Class notes for MAE 123: Introduction to Transport in Porous Media

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Chapter 1

Basic Concepts

This course describes *fundamentals* of mathematical modeling of physical and bio-chemical processes in subsurface environments. The importance of this subject is underscored by Figure 1.1. This figure also explains the genesis of groundwater. We will be concerned with its movement.

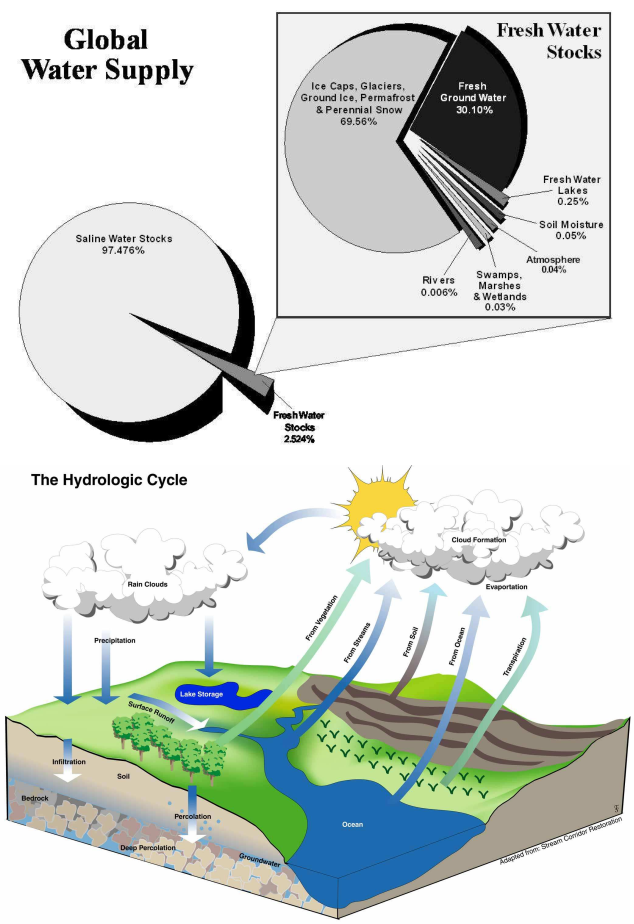


Figure 1.1: The distribution of global water supply (after www.internationalwaterlaw.org) and the hydrologic cycle (after www.buffer.forestry.iastate.edu).

1.1 Microscopic and Macroscopic Models

Flow and transport in porous media involve complex interactions between a solid matrix and a moving fluid. A detailed description of these processes forms the foundation of so-called *microscopic models*, which include Lattice Boltzman and Smooth Particle Hydrodynamics approaches. Such methods require, among other things, detailed knowledge of pore geometry, which is rarely available in practice.

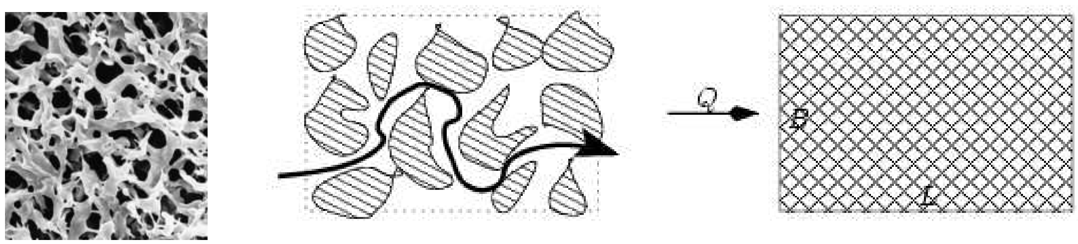


Figure 1.2: An example of porous media and its schematic representation. Both are replaced with a "black box" in macroscopic models.

Macroscopic models (which we will deal with in this class) overcome this conceptual difficulty by relying on a coarse, aggregate description of porous media. The following macroscopic properties of porous media are of interest.

Total porosity ω is defined as

$$\omega = \frac{\text{volume of the voids}}{\text{total volume of the medium}}, \qquad [\omega] = 1. \tag{1.1}$$

Void ratio ϵ is defined as

$$\epsilon = \frac{\text{volume of the voids}}{\text{volume of the solid}}, \qquad [\epsilon] = 1. \tag{1.2}$$

Surface porosity ω_s is defined as

$$\omega_s = \frac{\text{surface area of the voids in a cross-section}}{\text{total surface area of a cross-section}}, \qquad [\omega_s] = 1. \tag{1.3}$$

Specific surface area S_{sp} is defined as

$$S_{sp} = \frac{\text{total surface area of the voids}}{\text{total volume of the medium}}, \qquad [S_{sp}] = L^{-1}. \tag{1.4}$$

It is important to recognize that these and other macroscopic characteristics of porous media are always associated with some support volume V_T. Moreover, they typically vary with the size of V_T, as shown schematically in Figure 1.3. Since these parameters are used as coefficients in differential equations, they are treated mathematically as point values. This is accomplished by invoking a concept of the *Representative Elementary Volume* (REV), according to which macroscopic parameters at a point $\mathbf{x}$ are representative of a volume $V_T(\mathbf{x})$ surrounding this point. The REV is then defined as a volume that is both[1]

[1]De Marsily, 1986; p. 15

(i) "sufficiently large to contain a great number of pores so as to allow us to define a mean global property, while ensuring that the effects of the fluctuations from one pore to another is negligible;" and
(ii) sufficiently small to account for possible parameter variations from one domain to the next.

A porous medium is called *homogeneous* if the parameter values associated with the REV are constant in space, and *heterogeneous* otherwise.

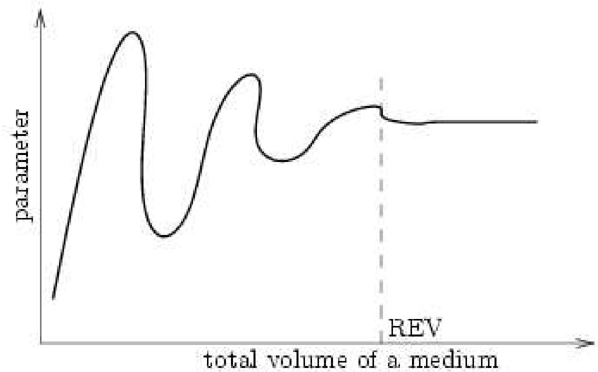


Figure 1.3: Parameter's variability with the volume of a sample. In homogeneous porous media, this variability diminishes when the sample becomes large enough. The smallest volume at which this occurs is called the Representative Elementary Volume (REV).

1.2 Darcy's Law

Darcy's law forms the foundation of macroscopic quantitative analyses of flow in porous media. It is an *empirical* law that was postulated in 1856 by Henry Darcy as a result of his experimental studies of fountains in the city of Dijon, France.

Consider a tube of cross-section A filled with a porous material, say sand (Figure 1.4). The tube is equipped with two piezometers located at elevations z_1 and z_2, a distance $\triangle z = z_1 - z_2$ apart. A fluid is introduced through the inlet at a constant rate Q. The medium is allowed to saturate, at which point the outflow rate equals the inflow rate Q and the elevations of the fluid levels in the piezometers are h_1 and h_2, respectively. Consider a quantity

$$q = \frac{Q}{A}, \tag{1.5}$$

which is variously known as Darcy's flux, specific discharge, or filtration velocity. Darcy observed that q is directly proportional to $\triangle h = h_1 - h_2$ for any fixed $\triangle z$, i.e.,

$$q = -K \frac{\triangle h}{\triangle z}. \tag{1.6}$$

The constant of proportionality K is called the *hydraulic conductivity* of a porous medium. Note that it is a property of both a porous medium and a filtrating fluid. The negative sign indicates that the fluid moves

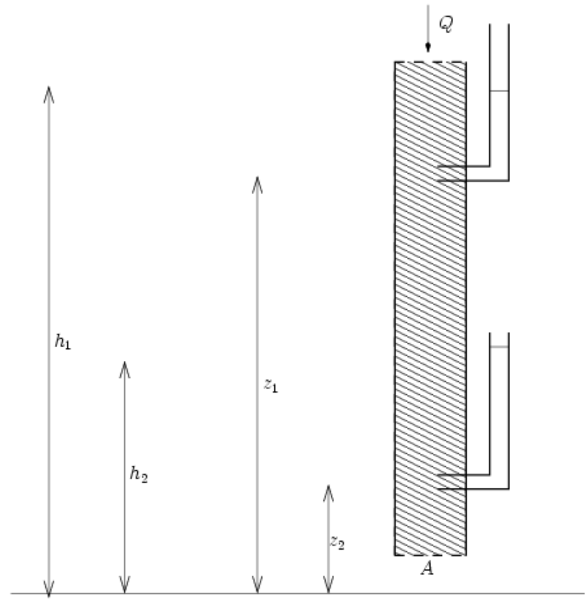


Figure 1.4: A schematic representation of Darcy's experiment.

from a point where the fluid elevation is higher to a point where it is lower. The experimental relation (1.6) can be written in differential form as

$$q = -K\frac{\mathrm{d}h}{\mathrm{d}z} \tag{1.7}$$

and further generalized to flow in two and three dimensions as

$$\mathbf{q} = -K\nabla h \tag{1.8}$$

(Note that the hydraulic conductivity scalar K should be replaced with a hydraulic conductivity tensor $\mathbf{K}$ if a medium is *anisotropic*.)

1.3 Hydraulic and Piezometric Head

Next we examine the physical meaning of the quantity h in Darcy's law (1.8). Following the standard practice in fluid mechanics, we examine the mechanical energy balance during the flow process.[2]

Consider a point M of a fluid, whose elevation is z. The work W_1 required to lift the mass m of a fluid from the elevation $z = 0$ (datum) to the point M at elevation z is

$$W_1 = mgz, \tag{1.9}$$

where g is the gravitational constant. The work W_2 required to accelerate the fluid from (datum) velocity $u = 0$ to velocity u is

$$W_2 = \frac{mu^2}{2}. \tag{1.10}$$

[2]Freeze and Cherry, 1979; Sec. 2.2 & de Marsily, 1986; Sec. 3.3

(Note that u is the *real* velocity of the fluid at point M.) Finally, the work W_3 required to raise the fluid pressure from $p = p_0$ at the datum to p at point M is

$$W_3 = m \int_{p_0}^{p} \frac{\mathrm{d}p}{\rho(p)}. \tag{1.11}$$

W_1, W_2, and W_3 represent the losses in potential, kinetic, and elastic energy respectively, caused by the movement of the fluid from the datum (a point at some standard state) to point M. The mechanical energy per unit mass, or the *fluid potential*, is $W = (W_1 + W_2 + W_3)/m$, which gives rise to the Bernoulli function

$$W = gz + \frac{u^2}{2} + \int_{p_0}^{p} \frac{\mathrm{d}p}{\rho(p)}. \tag{1.12}$$

The quantity $h = W/g$ is called *hydraulic head*,

$$h = z + \frac{u^2}{2g} + \int_{p_0}^{p} \frac{\mathrm{d}p}{g\rho(p)}. \tag{1.13}$$

According to Bernoulli's theorem, the head h decreases in the direction of the flow and the fluid is immobile if its head is constant in space. This is exactly what Darcy's law (1.8) predicts.

In porous media, the real fluid velocities u are exceedingly small, so that the dynamic head, the second term in (1.13), can be neglected. This reduces the hydraulic head to the static or *piezometric* head,

$$h = z + \int_{p_0}^{p} \frac{\mathrm{d}p}{g\rho(p)}. \tag{1.14}$$

In applications of porous-media flow to subsurface phenomena, it is common to select atmospheric pressure as a reference pressure, $p_0 \equiv p_{atm}$, and to express hydraulic heads in relation to the mean sea level. Finally, for incompressible fluids, such as water, (1.14) simplifies further to yield

$$h = z + \psi, \qquad \psi = \frac{p}{g\rho}, \tag{1.15}$$

where, in accordance with Darcy's experiment (Figure 1.4), z and ψ are called *elevation* and *pressure heads*, respectively.

Chapter 2

Single-Phase Flow in Porous Media

In this chapter, we will further investigate the physical foundation of Darcy's law (1.8), including the limits of its validity and the physical meaning of Darcy's flux $\mathbf{q}$ and hydraulic conductivity K. We will also derive a complete set of differential equations that describes single-phase (saturated) flow in porous media.[1]

2.1 Fundamentals of Fluid Mechanics

We begin by briefly reviewing the fundamentals of fluid mechanics relevant to flow in porous media. A general *equation of motion* (conservation of momentum) of a unit mass of fluid can be written as

$$\rho \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = \nabla \cdot \boldsymbol{\tau} - \nabla p + \rho \mathbf{g}. \tag{2.1}$$

The term on the left hand side of this equation is called *enertia*, with

$$\frac{\mathrm{D}}{\mathrm{D}t} \equiv \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \tag{2.2}$$

denoting a *substantial* (or *hydrodynamic* or *material*) derivative, and $\mathbf{u}$ being the fluid velocity. The first term on the right hand side of (2.1),

$$\nabla \boldsymbol{\tau} \equiv \left(\sum_{j=1}^{3} \frac{\partial \tau_{1j}}{\partial x_j}, \ldots, \sum_{j=1}^{3} \frac{\partial \tau_{3j}}{\partial x_j} \right)^T, \tag{2.3}$$

represents *viscous resistance* forces ($\boldsymbol{\tau}$ denotes the viscous stress tensor), which arise due to molecular cohesion and momentum transfer when the fluid is sheared. The remaining two terms, $-\nabla p + \rho \mathbf{g}$, represent the *driving force*, which consists of *hydrostatic pressure force* $-\nabla p$ and the gravitational force $\rho \mathbf{g}$ where $\mathbf{g} = (0, 0, -g)^T$.

Dynamic equilibrium is a state of no inertia, i.e., no acceleration,

$$0 = \nabla \cdot \boldsymbol{\tau} - \nabla p + \rho \mathbf{g}. \tag{2.4}$$

[1]The presentation here follows that of S. P. Neuman, U of A.

Hydrostatic conditions represent a state of no flow, i.e., the absence of both inertia and shear stress,

$$0 = -\nabla p + \rho \mathbf{g}. \tag{2.5}$$

These equations can be integrated to give

$$p = \text{constant along each horizontal plane } (x_1, x_2) \qquad \text{and} \qquad \frac{p}{\rho g} = c - x_3, \tag{2.6}$$

where c is a constant of integration. Hence pressure head $\psi \equiv p/\rho g$ increases linearly with depth.

Ideal fluids – Euler's equations (1775). Ideal fluids are fluids without viscous resistance. For ideal fluids, the equation of motion (2.1) becomes

$$\rho \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\nabla p + \rho \mathbf{g}. \tag{2.7}$$

Newtonian fluids – Navier-Stokes equations (1822). Newtonian fluids are fluids that have a constant viscosity at all shear rates at a constant temperature and pressure, and can be described by a one-parameter rheological model. For such fluids, the viscous stress $\boldsymbol{\tau}$ is a symmetric tensor whose components are given by (a rheological model)

$$\tau_{ii} = 2\mu \frac{\partial u_i}{\partial x_i} + \left(\frac{2}{3}\mu - \kappa \right) \nabla \cdot \mathbf{u} \tag{2.8a}$$

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \qquad i \neq j. \tag{2.8b}$$

Here μ is the *dynamic viscosity* of the fluid and κ is *bulk viscosity*, such that $\kappa \equiv 0$ for low-density mono-atomic gases and $\kappa \approx 0$ for dense gases and liquids.

We can now compute an expression for the viscous resistance forces in (2.1) and (2.3). Since the derivative of (2.8b) is

$$\frac{\partial \tau_{ij}}{\partial x_j} = \mu \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = \mu \frac{\partial^2 u_i}{\partial x_j^2} + \mu \frac{\partial^2 u_j}{\partial x_i \partial x_j}. \tag{2.9}$$

the i-th component of the vector $\nabla \boldsymbol{\tau}$ in (2.3) is

$$\sum_{j=1}^{3} \frac{\partial \tau_{ij}}{\partial x_j} = \mu \sum_{j=1}^{3} \frac{\partial^2 u_i}{\partial x_j^2} + \mu \sum_{j=1}^{3} \frac{\partial^2 u_j}{\partial x_i \partial x_j} \equiv \mu \nabla^2 u_i + \mu \frac{\partial}{\partial x_i} \nabla \cdot \mathbf{u}. \tag{2.10}$$

For homogeneous incompressible fluids, $\nabla \cdot \mathbf{u} = 0$ and we obtain a constitutive law

$$\sum_{j=1}^{3} \frac{\partial \tau_{ij}}{\partial x_j} = \mu \nabla^2 u_i \qquad \Longrightarrow \qquad \nabla \cdot \boldsymbol{\tau} = \mu \nabla^2 \mathbf{u}. \tag{2.11}$$

Substituting this expression into (2.1) yields Navier-Stokes equation

$$\rho \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = \mu \nabla^2 \mathbf{u} - \nabla p + \rho \mathbf{g}. \tag{2.12}$$

It is applicable to homogeneous incompressible Newtonian fluids under isothermal conditions.

Stokes flows. The inertial term in Navier-Stokes equations (2.12),

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} \equiv \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}, \tag{2.13}$$

introduces nonlinearity. However, if flow is slow, one can disregard the nonlinear term $\mathbf{u} \cdot \nabla \mathbf{u}$. The problem, of course, is that while $|\mathbf{u}|$ can be small in some units (say, in km/s) it might be quite large in other units (say, in $mm/year$). This is one of the reasons we need dimensionless analysis.

A standard dimensionless analysis in fluid mechanics is conducted as follows. Let B denote a characteristic length (e.g., the size of a container) and U a characteristic velocity (e.g., specific flow rate). Let us define the dimensionless variables,

$$\mathbf{x}_d = \frac{\mathbf{x}}{B}, \quad \mathbf{u}_d = \frac{\mathbf{u}}{U}, \quad t_d = \frac{tU}{B}, \quad p_d = \frac{p}{\rho U^2}, \quad \mathbf{g}_d = \frac{\mathbf{g}}{g} = (0,0,-1)^T, \qquad \nabla_d = B\nabla \tag{2.14}$$

Then Navier-Stokes equations (2.12) becomes

$$\frac{\partial \mathbf{u}_d}{\partial t_d} + \mathbf{u}_d \cdot \nabla_d \mathbf{u}_d = \frac{\mu}{\rho B U} \nabla_d^2 \mathbf{u}_d - \nabla_d p_d + \frac{Bg}{U^2} \mathbf{g}_d. \tag{2.15}$$

We have identified two dimensionless parameters, the Froude number Fr and the Reynolds number Re,

$$\mathrm{Fr} = \frac{U^2}{Bg} = \frac{\text{inertia}}{\text{gravity}}, \qquad \mathrm{Re} = \frac{BU}{\nu} = \frac{\text{inertia}}{\text{viscous resistance}}. \tag{2.16}$$

where $\nu = \mu/\rho$ is *kinematic viscosity*, $[\nu] = L^2 T^{-1}$. This gives a dimensionless form of Navier-Stokes equations,

$$\frac{\partial \mathbf{u}_d}{\partial t_d} + \mathbf{u}_d \cdot \nabla_d \mathbf{u}_d = \frac{1}{\mathrm{Re}} \nabla_d^2 \mathbf{u}_d - \nabla_d p_d + \frac{1}{\mathrm{Fr}} \mathbf{g}_d. \tag{2.17}$$

When $\mathrm{Re} \ll 1$, viscous forces dominate and inertia can be disregarded, leading to a *Stokes regime of slow viscous motion*,

$$\frac{\partial \mathbf{u}_d}{\partial t_d} = \frac{1}{\mathrm{Re}} \nabla_d^2 \mathbf{u}_d - \nabla_d p_d + \frac{1}{\mathrm{Fr}} \mathbf{g}_d. \tag{2.18}$$

It is, of course, linear.

2.2 Stokes Flow in Porous Media & Darcy's Law

In studies of flow in granular and porous media, it is more common to use an alternative way to dimensionalize Navier-Stokes equations (2.12). To begin with, we select the characteristic length and velocity as follows. Let the mean grain diameter d play the role of a characteristic length, and the external Darcy flux $q \equiv Q/A$ be a characteristic velocity. Then the Reynolds number is defined as

$$\mathrm{Re} = \frac{qd}{\nu}. \tag{2.19}$$

Next, recalling the definition of hydraulic head h in (1.15), we observe that Navier-Stokes equations (2.12) can be rewritten as

$$\frac{1}{g} \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = \frac{\mu}{\rho g} \nabla^2 \mathbf{u} - \nabla h. \tag{2.20}$$

In addition to dimensionless parameters x_d and u_d, we define the dimensionless time t_d and hydraulic head h_d as

$$t_d = \frac{\mu t}{\rho d^2}, \qquad h_d = \frac{\rho g d h}{\mu q}, \tag{2.21}$$

This gives an alternative dimensionless form of Navier-Stokes equations,

$$\frac{\partial \mathbf{u}_d}{\partial t_d} + \mathrm{Re}\ \mathbf{u}_d \cdot \nabla_d \mathbf{u}_d = \nabla_d^2 \mathbf{u}_d - \nabla_d h_d. \tag{2.22}$$

When $\mathrm{Re} \to 0$, we obtain a dimensionless form of Stokes equations,

$$\frac{\partial \mathbf{u}_d}{\partial t_d} = \nabla_d^2 \mathbf{u}_d - \nabla_d h_d. \tag{2.23}$$

Their dimensional form is

$$\frac{1}{g}\frac{\partial \mathbf{u}}{\partial t} - \frac{\nu}{g}\nabla^2 \mathbf{u} = -\nabla h. \tag{2.24}$$

Note that ν controls the rate at which viscous effects "diffuse" the momentum.

The *averaging* of Stokes equations (2.24) over a volume of the porous medium leads to macroscopic equations of motion,

$$\mathbf{q} + \frac{k\rho}{\omega\mu}\frac{\partial \mathbf{q}}{\partial t} - \frac{k\tilde{\mu}}{\omega\mu}\nabla^2 \mathbf{q} = -\frac{k\rho g}{\mu}\nabla h, \tag{2.25}$$

where k is intrinsic permeability (tensor), $[k] = L^2$; ω is porosity; and $\tilde{\mu}$ is effective viscosity. The first term on the left hand side of (2.25) results from the averaging of the viscous resistance term in Stokes equations (2.24). The second (transient) term comes from the inertia term in (2.24). The third term is known as *the Brinkman term*. It is the macroscopic shear term that accounts for viscous resistance near pores' surfaces. Finally, the term on the right hand side represents the macroscopic driving force.

The transient term might be important near rapidly fluctuating boundaries and sources, but is generally disregarded. The Brinkman term was introduced empirically by Brinkman (1947) to account for distortion of a velocity profile near boundaries of porous media (transfer of shear across such boundaries). Except for special flow scenario, it is also neglected. This gives the simplest form of Darcy's law,

$$\mathbf{q} = -\frac{k\rho g}{\mu}\nabla h. \tag{2.26}$$

Comparison of (2.26) and (1.8) reveals that hydraulic conductivity K is given by

$$K = \frac{k\rho g}{\mu}. \tag{2.27}$$

It now becomes apparent that K is indeed a property of both the porous medium (through its intrinsic permeability) and the fluid (through its density and viscosity).

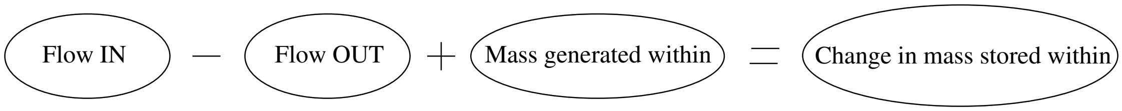


Figure 2.1: Mass conservation.

2.3 Continuity Equations

Equations of groundwater flow are derived by combining Darcy's law (2.26) with mass conservation law, i.e., with continuity equations.[2] Mass conservation is represented schematically in Figure 2.1. It is expressed mathematically as follows.

Inside a fully saturated porous medium, we select a small cube (Figure 2.2), whose dimensions are $\triangle x_1$, $\triangle x_2$ and $\triangle x_3$, and whose volume is $\triangle V = \triangle x_1 \triangle x_2 \triangle x_3$. The rate of fluid mass flow into the cube

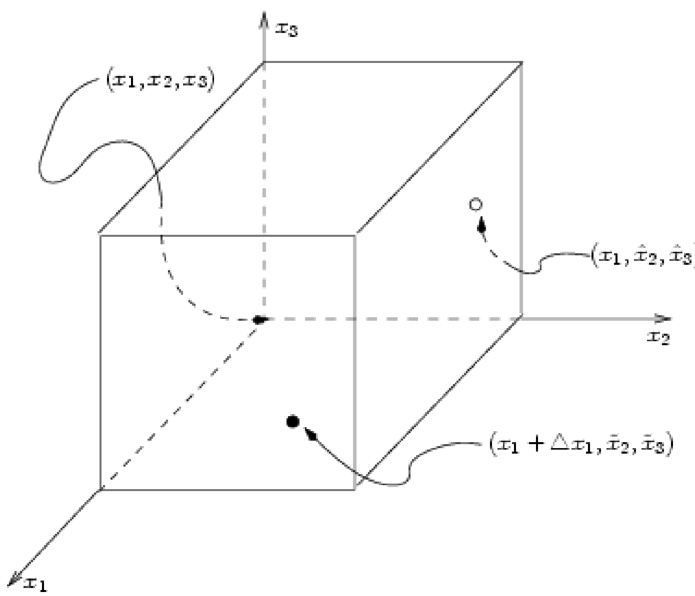


Figure 2.2: An elementary volume used to derive equations of groundwater flow.

through the side $x_1 + \triangle x_1$ during the time interval $[t, t + \triangle t]$ is $Q_1(x_1 + \triangle x_1) = \rho q(x_1 + \triangle x_1) \triangle x_2 \triangle x_2 \triangle t$. According to Darcy's law (1.8) this gives

$$Q_1(x_1 + \triangle x_1) = \rho K \frac{\partial h}{\partial x_1}(x_1 + \triangle x_1) \triangle x_2 \triangle x_3 \triangle t. \tag{2.28}$$

Likewise, the rate of fluid mass flow out of the cube through the side x_1 during the time interval $[t, t + \triangle t]$ is

$$Q_1(x_1) = \rho K \frac{\partial h}{\partial x_1}(x_1) \triangle x_2 \triangle x_3 \triangle t. \tag{2.29}$$

[2] See also Freeze and Cherry, 1979; Sec. 2.11

The rate of fluid mass $\triangle Q_1 = Q_1(x_1 + \triangle x_1) - Q_1(x_1)$ flowing into and out of the cube in the x_1 direction is

$$\triangle Q_1 = \left[\rho K \frac{\partial h}{\partial x_1}(x_1 + \triangle x_1) - \rho K \frac{\partial h}{\partial x_1}(x_1) \right] \triangle x_2 \triangle x_3 \triangle t. \tag{2.30}$$

In a similar manner, one can derive expressions for $\triangle Q_2$ and $\triangle Q_3$, the rate of fluid mass flow into and out of the cube in the x_2 and x_3 directions, respectively.

Mass generation inside the volume can be caused by the withdrawal, recharge or injection of fluid. Let $f(\mathbf{x}, t)$ denote the volumetric fluid rate per unit volume at each point. Note that f is defined on a macroscopic scale, such that $f > 0$ if fluid is added to the cube and $f < 0$ if it is withdrawn. The total mass flow rate added to the cube during the time interval $[t, t + \triangle t]$ is $Q_a = \rho f \triangle x_1 \triangle x_2 \triangle x_3 \triangle t$.

Finally, the change in fluid mass during the time interval $[t, t + \triangle t]$ is

$$\triangle m = m(\mathbf{x}, t + \triangle t) - m(\mathbf{x}, t) = [\rho\omega(t + \triangle t) - \rho\omega(t)] \triangle x_1 \triangle x_2 \triangle x_3. \tag{2.31}$$

The conservation of energy in Figure 2.1 can now be written as $\triangle H = \triangle Q_1 + \triangle Q_2 + \triangle Q_3 + Q_a$, or

$$\begin{aligned} \frac{\rho\omega(t + \triangle t) - \rho\omega(t)}{\triangle t} =& \frac{1}{\triangle x_1} \left[\rho K \frac{\partial h}{\partial x_1}(x_1 + \triangle x_1) - \rho K \frac{\partial h}{\partial x_1}(x_1) \right] \\ &+ \frac{1}{\triangle x_2} \left[\rho K \frac{\partial h}{\partial x_2}(x_2 + \triangle x_2) - \rho K \frac{\partial h}{\partial x_2}(x_2) \right] \\ &+ \frac{1}{\triangle x_3} \left[\rho K \frac{\partial h}{\partial x_3}(x_3 + \triangle x_3) - \rho K \frac{\partial h}{\partial x_3}(x_3) \right] + \rho f. \end{aligned} \tag{2.32}$$

Taking the limit as $\triangle x_i \to 0$ $(i = 1, 2, 3)$ and $\triangle t \to 0$ yields[3]

$$\frac{\partial \rho\omega}{\partial t} = \sum_{i=1}^{3} \frac{\partial}{\partial x_i} \left(\rho K \frac{\partial h}{\partial x_i} \right) + \rho f. \tag{2.33}$$

The left hand side of (2.33),

$$\frac{\partial \rho\omega}{\partial t} = \omega \frac{\partial \rho}{\partial t} + \rho \frac{\partial \omega}{\partial t}, \tag{2.34}$$

reflects both the compressibility of a fluid—the first term on the right hand side of (2.34)—and the compressibility of a porous medium—the second term on the right hand side of (2.34). Consider an equation of state of the fluid under isothermal conditions,

$$\rho = \rho_0 \mathrm{e}^{\beta_f p}, \tag{2.35}$$

where β_f is the compressibility coefficient of the fluid $[M^{-1}LT^2]$, and ρ_0 is the fluid density at the datum (atmospheric) pressure, which is here set to 0. For water, $\beta_f = 5 \times 10^{-10}$ Pa^{-1}. Then the first term on the right hand side of (2.34) can be written as

$$\frac{\partial \rho}{\partial t} = \beta_f \rho \frac{\partial p}{\partial t}. \tag{2.36}$$

[3]Here we disregard the displacement of the porous medium itself. A full derivation that accounts for this effect can be found in de Marsily, 1986; Sec. 5.3

The compressibility of porous media consists of two phenomena: (i) the compressibility of the solid grains and (ii) the compressibility of the solid matrix. Rigorous understanding of these processes requires some familiarity with solid mechanics. Here we simply assume that, in analogy with (2.35) and (2.36), we can write for the density of the solids ρ_s,

$$\frac{\partial \rho_s}{\partial t} = \beta_s \rho_s \frac{\partial p}{\partial t}. \tag{2.37}$$

The compressibility coefficient of the solid grains β_s is measurable on pure minerals. For quartz, $\beta_s \sim 2 \times 10^{-11}$ Pa^{-1}. Since the mass of the porous matrix of the elementary volume $m_s = \rho_s V_s$ remains constant,

$$\frac{\partial \rho_s V_s}{\partial t} = 0 \qquad \Rightarrow \qquad V_s \frac{\partial \rho_s}{\partial t} = -\rho_s \frac{\partial V_s}{\partial t} \tag{2.38}$$

Combining (2.37) and (2.38), we obtain

$$\frac{\partial V_s}{\partial t} = -\beta_s V_s \frac{\partial p}{\partial t}. \tag{2.39}$$

Next, we recall that the total volume of a porous medium $V_t = V_s + V_p$ consists of the volumes occupied by solids (V_s) and by pores (V_p), so that $V_s = (1-\omega)V_t$. Hence[4]

$$V_t \frac{\partial \omega}{\partial t} = \beta_s V_s \frac{\partial p}{\partial t} \qquad \Rightarrow \qquad \frac{\partial \omega}{\partial t} = (1-\omega)\beta_s \frac{\partial p}{\partial t}. \tag{2.40}$$

The quantity $\alpha = (1-\omega)\beta_s$ is called the compressibility of a porous medium, $[L^2 F^{-1}]$. For sandy aquifers, $\alpha = 10^{-7}$ – 10^{-9} Pa^{-1}. Substitution of (2.36) and (2.40) into (2.34) yields

$$\frac{\partial \rho \omega}{\partial t} = \rho \left(\alpha + \omega \beta_f\right) \frac{\partial p}{\partial t}. \tag{2.41}$$

Combining (2.41) with (2.33) and multiplying both sides of the resulting equation with g gives

$$S_s \frac{\partial p}{\partial t} = g \nabla \cdot (\rho K \nabla h) + \rho g f, \tag{2.42}$$

where the coefficient

$$S_s \equiv \rho g \left(\alpha + \omega \beta_f\right) \tag{2.43}$$

is called the *specific storage coefficient* of an aquifer, $[L^{-1}]$. Its physical meaning can be expressed as[5]

> The volume of water that a unit volume of aquifer releases from storage under a unit decline in hydraulic head h.

Neglecting the spatial variability of fluid density ρ, or assuming that $\nabla \rho \cdot \nabla (K \nabla h) \approx 0$, i.e., that density changes in the direction perpendicular to flow, yields

$$\frac{S_s}{\rho g} \frac{\partial p}{\partial t} = \nabla \cdot (K \nabla h) + f. \tag{2.44}$$

[4] Here we assumed that the total volume V_t remains constant in time. For a more rigorous derivation, which does not make this assumption, see de Marsily, 1986; Sec. 5.3

[5] Freeze and Cherry, 1979; p. 58

Finally, we recall the definition of hydraulic head (1.15) to observe that $p = \rho g(h - z)$ and

$$\frac{\partial p}{\partial t} = g(h - z)\frac{\partial \rho}{\partial t} + \rho g \frac{\partial h}{\partial t}. \tag{2.45}$$

Accounting for (2.36),

$$\frac{\partial p}{\partial t}\big[1 - g(h - z)\beta_f \rho\big] = \rho g \frac{\partial h}{\partial t}. \tag{2.46}$$

In most applications in subsurface hydrology, $g(h - z)\beta_f \rho \ll 1$ so that

$$\frac{1}{\rho g}\frac{\partial p}{\partial t} \approx \frac{\partial h}{\partial t}. \tag{2.47}$$

Substituting this expression into (2.44) yields the final form of the groundwater flow equation,

$$S_s \frac{\partial h}{\partial t} = \nabla \cdot (K \nabla h) + f. \tag{2.48}$$

This equation forms the foundation of modern groundwater modeling.

2.4 Groundwater Systems and Corresponding Boundary Conditions

Groundwater flow equations are routinely used to model water movement in aquifers in response, for example, to pumping. An *aquifer* is defined as[6]

> a layer, formation, or group of formations of permeable rocks, saturated with water and with a degree of permeability that allows economically profitable amounts of water to be withdrawn.

Aquifers rest on impermeable geologic units, e.g., bedrock. An aquifer is called *confined* if it is

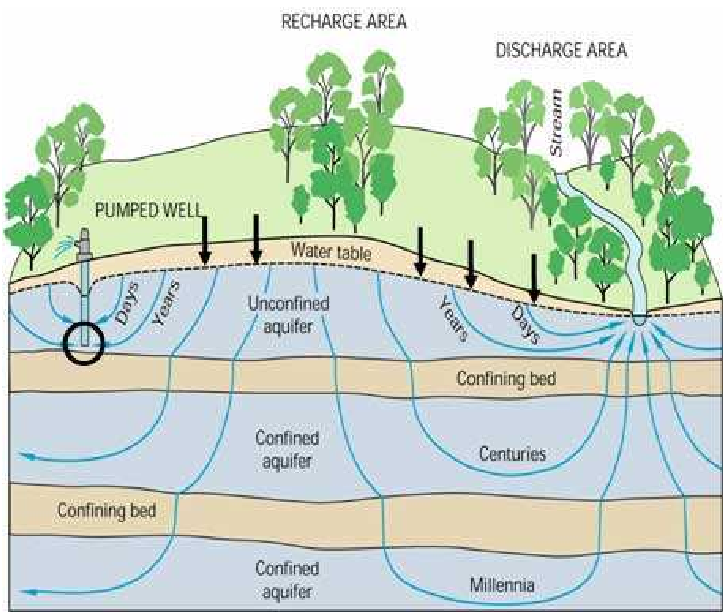
> overlaid by a formation with low (or zero) permeability and if the hydraulic head of the water it contains is higher than the elevation of the upper limit of the aquifer (see Figure 2.3).

As the definition suggests, a well drilled into a confined aquifer will be filled with water to the depth $h_0 > b$ which is larger than the depth b of the upper limit of the aquifer (see Figure 2.3). If the *piesometric surface* h_0 is higher than the ground, water will gush from the well without any pumping. Such aquifers are called *artesian*, and such wells are called *flowing*.

An *unconfined* aquifer is an aquifer in which the piesometric surface coincides with the free or *phreatic surface*, also known as *water table* (see Figure 2.3). Unconfined aquifers include

- *Valley aquifers*, which are formed by snow- or rainwater infiltrating into the soil. In such aquifers water flows towards outlets (e.g., springs and streams)—the low points in the topography.

[6] de Marsily, 1986; Chapter 6



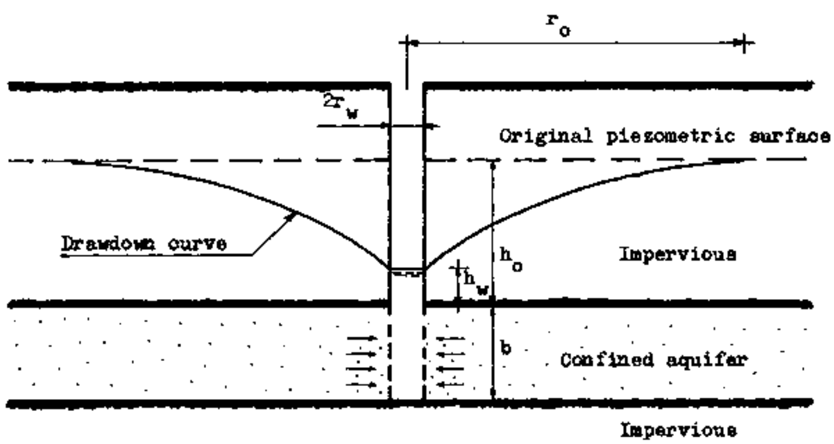


Figure 2.3: A schematic representation of aquifer types (http://www.epa.gov).

- *Alluvial aquifers* are unconfined aquifers situated in alluvial deposits along the course of a stream. Water in the aquifer is generally in equilibrium with the stream, which alternately drains or recharges it.

- *Coastal aquifers* which bring terrestrial fresh water contact with marine salt water.

- Etc. (see de Marsily, 1986; Sec. 6.1 from which the above description is copied almost verbatim.)

Since the same (or almost the same) groundwater flow equation (2.48) is used to model flow of water under these and many other field conditions, how do we formulate our model to reflect the reality? This is accomplished by specifying *boundary conditions* for (2.48). For example,

Prescribed head boundaries are boundaries Γ_D on which the hydraulic head h is determined by external forces rather than the processes occurring in the aquifer. Boundary conditions

$$h(\mathbf{x}, t) = H(\mathbf{x}, t), \qquad \mathbf{x} \in \Gamma_D$$

are called *Dirichlet's boundary conditions*. They occur along the surface where an aquifer comes into contact with open water, such as sea, lake or river.

Prescribed flux boundaries are boundaries Γ_N on which the normal hydraulic head gradient $\mathbf{n} \cdot \nabla h$ (or, equivalently the normal Darcy flux $\mathbf{n} \cdot \mathbf{q}$) is determined by external forces rather than the processes occurring in the aquifer. Boundary conditions

$$-K\mathbf{n} \cdot \nabla h(\mathbf{x}, t) = Q(\mathbf{x}, t), \qquad \mathbf{x} \in \Gamma_N,$$

where $\mathbf{n}$ is the unit normal vector to Γ_N, are called *Neumann's boundary conditions*. If the flux through the boundary Γ_N is zero, $Q = 0$, the boundary is called *impermeable* or *no-flow* boundary. A typical example are confining beds of a confined aquifer. An example of non-zero flux Q is given by an infiltration rate of the rainfall or artificial irrigation.

Free surface boundaries are boundaries γ that move in response to the flow conditions inside an aquifer. On such boundaries *two* boundary conditions are specified,

$$h(\mathbf{x}, t) = x_3, \qquad -K\mathbf{n} \cdot \nabla h(\mathbf{x}, t) = V_n$$

The first boundary condition implies that on the free surface the pressure $p = p_{atm} = 0$. The second condition is a form of mass conservation that defines the *dynamics* of the free surface. At equilibrium, $V_n = 0$. An example is the water table of an unconfined aquifer that moves in response to groundwater pumping.

For transient problems, it is also necessary to provide an *initial condition*, which specifies hydraulic head in an aquifer Ω at time $t = 0$,

$$h(\mathbf{x}, 0) = H_{in}(\mathbf{x}), \qquad \mathbf{x} \in \Omega.$$

Time $t = 0$ can correspond, for example, to the time at which groundwater pumping commenced.

A typical example of groundwater modeling that starts with identification of boundary conditions is shown in Figure 2.4.

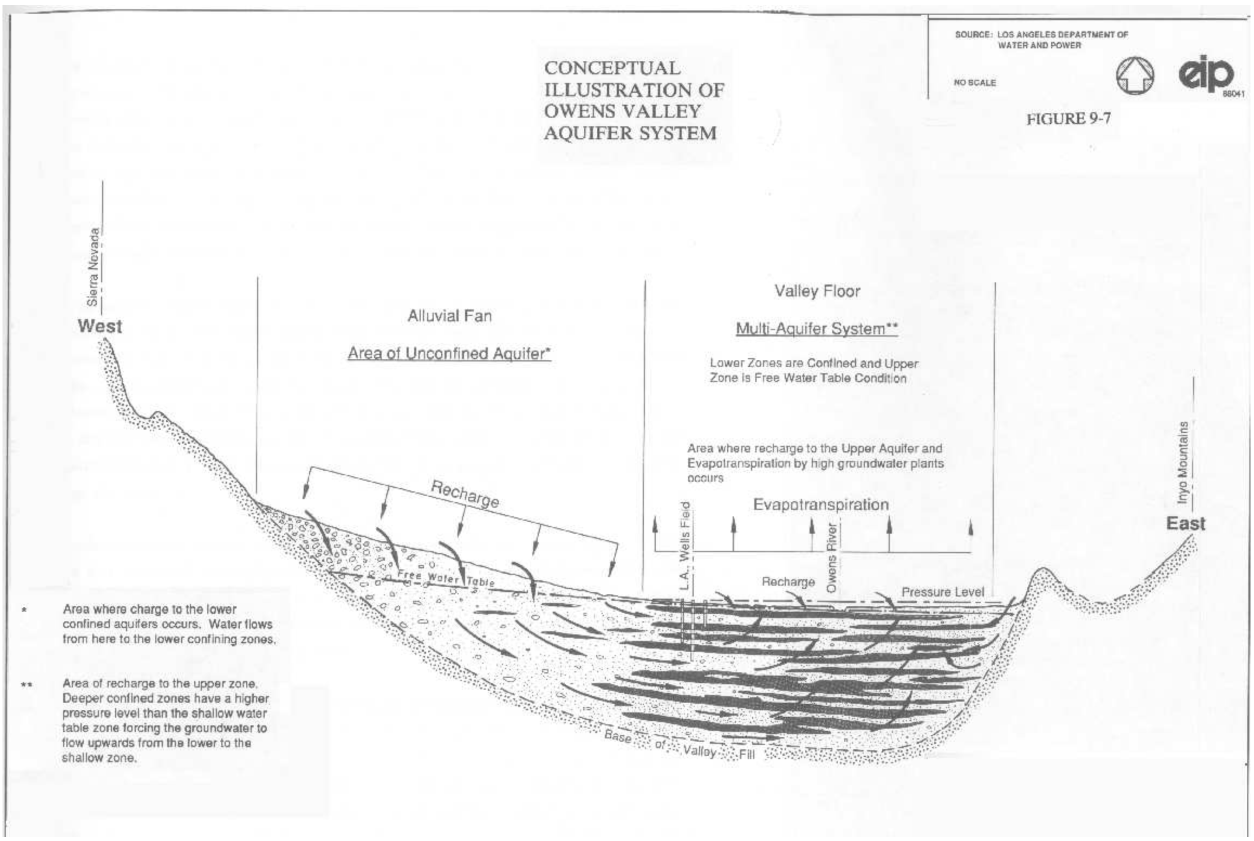


Figure 2.4: This figure is a reproduction of Figure 9-7 of the EIR to the LTWA (City of Los Angeles Department of Water and Power and County of Inyo, 1990).

2.5 Parameter Identification

Having derived the governing equations and boundary conditions, the only remaining thing is to parameterize our groundwater flow model, i.e., to select values of hydraulic conductivity K and specific storage S_s. Unfortunately, these parameters, and especially hydraulic conductivity, are highly variable (see Table 2.1) from one aquifer to another and within each aquifer. This section is devoted to the question of how to measure K.

$K\ (cm/s)$	10^2	10	10^0	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
Relative permeability	pervious				semi-pervious				impervious				
Aquifer	good					poor				none			
Unconsolidated sand & gravel	well sorted gravel		well sorted sand or sand & gravel			very fine sand, silt, loess, loam							
Unconsolidated clay & organic					peat		layered clay			fat / unweathered clay			
Consolidated rocks	highly fractured rocks				oil reservoir rocks			limestone sandstone		dolomite		granite	

Table 2.1: Table of saturated hydraulic conductivity K values found in nature. Values represent typical fresh groundwater conditions (http://en.wikipedia.org/wiki/Hydraulic_conductivity).

2.5.1 Laboratory determination of hydraulic conductivity

Permeameters are used for laboratory determination of hydraulic conductivity K from Darcy's law (Figure 2.5)[7].

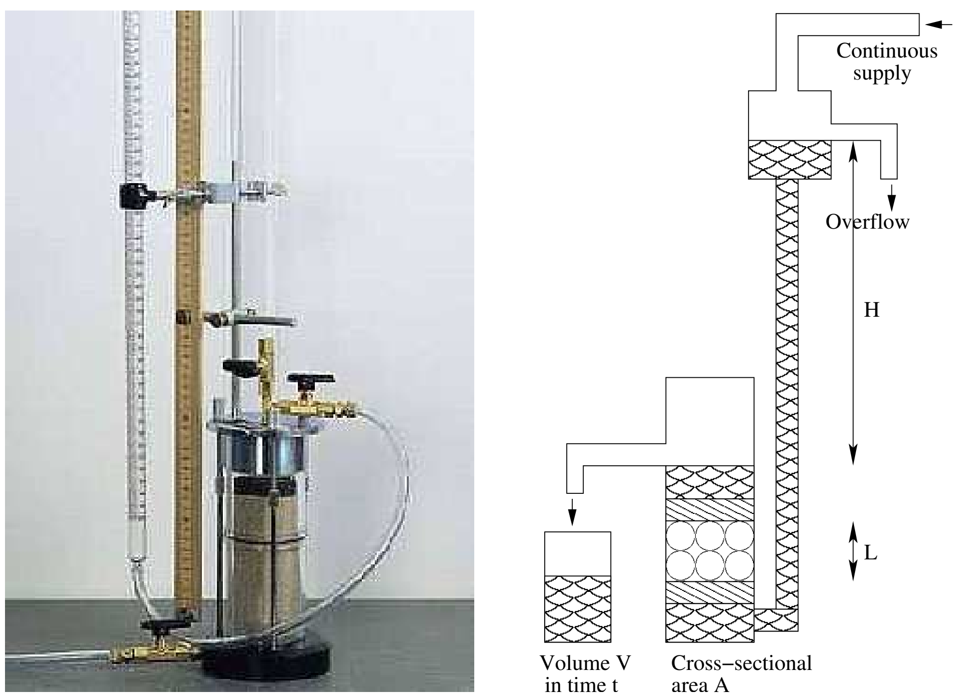


Figure 2.5: Permeameters are used to measure the hydraulic conductivity of a sample in the laboratory.

[7] see Section 8.4 of Freeze and Cherry, 1979

Constant-head permeameters refer to the experimental setup in which constant head differential $H = h_2 - h_1$ is maintained over the duration of the experiment and the volume of water V in the beaker is measured as a function of time. After the volumetric discharge through the sample $Q = V/t$ reaches steady state, the hydraulic conductivity K is readily determined from Darcy's law as

$$K = \frac{QL}{AH}. \tag{2.49}$$

Falling-head permeameters refer to the experimental setup in which head differential $H = h_2 - h_1$ is allowed to drop from the initial head differential H_0 at time $t = 0$ to some head differential H_1 at time t. Once again, Darcy's law is used to infer the hydraulic conductivity,

$$-K\frac{AH}{L} = Q(t). \tag{2.50}$$

However now $Q(t)$ is not measured, but is related to the velocity with which the head differential drops in the tube,

$$v(t) = -\frac{dH}{dt}. \tag{2.51}$$

If the cross-section of the tube is a, than the mass flux is $Q(t) = av(t)$, which gives

$$K\frac{AH}{L} = a\frac{dH}{dt} \qquad \Rightarrow \qquad K = \frac{aL}{At}\ln\left(\frac{H}{H_0}\right). \tag{2.52}$$

The constant-head experiments are typically used for porous media with relatively high hydraulic conductivity (e.g., $K > 0.01cm/min$), while the falling-head experiments are best suited for less permeable porous media.[8]

Regardless of the type, the laboratory experiments used to measure hydraulic conductivity suffer from a number of drawbacks. These include the large disparity of scales on which the values of conductivity are measured and used, and the virtual impossibility of collecting undisturbed core samples.

2.5.2 Field-scale experiments: Pumping tests

Pumping tests are among the most widely used tools to determine the hydraulic conductivity on a large scale. Selection of a particular pumping test is determined by the field conditions.

Pumping tests in fractured rocks. Suppose we drilled into a rock that is virtually impermeable, save for a fracture of width b (Figure 2.6)[9]. We wish to determine the permeability of this rock formation by measuring the amount of water Q injected into the formation. We assume that (i) the bore-hole is perpendicular to the fracture, (ii) flow is radial, and (iii) the hydraulic head within the borehole is constant.[10] This example allows us to relate the permeability of a subsurface environment to its geometric characteristics, such as fracture width b.

[8] Freeze and Cherry, 1979; p. 336
[9] Lecture notes by S. P. Neuman
[10] The presentation below follows that of S. P. Neuman

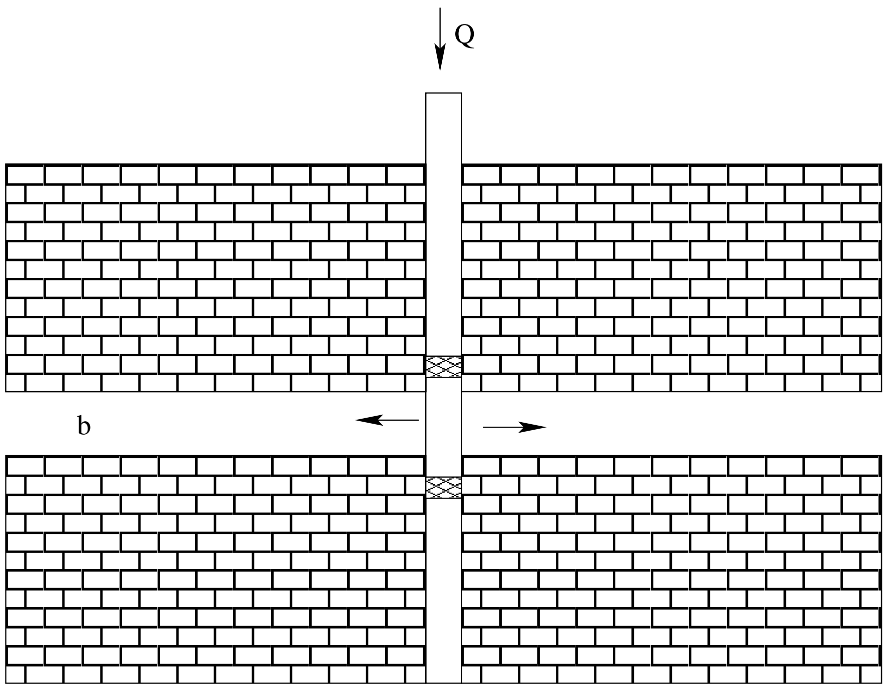


Figure 2.6: Pumping test in a fractured rock.

Darcy's law in the radial coordinates reads

$$q(r) = \frac{Q}{A} = -K_f \frac{dh}{dr}, \qquad A = 2\pi b r. \tag{2.53}$$

The question of finding the hydraulic conductivity K_f boils down to analyzing flow between two parallel plates. It is described by the steady-state Stokes equations (2.24),

$$\frac{\mu}{\rho g} \nabla^2 \mathbf{u} = \nabla h \tag{2.54}$$

or

$$\frac{\mu}{\rho g} \left(\frac{\partial^2 u_1}{\partial x_1^2} + \frac{\partial^2 u_1}{\partial x_2^2} \right) = \frac{\partial h}{\partial x_1} \qquad \text{and} \qquad \frac{\mu}{\rho g} \left(\frac{\partial^2 u_2}{\partial x_1^2} + \frac{\partial^2 u_2}{\partial x_2^2} \right) = \frac{\partial h}{\partial x_2}. \tag{2.55}$$

Since the surfaces of the fracture are impermeable, there is no flow in the vertical (x_2) direction, $u_2 \equiv 0$, $\partial h / \partial x_2 \equiv 0$, and the second equation vanishes. For incompressible fluids, $u_2 \equiv 0$ implies that

$$\frac{\partial^2 u_1}{\partial x_1^2} = \frac{\partial}{\partial x_1} \left(\frac{\partial u_1}{\partial x_1} \right) = \frac{\partial}{\partial x_1} \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} \right) = \frac{\partial}{\partial x_1} \left(\nabla \cdot \mathbf{u} \right) = 0. \tag{2.56}$$

Thus, the flow is described by

$$\frac{\partial^2 u_1}{\partial x_2^2} = \frac{\rho g}{\mu} J, \qquad J \equiv \frac{\partial h}{\partial x_1}. \tag{2.57}$$

The hydraulic head gradient J is the constant externally applied driving force induced by the injection of water at rate Q. Equation (2.57) can be readily integrated to yield

$$u_1 = \frac{\rho g}{2\mu} J x_2^2 + a_1 x_2 + a_2. \tag{2.58}$$

The constants of integration a_1 and a_2 are determined from the boundary conditions on the fracture's surfaces. Here we assume the no-slip boundary conditions

$$u_1\left(-\frac{b}{2}\right) = u_1\left(\frac{b}{2}\right) = 0, \tag{2.59}$$

although other conditions, e.g., those accounting for Klinkenberg effect with $u_1 \neq 0$, are also possible. With the boundary conditions (2.59), the *parabolic velocity profile* in (2.58) becomes

$$u_1(x_2) = -\frac{\rho g}{\mu}\frac{1}{2}\left(\frac{b^2}{4} - x_2^2\right)\frac{dh}{dx_1}. \tag{2.60}$$

One can think of (2.60) as a "pointwise Darcy's law", in which the intrinsic permeability $k = k(x_2)$. The actual Darcy's law is obtained by averaging (2.60) over the width of the fracture, so that Darcy's velocity

$$q_1 = \frac{1}{b}\int_{-b/2}^{b/2} u_1(x_2)dx_2. \tag{2.61}$$

This gives

$$q_1 = -\frac{\rho g}{\mu}\frac{b^2}{12}\frac{dh}{dx_1}, \tag{2.62}$$

which can be generalized to multiple dimensions,

$$\mathbf{q} = -\frac{\rho g}{\mu}\frac{b^2}{12}\nabla h. \tag{2.63}$$

Comparison with (2.26) reveals that the intrinsic permeability of a fracture is

$$k_f = \frac{b^2}{12}. \tag{2.64}$$

For fractures with *rough* walls, this expression can be modified to

$$k_f = f_L b^2, \qquad f_L \leq \frac{1}{12}, \tag{2.65}$$

where f_L is Lomize's roughness coefficient, and Darcy's law takes the form

$$\mathbf{q} = -K_f \nabla h, \qquad K_f = \frac{\rho g}{\mu} f_L b^2. \tag{2.66}$$

Combining (2.53) and (2.66), we obtain the so-called "cubic law"

$$Q = -2\pi r \frac{\rho g}{\mu} f_L b^3 \frac{dh}{dr}. \tag{2.67}$$

This equation can be integrated to give

$$\frac{Q}{2\pi f_L b^3 \rho g}\ln\left(\frac{r}{r_w}\right) = h_w - h(r), \tag{2.68}$$

where r_w is the radius of the well and h_w is the hydraulic head measured at the well. Assume there exists a *radius of influence* r_i at which $h(r_i)$ is negligibly small. Then

$$b^3 = \frac{Q}{2\pi f_L \rho g}\frac{\ln(r_i/r_w)}{h_w}. \tag{2.69}$$

If several fractures intersect the borehole, it is common to either

- assume all fractures are horizontal with the same f_L and b, or
- treat all fractures as a single "equivalent" horizontal fracture.

Pumping tests in confined aquifers: Theis solution. Developed in 1935, Theis solution remains the most widely used method for interpretation of pumping tests in *confined* aquifers (the second of Figures 2.3). The solution describes radial flow to a well and assumes that the aquifer is

1. bounded by horizontal perfectly impermeable surfaces,
2. homogeneous,
3. isotropic,
4. of infinite lateral extent, and
5. undisturbed by prior pumping, i.e., has a constant "original" piesometric surface;

and that the well

1. has zero radius,
2. fully penetrates the aquifer, and
3. has no internal storage.

Let Q denote the pumping rate, h_0 the initial piesometric head, $T = Kb$ the *transmissivity* of the aquifer, $S = S_s b$ the storativity of the aquifer; and $s(r,t) \equiv h_0 - h(r,t)$ the *drawdown*. Under the above assumptions, the groundwater flow equation (2.48) can be written in polar coordinates as

$$\frac{S}{T}\frac{\partial s}{\partial t} = \frac{\partial^2 s}{\partial r^2} + \frac{1}{r}\frac{\partial s}{\partial r}. \tag{2.70}$$

This equation is subject to the initial condition

$$s(r,0) = 0 \tag{2.71}$$

and the boundary conditions

$$s(r=\infty,t) = 0, \qquad \lim_{r_w \to 0} 2\pi r_w b K \frac{\partial s}{\partial r}(r_w) = -Q. \tag{2.72}$$

The second boundary condition follows directly from the application of Darcy's law at the well face, whose surface area is $2\pi r_w b$.

One way to solve (2.70) – (2.72) is to employ Boltzmann's transformation

$$\xi = \frac{r^2}{4Dt}, \qquad D \equiv \frac{T}{S}. \tag{2.73}$$

Since

$$\frac{\partial s}{\partial t} = \frac{\partial \xi}{\partial t}\frac{\mathrm{d}s}{\mathrm{d}\xi} = -\frac{r^2}{4Dt^2}\frac{\mathrm{d}s}{\mathrm{d}\xi} \tag{2.74a}$$

$$\frac{\partial s}{\partial r} = \frac{\partial \xi}{\partial r}\frac{\mathrm{d}s}{\mathrm{d}\xi} = \frac{r}{2Dt}\frac{\mathrm{d}s}{\mathrm{d}\xi} \tag{2.74b}$$

$$\frac{\partial^2 s}{\partial r^2} = \frac{1}{2Dt}\frac{\mathrm{d}s}{\mathrm{d}\xi} + \frac{r}{2Dt}\frac{\partial}{\partial r}\left(\frac{\mathrm{d}s}{\mathrm{d}\xi}\right) = \frac{1}{2Dt}\frac{\mathrm{d}s}{\mathrm{d}\xi} + \frac{r^2}{4D^2t^2}\frac{\mathrm{d}^2 s}{\mathrm{d}\xi^2}, \tag{2.74c}$$

Boltzmann's transformation (2.73) transforms the partial differential equation (2.70) into an ordinary differential equation (ODE)

$$\xi\frac{\mathrm{d}^2 s}{\mathrm{d}\xi^2} + (1+\xi)\frac{\mathrm{d}s}{\mathrm{d}\xi} = 0, \tag{2.75}$$

The initial condition and the boundary condition at infinity yield a single boundary condition

$$s(\xi = \infty) = 0. \tag{2.76}$$

The boundary condition at the well bore translates into

$$\lim_{\xi\to 0}\xi\frac{\mathrm{d}s}{\mathrm{d}\xi} = -\frac{Q}{4\pi bK}. \tag{2.77}$$

Let

$$u(\xi) \equiv \frac{\mathrm{d}s}{\mathrm{d}\xi}. \tag{2.78}$$

Then (2.75) and (2.77) yield a first-order ODE

$$\xi\frac{\mathrm{d}u}{\mathrm{d}\xi} + (1+\xi)u = 0 \tag{2.79}$$

subject to the boundary condition

$$\lim_{\xi\to 0}\xi u = -\frac{Q}{4\pi T}. \tag{2.80}$$

The corresponding solution is

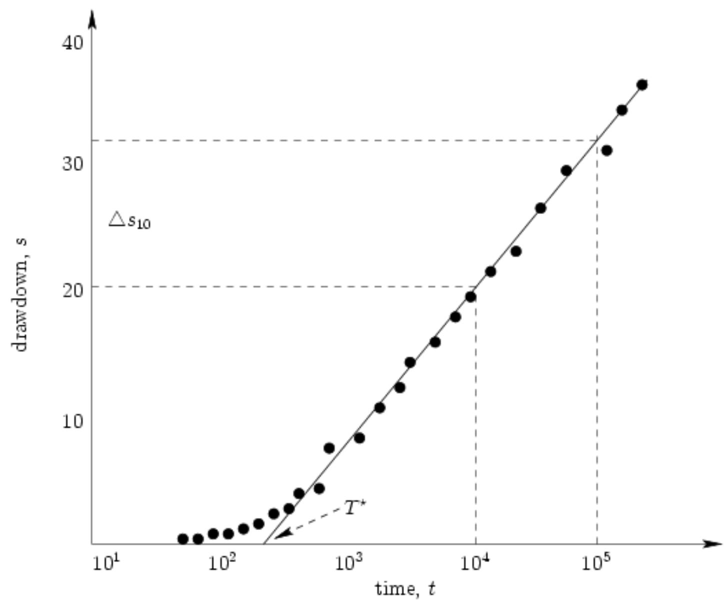
$$u(\xi) = -\frac{Q}{4\pi T}\frac{\mathrm{e}^{-\xi}}{\xi}. \tag{2.81}$$

Recalling the definitions of u in (2.78) and ξ in (2.73), and making use of the boundary condition at infinity, we obtain the *Theis equation*

$$s = \frac{Q}{4\pi T}\int_{1/4t_s}^{\infty}\frac{\mathrm{e}^{-\zeta}}{\zeta}\mathrm{d}\zeta, \qquad t_s = \frac{Dt}{r^2}. \tag{2.82}$$

The integral

$$E_1(u) = \int_u^{\infty}\frac{\mathrm{e}^{-\zeta}}{\zeta}\mathrm{d}\zeta \tag{2.83}$$



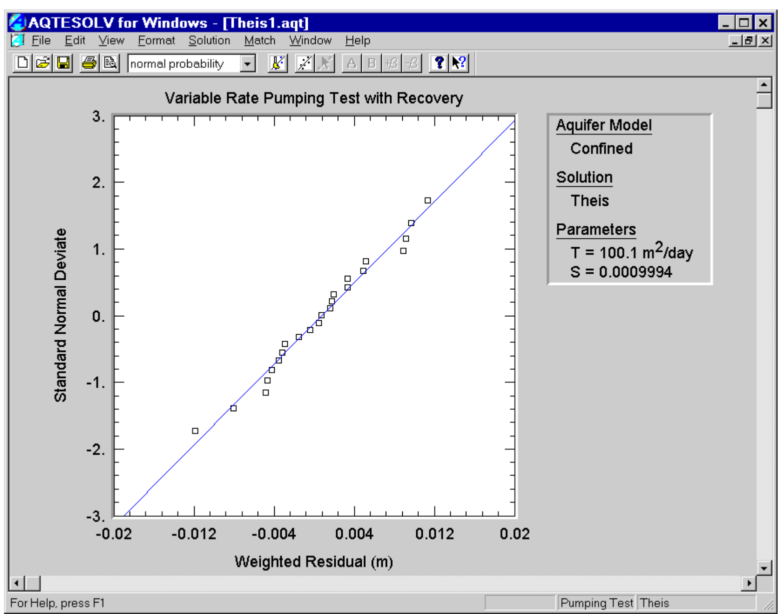


Figure 2.7: A screen-shot of a curve matching software AQTESOLV for analysis of pumping test data.

is called the *exponential integral* in mathematical literature, and is known an the *well function* to hydrogeologists.

Two approaches can be used to infer the transmissivity T and storativity S of a confined aquifer from the drawdown s versus time t data by means of Theis equation (2.82). In the first approach, which is known as a *type curve method*, the data are plotted on a log-log paper and compared with the log-log plot of the dimensionless drawdown[11]

$$s_d \equiv \frac{4\pi T s}{Q} = E_1 \tag{2.84}$$

versus the dimensionless time

$$t_d = \frac{Dt}{r^2}. \tag{2.85}$$

The latter curves are independent of the properties of an aquifer and hence can be used with any aquifer, which satisfies the assumptions discussed in the opening of this section—thus the term "type curve".

The straight-line fitting approach, also known as the Jacob-Cooper semi-log method, is based on the observation that, for large pumping times t, Theis equation (2.82) can be approximated by

$$\frac{4\pi T}{Q} s \approx -0.5772 + \ln(4t_d) = 2.303 \log_{10}(2.246 t_d). \tag{2.86}$$

This gives a straight line when the drawdown is plotted as a function of $\ln t$ (Figure 2.7a), from which

$$T = c_1 \frac{Q}{\triangle s_{10}} \quad \text{and} \quad S = c_2 \frac{T t^\star}{r^2}, \tag{2.87}$$

where $c_1 = 0.1833$ and $c_2 = 2.246$ if the cmg unit system is used. Note that to compute the storativity S one needs to have an observation well located a distance r from the pumping well. These methods are fully automated and available as software packages (Figure 2.7b).

Theis equation can also be used to estimate the extent of the *cone of depression* and other parameters of interest, if the hydraulic parameters of an aquifer (T and S) are known.

Pumping tests in unconfined aquifers. Unconfined aquifers are bounded from above by a water table (Figure 2.3) that changes its shape and position in response to pumping. The water table is accompanied by a *capillary fringe*, i.e., a region in which the saturation of a porous material varies from the full saturation in the aquifer to some residual saturation of an (almost) dry soil. We will study flow and transport in *partially (or unsaturated) porous media* in later chapters. Here it is enough to say that in the context of pumping in unconfined aquifers the capillary fringe can often be disregarded.[12]

Dupuit-Forchheimer approximation.[13] Consider groundwater flow in an unconfined homogeneous aquifer shown schematically in Figure 2.8. The flow is described by the groundwater flow equation (2.48)

$$S_s \frac{\partial h}{\partial t} = -\nabla \cdot \mathbf{q}, \qquad \mathbf{q} = -K \nabla h. \tag{2.88}$$

[11] See Section 8.3 of Freeze and Cherry for details.
[12] Freeze and Cherry, Chapter 8, pp. 324-325.
[13] After S. P. Neuman's class notes, U of A.

In the spirit of Theis' solution, we are interested in the vertically averaged behavior of the system. It is obtained by integrating (2.88),

$$S_s \int_{z_0(x)}^{\xi(x,t)} \frac{\partial h}{\partial t} dz = - \int_{z_0(x)}^{\xi(x,t)} \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right) dz. \tag{2.89}$$

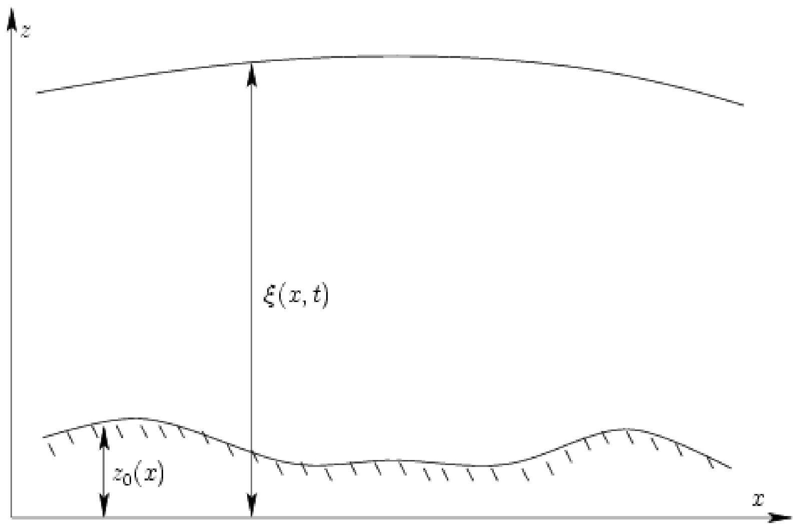


Figure 2.8: A schematic representation of unconfined aquifers.

Leibniz rule implies that

$$\int_{z_0(x)}^{\xi(x,t)} \frac{\partial h}{\partial t} dz = \frac{\partial}{\partial t} \int_{z_0(x)}^{\xi(x,t)} h dz - h(\xi, t) \frac{\partial \xi}{\partial t} \tag{2.90}$$

and

$$\int_{z_0(x)}^{\xi(x,t)} \frac{\partial q_x}{\partial x} dz = \frac{\partial}{\partial x} \int_{z_0(x)}^{\xi(x,t)} q_x dz + q_x(z_0) \frac{\partial z_0}{\partial x} - q_x(\xi) \frac{\partial \xi}{\partial x}. \tag{2.91}$$

Let $\tilde{h}$ and flux $\tilde{\mathbf{q}}$ denote the vertically averaged hydraulic head,

$$\tilde{h}(x,y,t) \equiv \frac{1}{b} \int_{z_0}^{\xi} h(x,y,z,t) dz, \qquad \tilde{\mathbf{q}}(x,y,t) \equiv \frac{1}{b} \int_{z_0}^{\xi} \mathbf{q}(x,y,z,t) dz = (\tilde{q}_x, \tilde{q}_y)^T, \tag{2.92}$$

where $b(x,y,t) = \xi(x,y,t) - z_0(x,y)$ is the width of the unconfined aquifer. Then (2.89)

$$S_s \left(\frac{\partial b \tilde{h}}{\partial t} - h(\xi, t) \frac{\partial \xi}{\partial t} \right) = -\hat{\nabla} \cdot (b \tilde{\mathbf{q}}) - \hat{\mathbf{q}}(z_0) \cdot \hat{\nabla} z_0 + \hat{\mathbf{q}}(\xi) \cdot \hat{\nabla} \xi - q_z(\xi) + q_z(z_0), \tag{2.93}$$

where $\hat{\nabla} \equiv (\partial/\partial x, \partial/\partial y)^T$ and $\hat{\mathbf{q}} \equiv (q_x, q_y)^T$. Note that this equation is exact, i.e., we have not made any approximations so far. It is also not particularly useful, and further progress requires some simplifying assumptions.

Let us assume that $h(z) \approx h(z_0) \approx h(\xi)$, which implies

- static equilibrium along each vertical,
- vertical equipotentials,
- horizontal flow.

Of course, all these flow characteristics mean the same thing. This assumption is due to Dupuit (1863) and Forchheimer (1930). *It remains valid as long as the drawdown remains much smaller than the total width of the unconfined aquifer.* Since $\partial\xi/\partial t = \partial b/\partial t$, this assumption yields

$$\frac{\partial b\tilde{h}}{\partial t} - h(\xi, t)\frac{\partial \xi}{\partial t} \approx \frac{\partial b\tilde{h}}{\partial t} - \tilde{h}\frac{\partial b}{\partial t} = b\frac{\partial \tilde{h}}{\partial t}. \tag{2.94}$$

Recalling the definition of storativity $S = S_s b$, we obtain from (2.93)

$$S\frac{\partial \tilde{h}}{\partial t} = -\hat{\nabla} \cdot (b\tilde{\mathbf{q}}) - \hat{\mathbf{q}}(z_0) \cdot \hat{\nabla} z_0 + \hat{\mathbf{q}}(\xi) \cdot \hat{\nabla}\xi - q_z(\xi) + q_z(z_0). \tag{2.95}$$

It remains to evaluate the boundary terms. The term $q_z(z_0)$ represents the leakage from the bottom impermeable (or low-permeable) layer. The term $\hat{\mathbf{q}}(z_0) \cdot \hat{\nabla} z_0$ represents the contribution of *uneven* bottom to the leakage. These two terms act as driving forces acting externally on the aquifer. The boundary terms on the water table ξ are trickier to deal with, since the position of the water table is determined from the solution of the problem.

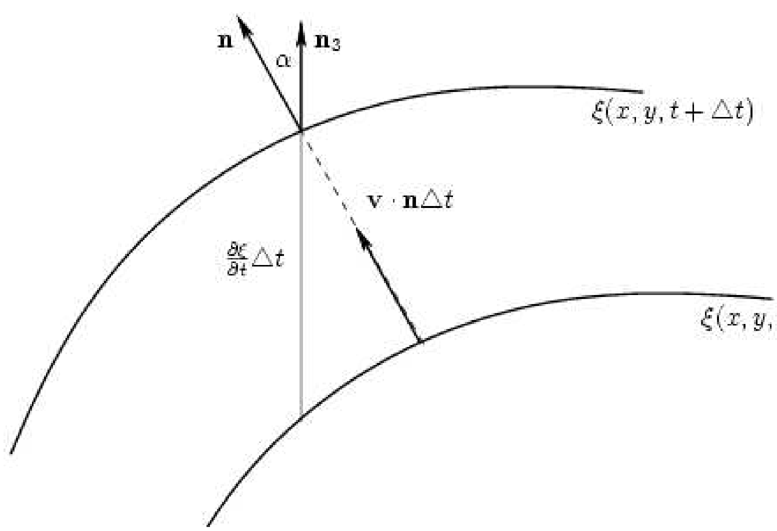


Figure 2.9: Derivation of the kinematic boundary condition on free surface (water table).

In section 2.4, we established that the pressure along the water table equals atmospheric pressure and can be set to zero. In other words, the hydraulic head on the water table equals the elevation of the water table,

$$h(x, y, z, t) = \xi(x, y, t). \tag{2.96}$$

The kinematic boundary condition is

$$\mathbf{q}(\xi) \cdot \mathbf{n} = V_n \tag{2.97}$$

where V_n denotes the *macroscopic* velocity of the moving water table. The macroscopic ($\mathbf{V}$) and microscopic ($\mathbf{v}$) velocities differ by a kinematic porosity S_y, i.e., $\mathbf{V} = S_y \mathbf{v}$. It is customary to use the *specific yield* of a medium as such a porosity. Hence V_n becomes

$$V_n = S_y \mathbf{v} \cdot \mathbf{n}. \tag{2.98}$$

Consider an infinitesimal segment of the water table that has moved from its position at time t to a new position at time $t + \triangle t$ (Figure 2.9). A point on the water table moved the distance

$$\mathbf{v} \cdot \mathbf{n} \triangle t, \tag{2.99}$$

and the vertical displacement of the water table is

$$\frac{\partial \xi}{\partial t} \triangle t. \tag{2.100}$$

One can see from Figure 2.9 that these two quantities are related by

$$\mathbf{v} \cdot \mathbf{n} \triangle t = \frac{\partial \xi}{\partial t} \triangle t \cos \alpha, \tag{2.101}$$

where α is the angle between the unit normal vector $\mathbf{n}$ and the vertical coordinate. If n_3 denotes the projection of the vector $\mathbf{n}$ onto the vertical coordinate, then $\cos \alpha = n_3$, and

$$\mathbf{v} \cdot \mathbf{n} = \frac{\partial \xi}{\partial t} n_3. \tag{2.102}$$

Combining (2.97), (2.98), and (2.102), we obtain the kinematic condition on the water table,

$$-\mathbf{q}(\xi) \cdot \mathbf{n} = S_y \frac{\partial \xi}{\partial t} n_3. \tag{2.103}$$

Finally, we recall that the elevation of the water table is $z = \xi(x, y, t)$, i.e., that its equation in three dimensions is $F(x, y, z, t) \equiv \xi(x, y, t) - z = 0$. The unit normal vector to such a surface is given by

$$\mathbf{n} = -\frac{\nabla F}{|\nabla F|} = \frac{1}{|\nabla F|} \left(-\frac{\partial \xi}{\partial x}, -\frac{\partial \xi}{\partial y}, 1 \right)^T. \tag{2.104}$$

Hence

$$\hat{\mathbf{q}}(\xi) \cdot \hat{\nabla} \xi - q_z(\xi) = -S_y \frac{\partial \xi}{\partial t}. \tag{2.105}$$

Substituting (2.105) into (2.95) yields

$$S \frac{\partial \tilde{h}}{\partial t} = -\hat{\nabla} \cdot (b \tilde{\mathbf{q}}) - \hat{\mathbf{q}}(z_0) \cdot \hat{\nabla} z_0 - S_y \frac{\partial \xi}{\partial t} + q_z(z_0). \tag{2.106}$$

Since $\tilde{h} \approx \xi$ and $\tilde{\mathbf{q}} = -K \hat{\nabla} \tilde{h}$,

$$(S + S_y) \frac{\partial \tilde{h}}{\partial t} = \hat{\nabla} \cdot (K b \hat{\nabla} \tilde{h}) - \hat{\mathbf{q}}(z_0) \cdot \hat{\nabla} z_0 + q_z(z_0), \tag{2.107}$$

This is the final form of the flow equation for unconfined aquifers *under Dupuit-Forchheimer approximation*. Further simplifications are obtained by assuming

- that the bottom is flat ($\hat{\nabla} z_0 = 0$) and impermeable ($q_z(z_0) = 0$), so that $b = \tilde{h}$; and
- that $S \ll S_y$.

Then

$$S_y \frac{\partial \tilde{h}}{\partial t} = \hat{\nabla} \cdot (K \tilde{h} \hat{\nabla} \tilde{h}), \tag{2.108}$$

which is known as Boussinesq's equation.

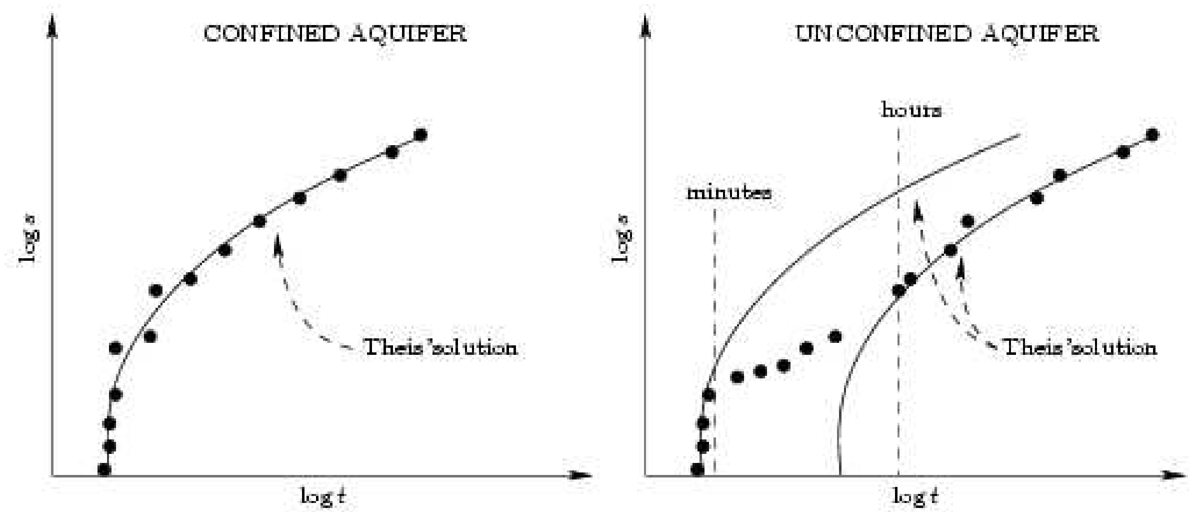


Figure 2.10: Water table response to pumping.

The response in an observation well located the distance r from the pumping well is shown in Figure 2.10. Note that it is possible to fit both the early- and late-time data to Theis' curves. It means that both yield the same transmissivity T, but different storativity S ($S_{\text{early}} < S_{\text{late}}$). This is because the storativity S of confined aquifers is constant, while the specific yield S_y of unconfined aquifers varies with time.

Chapter 3

Multi-Phase Flow in Porous Media

In the previous chapter, we considered flow in porous media that are fully saturated with one fluid. There are many situations where several fluids coexist in pores, e.g., air and water in soils; oil, gas and water in oil reservoirs; and water and DNAPLs in contaminated aquifers.

One can distinguish two types of multi-phase flows in porous media:[1]

- *Immiscible* flow in which a distinct fluid-fluid interface separates immiscible fluids, such as air and water; and
- *Miscible* flow of fluids that are completely soluble in each other, e.g., saltwater and freshwater mixing as a consequence of seawater intrusion into coastal aquifers.

The first type is the subject of this chapter. The second type, which is often referred to as *hydrodynamic dispersion*, will be discussed in the following chapters.

3.1 Basic Definitions

While the presentation below[2] is applicable to any number of phases and any fluids, we will use only two fluids, air and water, to be concrete (Figure 3.1). In addition to averaged quantities defined over the REV in Section 1.1, we define the following:

$$S_w = \frac{\text{volume of water}}{\text{volume of voids}} = \text{water saturation}$$

and

$$S_a = \frac{\text{volume of air}}{\text{volume of voids}} = \text{air saturation}$$

Of course,

$$S_a + S_w = 1. \tag{3.1}$$

[1] Bear, 1972, Sec. 9.1

[2] After S. P. Neuman's class notes, U of A.

In addition, let p_a and p_w denote the average pressure in air and water, respectively. The difference between the two,

$$p_c = p_a - p_w \tag{3.2}$$

is called *capillary pressure*. It is given by

$$p_c = \frac{2\sigma_{aw}}{r}, \tag{3.3}$$

where σ_{aw} is the interfacial tension between air and water, and r is the mean radius of the curvature of the air-water interface. In general, $p_c < 0$.

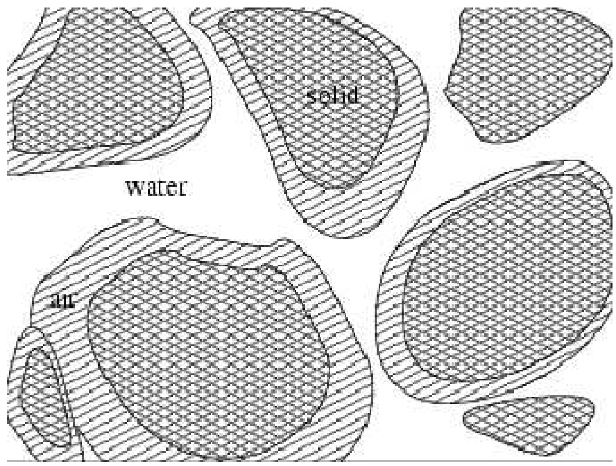


Figure 3.1: REV of a porous medium containing air and water.

3.2 Generalized Darcy's Law

In analogy to single-phase flow, we define water hydraulic head h_w and air hydraulic head h_a as

$$h_w = \frac{p_w}{\rho_w g} + z \qquad \text{and} \qquad h_a = \int_{p_0}^{p_a} \frac{\mathrm{d}p_a}{\rho_a g}. \tag{3.4}$$

Here both the compressibility of water and the weight of air are disregarded. In analogy to (2.26), we *postulate* the generalized Darcy's law for water and air

$$\mathbf{q}_w = -\frac{\rho_w g}{\mu_w} k_w \nabla h_w \qquad \text{and} \qquad \mathbf{q}_a = -\frac{\rho_a g}{\mu_a} k_a \nabla h_a = -\frac{k_a}{\mu_a} \nabla p_a. \tag{3.5}$$

Note that this result is *empirical*. Our derivation of Darcy's law from Stokes equations (Section 2.2) no longer holds, since it does not account for the compressibility of air.[3]

Since only a portion of the pores is available for flow of each fluid, the *permeabilities of the medium for water and air* (k_w and k_a, respectively) depend on saturation. The higher the water saturation S_w, the larger

[3] Volumetric averaging techniques typically result in systems of over 20 coupled differential equations...

portion of the pores is available for flow of water, and the larger the permeability for water k_w. Likewise, the higher the water saturation S_w, the smaller portion of the pores is available for flow of air, and the smaller the permeability for air k_a. This behavior is demonstrated schematically by Figure 3.2, which shows the dependence of *relative permeabilities for water ($k_{r_w} = k_w/k$) and air ($k_{r_a} = k_a/k$)* on water saturation S_w. Recall that k is the intrinsic permeability of the porous medium and is the property of the medium only. It represents the permeability of the medium at full saturation by either fluid.

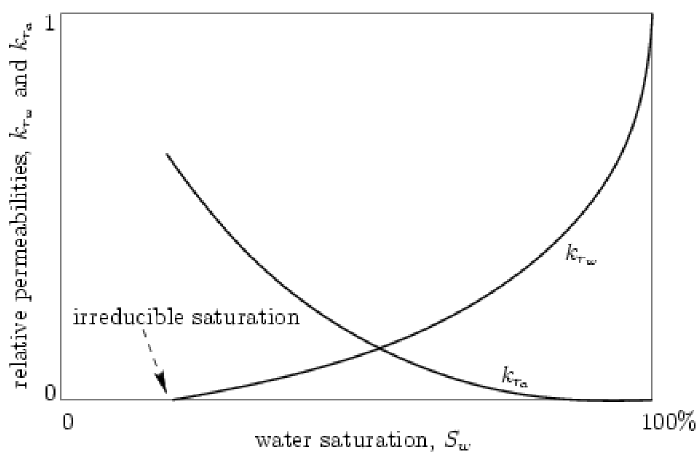


Figure 3.2: Dependence of relative permeabilities for water (k_{r_w}) and air (k_{r_a}) on water saturation S_w.

3.3 Governing Equations of Multi-Phase Flow

Multi-phase flow equations are obtained by combining the generalized Darcy's law with continuity equations. In analogy with their single-phase counterparts (Section 2.3), continuity (mass conservation) equations for water and air phases read

$$
\begin{aligned}
-\nabla \cdot (\rho_w \mathbf{q}_w) + f_w &= \omega \frac{\partial S_w \rho_w}{\partial t} \\
-\nabla \cdot (\rho_a \mathbf{q}_a) + f_a &= \omega \frac{\partial S_a \rho_a}{\partial t},
\end{aligned}
\tag{3.6}
$$

where the source terms f_w and f_a represent the internal rates of generation of mass of water and air per unit volume, respectively. The terms on the right hand sides of (3.6) correspond to the temporal change in the amount of the i-th fluid (mass per unit volume) $\rho_i S_i \omega$, where $i = w, a$. The quantities $\theta_w = \omega S_w$ and $\theta_a = \omega S_a$ are called *volumetric water and air contents*, respectively.

The right hand sides of (3.6) account for mass changes due to the two mechanisms, change in saturation and change in density. They do *not* account for any deformations of the porous medium. This becomes clear if one considers transient fully saturated flow of an incompressible fluid (water). In this case, the second equation vanishes, and the right hand side of the first is 0. This results in $\nabla \cdot \mathbf{q} = 0$, with the transient effects, caused by source and boundary fluctuations, propagating instantaneously through the system.

Combining generalized Darcy's law (3.5) with continuity equations (3.6), we obtain the multi-phase flow equations

$$\omega \frac{\partial S_w \rho_w}{\partial t} = \nabla \cdot (\rho_w K_w \nabla h_w) + f_w$$
$$\omega \frac{\partial S_a \rho_a}{\partial t} = -\nabla \cdot (\rho_a K_a \nabla h_a) + f_a, \tag{3.7}$$

where the hydraulic conductivities of porous media with respect to water (K_w) and air (K_a) are given by

$$K_w = \frac{\rho_w g}{\mu_w} k_w \qquad \text{and} \qquad K_a = \frac{\rho_a g}{\mu_a} k_a. \tag{3.8}$$

It is important to remember that these two equations are *coupled* through the relationships (3.1) and (3.2),

$$S_a + S_w = 1 \qquad \text{and} \qquad p_c = p_a - p_w. \tag{3.9}$$

This system of equations is closed by supplying *equations of state*, which specify

- the dependence of saturations S_w and S_a on capillary pressure p_c,
- the dependence of intrinsic permeabilities k_w and k_a on saturations S_w and S_a, and
- the dependence of densities ρ_w and ρ_a on pressures p_w and p_a.

The first two sets of dependencies can be determined experimentally, but often exhibit *hysteresis* (more on this later).

The latter set equations of state can be expressed by[4]

$$\rho = Ap^m \mathrm{e}^{cp}, \qquad c > 0. \tag{3.10}$$

- For liquids, $m = 0$.
  - Incompressible liquids: $c = 0$.
- For gases, $c = 0$.
  - Ideal gases:
    - Isothermal: $m = 1$, i.e.,
      $$\rho = \frac{pM}{RT},$$
      where $R = 8.3145 J/(mol\, K)$ is the universal gas constant, T is the absolute temperature, and M is the molecular weight (mass of $1 mole$).
    - Adiabatic (no heat exchange with the environment):
      $$m = \frac{\text{specific heat at constant volume}}{\text{specific heat at constant pressure}}.$$
  - Real gases:
    $$\rho = \frac{pM}{ZRT},$$
    where Z is the super-compressibility factor (Van der Waals corrections).

[4] refresh your thermodynamics

3.4 Flow in Partially Saturated Porous Media

The following assumptions are often made to model water movement in unsaturated (partially saturated) soils.

1. Air is immobile, i.e., $p_a =$ constant. This assumption is justified by an observation that air moves through porous media much easier than water and, hence, attains a state of equilibrium much faster.

2. Air pressure is at equilibrium with atmosphere, i.e., $p_a = p_{\text{atmospheric}} = 0$.

3. Water is incompressible, i.e., $\rho_w =$ constant.

The first assumption implies that flow in unsaturated soils (vadose zone) can be completely described by the first equation in (3.7),

$$\frac{\partial \theta \rho_w}{\partial t} = \nabla \cdot (\rho_w K_w \nabla h_w) + f_w, \tag{3.11}$$

where

$$\theta \equiv \omega S_w = \frac{\text{volume of water in pores}}{\text{total volume of the medium}} \tag{3.12}$$

is called the *volumetric water content*.

The second assumption implies that the capillary pressure in (3.2) and the hydraulic head of water in (3.4) become

$$p_c = -p_w \tag{3.13}$$

and

$$h_w = \psi + z, \qquad \psi \equiv \frac{p_w}{\rho_w g} = -\frac{p_c}{\rho_w g}, \tag{3.14}$$

respectively. The pressure head ψ is known in soil physics literature as *tension*, *suction*, or *matrix potential*.

The third assumption, combined with (3.14), allows one to rewrite (3.11) as

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (K_w \nabla \psi) + \frac{\partial K_w}{\partial x_3} + F, \tag{3.15}$$

where $F \equiv f_w / \rho_w$ is the volumetric source term, $[F] = T^{-1}$.

Equation (3.15), which is known as *Richards' equation*, has to be supplemented by two constitutive laws that specify the dependencies $\theta = \theta(\psi)$ and $K_w = K_w(\theta)$. These laws, whose general behavior is shown schematically in Figure 3.3, are determined experimentally (more on this later) and allow one to write Richards equation (3.15) in one of the following forms.

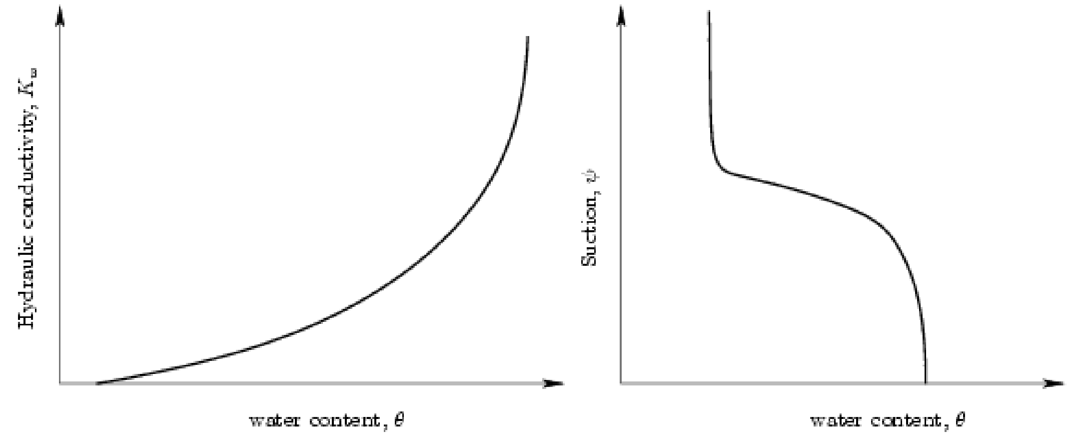


Figure 3.3: Dependence of hydraulic conductivity K_w and suction ψ on volumetric water content θ.

The ψ-based form. Since

$$\frac{\partial \theta}{\partial t} = C(\psi)\frac{\partial \psi}{\partial t}, \qquad C(\psi) \equiv \frac{\partial \theta}{\partial \psi}, \tag{3.16}$$

Richards' equation (3.15) can be expressed in the ψ-based form

$$C(\psi)\frac{\partial \psi}{\partial t} = \nabla \cdot [K_w(\psi)\nabla\psi] + \frac{\partial K_w}{\partial x_3} + F. \tag{3.17}$$

The function $C(\psi)$ is called the *specific moisture capacity*. It is a property of the medium, whose general behavior is shown in Figure 3.4.

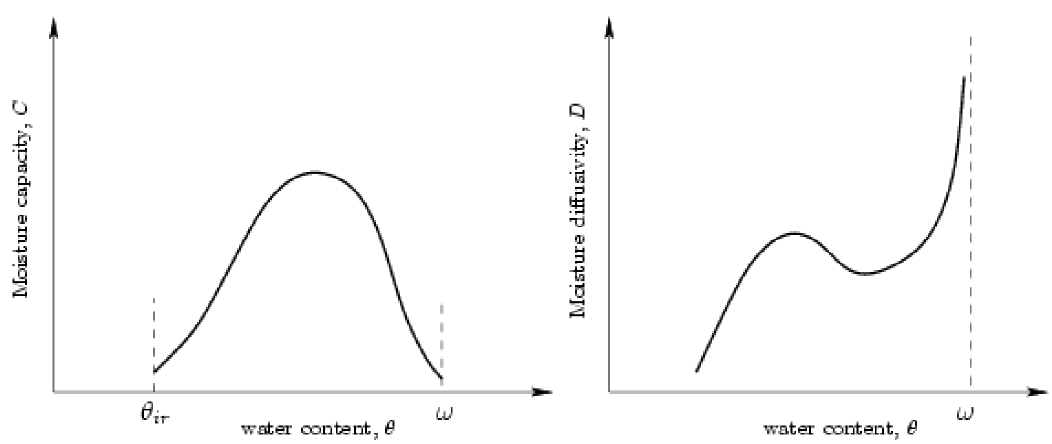


Figure 3.4: A schematic representation of the functional dependences of the specific moisture capacity $C(\theta)$ and moisture diffusivity $D(\theta)$.

The θ-based form. Since

$$\nabla\psi = \frac{\partial \psi}{\partial \theta}\nabla\theta, \tag{3.18}$$

Richards' equation (3.15) can be expressed in the θ-based form

$$\frac{\partial \theta}{\partial t} = \nabla \cdot [D(\theta)\nabla\theta] + \frac{\partial K_w}{\partial x_3} + F. \tag{3.19}$$

The function $D(\theta)$ is called the *moisture diffusivity*. It is a property of the medium, whose general behavior is shown in Figure 3.4.

Pros & cons of the two forms of Richards' equation. The advantages of the ψ-based form of the Richards' equation (3.17) are[5]

- Since equation (3.17) describes flow in both unsaturated and saturated regions of a porous medium, it can be used throughout a computational domain. There is no need to identify the transitional zone between the two regions.
- The continuity of the hydraulic head $h_w = \psi + z$ across a porous medium consisting of different materials facilitates numerical solutions of (3.17).

The disadvantage of the ψ-based form of the Richards' equation is that both its left and right hand side are nonlinear. Hence special care must be paid while solving it numerically.

The advantage of the θ-based form of the Richards' equation (3.19) is[6]

- Its left hand side is linear. This fact facilitates numerical solutions of (3.19) for infiltration into dry soils.

The disadvantages of the θ-based form of the Richards' equation (3.19) are

- One can see from Figure 3.4 that $D(\theta) \to \infty$ as $\theta \to \omega$. This invalidates equation (3.19) for regions close to saturation.
- Since θ is discontinuous across material interfaces, solving equation (3.19) for layered media is problematic.

3.5 Characterization of Vadose Zone

Here we provide a brief overview of some of the approaches used to measure various parameters describing flow in unsaturated regions (vadose zone)[7].

[5] de Marsily, 1986; Sec. 9.2.1, p. 215
[6] Neuman, Classnotes, U of A.
[7] After D. Hillel, Fundamentals of Soil Physics, 1980

3.5.1 Measurement of Water Content

Laboratory drying. Collect samples in the field and bring them to the lab. Place samples in an oven at $105°C$ for 24 hours. Determine the *mass (gravimetric) wetness* of the sample w as the ratio

$$w = \frac{\text{(wet weight) - (dry weight)}}{\text{(dry weight)}} = \frac{\text{weight loss in drying}}{\text{weight of dried sample}}. \tag{3.20}$$

Finally, use

$$\theta = \frac{\rho_b}{\rho_w} w \tag{3.21}$$

to determine the volumetric water content θ. Here ρ_w is the density of water, and $\rho_b = M_s/V_t$ is the *dry bulk density* (V_t denotes the total volume of the sample).

Field measurement: Electrical resistance. This method is based on an observation that the electrical resistance of a soil varies with its water content. To minimize the spurious effects of soil's composition, texture, and soluble salt concentration, electrodes are embedded in an electrical resistance block. After the block is placed in a soil, it equilibrated with the surrounding. As discussed earlier, it equilibrates with suction ψ rather than with water content θ. Hence the electrical resistance is usually calibrated against suction, and then water content is determined from the retention curve $\psi = \psi(\theta)$. Such a procedure is prone to hysteresis.

Field measurement: Neutron scattering. This method is based on an observation that the rate with which *alpha particles* slow down is proportional to the degree of the saturation of a soil. A typical *neutron moisture meter* consists of a probe that emits fast neutrons and a scaler that monitors the flux of slow neutrons. The neutrons are slowed down by the collisions with atoms of the soils and water. The slow neutron count rate N_w in a wet soil is linearly proportional to the volumetric moisture content θ,

$$N_w = m\theta + b, \tag{3.22}$$

where m and b are fitting parameters.

Laboratory & field measurement: Gamma-ray absorption. Gamma-ray scanners are based on the ideas similar to those discussed above for neutron moisture meters, except they use gamma particles. A typical devise consists of two probes: one hosting a source of gamma particles (e.g., radioactive cesium) and the other containing a detector (counter). The measurements are related to water content through the following relation,

$$N_w = N_d \mathrm{e}^{-\theta_m \beta_w b}, \tag{3.23}$$

where N_w and N_d are the radiation fluxes transmitted through wet and dry soils, respectively; θ_m is the mass of water per unit bulk volume of soil; β_w is the mass attenuation coefficient for water; and b is the soil's thickness.

3.5.2 Measurement of Suction

Tensiometers are often used for *in situ* measurements of hydraulic head and suction.[8] A tensiometer consists of a porous cup that is connected to a tube fully filled with water and equipped with a vacuum gauge (Figure 3.5). Without a contact with a soil, water in the tensiometer is in equilibrium with atmospheric pressure. After the tensiometer is inserted into an unsaturated soil in which water pressure is below atmospheric, suction pulls water out of the tensiometer. This creates a partial vacuum inside the tube that is read on the vacuum gauge. The dryer the soil, the higher the reading on the vacuum gauge.

Figure 3.5: Tensiometers are often used to measure suction in unsaturated soils.

3.5.3 Measurement of the Soil-Moisture Characteristic Curves

The soil-moisture characteristic (retention) curves specify the dependence of suction on water content (saturation), $\psi = \psi(\theta)$. Since we know how to measure both ψ and θ, experimental determination of $\psi = \psi(\theta)$ is a matter of plotting one versus the other.[9]

In a saturated sample, water content is $\theta = \omega$ and $\psi = p_{\text{atmospheric}} = 0$. When a slight suction is applied to water in a saturated sample, no outlflow may occur until suction increases a certain value ψ_e, at which the largest pores begin to empty. This critical suction is called the *air-entry suction*. As suction $\psi \geq \psi_e$ increases further, more water is drawn from the sample, i.e., its water content decreases. Since $\psi \sim r^{-1}$, a gradual increase in suction leads to the emptying of progressively smaller pores until the irreducible (residual) water content θ_r is reached. This process is shown schematically in the second of Figures 3.3.

A number of *empirical* relationships have been proposed to fit the $\psi - \theta$ data. These include Gardner's model

$$\psi = a\theta^{-b}, \tag{3.24}$$

[8]Hillel, p. 155, Sec. 7.N

[9]The following discussion follows verbatim Hillel, Sec. 7.L (p.148) and Sec 7.M (p.152). See also Sec. 7.N.3 (p.161)

and the Brooks and Corey model

$$\left(\frac{\psi}{\psi_e}\right)^\lambda = \frac{\omega - \theta_r}{\theta - \theta_r}. \tag{3.25}$$

Here the constants a, b, ψ_e, λ, and θ_r are fitting parameters determined by the data.

These and other relationships work well for some soils and fail for others. They are generally applicable to limited suction ranges. A typical experimental setup to conduct these experiments is called a tension plate assembly.

Hysteresis. The relationship between ψ and θ can be measured in two ways: (i) in *desorption*, by taking an initially saturated sample and applying increasing suction to gradually dry it while taking successive measurements of ψ and θ; and (ii) in *sorption*, by gradually wetting up an initially dry sample while reducing the suction. Unfortunately, these two alternatives often result in two different water retention curves (Figure 3.6). This phenomenon is called *hysteresis*.

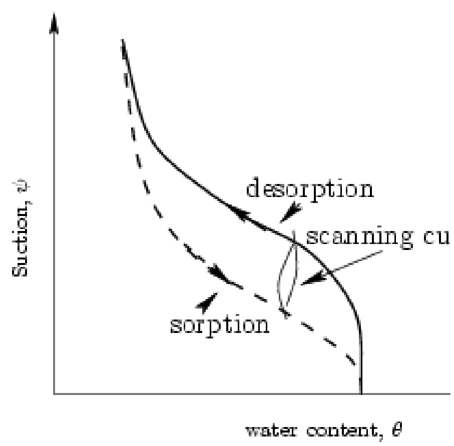


Figure 3.6: Hysteresis in the water retention curves $\psi = \psi(\theta)$.

Among many reasons for hysteresis are

- entrapped air, which decreases the water content of newly wetted samples; and
- the geometric nonuniformity of the individual pores, resulting in the so-called "inkbottle" effect.

Water retention curves that are generally reported represent the desorption curves, since they are easier to determine experimentally than the sorption curves.

3.5.4 Measurement of Unsaturated Hydraulic Conductivity

Unsaturated hydraulic conductivity $K(\psi)$ is often expressed as the product of saturated (K_s) and relative (K_r) hydraulic conductivities, $K(\psi) = K_s K_r(\psi)$. When the medium becomes saturated, $\theta = \omega$, $\psi = 0$, and $K_r(\psi = 0) = 1$. Both laboratory and field setups for measuring unsaturated hydraulic conductivity in Hillel, Sec. 9 (Subsections H and I, respectively).

Here we will consider a hypothetical Darcy's experiment with an unsaturated soil.[10] Consider an unsaturated soil sample ensconced in a tube of length L. Suction $\psi(x = 0) = \Psi_1$ and $\psi(x = L) = \Psi_2$ is maintained at the two ends of the tube (sample). As established above, the variation in suction along the length of the sample causes the saturation and relative hydraulic conductivity to do the same. We therefore make an assumption that the sample is sufficiently short to allow us to evaluate an average conductivity for the whole sample from Darcy's law $q = K\triangle\psi/L$. For various average suctions $\overline{\Psi} = (\Psi_1 + \Psi_2)/2$, one can measure the flux q and compute the unsaturated hydraulic conductivity as $K = qL/\triangle\psi$. The result is shown in Figure 3.7.

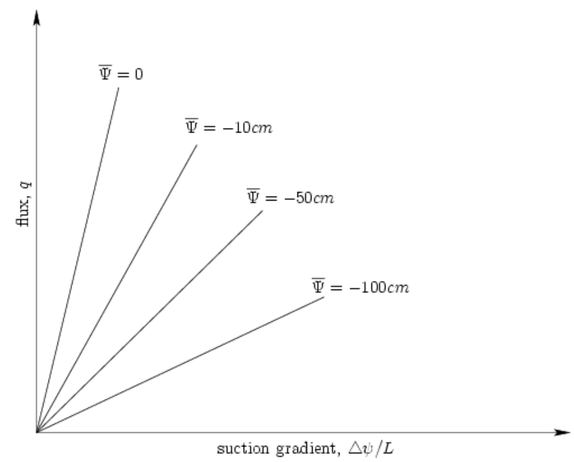


Figure 3.7: Unsaturated hydraulic conductivity is given by the slope of the q versus $\triangle H/L$ lines. It depends on average suction $\overline{\Psi}$.

3.6 Horizontal wetting of porous media

Steady-state regime. Consider a horizontal column of an unsaturated soil in equilibrium with water in a container that is located at the column's inlet $x = 0$. The length of the column is L. The soil remains dry at the outlet $x = L$. Our goal is to find the distribution of moisture inside the soil sample.

The state of equilibrium implies a steady-state regime. Since the column is horizontal, this implies that the distribution of moisture in the sample is described by the steady-state version of (3.19),

$$0 = \frac{\mathrm{d}}{\mathrm{d}x}\left[D(\theta)\frac{\mathrm{d}\theta}{\mathrm{d}x}\right]. \tag{3.26}$$

The physical conditions at the inlet and outlet of the column imply the following boundary conditions,

$$\theta(x = 0) = \omega, \qquad \theta(x = L) = \theta_r. \tag{3.27}$$

[10] After Hillel, Sec. 9.C, p. 198

Integrating (3.26), while accounting for the first boundary condition, we obtain

$$\int_{\omega}^{\theta} D(\theta')\mathrm{d}\theta' = cx, \tag{3.28}$$

where c is a constant of integration. The detailed distribution of moisture inside the sample depends of the functional form of moisture diffusivity $D(\theta)$. It is quite a complex function, whose behavior is shown in Figure 3.4. For simplicity, we assume that the moisture diffusivity increases exponentially with water content, i.e, that $D = \exp(\theta)$. This results in

$$\theta = \ln(cx + \mathrm{e}^{\omega}). \tag{3.29}$$

Using the boundary condition at $x = L$ to determine c, we obtain the final expression for the moisture profile,

$$\theta(x) = \ln\left[(\mathrm{e}^{\theta_r} - \mathrm{e}^{\omega})\frac{x}{L} + \mathrm{e}^{\omega}\right]. \tag{3.30}$$

Transient regime. Consider a horizontal column of an unsaturated soil that, at time $t = 0$, has been brought in contact with water in a container that is located at the column's inlet $x = 0$. Our goal is to model the wetting of the soil sample. We will look at an early time period during which only a part of the sample gets wet, i.e., we can assume that the length of the column is infinite so that the soil remains dry at $x = \infty$.

The wetting process is described by (3.19),

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}\left[D(\theta)\frac{\partial \theta}{\partial x}\right]. \tag{3.31}$$

The physical conditions at the inlet and outlet of the column imply the following initial and boundary conditions,

$$\theta(x, 0) = \theta_r, \qquad \theta(0, t) = \omega, \qquad \theta(\infty, t) = \theta_r. \tag{3.32}$$

Boltzmann's transformation

$$\xi = \frac{x}{\sqrt{t}} \tag{3.33}$$

transforms the partial differential equation (3.31) into an ordinary differential equation

$$-\frac{\xi}{2}\frac{\mathrm{d}\theta}{\mathrm{d}\xi} = \frac{\mathrm{d}}{\mathrm{d}\xi}\left[D(\theta)\frac{\mathrm{d}\theta}{\mathrm{d}\xi}\right]. \tag{3.34}$$

The three initial and boundary conditions (3.32) are transformed into two boundary conditions

$$\theta(\xi = 0) = \omega \qquad \theta(\xi = \infty) = \theta_r. \tag{3.35}$$

For general functional relations of moisture diffusivity $D(\theta)$, the boundary value problem (3.34) – (3.35) has to be solved numerically. The advantages of using Boltzmann's transformation are twofold. First, the ordinary differential equation (3.34) is easier and computationally less expensive to solve numerically than the partial differential equation (3.31). Second, it shows that water content θ depends on space x and time t only in combination $\xi = x/\sqrt{t}$, rather than separately. This implies that the wetting front moves through the column in a self-similar manner, i.e., without changing its shape (Figure 3.8).

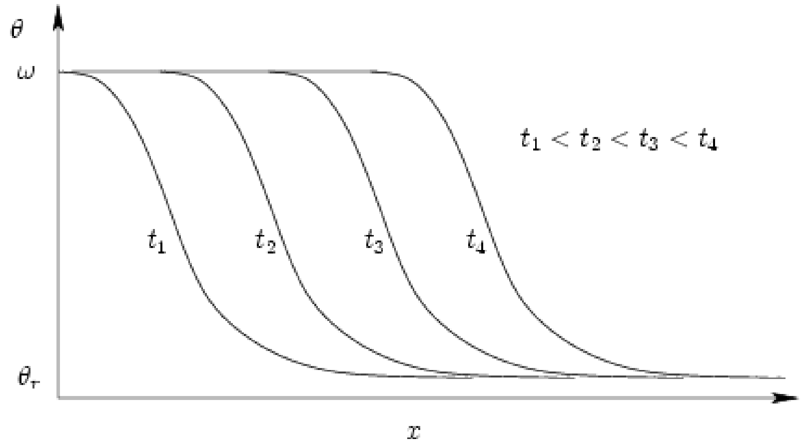


Figure 3.8: Propagation of a self-similar wetting front.

3.7 Vertical Wetting of Porous Media: Infiltration

Consider infiltration into an initially dry homogeneous soil of large (infinite) vertical extent. The process is described by the one-dimensional Richards equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K\frac{\partial \psi}{\partial z}\right) + \frac{\partial K}{\partial z} \tag{3.36}$$

subject to the initial and boundary conditions

$$\theta(z,0) = \theta_r, \qquad \theta(0,t) = \omega, \qquad \theta(\infty,t) = \theta_r. \tag{3.37}$$

Due to the highly nonlinear nature of Richards' equation introduced by the dependencies $K(\theta)$ and $\psi(\theta)$, it has to be solved numerically in all but a few special cases. Here we consider one such a case, which employs the following exponential relations

$$K(\psi) = K_s \mathrm{e}^{\alpha\psi}, \qquad \text{and} \qquad \theta = \mathrm{e}^{\alpha\psi}. \tag{3.38}$$

Substituting (3.38) into (3.36) and introducing a new dependent variable

$$\Phi = \mathrm{e}^{\alpha\psi}, \tag{3.39}$$

we obtain

$$\frac{\partial \Phi}{\partial t} = \frac{K_s}{\alpha}\frac{\partial^2 \Phi}{\partial z^2} + \frac{\partial \Phi}{\partial z}. \tag{3.40}$$

This linear differential equation can be solved by a variety of standard techniques, e.g., by Laplace transform. The resulting solution is a sigmoidal moisture profile $\theta(z,t)$ propagating downward with time.

Green and Ampt (1911) model of infiltration. The problem can be significantly simplified by approximating the shape of a wetting front. Green and Ampt's model replaces an actual sigmoidal wetting front with a step function. This approach ignores the transitional zone wherein water content gradually decreases from ω to θ_r.

Let $z_f(t)$ be the position of the wetting front at time t. Let $h_f = \psi_f + z_f$ denote the hydraulic head on the wetting front, and $h_0 = \psi_0$ denote the hydraulic head on the soil's surface $z = 0$. The flux i, which is called *infiltration rate*, is determined from Darcy's law as

$$i = -K_s \frac{h_f - h_0}{z_f} = -K_s \frac{\psi_f + z_f - \psi_0}{z_f}. \tag{3.41}$$

On the other hand, the velocity of the wetting front is $v_f = -\mathrm{d}z_f/\mathrm{d}t$, where the minus sign indicates that the movement is downward, while the vertical z coordinate is positive upward. The corresponding mass flux is

$$i = -\triangle\theta \frac{\mathrm{d}z_f}{\mathrm{d}t}, \tag{3.42}$$

where $\triangle\theta = \omega - \theta_r$ is the change in water content between the wet and dry states. Equating the two expressions gives a differential equation

$$\triangle\theta \frac{\mathrm{d}z_f}{\mathrm{d}t} = K_s \frac{\psi_f - \psi_0 + z_f}{z_f}, \qquad z_f(t=0) = 0, \tag{3.43}$$

whose solution is

$$z_f - (\psi_f - \psi_0) \ln\left(1 + \frac{z_f}{\psi_f - \psi_0}\right) = \frac{K_s}{\triangle\theta} t, \tag{3.44}$$

This solution describes the evolution of the wetting front $z_f(t)$. The suction on the wetting front is yet unknown. It is specified empirically, e.g., as (Bower, 1964)

$$\psi_f = -\int_{\psi_{\mathrm{dry}}}^{0} K_r(\psi)\mathrm{d}\psi. \tag{3.45}$$

3.8 Evapotranspiration

Two main physical mechanisms of extracting water from the vadoze zone are *evaporation* and *transpiration* (root uptake).[11] Water extraction is modeled by a source term F in the Richards equation (3.15)

$$\frac{\partial\theta}{\partial t} = \nabla \cdot (K_w \nabla\psi) + \frac{\partial K_w}{\partial x_3} - F, \qquad F = T + E. \tag{3.46}$$

The minus sign in front of F indicates that water is being extracted from the system. Physical intuition suggests that both transpiration flux T and evaporation flux E should depend on saturation and vary with depth. There exist a number of alternative *phenomenological* models that describe these dependences[12]. A few of them are described below.

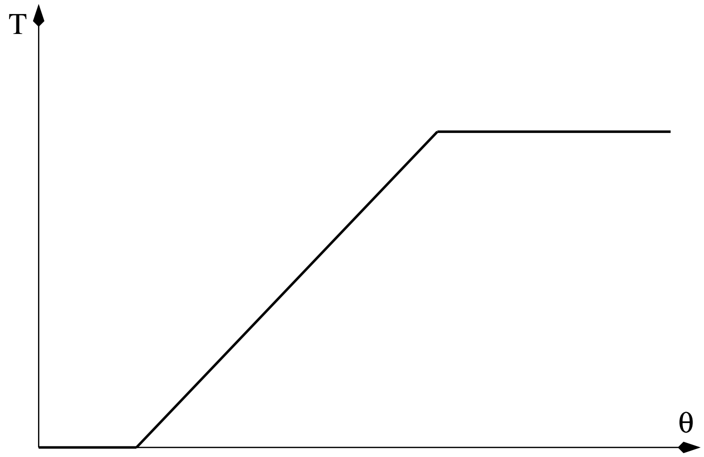


Figure 3.9: A piece-wise linear model of the dependence of transpiration T on water content θ.

3.8.1 Models for Transpiration

A piece-wise linear model. It is shown in Figure 3.9 and assumes that (i) there is no transpiration below the so-called wilting saturations S_w (plants die) and (ii) above some saturation S_s transpiration is constant.

Root resistivity model. According to Darcy's law, water will flow towards a plant's roots if $\psi_{\text{roots}} < \psi_{\text{soil}}$. The corresponding transpiration flux is given by Darcy's law,

$$T = -K_{r,s} \nabla \psi = \frac{\psi_{\text{soil}} - \psi_{\text{roots}}}{r_{\text{soil}} + r_{\text{roots}}}, \tag{3.47}$$

where r_{soil} and r_{roots} are the resistivities of the soil and roots, respectively. The resistivities are inversely proportional to the corresponding conductivities and represent resistance to flow exerted by the soil and roots.

It is reasonable to assume that resistance to flow is inversely proportional to the root density ρ_{roots},

$$r_{\text{roots}} = \frac{C_{\text{r}}}{\rho_{\text{roots}}}, \qquad r_{\text{soil}} = \frac{C_{\text{s}}}{\rho_{\text{roots}} K(\theta)}, \tag{3.48}$$

where C_{r} and C_{s} are fitting parameters.

3.8.2 Models for Evaporation

These have analogous forms to the transpiration models described above.

3.8.3 Lumped-parameter Models

If one is concerned with the vadoze zone only as a conduit of water from the soil surface to the water table, the so-called *lumped-parameter* parameter models might be sufficient. Such models are essentially a mass

[11]The presentation below is based on Ch. 11.3.4 of *Subsurface hydrology* by Pinder and Celia.
[12]See Ref [19] in *Pinder and Celia*.

balance for the vadoze zone and do not yield a spatial distribution of saturation. A typical lumped-parameter model can be obtained by spatial averaging of Richards equation.

For vertical (i.e., one-dimensional) infiltration, this gives

$$\int_0^R \frac{\partial \theta}{\partial t} \mathrm{d}z = -\int_0^R \frac{\partial q_z}{\partial z} \mathrm{d}z - \int_0^R F \mathrm{d}z, \tag{3.49}$$

where R is the averaging length scale, e.g., the depth of a root zone or depth to the water table. This leads to

$$R \frac{\partial \theta_{\mathrm{av}}}{\partial t} = -q_{\mathrm{inf}} + q_{\mathrm{leak}} - ET_{\mathrm{tot}}, \tag{3.50}$$

where

$$\theta_{\mathrm{av}} = \frac{1}{R} \int_0^R \theta \mathrm{d}z \tag{3.51}$$

is the average water content in the vadoze zone, $q_{\mathrm{inf}} = q_z(0)$ is the infiltration rate, $q_{\mathrm{inf}} = q_z(R)$ is the downward leakage rate, and

$$ET_{\mathrm{tot}} = \frac{1}{R} \int_0^R F \mathrm{d}z = R(T_{\mathrm{av}} + E_{\mathrm{av}}) \tag{3.52}$$

is the total evapotranspiration.

Chapter 4

Dispersion of Contaminants

The presence of a soluble contaminant (solute) in water in general, and in subsurface water in particular, can be quantified by its concentration $C(\mathbf{x}, t)$. We will use the following definition of (volumetric) concentration,

$$C = \frac{\text{mass of solute}}{\text{volume of solution}} = \frac{[M]}{[L^3]}.$$

Migration of subsurface contaminants is described by the evolution of concentration in space and time. The latter is governed by transport equations.

4.1 Derivation of Transport Equations

A solute in porous media can be affected by the following processes:

a) Advection,

b) Molecular diffusion,

c) Kinematic dispersion,

d) Biochemical reactions, etc.

These processes are combined with mass conservation to derive a transport equation.[1]

Advection. The migration of a dissolved substance due to the movement of water is called *advection*. Recalling that the Darcy velocity $\mathbf{q}$ is a volumetric flux, we can write *mass flux* of the transported substance as

$$\mathbf{J}_a(\mathbf{x}, t) = \mathbf{q}(\mathbf{x}, t)C(\mathbf{x}, t). \tag{4.1}$$

If one releases a particle of substance at a point $\mathbf{X}$ at time $t = 0$, in time $\triangle t$ it will end up at a point $\mathbf{Y} = \mathbf{X} + \mathbf{q}\triangle t$. Releasing many particles with total concentration C results in (4.1). A contaminant plume

[1] The following derivation is based on de Marsily, Chapter 10.

of shape Ω will be transported to another location (the displacement vector is $\mathbf{q}\triangle t$) without changing its shape.

Molecular diffusion. This is a mixing process by which a substance migrates even in the absence of flow. It is based on movement of molecules of a substance among molecules of water (the so-called Brownian motion). This process is described by Fick's law $\mathbf{J}_m(\mathbf{x},t) = -D_m \nabla C(\mathbf{x},t)$, where $\mathbf{J}_m$ is the molecular flux of substance and D_m is the molecular diffusion. In porous media, the molecular diffusion coefficient is smaller than its counterpart in a free fluid, since solute particles diffuse in the solid matrix much slower (if at all) than in the fluid. Fick's law can be modified to account for this effect,

$$\mathbf{J}_m(\mathbf{x},t) = -\omega D_m \nabla C(\mathbf{x},t). \tag{4.2}$$

Diffusion occurs even in the absence of flow and manifests itself through spreading of a solute plume.

Kinematic dispersion. This mixing process is due to the variability of the velocities both within a single pore (Poiseuille formula) and within a pore network. Numerous experimental and theoretical studies[2] have shown that the dispersive flux $\mathbf{J}_d$ can be written in analogy to the molecular flux (4.2) as[3]

$$\mathbf{J}_d(\mathbf{x},t) = -\mathbf{D}_d \nabla C(\mathbf{x},t), \tag{4.3}$$

where the coefficient $\mathbf{D}_d$ is called a *dispersion coefficient*. The dispersion accounts for the spread of a solute plume.

The similarity between (4.2) and (4.3) can be misleading. First, the dispersive flux $\mathbf{J}_d$ is induced by the fluid's velocity, e.g., by the Darcy velocity $\mathbf{q}$. As such, it should depend on $\mathbf{q}$. In (4.3), this dependence can only by accounted for by stipulating that the dispersion coefficient $\mathbf{D}_d$ is a function of $\mathbf{q}$. Second, experimental studies have shown that a plume spreads more in the mean direction of the flow (longitudinal direction) than in the direction perpendicular to flow (transverse direction). In other words, the dispersion coefficient D_{d_L} in the longitudinal direction is large than the dispersion coefficient D_{d_T} in the transverse direction, $D_{d_L} > D_{d_T}$. This means that the dispersion coefficient $\mathbf{D}_d$ is a *tensor*.

To analyze the dependence of the dispersion coefficient tensor on flow velocity, one can introduce a dimensionless Peclet number,

$$Pe = \frac{|\mathbf{q}| l}{\omega D_m}, \tag{4.4}$$

which compares the diffusive and advective transport mechanisms. The parameter l is a characteristic length of a porous media, e.g., the mean radius of pores or grains. For a typical range of flow regimes in porous media, $Pe > 10$ and the following relations have been observed,

$$D_{d_L} = \lambda_L |\mathbf{q}|, \qquad D_{d_T} = \lambda_T |\mathbf{q}|. \tag{4.5}$$

The coefficients λ_L and λ_T are called the *longitudinal and transverse dispersivities*, respectively. They have units of length and $\lambda_L > \lambda_T$. A typical ratio between the two, λ_T/λ_L, is on the order of 0.1.

The total mass flux of a solute migrating in porous media is

$$\mathbf{J} = \mathbf{J}_a + \mathbf{J}_m + \mathbf{J}_d. \tag{4.6}$$

[2] E.g., G. I. Taylor (1953).

[3] Alternative theories that dispute this relation also exist.

Consider an elementary volume in a coordinate system, whose x coordinate is aligned with the Darcy velocity $\mathbf{q}$ (Fig. 4.1). The mass of solute contained within this volume is

$$M(\mathbf{x},t) = C(\mathbf{x},t)\omega\triangle x\triangle y\triangle z. \tag{4.7}$$

According to mass conservation, the change in mass of the solute $\triangle M(\mathbf{x},t) \equiv M(\mathbf{x},t+\triangle t) - M(\mathbf{x},t)$

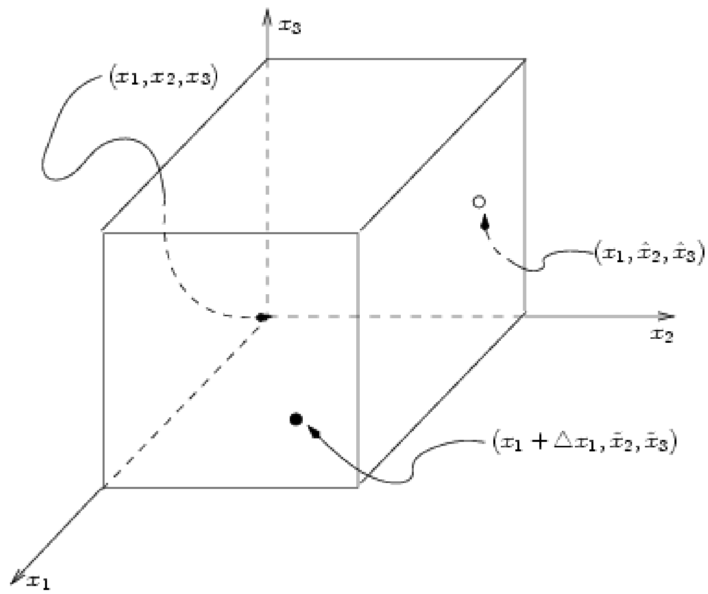


Figure 4.1: An elementary volume used to derive transport equations.

during time interval $\triangle t$ must be balanced by the influx and outflux of the solute and, if present, biochemical reactions $R(C)$. This balance gives

$$\omega\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(\tilde{D}_L\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\tilde{D}_T\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(\tilde{D}_T\frac{\partial C}{\partial z}\right) - \frac{qC}{\partial x} + R(C), \tag{4.8}$$

where

$$\tilde{D}_L = \omega D_m + \lambda_L|\mathbf{q}|, \qquad \tilde{D}_T = \omega D_m + \lambda_T|\mathbf{q}|. \tag{4.9}$$

For transport in porous media with constant porosity, it is common to rewrite these equations as

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_L\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_T\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_T\frac{\partial C}{\partial z}\right) - \frac{uC}{\partial x} + \frac{1}{\omega}R(C), \tag{4.10}$$

where

$$D_L = D_m + \lambda_L|\mathbf{u}|, \qquad D_T = D_m + \lambda_T|\mathbf{u}|. \tag{4.11}$$

Here $\mathbf{u} \equiv \mathbf{q}/\omega$ is called the *mean microscopic flow velocity*. For an arbitrary orientation of the elementary volume relative to the direction of flow, these equations are generalized to give

$$\frac{\partial C}{\partial t} = \nabla\cdot(\mathbf{D}\nabla C) - \nabla\cdot(\mathbf{u}C) + R(C), \tag{4.12}$$

4.2 Adsorption of a Chemically Reactive Solute

The term $R(C)$ in (4.12) can account for chemical reactions that remove(add) the solute from(to) the solution. Here we consider an example of such a process: adsorption of the solute onto the pores's surface. Since this phenomenon removes the solute from the solution, $R < 0$.

Let F denote the mass concentration of the adsorbed substance,

$$F = \frac{\text{mass of adsorbed solute}}{\text{unit mass of solid}}.$$

Since the mass of solids in a unit volume of the porous medium is

$$(1-\omega)\rho_s = \frac{\text{unit mass of solids}}{\text{unit volume of porous media}},$$

the mass of substance bound to solids in unit volume of porous media is $(1-\omega)\rho_s F$. Thus the change in mass per unit volume per unit time is

$$R = -(1-\omega)\rho_s \frac{\partial F}{\partial t} \tag{4.13}$$

so that (4.12) becomes

$$\omega \frac{\partial C}{\partial t} + (1-\omega)\rho_s \frac{\partial F}{\partial t} = \nabla \cdot \left(\tilde{\mathbf{D}} \nabla C \right) - \nabla \cdot (\mathbf{q} C). \tag{4.14}$$

Note that this formulation does not account for a possible clogging of pores. If adsorption is *instanteneous*, it might be possible under some conditions to write

$$F = K_d C, \tag{4.15}$$

where K_d is the distribution coefficient of the substance in relation to the porous medium. Its units are $[K_d] = L^3 M^{-1}$. Then, introducing the retardation coefficient R_c,

$$\omega R_c \frac{\partial C}{\partial t} = \nabla \cdot \left(\tilde{\mathbf{D}} \nabla C \right) - \nabla \cdot (\mathbf{q} C), \qquad R_c = 1 + \frac{1-\omega}{\omega} \rho_s K_d. \tag{4.16}$$