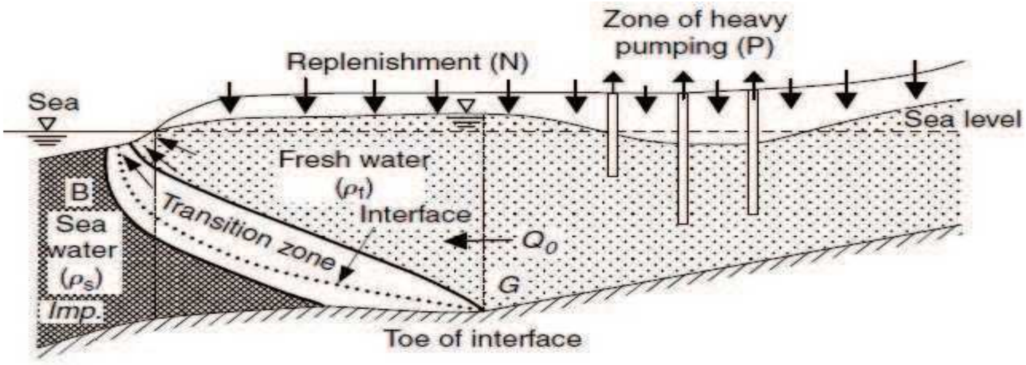


Figure 6. A typical cross section of sea water intrusion in a coastal aquifer. (Bear, I979)

Figure 7a shows a vertical cross section normal to the coast, with a sharp interface separating the two fluids as envisaged by the Ghyben– Herzberg assumption. Essentially, Ghyben and Herzberg assumed that under steady-state conditions, a static equilibrium exists, with stationary sea water and a hydrostatic pressure distribution in the seaward-flowing fresh water. This means that the flow is (essentially) horizontal and the equipotentials (i.e., surfaces of equal piezometric head) are vertical. This, in fact, is identical to the Dupuit assumption of essentially horizontal flow in aquifers.

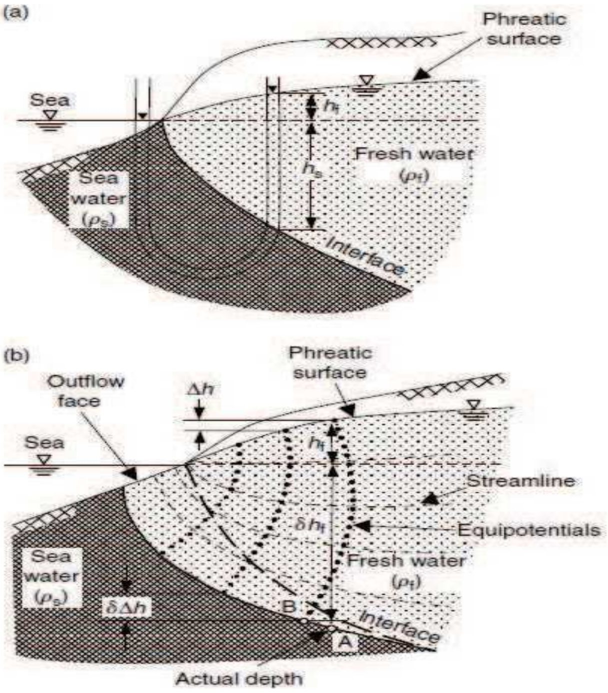


Figure 7. (a) The Ghyben–Herzberg approximation, and (b) the actual sharp interface

In the past, the sharp interface approximation was introduced, primarily, to enable relatively easy solutions, both analytical and numerical, of certain simple sea water intrusion problems of practical interest. However, nowadays, with the availability of new improved numerical techniques, including methods for coping with the nonlinearities that are inherent in the transition zone model, and with fast and large memory computers (even PCs), numerical solutions of 3D models that take the transition zone into account should not pose special difficulties. There is also no reason to limit the models to (vertical) two-dimensional (2D) flow domains. Indeed, a number of models and computer codes that consider sea water intrusion as a solute transport problem have already been developed (Sorek and Pinder, I999). A number of typical sea water intrusion cases solved by the computer code FEAS (Zhou, I999; Bensabat et al., 2000; Bear et al., 200I; Zhou et al., 200I, 2005).

Plenty of information on sea water intrusion into coastal aquifers (e.g., the management problem, modeling with the sharp interface approximation, analytical solutions, modeling as a variable density flow and transport problem, numerical solutions, and discussions on specific numerical codes) can be found in Bear et al. (I999).

As already mentioned in the introduction, in reality, the aquifer domain occupied by only sea water, and the aquifer domain occupied by only fresh water are separated by a transition zone. This is a consequence of the fact that the two “miscible” liquids are, actually, single liquid— water—with different concentrations of dissolved salts. The width of the transition zone is dictated by three phenomena (a) advection of fresh water towards the sea (or, under certain conditions, landward), (b) recirculation of sea water and mixed water, and (c) hydrodynamic dispersion (dispersion and molecular diffusion) in the transition zone. Across it, the salinity of the water varies from that of fresh water to that of sea water. The width of this zone grows as it is being displaced in response to changes in the flow regime and in the discharge of water to the sea. The transition zone is also fed by a flux of salt from the sea water zone.

Figure 8 shows a phreatic coastal aquifer with a transition zone between sea water and fresh water. The considered flow domain is ABCDEMFA. The new features here are that the flow and the solute transport models are coupled as the density of the liquid continuously varying in response to the changes in dissolved salt concentration, and that here we apply these models to the particular case of sea water intrusion in a coastal aquifer.We usually refer to such a model as “variable density flow and transport model.” In what follows, we shall present this model, assuming isothermal conditions. The mathematical model describing sea water intrusion in a coastal aquifer consists of *(a)* mass balance equation for the water, *(b)* flux equation for the water of variable density (Darcy’s law), *(c)* mass balance equation for the dissolved salts, and (d) flux equation for the dissolved salts. The first two equations are often combined as a single flow equation for the water. The last two equations may be combined to form a single mass balance equation for the dissolved salts, often referred to as the advection–dispersion equation, or the transport equation.

In addition, the complete model includes (a) constitutive equations that relate the liquid's density and dynamic viscosity to the total dissolved salt concentration, and (b) initial and boundary conditions (Bear, 1999; Zhou, 1999; Zhou et al., 2005).

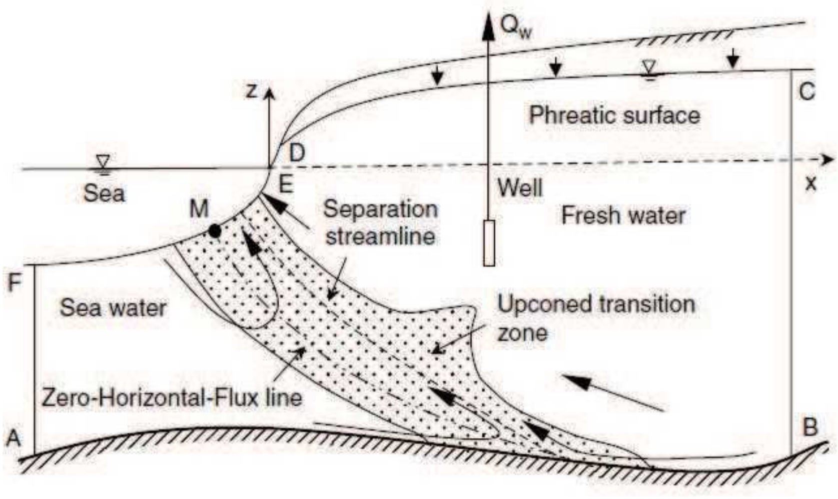


Figure 8. The transition zone with upconing in a simplified vertical cross section of a coastal aquifer, normal to the coast line

Modelling seawater intrusion (SWI) has evolved from a tool for understanding to a water management need. Yet, it remains a challenge. Difficulties arise from the assessment of dispersion coefficients and the complexity of natural systems that results in complicated aquifer geometries and heterogeneity in the hydraulic parameters.

Deterministic modeling considers that the model parameters describing the aquifer system are known and that the response of the system to stresses can be determined through the modeling effort. The most classical deterministic odeling of saltwater intrusion is based on the Ghyben- Herzberg (1901) relation of the position of the (sharp) interface between the fresh and the saline water (Todd, 1980; Bear, 1979). The Ghyben-Herzberg relation ship was conceptualized by assuming hydrostatic balance, immiscible fluids and the existence of a sharp interface between the fresh and the saltwater. Numerical saltwater intrusion models have traditionally been developed for areal- and cross-sectional simulations by assuming this sharp interface-approach between fresh- and saltwater (Todd, 1980; Merritt, 1996; Cheng and Chen, 2001). Mercer et al. (1980) were one of the first authors to present a numerical model that solves the partial differential equations describing the motion of saltwater and freshwater separated by such a sharp interface. Their 2D areal approach was based on the Dupuit approximation.

Voss (1984) developed SUTRA which simulates fluid movement and transport of either energy or solute in a subsurface environment. It employs a two-dimensional hybrid finite-element and integrated-finite-difference method. Essaid (1990) presented a quasi-three-dimensional, finite difference sharp interface model in a multiple-layered coastal aquifer system. Gangopadhyay (1993) modified the SUTRA model to a quasi three-dimensional model to simulate saltwater encroachment in a multiple-aquifer system. A preliminary groundwater flow model was constructed using the SWIP code as modified by Merritt (1994). The model solved groundwater flow equation accounting for fluid density and viscosity dependence on temporal changes of pressure, temperature and solute transport. Putti and Paniconi (1995) applied Picard and Newton linearization for the coupling between the flow and transport equations of saltwater intrusion. Craig et al. (2004) used SUTRA for an idealized evaporating Salt Lake, the results of which are compared with an equivalent laboratory Hele-Shaw cell system. Koch and Zhang (1998) investigated saltwater seepage from coastal brackish canals in Southeast Florida with the SUTRA model. Cheng and Chen (2001) developed a three-dimensional variable density flow and transport model to study saltwater intrusion. Its transport equation is solved by a coupled Eulerian-Lagrangian method. Guo and Langevin (2003) developed the SEAWAT-2000 model to simulate three-dimensional, variable- density, transient ground-water flow in porous media. The source code for SEAWAT-2000 was developed by combining MODFLOW-2000 (Harbaugh et al., 2000) and MT3DMS (Zheng and Wang, 1999) into a single program that either solves the coupled flow and solute-transport equations or uncoupled ones. Voss and Koch (2001) simulated effects of groundwater pumping on saltwater upconing in the state of Brandenburg, Germany, using several 2D and 3D flow and transport models, with and without density effects included. This, in order understands their origins, namely, if they are (1) derived from a major leaching salt dome in the study area or, (2) are just ancient regional formation water. They found that, due to the shallowness of the aquifer system, the surficial topography has a large effect on the flow and migration patterns and, especially, gives rises to upwelling flow underneath the discharge area underneath the major river in the region. Comparing models with and without density effects included, they then investigated possible saltwater upconing due this natural discharge flow pattern. Eventually the accentuated effects of a newly proposed well field on the upconing process were simulated, using both classical non- density-dependent and density-dependent models. Based on these results, their final objective of the investigation was to provide the water agencies with a proper management plan to secure the long-term quality of the extracted groundwater in that part of the country Bakker (2003) adopted the Dupuit approximation for the simulation of three-dimensional regional seawater intrusion, but diffusion and dispersion are not taken into account. The formulation is based on a vertical discretization of the groundwater into zones of either constant density (stratified flow) or continuously varying density (piecewise linear in the vertical direction). During a simulation both the change of the elevations of the surfaces and the change in head are computed through consistent application of continuity of flow; a simple tip and toe tracking algorithm is applied to simulate the horizontal movement of the surfaces. The main advantage is the tremendous reduction of the number of cells needed for a simulation because every aquifer may be represented by a single layer of cells.

The investigation of groundwater resources in the Bangkok area started in I969 by Camp, Dresser and McKee (I970) who reported that chloride concentrations in some wells had increased from I0 ppm in I959 to 600 ppm in I969 and that they were ranging from 500 ppm to thousands of ppm in depths of only about 35 m. Bashir(I978) applied a ID finite-difference (FD) model to investigate saltwater intrusion in the Nakhon Luang aquifer. His results showed that saltwater had intruded into the aquifer from a connate water body located on the western side of Chao Praya River and also from the Gulf of Thailand. Yapa(I979) formulated a 2D FD model and investigated the saltwater intrusion in the Phra Pradang Aquifer and provided an approximate location for the connate water bodies. He further stated that the saltwater contamination may not only be due to seawater intrusion, but also due to vertical leakage of saline water from adjoining aquifers. Gunasekara(I980) developed a saltwater intrusion model by coupling the 2D hydrodynamic and 2D convection-diffusion equations to simulate saltwater movement in the aquifer. The model was calibrated and applied to different pumping scenarios in the Nakhon Luang aquifer to study the response of the aquifer system and the saltwater intrusion. De Mel (I982) formulated a multiple-aquifer solute transport model which takes into account the interaction between aquifers. A multi-aquifer hydrodynamic model is coupled with the solute transport model to study the cause of saltwater intrusion in the Bangkok and Phra-Padang aquifers considering intrusion caused by sea, seepage from Tha-Chin and Chao-Praya River and connate water bodies. The study results showed that the seepage of saltwater from the two rivers is not the only cause of contamination in the aquifers, but the connate water bodies entrapped in both aquifers may also be responsible. Especially, for the Phra-Padang aquifer the seepage of saline water from the overlying Bangkok clay aquifer is found to be significant in areas where the two layers interconnect as evidenced by a detailed geological investigation. Gupta and Yapa (I982) applied both analytical and numerical models for assessing the saltwater intrusion phenomenon in the Phra Pradaeng aquifer. They considered only longitudinal dispersion to assess the contamination sources and used also numerical modeling to identify the sources of contamination and to evaluate the effectiveness of the present water quality monitoring network. From their study they could conclude that saltwater intrusion in the Phra Pradaeng aquifer does not occur only from the sea but also from the infiltration of connate water bodies entrapped in sediments from the time of deposition under marine conditions, leading to a contamination of fresh water supplies. These bodies are to the west and southwest of the Chao Praya River. Either vertical leakage of saltwater from the upper aquifer of brackish-water content occurs, or some wells from which water samples had been collected were improperly grouted. Possibly both of these conditions have prevailed. Sabanathan (I984) developed a computer program which solved the partial differential equation describing the process of solute transport in the groundwater flow and coupled it to the flow model. This model was applied to the Bangkok, Phra-Pradaeng and Nakhon Luang aquifers and the results showed that the main sources of saltwater intrusion into these aquifers are the connate water body entrapped in the western side of Chao Praya river and the vertical leakage of salt water from the Chao Praya itself, especially in places where the aquifers are vertically interconnected. Furthermore, this connate water body had a very high concentration in the southwest corner of the model area. This may be because of its location closer to the sea where horizontal seawater intrusion becomes more influential. Buapeng (I985) reviewed the previous studies and the observed data in the Bangkok aquifer system. According to these publications he concludes that the groundwater is mainly withdrawn from the Phra Pradaeng, Nakhon Luang and Nonthaburi aquifers. The water levels have dropped around 50- 5Im below the ground surface in the Nakhon Luang aquifer, 34-35 m in the Phra Pradaeng aquifer and 50-5Im in the Nonthaburi aquifer. In the Bangkok aquifer, water was found to be salty with a chloride content ranging from 500 mg/l to several thousands' mg/l throughout most of the area. The Nakhon Luang and Nonthaburi aquifers contained freshwater in the east bank of the Chao Praya river and in the extreme westerly parts of the multiple-aquifer system. Salty water has been found almost all along the north-south direction of the western bank of the Chao Praya river. From the observations and the interpretation of the hydrochemistry of the water it was deduced that actual sea water intrusion occurs only in areas near the shore, whereas connate water entrapped under marine conditions after the time of their deposition is the predominant contaminating source of the fresh groundwater supply. Gupta (I986) applied analytical and numerical modeling procedures to simulate hydrodynamic dispersion and analyzed the saltwater contamination in the Nakhon Luang aquifer. A preliminary evaluation of the approximate locations of the contaminating sources was performed by simulating one-dimensional transport along selected streamlines. The study showed that (I) the connate water bodies were the predominant source of contamination; (2) the contaminating sources are widespread and located on the western side of the Chao Praya River and, (3) with the current pumping rates, the highest rate of intrusion is from the northwest direction towards the main pumping center. The author recommended further studies to investigate the possibility of contamination due to vertical leakage of saltwater from the Bangkok aquifer through the abandoned deep wells. Gangopadhyay (I993) modified the SUTRA to a quasi-three-dimensional model and then applied it to simulate groundwater flow and chloride movement in the Phra Pradaeng and Nakhon Luang aquifers. His study results revealed that in both aquifers the predominant saltwater front invades from the west, south-west, and north-west toward the central Bangkok region where the maximum pumped zones are located. Also, the critical regions can be identified to be in the south-west, south- east and north of the Chao Phraya River, namely, Samut Sakorn province, Samut Prakarn province and the western part of Prathumtani province. Kokusai Kogyo (1995) has performed the most comprehensive study up to date. They investigated groundwater flow, land subsidence and saltwater intrusion in the Bangkok area and its vicinity, in order to establish a groundwater management system and to set up scenarios to mitigate land subsidence and saline water intrusion in the study area. The results of this exhaustive study revealed that, (1) according to a well inventory database, the total groundwater extraction rate in the Bangkok aquifers system amounts to around 1.5 million m3/day, (2) piezometric heads in the Phra Pradaeng, Nakhon Luang and Nonthaburi aquifers have declined from 30 m to 60 m below MSL in Pathum Thani, Samut Sakhon and from eastern Bangkok to Samut Prakarn, (3) land subsidence occurred at a rate of more than 20 mm/year underneath Bangkok metropolis, Samut Prakarn, Samut Sakhon, and the central part of Pathum Thani and parts of Nonthaburi and, (4) high chloride concentrations exist underneath the areas from Samut Sakhon to Pathum Thani along the western side of Chao Praya River and in the coastal rea of Samut Prakarn. In some areas of the Phra Pradaeng aquifer these saline concentrations are over 5,000 mg/L, between 3,000 to 16,000 mg/L in the Nakhon Luang aquifer and between 2,400 to 13,000 mg/L in the Nonthaburi aquifer. Chaowiwat (1999) used a coupled version of the MODFLOW and MT3D program to simulate groundwater flow and saltwater intrusion in the Nonthaburi aquifer. The study results revealed that the total salt mass transport in the Nonthaburi aquifer is due to seawater intrusion for as much as 84%, and by vertical leakage from the Nakhon Luang aquifer by only 16 %. The author recommended that a further study should investigate the possibility of artificial groundwater recharge along the coast of gulf of Thailand to remedy seawater intrusion which, as stated, is one of the major objectives of the present Ph.D. thesis.

Density effects on solute transport Experimental effects of the impacts of density dependence on the migration of a contaminated plume have been discovered by Paschke and Hoopes (1984) who investigated the leaching of a sodium chloride plume of very high concentration in a sand tank model. Schincariol and Schwartz (1990) investigated the mixing of a variable density plume in a porous medium, Hayworth et al. (1991), show significant vertical plume movements for already relatively low concentrations.

The observed plume delineations of these experiments also disclosed several significant features of hydrodynamic instability and viscous fingering phenomena in a porous medium. Koch (1992) investigated numerically interface instabilities for unfavorable density contrasts between (a) two superposed immobile layers and (b) at boundaries of advected solute plume which is of some environmental interest. The numerical results showed, at least qualitatively, agreement with some of the predictions of a theoretical scaling analysis and with experiments. He disclosed that the onset and evolution of these interface instabilities is mostly affected by the competition of the unfavorable density contrast (destabilizing) and the hydrodynamic dispersion (destabilizing). The latter and here especially the transversal dispersion governs morphology and growth of the finger regime in a non-deterministic way. The author indicated, additionally, that the problem of interface instabilities has to be treated as a classical nonlinear dynamical system. Koch and Zhang (1992) illustrated that the migration of a miscible solute phase is not only due to forced advection by hydraulic gradients and to dispersion, but is also driven by free convective motions due to the density differences. Whether density effects are important or not depends on a variety of hydraulic parameters of the aquifer model. Furthermore, they found that the combined influence of the various model parameters above can be very different, depending on whether the plume is still near the source or has already extended into the region far away from it. In some cases, variable density might have an effect on the plume migration for even moderate density contrasts of ~ 0.3% (which corresponds to a concentration of ~ 2160 mg/l NaCl). Again, hydrodynamic dispersion tends to reduce the density effects.

Koch (1993) investigated numerically the dynamics of viscous fingering arising at a miscible interface in a unstably density-stratified fluid in porous media. The study results unveiled that the onset, evolution and morphology of the instability are mostly affected by the dispersivity of the porous medium. The analysis of S-curves of the vertical plume movement demonstrated that the onset of instability is mainly governed by the longitudinal dispersion, whereas transversal dispersion is more responsible for the dynamics of the mature fingers. The finger instabilities show the typical behavior of a nonlinear dynamical system whose response depends essentially on the initial conditions imposed. Koch (1994) extended his earlier study to include stochastic heterogeneity of the porous media. Both a deterministic and a random heterogeneous (stochastic) porous medium are considered. The results of the simulations showed that unlike in a homogeneous porous medium where the evolution and the morphology of finger instabilities are mostly affected by the initial perturbation, for a random medium it is its stochastic realization that determined the fate of the fingers; i.e., the medium has an ordering effect on the finger pattern and fingers are essentially channeled through local sections of reduced hydraulic conductivity. Koch and Zhang (1998) modeled the phenomenon of density-driven vertical saltwater intrusion from a brackish, tidally-affected open sea-canal in southeast Florida with the density-coupled groundwater flow and transport model SUTRA.

Their results showed that brackish canal water intrusion depends on the adjacent groundwater table elevation: lowering the latter during a dry season may trigger the seepage process which then becomes essentially irreversible. Moreover, the authors reveal a significant influence of the short-term tidal fluctuations on the long-term dispersion of the vertical saltwater plume in the aquifer. Then possible mitigation plans were simulated which show that a minimum of threshold water level must be maintained in the well field during dry seasons. However, raising the water table can not be achieved by artificial injection of reclaimed wastewater, but may be succeeded by placing a freshwater canal along the brackish tidal canal. Voss and Koch (2001) modeled the effects of groundwater pumping on saltwater upconing in the state of Brandenburg, Germany, using several 2D flow and transport models, with and without density effects included. A sensitivity study of the hydrodynamic dispersion and of the hydraulic anisotropy of the aquifer was carried out. The model results revealed that density effects are diminishing for large values of the dispersivity and high anisotropy ratios. Koch and Starke (2001; 2002; 2003; 2006) investigated the macro-dispersion in density- dependent transport in a heterogeneous medium by both experiments and numerical modeling. Their results showed that both experiments and numerical models exhibit for the same density contrast a larger sinking of the mixing layer with decreasing inflow velocity and, at the same time, an apparent increase of the lateral dispersion coefficient DT.

All of these studies above do, indeed, indicate that density effects on solute transport are, in principal not to be dismissed. Even so, as density-dependent flow and transport modeling poses, at least in many practical applications, a tremendous burden on the computational resources available, the question still remains as for their indispensable need in the every-day modeling of groundwater quantity and quality in a particular real aquifer situation, i.e. to forgo exact representation of the physical system dynamics for computational expediency. The present thesis will attempt to provide some further arguments in this debate.

MODELING GROUNDWATER FLOW AND POLLUTION

The French engineerHenry Darcy (Figure 9) performed experiments on the filtration of water through sand columns. His finding that the rate of flow through a sand column is proportional to the loss of head appeared in an appendix to his treatise on the public fountains of the city of Dijon (Darcy, 1856). Henry Philibert Gaspard Darcy (1803–1858) was a mechanical and hydraulic engineer who was, among others, concerned with water-supply systems. His treatise on the successful design and construction of Dijon's public water supply, published in 1856, contains the results of his famous experiments on ground water percolation through sand filters. From this study he derived his well-known linear law of groundwater flux and hydraulic gradient, which became the foundation of quantitative groundwater hydrology. This law of groundwater flow through porous media shows similarity with the Hagen–Poisseuille equation for laminar viscous flow through small-diameter pipes, developed earlier by the French physician Jean Louis Poisseuille (1799–1869) and the German hydraulic engineer Gotthilf Heinrich Ludwig Hagen (1797–1884). Darcy, who had a sound theoretical background, was certainly aware of this analogy (Biswas, 1970). Other important contributions to water science at the beginning of the 19th century were discovery of the composition of the water molecule, $H2O$, by J ns Jacob Berzelius (1779–1848), and the fundamental law of evaporation by diffusive and turbulent transport of vapor, formulated in 1804 by the founder of atomic chemistry, John Dalton (1766–1844).

Figure 9 Henry Philibert Gaspard Darcy (1803–1858). Portrait by Perrodin, Collection of the Bibliothèque Municipale de Dijon.

A quantitative approach to groundwater hydrology began with the previously mentioned work of the French engineer Henry Darcy (Figure 9). In the framework of his ingenious work for the Dijon central drinking water supply system, he carried out percolation experiments using purification filters as depicted in Figure 10. From these investigations, he derived his well-known law for the linear relation between hydraulic gradient and groundwater flux, which he published as an appendix to his monumental treatise on the water-supply scheme (Darcy, 1856). This work not only revealed Darcy's technical skills, but also accounted for his thorough understanding of the role of topography and geology for the groundwater conditions and their meaning for his water-supply scheme (Brown et al., 2003). The French engineerHenry Darcy performed experiments on the filtration of water through sand columns. His finding that the rate of flow through a sand column is proportional to the loss of head appeared in an appendix to his treatise on the public fountains of the city of Dijon (Darcy, 1856). Figure 11 shows the original set up utilized by Darcy and Figure 12 shows some of his experimental results as plotted by Hubbert (1956) from Darcy's data. Darcy's law states that the volumetric flow rate, Q [L3T–1], across a gross area A of a formation with a hydraulic conductivity K [LT^{-1}], under a hydraulic gradient i = –&h/&s in the s direction is given by

$$Q = qA = -kA\frac{\partial h}{\partial s} = KAi = \frac{k\rho g}{\mu}Ai \qquad (1)$$

where q is a conceptual velocity called the specific discharge or flow rate per uni t area [LT–I] also known as the Darcy velocity, µ is the dynamic viscosity, and k is the intrinsic permeability. The hydraulic head, h, is the sum of the elevation head z and the pressure head p/γw. The minus sign in Equation (I) indicates that the flow takes place from high to low head, namely in the direction of decreasing head. The pore velocity i s given by v = q/ne, where ne is the effective porosity, namely the porosity available for the fluid flow, and v is the average flow velocity in the pores, usually called the seepage velocity.

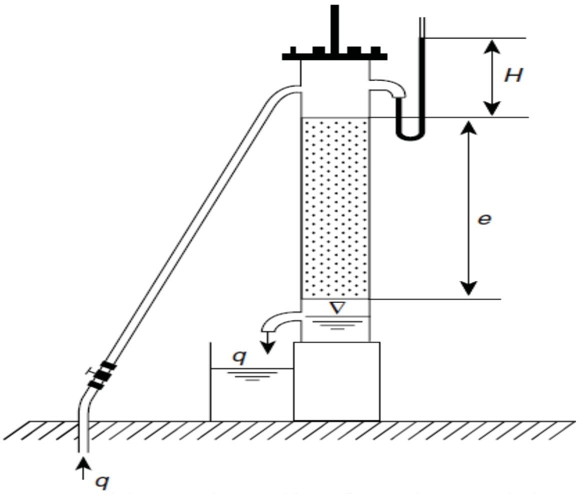


Figure 10 Principle of Darcy's percolation experiment with outflow under atmospheric (=zero) pressure. The results are formulated for the case that the lower boundary of the column is chosen as reference elevation level, so that elevation head and pressure head are both zero at the outflow surface.

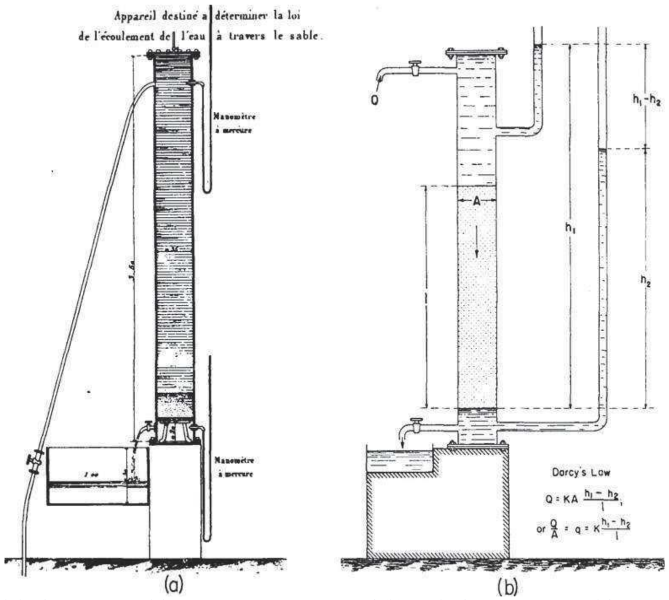


Figure 11 (a) Darcy's original apparatus with mercury manometer and (b) equivalent apparatus with water manometers. (Hubbert, I953).

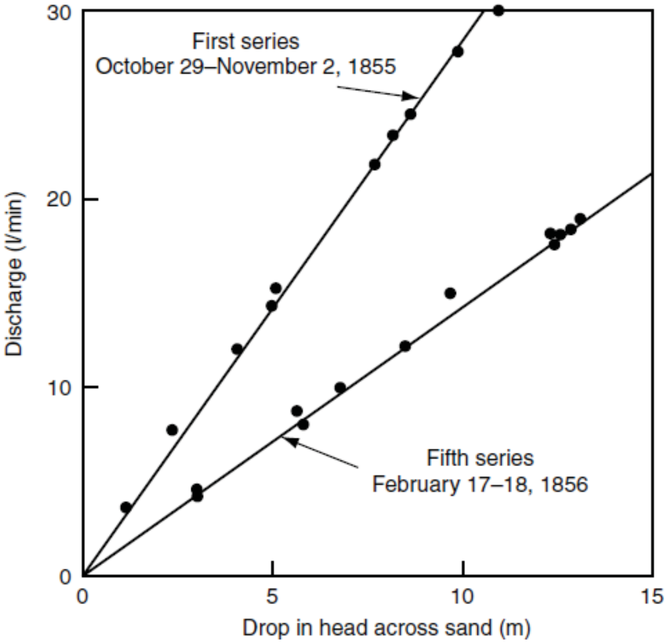


Figure 12 Darcy's data plotted by Hubbert. (Hubbert, I956.)

A groundwater model is a representation of reality and, if properly constructed, it can be a valuable predictive tool used for management of groundwater resource. A mathematical model simulates groundwater flow indirectly by means of governing equation that represents the physical processes that occur in the system, together with equations that describe heads or flows along the boundaries of the model. For time-dependent problems, an equation describing the initial distribution of heads in the system is also needed. Differential equations that govern the flow of groundwater flow can essentially represent the groundwater flow system derived from the basic principles of groundwater flow hydraulics.

The three dimensional movement of groundwater of constant density through porous earth media may be described by the partial – differential equation (MODFLOW, McDonald and Harbaugh, I988): The main flow equation for saturated groundwater flow is derived by combining a water balance equation with Darcy's law, which leads to a general form of the 3-D groundwater flow governing equation:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-w=S_S\frac{\partial h}{\partial t} \tag{2}$$

Where
Kxx, Kyy and Kzz are values of hydraulic conductivity along the x, y and z coordinate axes (LT-I),
h is the potentiometric head (L),
w a volumetric flux per unit volume and represents sources and/or sinks of water (T-I),
Ss is the specific storage coefficient of the porous media (L-I)
t is the time (T).

Under steady state conditions, Eq. (2) is equal to zero as continuity requires that the amount of water flowing into a representative elemental volume is equal to the amount flowing out, this leads to Eq. (3)

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)+w=0 \tag{3}$$

In transient conditions the general flow equation is formulated by applying the law of conservation of mass over an elemental volume of an aquifer situated in the flow field in function of time. Continuity requires that the net inflow into the elemental control volume must be equal to the rate at which water is accumulating within the volume under investigation, which is outflow minus inflow equals change in storage. The change in storage is represented by the specific storage, or specific storage coefficient, Ss, which is defined asthe volume of water released from storage pervolume of soil for a unit decline in hydraulic head. The flow of groundwater is taken to be governed by Darcy's law, which states that the velocity of the flow is directly proportional to the hydraulic gradient. A similar statement in an electrical system is Ohm's law andin a thermal system, Fourier's law. The grandfather of all such relations is Newton's law of motion. Table I presents some other points of similarity. Prior to I856, the formidable nature of the flow through porous media defied rational analysis. In that year, Henry Darcy publisheda simple relation basedon his experiments on the flow of water in vertical sandfilt ers in Les Fontaines Publiques de la Ville de Dijon, namely.

$$v = ki = -k\frac{dh}{ds} \qquad (4)$$

Table I Some Similarities of Flow Models

Form of Energy	Name of Law	Quantity	Storage	Resistance
Electrical	Ohm's law	Current (voltage)	Capacitor	Resistor
Mechanical	Newton's law	Force (velocity)	Mass	Damper
Thermal	Fourier's law	Heat flow (temperature)	Heat capacity	Heat resistance
Fluid	Darcy's law	Flow rate (pressure)	Liquid storage	Permeability

Equation (4), commonly called Darcy's law, demonstrates a linear dependency between the hydraulic gradient and the discharge velocity v. The discharge velocity, v = nv˙, is the product of the porosity n andthe seepage velocity v˙,v . The coefficient of proportionality k in Equation (4) is called by many names depending on its use; among these are the coefficient of permeability, hydraulic conductivity, and permeability constant. As shown in Equation (4), k has the dimensions of a velocity. It should be carefully noted in this equation that flow is a consequence of differences in total headandnot of pressure gradients. This is demonstratedin Figure I3 where the flow is directedfr om A to B, even though the pressure at point B is greater than that at point A. Defining Q as the total volume of flow per unit time through a cross-sectional area A, Darcy's law takes the form

$$Q = Av = Aki = -Ak\frac{dh}{ds} \qquad (5)$$

Darcy's law offers the single parameter k to account for both the characteristics of the medium

and the fluid. It has been found that k is a function of γw, the unit weight of the fluid, μ, the coefficient of viscosity, and n, the porosity, as given by

$$K = C\frac{\gamma_w n}{\mu} \qquad (6)$$

Where C (dimensionally an area) typifies the structural characteristics of the media independent of the fluid properties. The principal advantage of Equation (6) lies in its use when dealing with more than one fluid or with temperature variations. When employing a single relatively incompressible fluid subjected to small changes in temperature, such as in groundwater and seepage-related problems, it is more convenient to use k as a single parameter. Some typical values for k are given in Table 2.

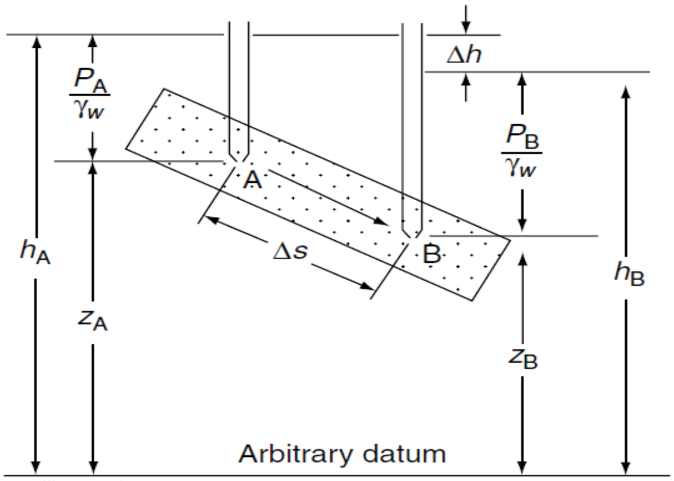


Figure 13. Heads in Bernoulli's equation

Although Darcy's law was obtained initially from considerations of one-dimensional macroscopic flow, its practical utility lies in its generalization into two or three spatial dimensions. Accounting for the directional dependence of the coefficient of permeability, Darcy's law can be generalized to where ks is the coefficient of permeability in the "s" direction, and vs and &h/&s are the components of the velocity and the hydraulic gradient, respectively, in that direction.

Table 2 Some Typical Values of Coefficient of Permeability

Soil type	Coefficient of Permeability k, cm/sec
Clean gravel	1.0 and greater
Clean sand (coarse)	1.0–0.01
Sand (mixtures)	0.01–0.005
Fine sand	0.05–0.001
Silty sand	0.002–0.0001
Silt	0.0005–0.00001
Clay	0.000001 and smaller

In differential form, Darcy.s law is expressed as: q = - K . grad (h)

where q is the groundwater flux (LT-I) K is the conductivity tensor (LT-I) grad (h) is the gradient operator.

This equation clearly shows that the cause of groundwater movement is the difference in the hydraulic potential. The potential is a function of all three space coordinates, that is h = h (x,y,z), the rate of change of head with position giving the gradient, which multiplied by the conductivity yields the groundwater flux. The hydraulic conductivity is represented by a second order tensor that takes into account anisotropic conditions. Usually, anisotropy is only considered in the vertical and horizontal direction, hence.

Where:

$$q_x = -K_x \frac{\partial h}{\partial x} \qquad q_y = -K_y \frac{\partial h}{\partial y} \qquad q_z = -K_z \frac{\partial h}{\partial z}$$

Where qx, qy, qz are the three components of the flux, and Kx, Ky, Kz the hydraulic conductivity values in the horizontal (x,y) and vertical (z) direction. In case of isotropic conditions, Kx = Ky = Kz each component of q is the same scalar multiple K of the corresponding component of -grad (h), such that the vectors q and -grad (h) both point in the same direction.

A spatial discretization of an aquifer system with a mesh of blocks called cells, the locations of which are described in term of rows, columns and layers. An i, j, k indexing system is used. For a system consisting of "nrow" rows, "ncol" column, and "nlay" layers, i is the row index, i = 1,2,....nrow; j is the column index, j = 1,2,. ncol; and k is the layer index, k = 1,2,.. n layer (Figure 14). Finite difference formulation The groundwater flow equation in finite difference form follows from the application of the continuity equation: the sum of all flows into and out of the cell must be equal to the rate of change in storage within the cell. Under the assumption that the density of groundwater is constant, the continuity equation expressing the balance of flow for a cell is

$$\sum Q_i = S_S{}^{\Delta h}\Delta v \tag{3}$$

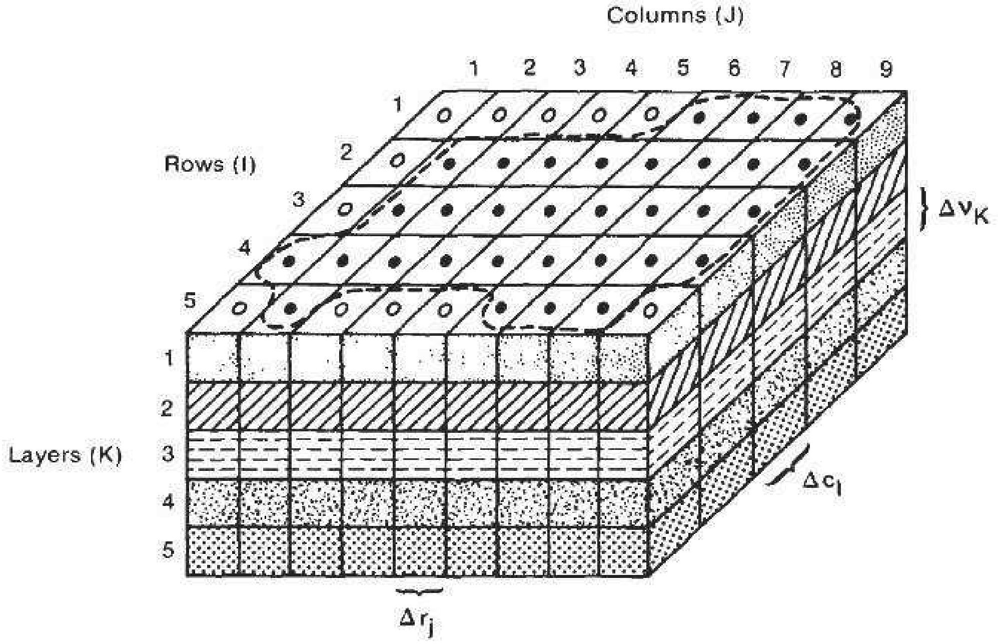


Figure 14. A discretized hypothetical aquifer system; ------- aquifer boundary, • active cell, ..inactive cell, OrJ dimension of cell along the row direction; subscript (J) indicates the number of the column, Ori dimension of cell along the column direction; subscript (I) indicates the number of row, and Ovk dimension of the cell along the vertical direction;subscript (K) indicates the number of the layer.

where Qi is a flow rate into the cell (L3T-I); SS has been introduced as notation for specific storage in the finite difference formulation; its definition is equivalent to that of Ss in equation (3)—i.e., it is the volume of water which can be injected per unit volume of aquifer material per unit change in head (L-I); OV is the volume of the cell (L3); and Oh is the change in head over a time interval of length Ot.

Figure 15 depicts a cell i, j, k and six adjacent aquifer cells, i-I, j, k; i+I, j, k; i,j-I,k; i,j+I,k; i, j, k- I; and i, j, k+I. To simplify the following development, flows are considered positive if they are entering cell i, j, k; and the negative sign usually incorporated in Darcy's law has been dropped from direction from cell i, j-I, k (Figure 5.I6), is given by Darcy's law as

$$q_{i,j-\frac{1}{2},k} = KR_{i,j-\frac{1}{2},k}\Delta c_j \Delta v k \frac{(h_{i,j-1,k} - h_{i,j,k})}{\Delta v_{j-1/2}} \tag{4}$$

where , hi,j,k is the head at node i,j,k and hi,j-I,k that at node i,j-I,k; qi,j-I/2,k is the volumetric fluid discharge through the face between cells i,j,k and i, j-I,k (L3T-I); KRi,j-I/2,k is the hydraulic conductivity along the row between nodes i, j, k and i, j-I, k (LT-I); Oci Ovk is the area of the cell faces normal to the row direction; and Orj-I/2 is the distance between nodes i, j, k and i, j-I, k (L).

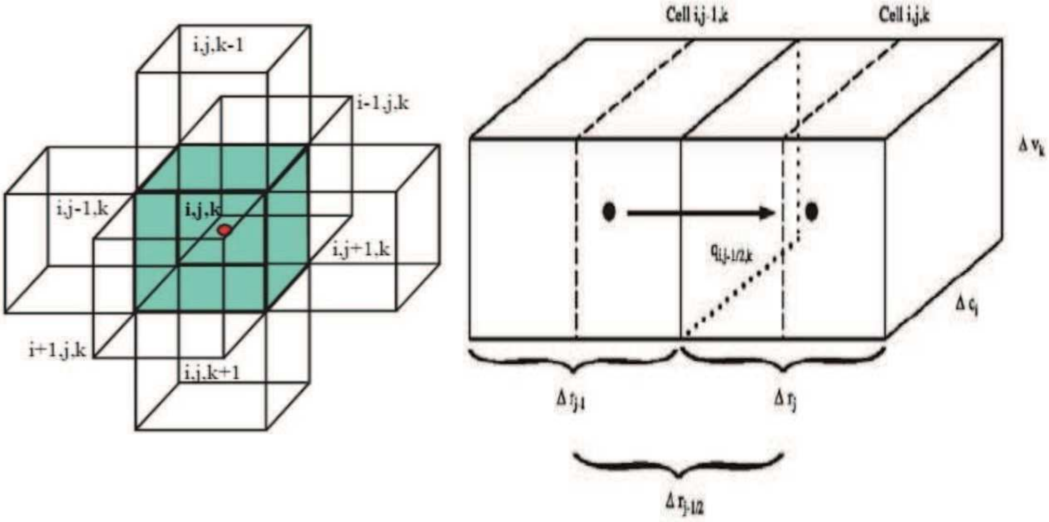


Figure 15. Cell i, j, k and indices for the six adjacent cells.

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