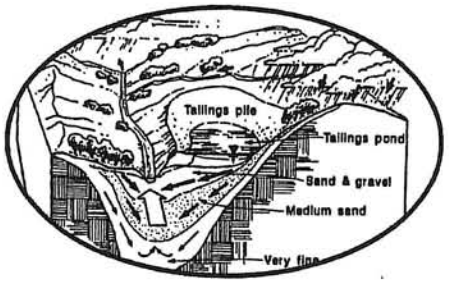
transport conditions. They also help in the understanding of inadequacies in the existing database.

- Numerical models are widely applied to study various specific groundwater problems such as saltwater intrusion, heat transport, land subsidence, displacement of immiscible fluids, or solute transport in fractured rock.
- Once a working model has been prepared it also can be used to support groundwater management decisions such as apportioning liability for contamination, estimating liability based on cleanup costs, and focusing negotiations with regulatory agencies or the public.

Since model predictions may be used to optimize future investigations or operations, it can be argued that the expense of modeling efforts is actually an overall cost saving.

1 Understanding Groundwater Modeling



In most groundwater investigations it is not practical to monitor all aspects of the groundwater flow and solute distribution. Information between and beyond monitoring locations and in the future are needed to understand the site and make informed decisions. Groundwater models, which replicate the processes of interest at the site, can be used to complement monitoring and laboratory bench-scale studies in evaluating and forecasting groundwater flow and transport. However, every reliable model is based on accurate field data.

In designing a groundwater model, the model user combines numerous modeling components. These components, listed in Table 1.1, are:

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

As the table indicates, the term "model" has different meanings. "Groundwater model" usually stands for the combination of all model components, but the term "model" is also used in the context of the various solution methods.

TABLE 1.1 Modeling Components

Component	Key Elements	Examples
Natural System	Geometry	Lateral extent, thickness, source volume
	Dimensionality	One-, two-, three-dimensional
	State	Transient, steady
	Hydrogeology	
	Material properties	Porosity, hydraulic conductivity, dispersivity, storativity, chemical properties
	Observed responses	Water level, concentration
Conceptual Model	Groundwater problem	Extraction, contamination
	Idealized system	
	Relevant units	Aquifer, aquitard, aquiclude
	Boundary and initial conditions	Initial condition
	Controlling processes	Flow, capillarity, gravity, transport, chemical reactions
Mathematical Model	Physical laws	Conservation of mass Conservation of energy Equilibrium of forces Constitutive relationships Material relationships
	Differential equations	Laplace equation
	Boundary conditions	First-kind condition Second-kind condition Third-kind condition
	Initial conditions	Specified head or concentration
Solution	Analytical model	
	Porous media (bench-scale) model	
	Analog model	Viscous fluid model Membrane model Electrical analog model
	Empirical model	
	Mass balance (single-cell) model	
	Numerical model	Finite-difference model Finite-element model Random walk model Method of characteristics Boundary element method
Calibration	Solution versus observation	
	Adjustment of model input data	
Validation	Testing of model predictions versus observations not used in calibration	
Simulations	Parameter sensitivity Predictive simulations Analysis of uncertainty	

Section 1.1 reviews different solutions, or models. The value of the model review lies in fostering the understanding of numerical modeling. Numerical models, being the most versatile approach to complex groundwater systems, have outclassed all other models. Section 1.2 introduces the main phases in numerical model design stipulated by the modeling components.

1.1 REVIEWING GROUNDWATER MODELS

The role of groundwater models in the study of groundwater flow and transport has long been a topic of interest for earth scientists. Among the numerous models developed, we will consider these eight:

- Analytical models
- Porous media models
- Viscous fluid models
- Membrane models
- Electrical analog models
- Empirical models
- Mass balance models
- Numerical models.

Advantages and disadvantages of each model are discussed briefly in the following subsections.

1.1.1 Using Analytical Models

The use of traditional analytical solutions is restricted, due to the rigorous simplification of the real world that is required. Whenever analytical solutions for the investigated groundwater problem exist, however, they are in general more efficient than other model types. The influence of individual parameters can be studied with little effort, and the method is often simple and time efficient. Traditionally analytical solutions were widely used in the analysis of pump tests (Kruseman and de Ridder 1970). Analytical solutions also find wide application in describing two-dimensional steady-state flow in a homogeneous flow system. Model users benefit from the fact that the Laplace equation, the governing flow equation, is the most studied differential equation in mathematics and physics. Solutions derived for problems in other engineering disciplines that follow the same differential equation can be easily adopted for the investigated groundwater problem. This holds true for the analogy between heat and groundwater flow. Numerous helpful analytical solutions addressing heat transport in solids are combined in Carslaw and Jaeger (1959). For solutions of the groundwater flow equation, refer to Polubarinova-Kochina (1952) or Strack (1989).

In transport problems, analytical solutions often become so complex and unwieldy that the advantages of the analytical approach, over a simple numerical solution, shrink. Examples of relatively simple analytical solutions that enjoy broad application are the one-dimensional solution of longitudinal transport of Ogata and Banks (1961) and the one-dimensional solution for transverse spreading of Harleman and Rumer (1963). Other helpful solutions are combined in Bear (1972) and Freeze and Cherry (1979).

1.1.2 Using Porous Media Models

Porous media or bench-scale models belong to the group of hydraulic models widely used in hydraulic engineering. The groundwater system is represented in an appropriate scale in the laboratory with its boundary included, as shown for one-dimensional flow in Figure 1.1. Figure 1.1 also gives examples of the viscous fluid, the membrane, the electrical analog, the mass balance, and the numerical model discussed in the following subsections. In the porous media model, the hydrogeological properties are distributed in space and magnitude according to the natural system. The porous media model is then manipulated and the flow system responses recorded, yielding insight into the behavior of the real system. When studying unconfined groundwater flow, corrections for the capillary rise are necessary, since it is disproportionately large in the model compared to field conditions. Streamlines can be produced by injecting dye.

Similarities between the natural and model system are defined by

Geometry (linear scale ratio L_r):

$$L_r = \frac{L_n}{L_m} \tag{1.1}$$

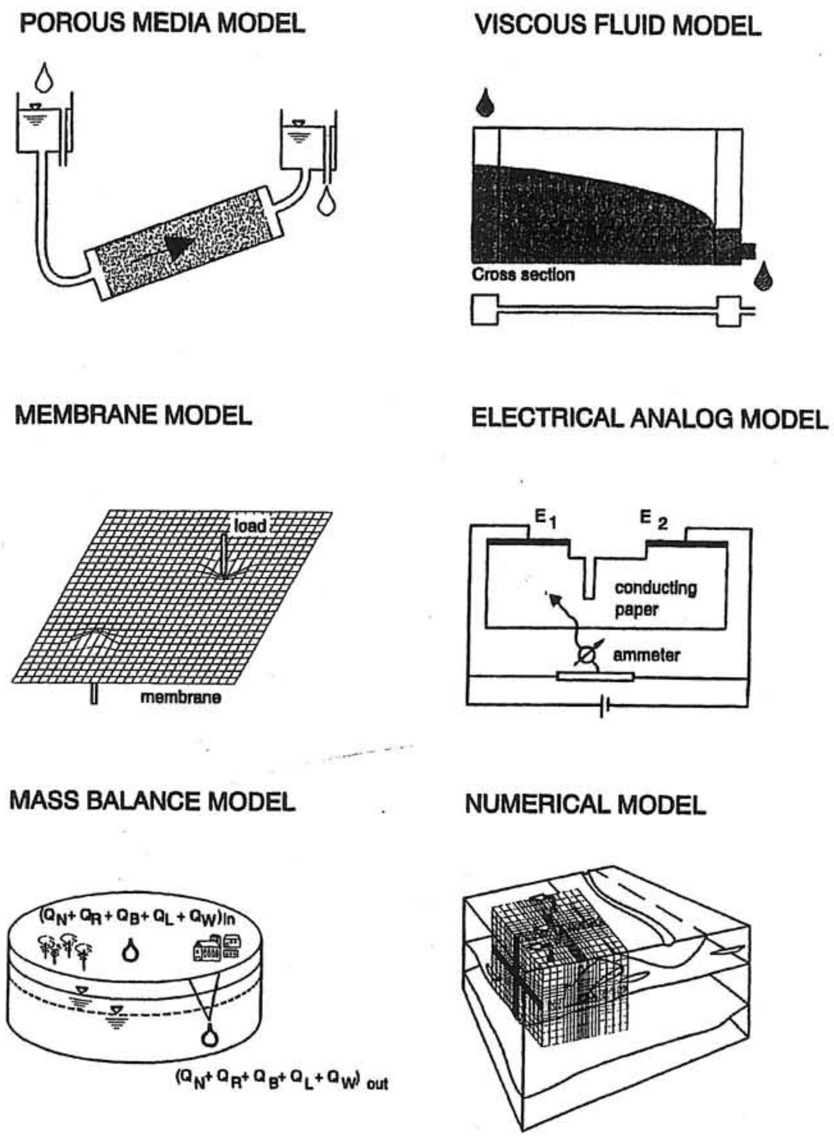


Figure 1.1 Examples of groundwater models.

Area (A_r):

$$A_r = L_r^2 \tag{1.2}$$

Specific discharge (Darcy flux q_r):

$$q_r = K_r i_r \tag{1.3}$$

Total flux (Q_r):

$$Q_r = K_r i_r L_r^2 \tag{1.4}$$

Time (t_r):

$$t_r = \frac{n_e L_r}{K_r i_r} \tag{1.5}$$

where

n = subscript for natural groundwater system
m = subscript for model groundwater system
r = subscript for the nature-model ratio
L = length in [L]
K = hydraulic conductivity in [L/T]
i = hydraulic gradient in [1]
n_e = effective porosity in [1]

The studies of Darcy (1856) can be regarded as the first groundwater model study. Porous media models such as sand models are still used extensively in research. They allow the study of special aspects of groundwater flow and transport under almost natural conditions. Large-scale physical models are used in practical application to evaluate particular flow or transport problems, such as three-dimensional flow toward monitoring wells in complex geological settings or multiphase transport. Otherwise, porous media models are used today only as a demonstration tool for students in teaching. In the study of field problems, porous media models have largely been replaced by numerical models.

1.1.3 Using Viscous Fluid Models

Hele-Shaw or parallel plate models are synonyms for the viscous fluid model. Figure 1.1 shows a Hele-Shaw model in its simplest form. The Hele-Shaw model makes use of the analog of the movement of a viscous fluid, such as

glycerine between two closely spaced parallel plates, and two-dimensional groundwater flow. A similar analogy is Ohm's law in an electrical system and Fourier's law in a thermal system. The most prominent equation of this type is Newton's law of motion. Figure 1.2 presents these and other points of similarity in analog models.

The specific flux q in the viscous fluid model is given by Poiseuille's equation:

$$q_m = -\frac{ga^2}{12\nu_m} i_m \tag{1.6}$$

Equation 1.6 is analogous to Darcy's law (see Section 2.2), describing groundwater flow:

$$q_n = -\frac{\rho_n g}{\mu_n} k i_n = -\frac{g}{\nu_n} k i_n \tag{1.7}$$

where

n = subscript for groundwater system
m = subscript for viscous fluid system

Model Task \ Model Type	Porous Media Model	Numerical Model	Viscous Fluid Model	Electrical Analog Model: Electrolytic	Electrical Analog Model: RC-Network	Membrane Model
DIMENSIONALITY						
two-dimensional	●	●	●	●	●	●
three-dimensional	●	●	○	●	●	○
FLOW PROBLEM						
steady	●	●	●	●	●	●
unsteady	●	●	●	○	●	○
phreatic	●	●	◐	◐	○	○
anisotropy	●	●	●	●	●	●
heterogeneity	●	●	●	●	●	○
variably saturated	●	●	◐	○	○	○
TRANSPORT PROBLEM						
stream-/pathlines	●	●	●	○	○	○
advection	●	●	●	○	○	○
dispersion	●	●	○	○	○	○
sorption	●	●	○	○	○	○
decay/reactions	●	●	○	○	○	○

● Yes ◐ With certain constraints ○ No

Figure 1.2 Applicability of models and analogs (after Bear 1972).

g = acceleration due to gravity in [L/T^2]
ρ = density in [M/L^3]
μ = dynamic viscosity in [M/LT]
ν = kinematic viscosity in [L^2/T]
i = hydraulic gradient in [1]
k = permeability of porous medium in [L^2]
a = distance between plates in [L]

The corresponding scaling factors are

Geometry (linear scale ratio L_r):

$$L_r = \frac{L_n}{L_m} \tag{1.8}$$

Flux (q):

$$q_r = \frac{12k}{\nu_r a^2}\, i_r \tag{1.9}$$

Time (t):

$$t_r = \frac{L_r}{q_r} \tag{1.10}$$

where r represents the subscript for nature-model ratio. Thus the plate spacing and fluid can be selected to correspond to a required permeability.

Although the viscous fluid model can be of a horizontal or vertical type, the latter has found greater application. Hele-Shaw models have been introduced to study flow and seepage through dams, saltwater intrusion, and other phenomena. They have been applied by Schwille (1988) to model groundwater flow and transport in fractured rock. One major advantage of the Hele-Shaw method is that it solves problems concerning the phreatic surface for steady and transient flow situations. The water table can be observed and path lines produced if dye is added to the viscous liquid at discrete points. Permeability represented by viscous plate models is isotropic, but local variation of permeability can be achieved either by varying the width of the interspace or by placing obstructions between the plates. Storage can be simulated by connecting small storage reservoirs to the interspace. Numerical models have decreased the importance of Hele-Shaw models. However, since the method is very illustrative, Hele-Shaw models are still used for demonstration purposes.

1.1.4 Using Membrane Models

Membrane models were used in engineering laboratories before computers were available. A membrane model consists of a mechanism for depressing a membrane covering a frame, and a device to measure deformations precisely. For example, to represent a single well, a nail can be applied to depress the membrane at a discrete point. The strength of the well can be adjusted by pulling in on the nail. For a pumping well the top of the membrane is depressed, while for an injection well the nail is placed beneath the membrane and is pushed upward as shown in Figure 1.1. Sinks and line or area sources can be represented by depressing the membrane by line or area loads. The deformation of the membrane is then directly related to known equations from groundwater hydraulics. V. E. Hansen (1949) describes the analogy of the deformation of the water table due to water extraction from wells and the deflection of thin membranes due to vertical displacement at discrete point. The equation describing the deflection of a thin stretched membrane is

$$\frac{d^2z}{dr^2} + \frac{1}{r}\frac{dz}{dr} = -\frac{W_m}{T_m} \tag{1.11}$$

where

z = elevation of membrane surface in [L]
r = radial distance from the coordinate origin in [L]
W_m = weight of the membrane per unit area in [M/L^2]
T_m = uniform membrane tension in [M/L]

The equation describing steady, axially symmetrical flow in a homogeneous, isotropic groundwater system is

$$\frac{d^2h}{dr^2} + \frac{1}{r}\frac{dh}{dr} = -\frac{N}{Kh} \tag{1.12}$$

where

h = water-table elevation in [L]
N = groundwater recharge per unit area in [L/T]
K = hydraulic conductivity in [L/T]

The analogy is also true for groundwater flow without natural recharge if the weight of the membrane is small. Today the value of membrane models lies more in the illustration of the deflection of the water table in the vicinity of wells rather than in the solution of real field studies. It is, however, an inexpensive tool to use to visualize groundwater stress, helping the inexperienced earth scientist to understand groundwater hydraulics.

1.1.5 Using Electrical Analog Models

Among the analog models, those types based on the analogy between electrical and groundwater flow were very popular before the dominance of numerical models. The electrical conductive medium in which flow is studied can be conducting paper, an electrolytic tank, or a resistance capacitance (RC) network. Conducting paper is a simple tool for simulating two-dimensional groundwater flow. The paper is cut into the form of the groundwater system under investigation. A simple model to simulate groundwater flow underneath a hydraulic structure with a cutoff wall is shown in Figure 1.1. Free edges of the conducting paper represent the impermeable boundaries. Equivalent voltage E is imposed on boundaries with prescribed heads by clamping copper strips with controlled voltage to the relevant edges of the conducting paper. Lines of constant potential drop represent lines of constant heads and can easily be measured. Regions with different hydraulic conductivities are represented by different types of conducting paper or by perforating the paper. In RC networks the groundwater system is represented by electrical elements. Each element represents a specific volume of the groundwater system. The elements are connected at nodes and even complex three-dimensional systems can be reproduced. Voltage measuring devices assess the voltage distribution within the network, which again reflects the head distribution in the simulated groundwater system.

According to Walton (1970) four scale factors show the relation of electrical units associated with the analog model to hydraulic units associated with the groundwater system. These scaling factors are given by Walton (1970) as

$$k_1 = \frac{\text{quantity of water (gallons)}}{\text{resistance (coulombs)}} \tag{1.13}$$

$$k_2 = \frac{\text{potentiometric head (feet)}}{\text{voltage (volts)}} \tag{1.14}$$

$$k_3 = \frac{\text{flux (gallons per day)}}{\text{current (amperes)}} \tag{1.15}$$

$$k_4 = \frac{\text{time}_n\text{ (days)}}{\text{time}_m\text{ (seconds)}} \tag{1.16}$$

with

$$k_1 = k_3 k_4 \tag{1.17}$$

The relation between hydraulic conductivity K and electrical conductivity σ—which is equivalent to the reciprocal of electrical resistance R—can be calculated by substituting Ohm's law and Darcy's law in these four scaling factors. This relationship calculation is written as

$$\sigma = \frac{1}{R} = \frac{k_2}{k_3} K \tag{1.18}$$

For discontinuous electrical analog models (network), the hydraulic conductivity in Equation 1.18 is replaced by the transmissivity of the volume of the groundwater system, represented by electrical resistance in the model.

1.1.6 Using Empirical Models

Also referred to as *lumped parameter models*, empirical models are used to represent physical or chemical processes by generalities, simplifications, or at a scale larger than the process itself. These models fill a useful gap between the simpler analytical models and the more sophisticated numerical models. Empirical models are of two types: models representing individual processes or mechanisms and models representing an entire groundwater problem.

Examples of the first type of model include Darcy's law described in Section 2.2, Fick's law described in Section 3.2.3, and adsorption isotherms described in Section 3.2.4. These empirical models are embedded in analytical and numerical models and impact the accuracy of the model predictions. They are used when detailed site-specific data are lacking, or when it is impractical to simulate fine-scale processes. This type of empirical model indicates a lack of understanding of the processes involved and is a temporary solution to aid analysis.

Empirical models representing an entire groundwater problem invoke a series of physical laws, empirical laws, and conservative assumptions to represent a flowpath of interest. Examples of such models include the organic leachate model (51 Fed. Reg. 21,653, 1986), the landfill analysis model HELP (Schroeder 1994), and the exposure assessment model, MULTIMED (USEPA). These models can be misused or misunderstood because they are easy to use; they are applicable only in limited circumstances, and they mask their limitations by lumping processes together.

1.1.7 Using Mass-Balance Models

The mass-balance model, also known as the black box or single-cell model, is regarded as a numerical model in its simplest form. Mass fluxes, either of groundwater (water balance) or of some constituent (solute balance) are balanced over large volumes as schematically shown in Figure 1.1. For illustration, consider a groundwater basin of horizontal area A, bounded by impermeable boundaries. Groundwater recharge is from natural replenishment N, and groundwater discharge is from pumping wells with a total discharge rate Q. The difference of total N and Q for a given time period causes either an increase or decrease of the average water level in the cell. No variations of groundwater levels within the groundwater system are calculated except the average water level. Due to the simplicity of black box models, evaluation of field data is only concerned with fluxes in and out of the system. Except for storativity, no other feature of the groundwater system needs to be considered. Therefore averaging over the entire area is a crude approximation, especially for solute balances. It means, for example, that as various sources contribute solutes to the groundwater system, complete mixing of the solute within the entire system takes place.

Despite its simplicity, the black box model is useful, since it leads to an examination of the global mass balance. In numerical modeling, single-cell models are best fitted to complement modeling efforts, providing a comparison of mass balances in the early stages of the calculations. Single-cell models are discussed in Chapters 5 and 6.

1.1.8 Using Numerical Models

All groundwater models discussed in the previous subsections are strongly restricted in their scope of application, as shown in Table 1.2 which compares the model tasks and model types. With the exception of the analytical solution methods and possibly the conducting paper models, the discussed groundwater models are not easily applied. For example, constructing an RC network for a given scenario is time-consuming and the hardware model is voluminous. Then comes the tedious simulation of different scenarios that further requires extensive experience in interpreting the results.

The simulation of groundwater flow and transport by numerical models is a relatively recent development dating from the early 1970s. Today numerical models dominate the study of complex groundwater problems. Numerical models basically represent an assembly of many single-cell models. Tremendous advances in computer technology have made them the standard procedure for the solution of groundwater flow and mass transport problems. Computer programs for most common flow and transport problems are available and the model user can apply a relevant computer program to an investigated scenario without writing any computer code. The numerical model solves both simple and complex problems. Theoretically numerical models impose no restrictions on the boundary type, the initial conditions, the characteristics of the groundwater system, or the characteristics of the investigated solute. Once the numerical model is completed, various scenarios can be realized without undue effort. The dominance of the numerical models has led to the use of "groundwater model" as a synonym for numerical groundwater models.

TABLE 1.2 Analogy in Physics

Physical Process	Law		Conservation Law	Quantity	Potential	Proportionality Factor
Groundwater flow	Darcy	$q = -K \nabla h$	$\nabla^2 h = 0$	Darcy flux q	Potentiometric head h	Hydraulic conductivity K
Viscous fluid flow	Poiseuille	$v = -f_r \nabla h$	$\nabla^2 h = 0$	Velocity v	Potentiometric head h	Conductivity of fracture f_r
Electricity flow	Ohm	$I = -\sigma E$	$\nabla^2 E = 0$	Current I	Voltage E	Electrical conductivity σ
Heat flow	Fourier	$Q_\theta = -\lambda \nabla \theta$	$\nabla^2 \theta = 0$	Heat flow Q_θ	Temperature θ	Thermal conductivity λ
Force field	Newton	$f = m \nabla U$	$\nabla^2 U = 0$	Force f	Potential U	Mass m
Diffusion	Fick	$q_0 = -D_0 \nabla c$	$\nabla^2 c = 0$	Diffusive flux q_0	Concentration c	Diffusion coefficient D_0
Incompressible flow of a frictionless fluid		$v = -\nabla \phi$	$\nabla^2 \phi = 0$	Velocity v	Velocity potential ϕ	1

In the following text we will refer to numerical groundwater modeling. The term "groundwater model," is used equivalently to the term "numerical model," which is the combination of the mathematical description, the numerical computer code, and its application to the specific groundwater problem. The same meaning is accepted when we discuss "groundwater modeling."

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

1.2 DESIGNING NUMERICAL MODELS

Alternate numerical theories for solving partial differential equations lead to different types of numerical models, but there are no fundamental differences in the overall model approach to a given problem. The modeling components listed in Table 1.1 result in the following main phases in model design:

- Compiling and interpreting field data.
- Understanding the natural system.
- Conceptualizing the groundwater system.
- Selecting the numerical model.
- Calibrating and validating the model.
- Applying the model.
- Presenting the results.

This section provides some introductory information on each phase in the design of numerical models. Details are discussed in the following chapters.

1.2.1 Compiling and Interpreting Field Data

Field data are essential to understand the natural system, to specify the investigated groundwater problem, to facilitate selection of computer code, and to derive model input data. The computer code of a numerical model is a tool for solving the governing flow or transport equation. It can be used for any model study as long as the flow or transport follows the mathematical model approximated by the computer code. The numerical model actually develops into a site-specific groundwater model when real field parameters are assigned. The accuracy of the modeling results is not primarily a question of the sophistication of numerical code, long calculation time, fine discretization, or large memory requirements. The quality of the simulations depends in large part on

the validity of the model physics and on the quality of the input data. The gigo rule, "garbage in, garbage out," also applies to groundwater modeling.

Generally, field data do not directly provide the parameters required for the model such as transmissivity or groundwater recharge per model segment. Model parameters must be derived from field data. Consider a pumping test. The measured field data are well discharge, time, and drawdown. The calculated model parameters are transmissivity and storage coefficient. In addition the same regional parameters must be assigned to each model segment. The time needed to perform a model study will depend significantly on the time required to collect and prepare the model input data.

It is wrong in many groundwater studies to first evaluate a huge volume of field data and then to design the groundwater model. Due to its strength in combining field data, a groundwater model will help to guide the evaluation of new meaningful data.

1.2.2 Understanding the Natural System

To ensure accurate modeling, the model user should make an effort to gain an appreciation of the natural system. This is the next phase in model design. Distribution of geological parameters and boundary conditions are identified as shown in Figure 1.3. Having a clear definition of the flow or transport problem is important. In only a few investigations will the model user apply a general groundwater model to simulate flow or transport in detail. More often the simplest, most appropriate approach is acceptable, depending on the problem to be solved. Stating the problem properly is often half the battle. Quite often, this will allow the model user to accomplish the analysis of a complex groundwater system with individual solutions for well-defined tasks. These tasks may then be solved independently assuming simplified configurations (two-dimensional instead of three-dimensional, analytical instead of numerical, etc.). Solutions to groundwater problems do not necessarily require the most sophisticated model. In each case the most appropriate model is the one that addresses the investigated problem with as little effort as necessary to represent the real system. The model should be simple enough to facilitate model efforts but not too simple so as to exclude features dominant to the investigated groundwater problem. In summary, the natural system must be well understood to design the best-fitted model in view of needs, cost, and the availability of data to develop and calibrate the model.

1.2.3 Conceptualizing the Natural System

In each model study the natural system is represented by a conceptual model, as shown schematically in Figure 1.3, for which an approximate solution is applied. To design and construct equivalent but simplified conditions, extensive information is required on the natural system. Transferring the real world

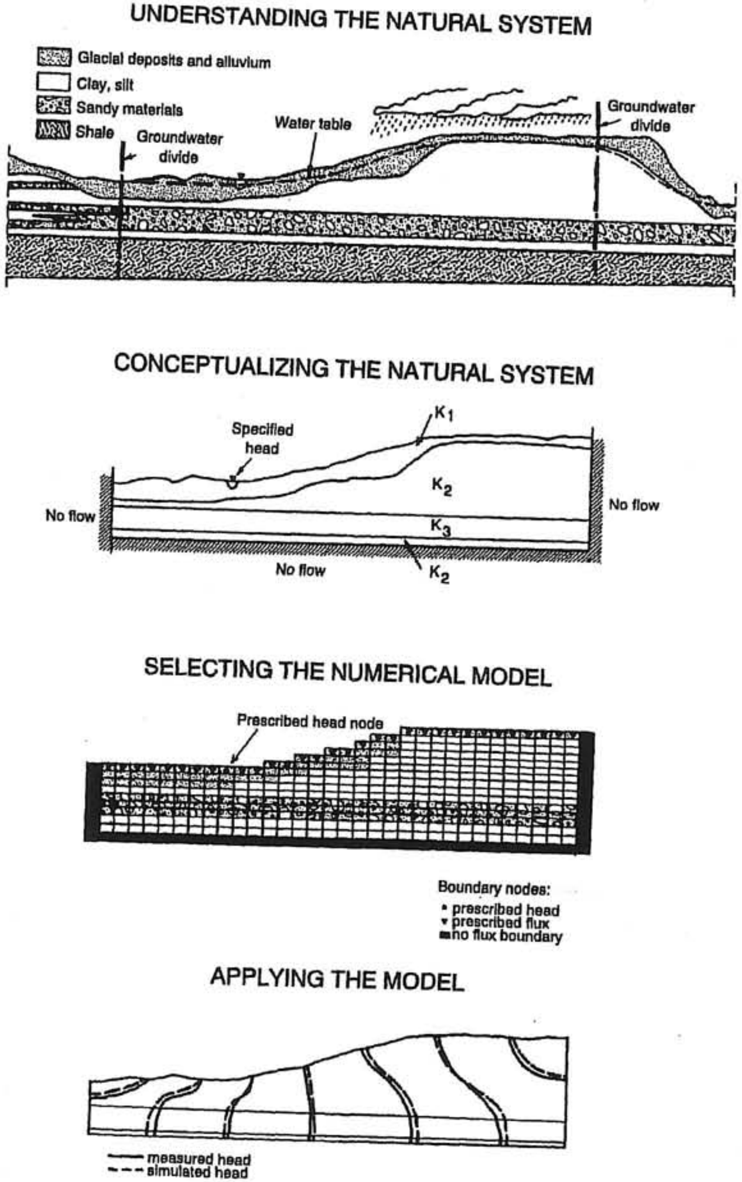


Figure 1.3 Examples of some of the main phases in model design.

into an equivalent model system, which can then be solved using existing program codes, is a crucial step in groundwater modeling. Errors in the conceptual model cannot be corrected during the model calibration or at any later stage of the model study without major revisions.

To illustrate the importance of an appropriate conceptual model, consider a flow problem with significant three-dimensional flow components such as the flow in the vicinity of a partially penetrating well. In approximating the flow field close to the well with a depth-integrated model such as a two-dimensional horizontal model, strong discrepancies between the real and the simulated groundwater flow must be expected.

Problems with approximating reality are magnified in transport modeling. Besides simplifying flow, solute transport processes are reduced to a few transport mechanisms considered dominant. It is the number and complexity of controlling processes in solute transport that generally make transport modeling so difficult in comparison to flow modeling and, in particular, require a sound and solid understanding of the relevant natural transport processes at this stage of modeling. The numerical model is only as good as the underlying assumptions or as the conceptual model allows.

1.2.4 Selecting the Numerical Model

Consider numerical models in the same way as analytical solutions. Both give meaningful results only for well-defined questions. No existing model is applicable to all types of flow and transport problems. Consequently, by this stage of the model study, the model user must decide which computer code to use for the calculation of a particular groundwater problem. Sometimes model users are not aware of what models are available. For sources of groundwater models, see Chapter 9.

Most numerical models are similar in that the investigated area is subdivided into either rectangular or irregular polygonal segments, as shown in Figure 1.3. The handling of the input and output data, which are referred to as pre- and postprocessing, determines if the computer code is "user friendly."

Today all popular and well-tested programs provide results of a similar accuracy for their range of application. Some models like the ones based on the finite element theory have proved to be more versatile. In each model the choice of the discretization of space and time basically controls the computational accuracy.

1.2.5 Calibrating and Validating the Model

Model calibration and validation are required to overcome the lack of input data, but they also accommodate the simplification of the natural system in the model. Calibration and validation will become meaningless, fail, or yield inadequate results if significant features of the natural system are excluded from the model.

In model calibration, simulated values like potentiometric surface or concentrations are compared with field measurements. The model input data are altered, within observed ranges, until the simulated and observed values are fitted within a chosen tolerance. Input data and comparison of simulated and measured values can be altered either manually (trial-and-error adjustment) or automatically (inverse or parameter estimation models). Be prepared to quantitatively assess model calibration. The more convincing the calibration, the more useful will be the model validation. Model calibration is time-consuming and can easily take up half of the time required for the whole study.

Model calibration represents a crucial stage in groundwater modeling. Model calibration tries to demonstrate that the site-specific groundwater model is capable of reproducing observed responses by the natural system. The observed responses of the natural system or the behavior of a particular solute in the subsurface environment may have different causes. The bend of a streamline, for example, may be caused by a change in hydraulic conductivity or by areal discharge or recharge. Relationships are much more complex in transport problems. Decline of concentration may be due to dispersion, decay, or variation of the source strength. To calibrate by trial-and-error adjustment or by inverse models, the model user has to judge, based on the understanding of the investigated problem, if calibrated data represent the natural system. A good fit to historical data based on unrealistic input data is not only wrong but misleading if the same model is applied for predictions.

Model validation has different meaning for different people. A model can sometimes be calibrated to match observed conditions based on arbitrary input parameters. Model validation is required to demonstrate that the model can be reliably used to make predictions. At present, no standard criteria exist on how to demonstrate model accuracy, neither will they be established easily in the near future due to limited data collection in field investigations. A one-time fit of calculated and measured values does not guarantee accuracy. In most model studies there are a large number of adjustable values compared with a small number of field observations. A common practice in validation is the comparison of the model with a data set not used in model calibration. This procedure is more useful when the simulated conditions differ significantly from the one used in calibration. If the calibrated groundwater model does not reproduce accurate results in model validation, model data are recalibrated using both data sets. Then other approaches to validation must be used. Calibration and validation are accomplished if all known and available groundwater scenarios are reproduced by the model without varying the material properties or aquifer characteristics supplied to the model. Model calibration and validation are two of the critical steps that precede model application and are discussed in more detail in Chapter 8.

1.2.6 Applying the Model

Model application is the part of the study in which the numerical model demonstrates its dominance over all other models. Alternative scenarios for a given area may be assessed efficiently. When applying numerical models in a predictive sense, however, limits exist in model application. Predictions of a relative nature are often more useful than those of an absolute nature. The outcome of a numerical model, must be reviewed critically.

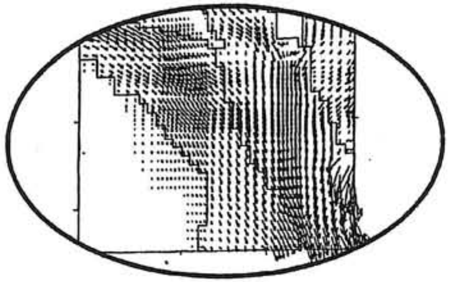
It makes a difference whether model users forecast water levels or concentrations for one week or some years into the future. Predictions into the far future are generally more uncertain. As in statistics, extrapolations into the future are more accurate if they are based on a long-term series of observed events in the past. There is a saying in geology that applies here: "The past is the key to the future." The larger the historical "key," the better is our ability to predict the future. Groundwater models calibrated on field data observed within a couple of weeks are not suitable for predictions over 100 years and more.

Another kind of limitation on predicting responses of a groundwater system exists. Flow or transport conditions during predictive runs may stress system parameters that have been irrelevant for model calibration or validation. Assume that a model calibrated to a steady-state condition is applied for predicting system behavior under unsteady conditions. Specific yield or storativity would not be a concern. Predictions would have to be based on best-guess values, and model results must be reviewed carefully. Thus sensitivity analyses become important. Sensitivity analysis helps to rank the input data in terms of its influence on model predictions and gives answers to "what if" questions. Sensitivity analysis also allows one to assess unforeseeable groundwater stresses in the future. Unknown future landuse may, for example, change natural groundwater recharge.

1.2.7 Presenting the Results

When reviewing modeling results, appreciate the presentation but trust the numbers. The output of numerical models is numbers such as hydraulic heads at discrete points of the solution domain at a given time. Model output normally undergoes postprocessing to produce modeling output that is understandable to nonmodel users. Such effort is necessary but postprocessors are not a substitute for lack of modeling experience. Modern postprocessors such as plot software packages, commercial or in-house codes, are unique tools in presenting modeling results illustratively and informatively. However, there is the chance of misuse or misinterpretation. Professional presentation of output-model data may infer an accuracy that does not exist. Interpolation and extrapolation of data in order to facilitate data interpretation are necessary, but manipulating output data to cover uncertainty in model results should never occur. Graphical interpolation programs actually weaken the accuracy of data presentation. Plots of measured potentiometric surface presented as isolines should include the number and location of observation points used for the interpolation. Section 8.10 is devoted to the topic of presenting modeling results.

2 Reviewing the Mathematical Model for Flow



This chapter deals with the description of groundwater flow. Topics are presented from the model user's view, to create a good understanding for applying groundwater flow models and for grasping solute transport caused by groundwater movement. After introducing subsurface water and porous bodies, emphasis is on the mathematical model for the description of groundwater flow: Darcy's law, the water balance equations, and the definition of suitable hydrogeological boundary conditions. Acknowledging its growing importance in groundwater modeling, multiphase flow is briefly discussed in Section 2.5.

2.1 IDENTIFYING GROUNDWATER AND AQUIFERS

To use models, the several forms of occurrence of water in the subsurface and the various openings in soil and rocks that allow water movement must be understood. The model user must also be able to identify characteristic regions of the groundwater system. The following sections are devoted to these topics:

- Defining water in the subsurface
- Classifying voids in soil and rock
- Identifying hydrologic units and aquifers.

2.1.1 Defining Water in the Subsurface

Subsurface water occurs in the following several forms:

- Mobile water. Water in interconnected pore space. The water is transmitted freely through the pores of rock or soil or, alternatively, through fractures in rocks.
- Immobile water. Crystalline water contained in minerals. Such adsorbed water is referred to as hygroscopic water; it is bound by electrostatic and van der Waal's forces on the grain or water enclosed in disconnected voids.
- Water vapor. Gaseous water distributed in the unsaturated groundwater zone.

The model user is particularly concerned with mobile water. One exception is in transport simulations where immobile water may influence the transport behavior of the solute under investigation due to diffusive mass exchange between the mobile and immobile water zone.

To allow significant horizontal water flow, groundwater must occupy the entire pore space forming one continuous water body called the *saturated zone*. The saturated zone may be bounded from above by the water table which is the interface with the unsaturated zone where water and air fill the pores. The water table is defined as the surface of the zone of saturation. Even though there is no strict relationship, the water table often follows a pattern flatter than the profile of the land surface. If groundwater is restrained in its movement by an impervious layer on the top, the water table in the above sense does not exist. Groundwater movement is confined and is described by defining an imaginary surface called the *potentiometric* surface to which water will rise when tapping the confined or semiconfined groundwater zone.

In the unsaturated zone, gravity is the driving force causing predominantly vertical flow and, consequently, vertical transport. This book primarily focuses on flow and transport in the saturated zone where the model study is not restricted to a vertical profile. The importance of flow and transport in the unsaturated zone in specific groundwater problems is briefly discussed.

2.1.2 Classifying Voids in Soil and Rock

Voids in soil and rock are fundamental hydrologic parameters. The fraction of voids in soil and rock are expressed by porosity and defined as a ratio of void volume to total soil or rock volume. Soil and rock with little void volume have little capacity to hold water. Openings in solids are necessary to allow water movement. The model user classifies voids in soil and rock into the following four groups, as shown in Figure 2.1:

- Matrix porosity. Soils and rocks are granular and yield intergrain pores (gravel, sand, silt, clay, sandstone, etc.). The rock or soil grains themselves may be porous (leading to higher overall porosity), or the aggregate porosity may be reduced by mineral deposition in pores.
- Fractured porosity. Rocks contain joints and fractures, regular or irregular.
- Karstic fractures and solution cavities. Rocks are characterized by distinguishable solution cavities.
- Fracture and matrix porosity (dual porosity). Such formations are porous units of the granular type such as clay or sandstone units, but they also contain fractures.

Figure 2.2 shows the typical range of porosity of various geological formations. Additionally porosity values of different soils and rocks are compiled in Appendix B.1. Even though porosity is essential for groundwater flow, the capacity of soil or rock to transmit water is not only a function of porosity but also a function of void geometry and internal forces (see also Section 2.2.4). For practical purposes the percentage of void volume that contributes to percolation (called *effective porosity*) is equivalent to the specific yield. This yield is the volume of water released from a unit volume of saturated soil or rock material drained by a falling water table of a unit height. Specific yield, or the effective porosity, is always less than the total porosity as indicated in Figure 2.2. For a compilation of values of specific yield see Appendix B.2.

Traditionally groundwater mathematics and numerical models have focused on the description of flow and transport in matrix porosity or in sand and gravel. Frequently the model user investigating a groundwater problem in groundwater systems other than the granular type tries to adopt these solutions established for granular medium flow and transport. This is an assumption that approximates reality with varying degrees of success and should be justified on a case-by-case basis. If model calculation cells contain many well-connected fractures and no large-scale discontinuities, then the assumption of porous-media-like behavior may be justifiable.

2.1.3 Identifying Hydrologic Units

Groundwater modeling represents an approximation of natural features and observations. The groundwater system is not described in detail but as units with similar characteristics. The ability to identify main hydrologic units is essential in the conceptualization of the groundwater system. Hydrologic units fall into the following three groups:

- Aquifer. A permeable unit that can yield water in usable quantities when tapped by a well. Common aquifers are geological units of unconsolidated sand and gravel or fractured rock.

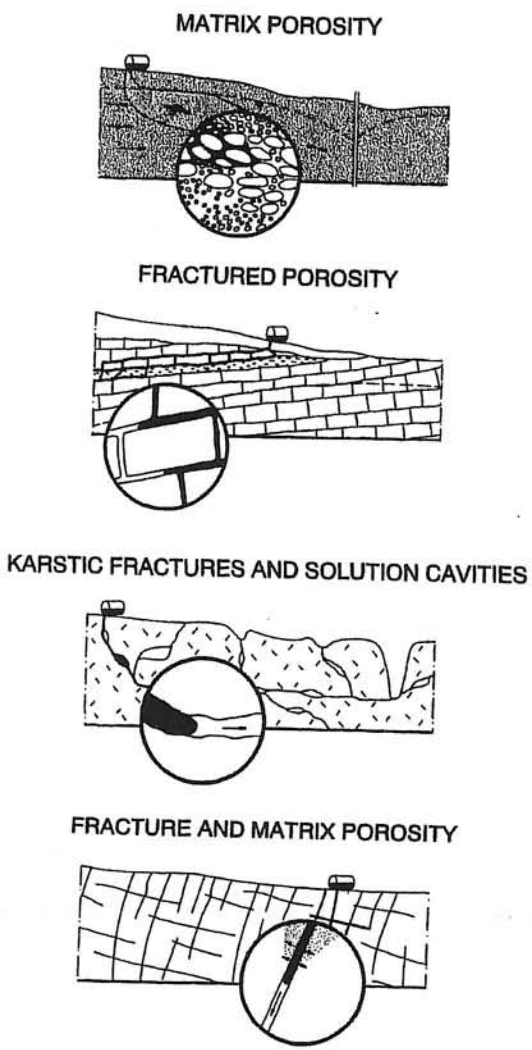


Figure 2.1 Classification of voids in soils and rocks according the type of porosity.

- Aquiclude. A very low permeability unit that will not transmit water freely. In an aquiclude, groundwater flow is often assumed to be zero. Solute transport, however, may not be zero. Common aquicludes are thick clay layers or solid rocks.
- Aquitard. A low permeability unit that falls between aquifers and aquicludes. Water cannot be produced economically through wells, but flow is

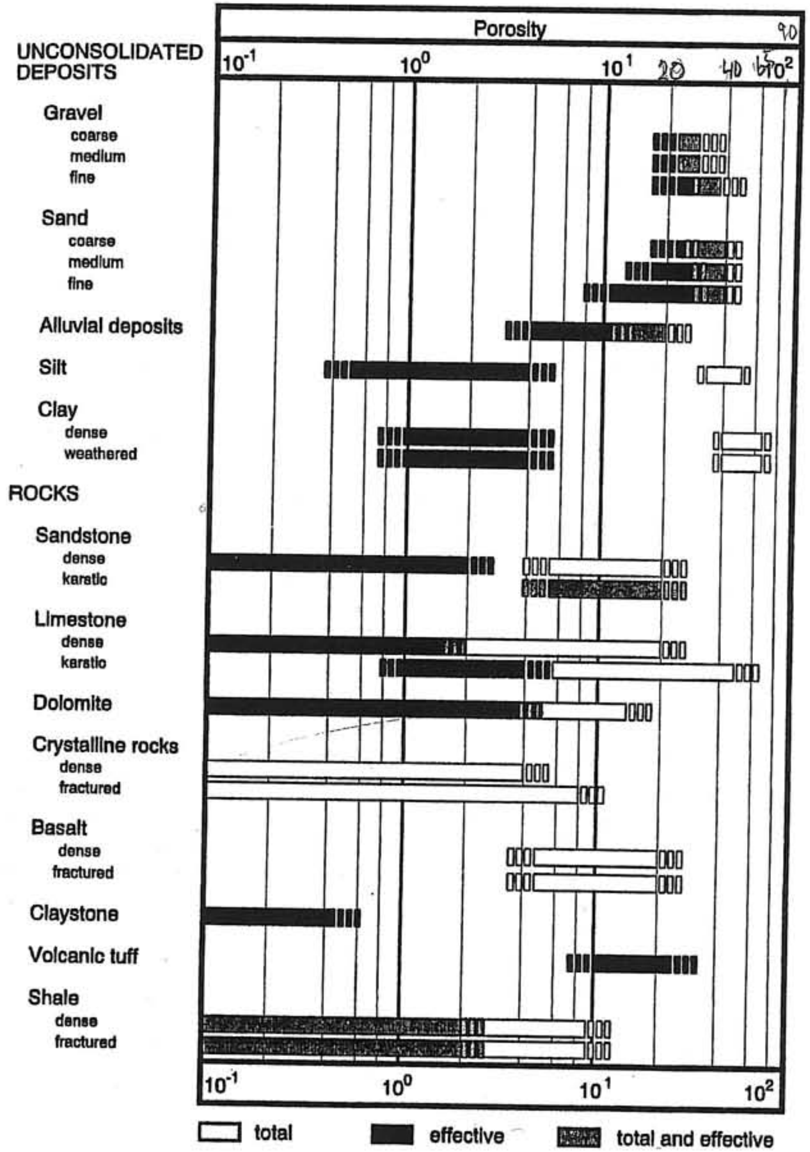


Figure 2.2 Range of porosity of geological formations.

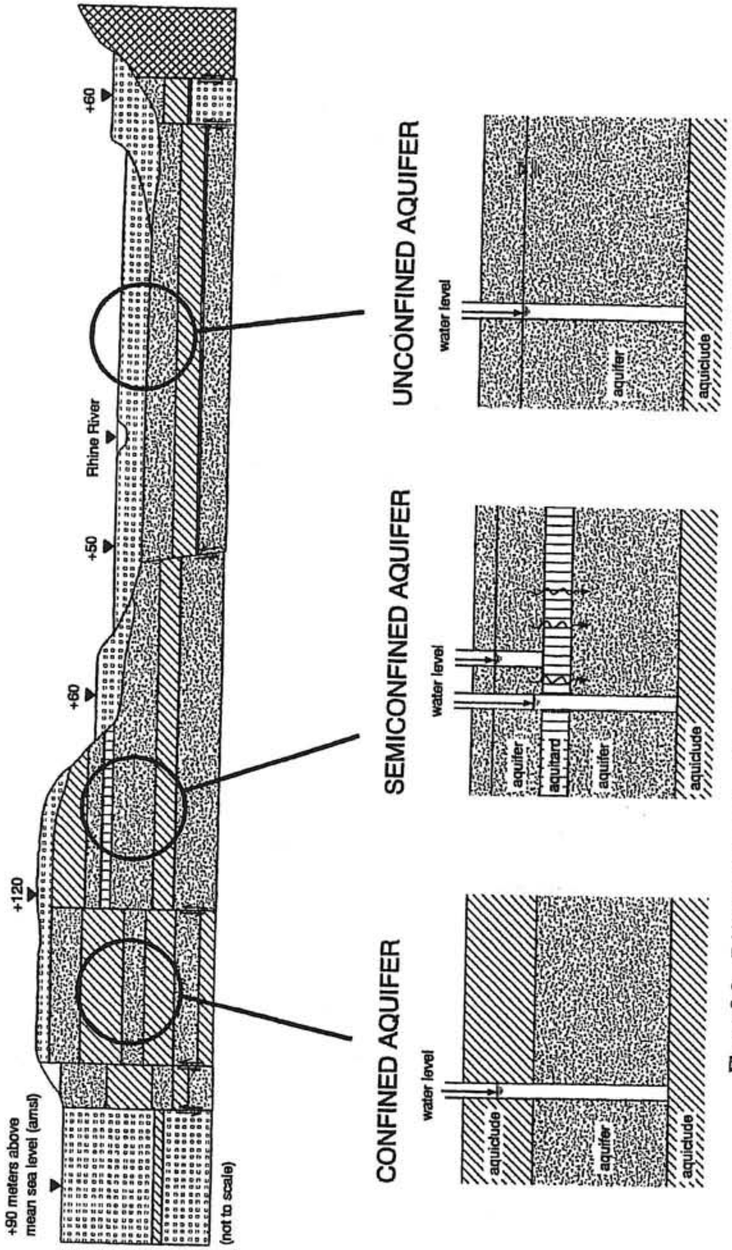


Figure 2.3 Different types of aquifers illustrated on a cross section of the Rhine River Valley at Cologne.

significant enough to feed adjacent aquifers. It is generally assumed that groundwater flow in an aquitard is predominantly vertical. Common aquitards are clay layers.

Figure 2.3 gives an example of how the model user can simplify the groundwater system in the conceptual model by identifying main hydrologic units. The given cross section of the Rhine valley at Cologne identifies schematically individual characteristic units relevant for a model study. The group in which a rock or sand formation falls (aquifer, aquiclude, or aquitard) depends on total porosity, specific yield, and hydraulic conductivity.

Modeling is often primarily concerned with flow in aquifers, even though flow, and transport, in aquitards may also on occasion become the subject of groundwater studies. In view of their hydraulic behavior, aquifers can be classified into three types shown in Figure 2.3:

- Confined aquifer. The aquifer is confined at the top and base and, in terms of its steady-state hydraulic behavior, is comparable to a pipeline. The saturated thickness is independent of flux or boundary conditions, unless these conditions cause the aquifer to become unconfined.
- Leaky or semiconfined aquifer. The aquifer receives or loses water to adjacent aquifers through an aquitard. In the case of an overlying aquitard, the aquitard may be only partly saturated. The leaky aquifer can, in many cases, be visualized as a pipeline with porous walls.
- Unconfined or phreatic aquifer. The unconfined aquifer has a free water table. A change in flux results in a change of the saturated thickness. Flow can often be compared to flow in an open channel. Leakage may, or may not occur across the base of a phreatic aquifer.

2.2 REVIEWING DARCY'S LAW

Darcy's law allows us to assess groundwater flow by means of graphical, analytical, and numerical models. The following sections illustrate Darcy's experiment and discuss the general form of Darcy's law.

2.2.1 Remembering Darcy's Experiment

The first groundwater model, a porous media model, was developed in a scientific application in 1856 by the French hydraulic engineer Henry Darcy (Darcy 1856). Figure 2.4 illustrates Darcy's original model design and its extension to study flow in each direction. Darcy had been enlarging and modernizing the water works in Dijon, France. While designing sand filters, he encountered a problem with the physics of flow through porous media for which no published information existed. The detailed description of flow at

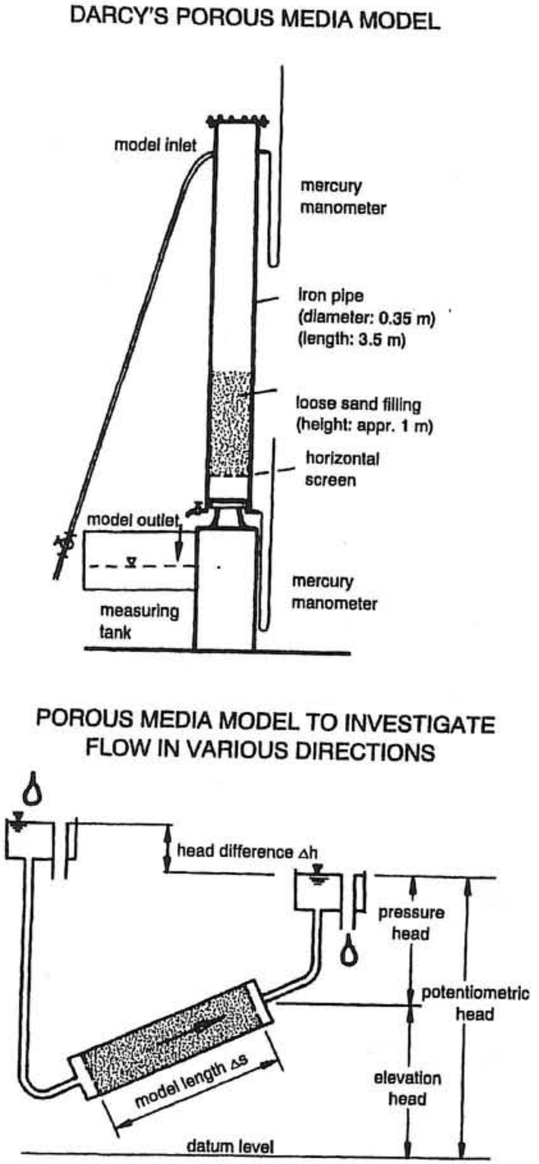


Figure 2.4 The first groundwater model: Porous media model to elaborate Darcy's law.

pore scale in a porous media was too complex to be practically applicable. To gain information about groundwater flow, Darcy constructed a porous media model.

In Darcy's experiment, fully saturated flow through a vertical experimental tank filled with porous material is generated by imposing different pressures on the model inlet and outlet. Darcy's law in its simplest form shows the relationship between flux, pressure gradient, and an empirical coefficient called the *hydraulic conductivity*, that depends on the characteristics of the porous material and of the water. This relationship is shown in Equation 2.1:

$$q = -K \frac{\Delta h}{\Delta s} = -Ki \qquad (2.1)$$

where

q = Darcy flux or specific discharge in [L/T]
K = hydraulic conductivity in [L/T]
Δh = head difference in [L]
Δs = length in [L]
i = hydraulic gradient in [1]

Hydraulic conductivity is a measure of the capacity of the porous media for transmitting water. Since the hydraulic gradient is dimensionless, K has the dimension of velocity. Flux is proportional to hydraulic gradient. The simple relationship illustrates, for example, that flux is doubled either by doubling the hydraulic gradient or doubling the hydraulic conductivity.

In the literature the Darcy flux q is often referred to as the *Darcy velocity*. Velocity is the rate of unit flow over unit cross-sectional area perpendicular to the flow direction. In groundwater flow, however, only a portion of the unit cross section of the aquifer has the capacity to transmit water while the remainder is solid material. Therefore the term velocity is misleading. Darcy velocity does not represent the velocity of water molecules. In groundwater flow studies which by nature are concerned with water quantities, the actual velocity of water in the irregular pore space is of no interest. In contrast, the true velocity of water-carrying solutes is necessary when studying solute transport. Thus in transport modeling the problem of approximating the true velocity based on known Darcy fluxes arises. This is discussed in more detail in Section 3.2.1.

2.2.2 Generalizing Darcy's Law

The hydraulic conductivity K depends on the permeability of the porous media k, on the physical properties of the fluid, on the density ρ, and on the dynamic viscosity μ or the kinematic viscosity ν:

$$K = \frac{\rho g}{\mu} k = \frac{g}{\nu} k \qquad (2.2)$$

where

- K = hydraulic conductivity in [L/T]
- k = permeability in [L^2]
- ρ = density in [M/L^3]
- g = acceleration due to gravity in [L/T^2]
- μ = dynamic viscosity in [M/LT]
- ν = kinematic viscosity in [L^2/T]

In most cases the permeability k varies from point to point in an aquifer; this is called *heterogeneity*. In addition, if permeability also depends on the direction of measurement, the aquifer is called *anisotropic*. The aquifer is called *homogeneous* if k is independent of the position of measurement. If k is independent of the direction of measurement at any point of the investigated aquifer, the aquifer is called *isotropic*. Mathematically speaking, the permeability, or respectively, hydraulic conductivity, is a second rank tensor with nine components.

Incorporating Equation 2.2 into Darcy's law, and expressing the hydraulic gradient in terms of elevation and pressure components, the general Darcy law is represented as

$$q_i = -\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} + \rho g \delta_j\right) \qquad (2.3)$$

where

- i,j = 1, 2, 3 (principal coordinate directions)
- q = Darcy flux in [L/T]
- p = pressure in [M/LT^2]
- x = space coordinate in [L]
- δ_j = 0 in horizontal flow direction
- δ_j = 1 in vertical flow direction

In Equation 2.3, and hereafter, the summation using double indexes is used (Einstein's convention of summation).

In modeling studies where the properties of water change with time or space (saltwater intrusion, migration of highly contaminated groundwater, warm water injection, etc.), the numerical formulation of groundwater flow must be based on the general Darcy law. The only remaining parameter in the general flow equation that is independent of water properties is permeability, characterizing the shape of the passages through which flow occurs.

2.2.3 Underlying Assumption of Darcy's Law

Darcy's law is established by experiments with various sands and gravels. The Darcian approach is to replace the actual aquifer with a representative continuum in order to use macroscopic law to describe flow at microscopic scale (Bear 1972). Groundwater flow is expressed by a simple relationship ignoring the complex flow configuration at pore scale. The macroscopic equation is also applicable for fractured or karstic material, assuming that the scale applied is large enough to eliminate the dominance of single fractures within the system. This restriction is important when describing flow in fractured or karstic aquifers. While numerous experiments demonstrate that Darcy's relationship holds true for unconsolidated media, as soon as one averages over a certain distance, similar rules do not exist for fractured or karstic formations. Averaging distances as large as several kilometers, beyond the size of the aquifer under investigation, may be required.

2.2.4 Summarizing Hydraulic Conductivities of Soils and Rocks

Since the first experiment by Darcy (1856), numerous laboratory and field studies have contributed to sketch a picture of hydraulic conductivities for natural rocks and unconsolidated deposits, facilitating the estimation of the hydraulic conductivity for a given aquifer. Figure 2.5 gives the range of hydraulic conductivity of various geological formations. A detailed compilation of relevant data concerned with the hydraulic conductivity is presented in Appendixes B.3 and B.4.

The hydraulic conductivity is a key factor when solving for groundwater flow. Although numerous approximate formulas exist to estimate the value theoretically, it is always preferable to rely on accurate field measurements rather than on calculation. When modeling at a regional scale, aquifer pumping tests giving conductivity values integrated over larger distances provide more helpful estimates of the hydraulic conductivity than local point measurements such as slug tests. Hydraulic conductivities of unconsolidated materials are considerably higher than those of most rocks. For rocks, K depends either entirely on the secondary porosity of the rock (fractures, weathering, etc.) or, in the case of sandstone, on the degree of cementation of pore space. High porosity environments such as karstic systems yield high conductivity values (as long as Darcy's law holds). Generally, horizontal hydraulic conductivities in sandy aquifers are in the region of a factor 10 to 100 higher than the vertical ones. The reason for larger horizontal conductivities lies in the bedding of grains during the geological formation of the aquifer.

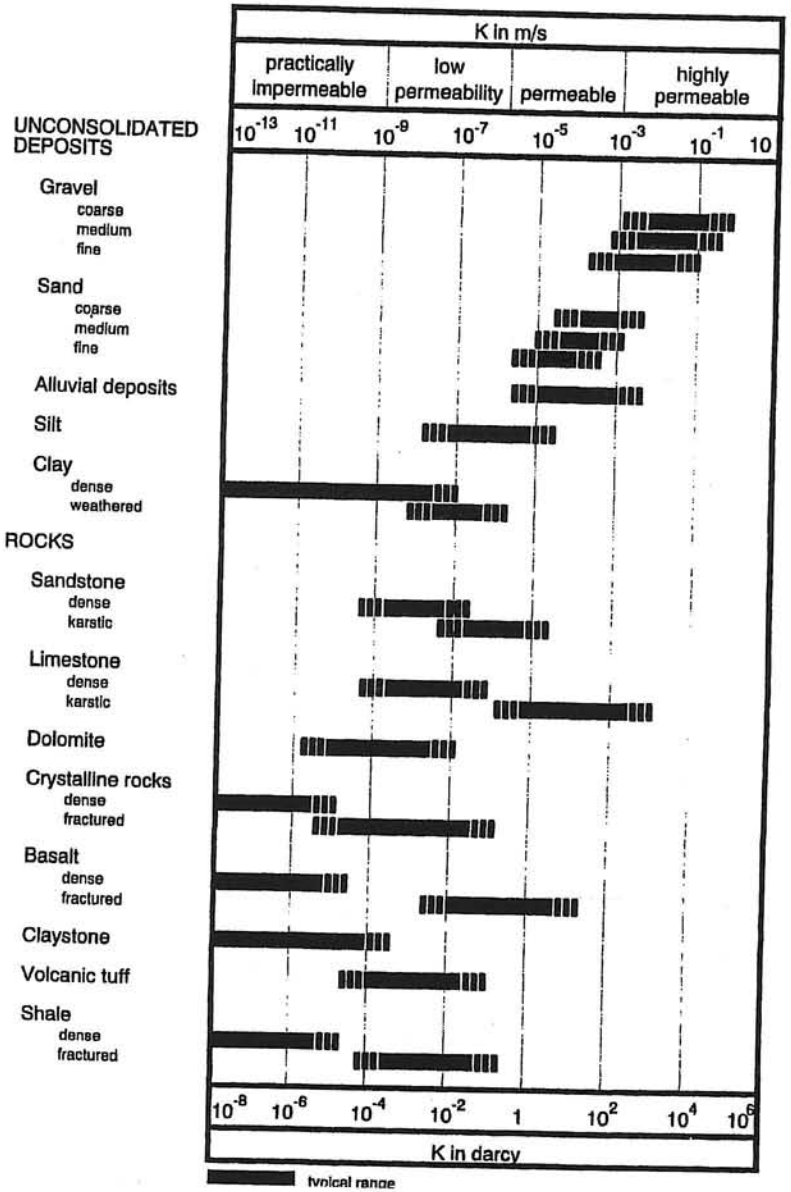


Figure 2.5 Range of hydraulic conductivity of geological formations.

There is no strict relationship between porosity and hydraulic conductivity despite the fact that rock of very low porosity is likely to have low hydraulic conductivity. Such correlation, however, does not necessarily hold true in the opposite case of materials with high porosity. Apart from the total amount of pore space, hydraulic conductivity depends on the openings or the geometry of pore space. Clay is commonly considered impermeable, even though its porosity is high. In clay, interconnecting tubes are small and hydraulic conductivity is low due to molecular attraction of water on the solid materials. In gravel, or reasonably coarse sediments, the force of molecular attraction between water and soil grains does not encompass or bridge the wide pore opening, and water is free to move in response to differences in potential. As long as the influence of molecular attraction is of the second order, hydraulic conductivity in unconsolidated deposits and sandstones follows trends in relation to porosity. Hydraulic conductivity increases with an increase of porosity, as can be seen by comparing Figure 2.2 and Figure 2.5.

Limestone reveals characteristics similar to sandstone. Dense limestone has low porosity and low hydraulic conductivity. However, limestone formations altered due to dissolution along fractures (karstic limestone) may transmit large quantities of water. Flow velocities in karstic systems may be on the order of flow velocities found in surface water.

2.3 FORMULATING THE GENERAL FLOW EQUATION

Darcy's law alone is not enough to describe groundwater flow, unless the head distribution within the entire flow system under review is measured. When modeling groundwater flow, however, the aim is to predict the head distribution under various groundwater stress situations. The head distribution known beforehand serves as initial conditions in a transient groundwater study.

The general flow equation for saturated groundwater flow is derived in numerous excellent textbooks such as Bear (1972). In most analyses the general flow equation is formulated by applying the law of conservation of mass over a control volume of an aquifer situated in the flow field. The net inflow into the volume must equal the rate at which water is accumulating within the volume under investigation, which leads to

$$\frac{\partial}{\partial x_i}\left(K_{ij}\,\frac{\partial h}{\partial x_j}\right) = S_s\,\frac{\partial h}{\partial t} + Q \qquad (2.4)$$

where

i,j = 1, 2, 3 (principal coordinate directions)
K = hydraulic conductivity in [L/T]
h = head in [L]