INTRODUCTION TO GROUNDWATER MODELING

Finite Difference and Finite Element Methods

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UNIVERSITY OF WISCONSIN, MADISON

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Preface

Mathematical models of groundwater flow have been used since the late 1800s. A mathematical model consists of a set of differential equations that are known to govern the flow of groundwater. The reliability of predictions from a groundwater model depends on how well the model approximates the field situation. Inevitably, simplifying assumptions must be made in order to construct a model because the field situation is too complex to be simulated exactly. Usually, the assumptions necessary to solve a mathematical model analytically are fairly restrictive—for example, many analytical solutions require that the medium be homogeneous and isotropic. To deal with more realistic situations, it is usually necessary to solve the mathematical model approximately using numerical techniques. Since the 1960s, when high-speed digital computers became widely available, numerical models have been the favored type of model for studying groundwater. The subject of this book is the use of numerical models to simulate groundwater flow and contaminant transport.

This book offers a fundamental and practical introduction to finite difference and finite element techniques. Our goal is to enable readers to solve groundwater flow problems with the digital computer, and every topic is developed with the aim of conveying a full understanding of the steps leading to the short sample computer programs included as part of the text. The programs can be run on any computer with a FORTRAN compiler. (On the University of Wisconsin

Univac 1100, job charges were about 75¢ per program.) Several of the sample problems appear in different forms throughout the text to illustrate various methods and assumptions. Problems at the ends of chapters are designed to reinforce the principles presented in the text.

The book covers five major topics. In Chapter 1, we review some fundamental principles of groundwater flow. In Chapters 2 and 3, we present an introduction to the finite difference method as applied to steady-state problems. Our method is to present selected applications for which numerical solutions are compared with analytical solutions. This method is used to verify the accuracy of the numerical solution. Once we have established confidence in the numerical solution technique, the numerical model can be used to solve problems for which no analytical solutions are available.

In Chapters 4 and 5, the method of finite differences is applied to transient flow problems. Governing equations used in Chapters 1 through 5 are derived as needed. Chapters 6 and 7 contain an introduction to the method of finite elements as applied to steady-state and transient flow problems, respectively. Finally, Chapter 8 contains a discussion of contaminant transport. We derive the advection-dispersion equation, which governs the movement of contaminants through a groundwater system, and we use the finite element method to solve a sample problem.

The subject matter becomes progressively more difficult in the later chapters of the book, and readers should expect to spend more time comprehending material in Chapters 4 and 5 than in Chapters 1 through 3. Likewise, the material in Chapters 6 through 8 is intrinsically more difficult than that in the earlier chapters.

Our book can serve as the first introduction for readers headed towards advanced work in numerical modeling of groundwater systems, or it can serve as a complete course for readers headed towards related areas of water resources who need a basic grasp of modeling concepts. Calculus, physics, FORTRAN programming, and a brief introduction to matrices are necessary prerequisites. The book can be used in a one-semester senior or graduate level course in geology or engineering. It could also supplement more general courses in hydrogeology or fluid mechanics. Professional engineers and geologists who desire an introduction to groundwater modeling should find the book readable and useful, especially if they have access to a computer.

We are especially grateful to Irwin Remson, who critically reviewed several versions of the entire manuscript. John Bredehoeft, Jay Lehr, Debu Majumdar, and Evelyn Roeloffs also made helpful suggestions. Thanks also go to the many students who commented on early versions of the manuscript.

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CHAPTER 1

Introduction

1.1 MODELS

A model is a tool designed to represent a simplified version of reality. Given this broad definition of a model, it is evident that we all use models in our everyday lives. For example, a road map is a way of representing a complex array of roads in a symbolic form so that it is possible to test various routes on the map rather than by trial and error while driving a car. A road map could be considered a kind of model (Lehr, 1979) because it is a way of representing reality in a simplified form. Similarly, groundwater models are also representations of reality and, if properly constructed, can be valuable predictive tools for management of groundwater resources. For example, using a groundwater model, it is possible to test various management schemes and to predict the effects of certain actions. Of course, the validity of the predictions will depend on how well the model approximates field conditions. Good field data are essential when using a model for predictive purposes. However, an attempt to model a system with inadequate field data can also be instructive as it may serve to identify those areas where detailed field data are critical to the success of the model. In this way, a model can help guide data collection activities.

Types of Groundwater Models

Several types of models have been used to study groundwater flow systems. They can be divided into three broad categories (Prickett, 1975): *sand tank models*, *analog models*, including viscous fluid models and electrical models, and *mathematical models*, including analytical and numerical models. A sand tank model consists of a tank filled with an unconsolidated porous medium through which water is induced to flow. A major drawback of sand tank models is the problem of scaling down a field situation to the dimensions of a laboratory model. Phenomena measured at the scale of a sand tank model are often different from conditions observed in the field, and conclusions drawn from such models may need to be qualified when translated to a field situation.

As we shall see later in the book, the flow of groundwater can be described by differential equations derived from basic principles of physics. Other processes, such as the flow of electrical current through a resistive medium or the flow of heat through a solid, also operate under similar physical principles. In other words, these systems are analogous to the groundwater system. The two types of analogs used most frequently in groundwater modeling are viscous fluid analog models and electrical analog models.

Viscous fluid models are known as Hele–Shaw or parallel plate models because a fluid more viscous than water (for example, oil) is made to flow between two closely spaced parallel plates, which may be oriented either vertically or horizontally. Electrical analog models were widely used in the 1950s before high-speed digital computers became available. These models consist of boards wired with electrical networks of resistors and capacitors. They work according to the principle that the flow of groundwater is analogous to the flow of electricity. This analogy is expressed in the mathematical similarity between Darcy's law for groundwater flow and Ohm's law for the flow of electricity. Changes in voltage in an electrical analog model are analogous to changes in groundwater head. A drawback of an electrical analog model is that each one is designed for a unique aquifer system. When a different aquifer is to be studied, an entirely new electrical analog model must be built.

A mathematical model consists of a set of differential equations that are known to govern the flow of groundwater. Mathematical models of groundwater flow have been in use since the late 1800s. The reliability of predictions using a groundwater model depends on how well the model approximates the field situation. Simplifying assumptions must always be made in order to construct a model because the field situations are too complicated to be simulated exactly. Usually the assumptions necessary to solve a mathematical model analytically are fairly restrictive. For example, many analytical solutions require that the medium be homogeneous and isotropic. To deal with more realistic situations, it is usually necessary to solve the mathematical model approximately using numerical techniques. Since the 1960s, when high-speed digital computers became widely available, numerical models have been the favored type of model for studying groundwater. The subject of this book is the use of numerical methods to solve mathematical models that simulate groundwater flow and contaminant transport.

We consider two types of models—finite difference models (Chapters 2 through 5) and finite element models (Chapters 6 through 8). In either case, a system of nodal points is superimposed over the problem domain. For example, consider the problem shown in Figure 1.1. The problem domain consists of an aquifer bounded on one side by a river (Figure 1.1a). The aquifer is recharged areally by precipitation, but there is no horizontal flow out of or into the aquifer except along the river. Two finite difference representations of the problem domain are illustrated in Figures 1.1b and 1.1c, and a finite element representation is shown in Figure 1.1d.

The concept of elements (that is, the subareas delineated by the lines connecting nodal points) is fundamental to the development of equations in the finite element method. Triangular elements are used in Figure 1.1d, but quadrilateral or other elements are also possible. In the finite difference method, nodes may be located inside cells (Figure 1.1b) or at the intersection of grid lines (Figure 1.1c). The finite difference grid shown in Figure 1.1b is said to use block-centered nodes, whereas the grid in Figure 1.1c is said to use mesh-centered nodes. Aquifer properties and head are assumed to be constant within each cell in Figure 1.1b. In Figure 1.1c, nodes are located at the intersections of grid lines, and the area of influence of each node is defined following one of several different conventions. Regardless of the representation, an equation is written in terms of each nodal point because the area surrounding a node is not directly involved in the development of finite difference equations.

The goal of modeling is to predict the value of the unknown variable (for example, groundwater head or concentration of a contaminant) at nodal points. Models are often used to predict the effects of pumping on groundwater levels. For example, consider the aquifer shown in Figure 1.1. In this example, a model could be used to predict the effects of pumping the three wells in the well field on water levels in the four observation wells or to predict the effects of installing additional pumping wells. The model could also be used to determine how much water would be diverted from the river as a result of pumping. However, before a predictive simulation can be made, the model should be calibrated and verified. The process of calibrating and verifying a model is discussed in Chapter 5.

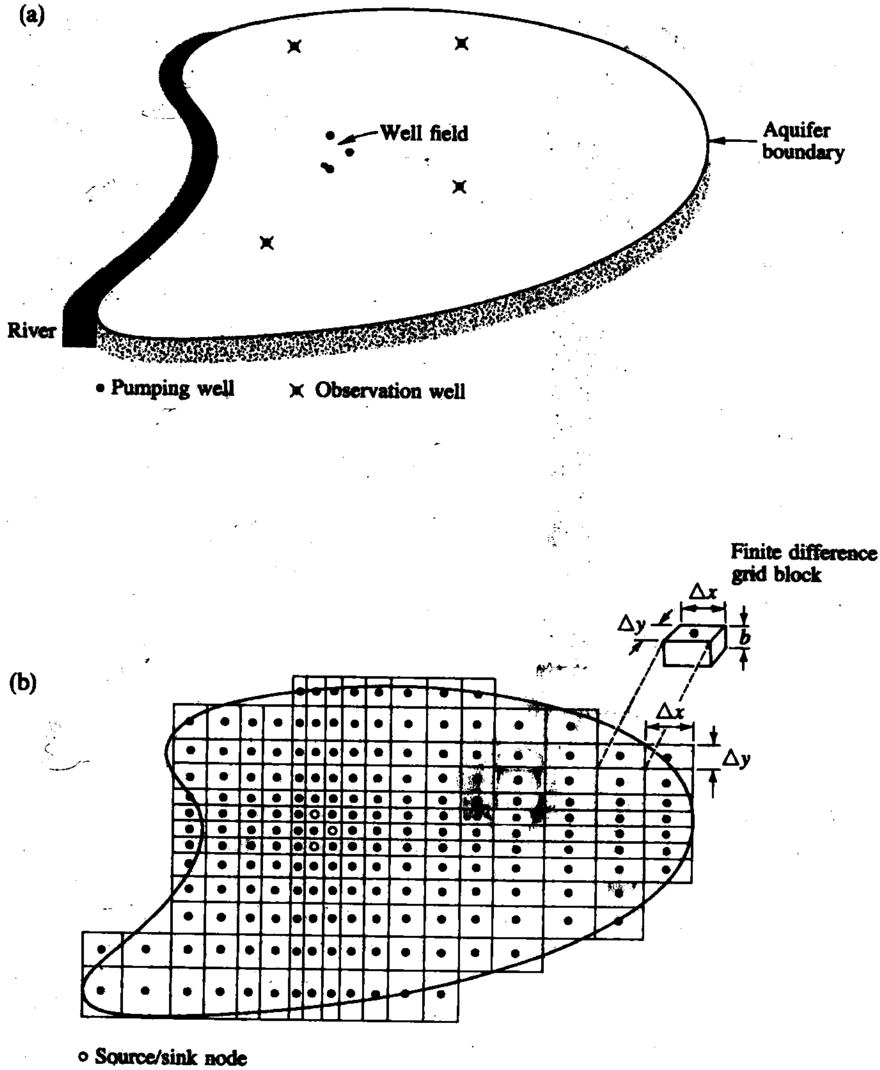
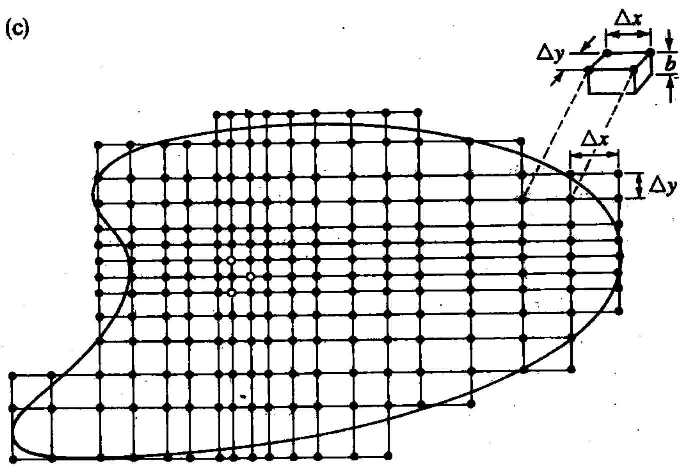


Figure 1.1
Finite difference and finite element representations of an aquifer region.
(a) Map view of aquifer showing well field, observation wells, and boundaries.
(b) Finite difference grid with block-centered nodes, where Δx is the spacing in the x direction, Δy is the spacing in the y direction, and b is the aquifer thickness.

(c)



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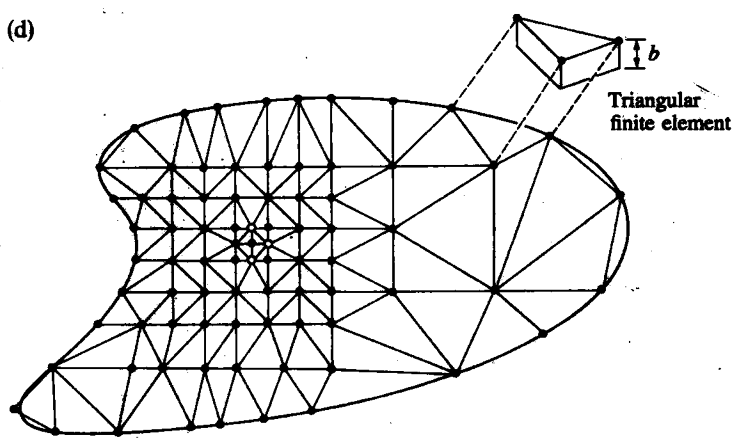
(d)



o Source/sink node

(c) Finite difference grid with mesh-centered nodes.
(d) Finite element mesh with triangular elements where b is the aquifer thickness.
(Adapted from Mercer and Faust, 1980a.)

1.2 PHYSICS OF GROUNDWATER FLOW

Darcy's Law

Darcy set out to find experimentally what factors govern water flow through a sand filter (Figure 1.2). He measured the discharge by timing the rate at which water filled a 1 square meter basin at the outlet, and he measured the head drop across the sand. Darcy defined head to be the height, relative to the elevation of the bottom of the sand, to which water rises in each U-shaped tube. Although Darcy used mercury-filled manometers, he always reported his head data in terms of the equivalent water height. We shall demonstrate that head is proportional to the sum of the pressure potential of the mercury (or any fluid) in the U-shaped tube plus the elevation potential relative to the

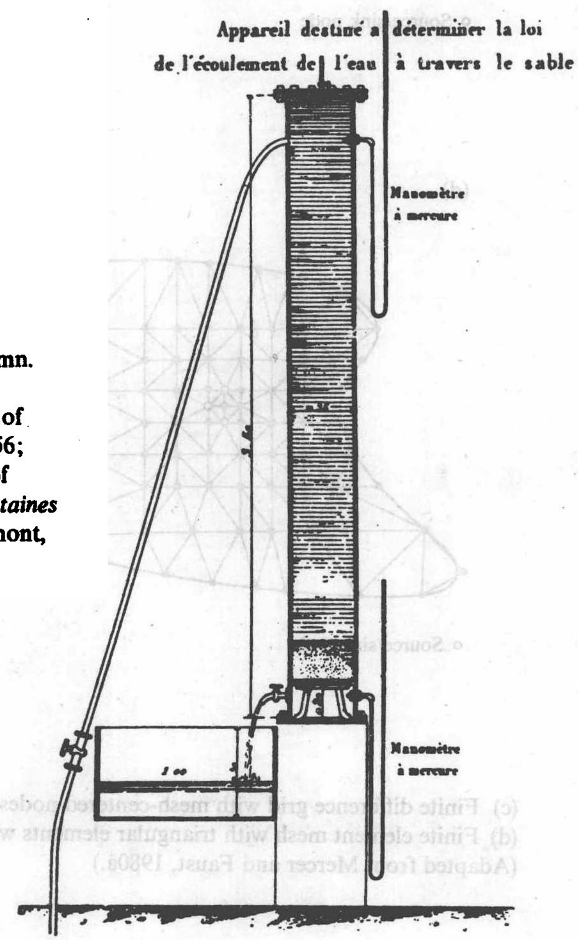


Figure 1.2
Darcy's experimental sand column. (From Hubbert, 1969. © 1956, Society of Petroleum Engineers of AIME, published *JPT*, Oct. 1956; *Trans.* AIME, 1956. Facsimile of Fig. 3 in Darcy, Henry, *Les Fontaines de la Ville de Dijon*, Victor Dalmont, Paris, 1856.)

base level. Applying the term head to the height above sea level of water in a well is the correct field use in Darcy's original sense of the term.

By a series of experiments, Darcy established that, for a given type of sand, the volume discharge rate Q is directly proportional to the head drop $h_2 - h_1$ and to the cross-sectional area A, but it is inversely proportional to the length difference $\ell_2 - \ell_1$. Calling the proportionality constant K the hydraulic conductivity gives Darcy's law:

$$Q = -KA \frac{h_2 - h_1}{\ell_2 - \ell_1} \tag{1.1}$$

The negative sign signifies that groundwater flows in the direction of head loss. Figure 1.3 is a graph showing Darcy's experimental data. It illustrates the linear relationship between discharge rate and head drop for two different sands.

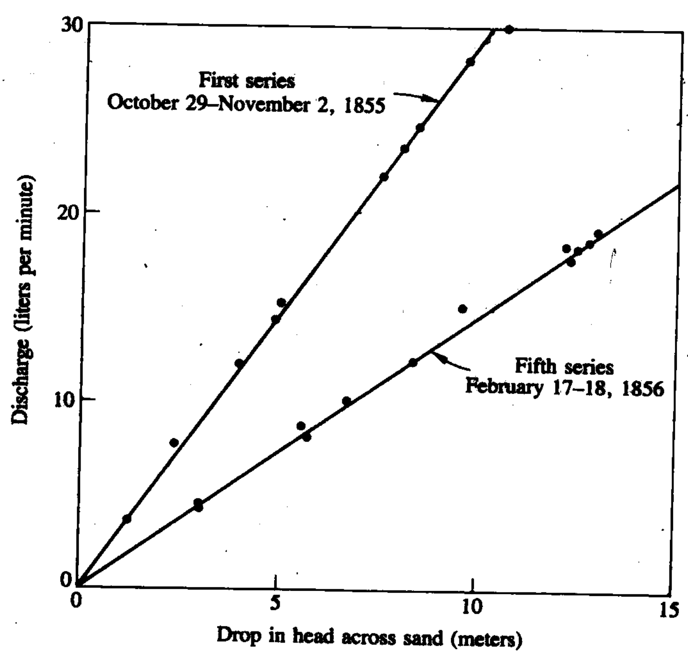


Figure 1.3
Darcy's data showing that discharge is proportional to head drop for two different sands. (From Hubbert, 1969. © 1956, Society of Petroleum Engineers of AIME, published *JPT*, Oct. 1956; *Trans.* AIME, 1956.)

Hubbert's Force Potential

Groundwater flows in response to pressure differences and elevation differences. Numerous persons made the error of equating head to pressure and neglecting elevation. Hubbert (1940) clarifies the concept of groundwater potential and its relationship to Darcy's head by deriving it from basic physical principles. Groundwater potential at a given point is the energy required to transport a unit mass of water from a standard reference state to that point. Differences in potential give rise to groundwater flow; that is, water moves from higher potential to lower potential. The potential is called a force potential because its space derivative has units of force per unit mass.

We now follow Hubbert's derivation of the groundwater potential. Two separate force potentials—pressure and elevation—act on a unit mass of groundwater. Suppose we have a sand-filled tube saturated with water, and the pressure is P at a height z. The potential energy per unit mass of water is defined to be the work required to bring a unit mass of water from a reference position z_{ref} to its actual position z. If we consider the pressure at the reference position to be zero, then the pressure P is in gage pressure, the pressure above atmospheric.

We consider separately the work required to raise the unit mass of water to pressure P and to raise the unit mass to elevation z. The work per unit mass required to raise the water pressure is

$$W = \frac{1}{m}\int_0^P V\,dP \tag{1.2}$$

where m is the water mass and V is the water volume. The volume V is m/ρ_w, where ρ_w is the density of water. If the water is assumed to be incompressible, that is, density is the same at all pressures, then the work per unit mass to raise the water pressure to P is P/ρ_w. The work per unit mass required to raise the fluid to elevation z is $g(z - z_{ref})$, where g is the acceleration of gravity. Therefore, the total groundwater potential is

$$\phi = \frac{P}{\rho_w} + g(z - z_{ref}) \tag{1.3}$$

We have expressed the sought-for potential for groundwater flow in fundamental physical terms. How is the potential ϕ related to Darcy's head h? That is, how do the terms of Equation 1.3 relate to the physically measured quantities in Darcy's experiment? Refer to Figure 1.4. Let the elevation reference datum