

MULTIPHASE FLUID FLOW IN POROUS MEDIA

(i.e. Fluid-Solid Interactions in Environmental Engineering)

Syllabus

1-Basic characteristics of rocks (Porosity, Permeability, Fluid saturations).

2-Properties of porous media containing multiple fluid saturations (Surface forces and capillary pressure, Effective and relative permeability).

3-Immiscible fluid displacement mechanism.

4-Miscible displacement.

5-Simultaneous flow of multiple phases in porous media.

References

1. "Numerical Computation of Multiphase Flows in Porous Media" Peter Bastian Heidelberg, June 1999.
2. "Upscaling Multiphase Flow in Porous Media" D.B. DAS and S.M. HASSANIZADEH, ISBN 1-4020-3513-6 (HB), 2005 Springer.

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. This figure also explains the genesis of groundwater. We will be concerned with its movement.

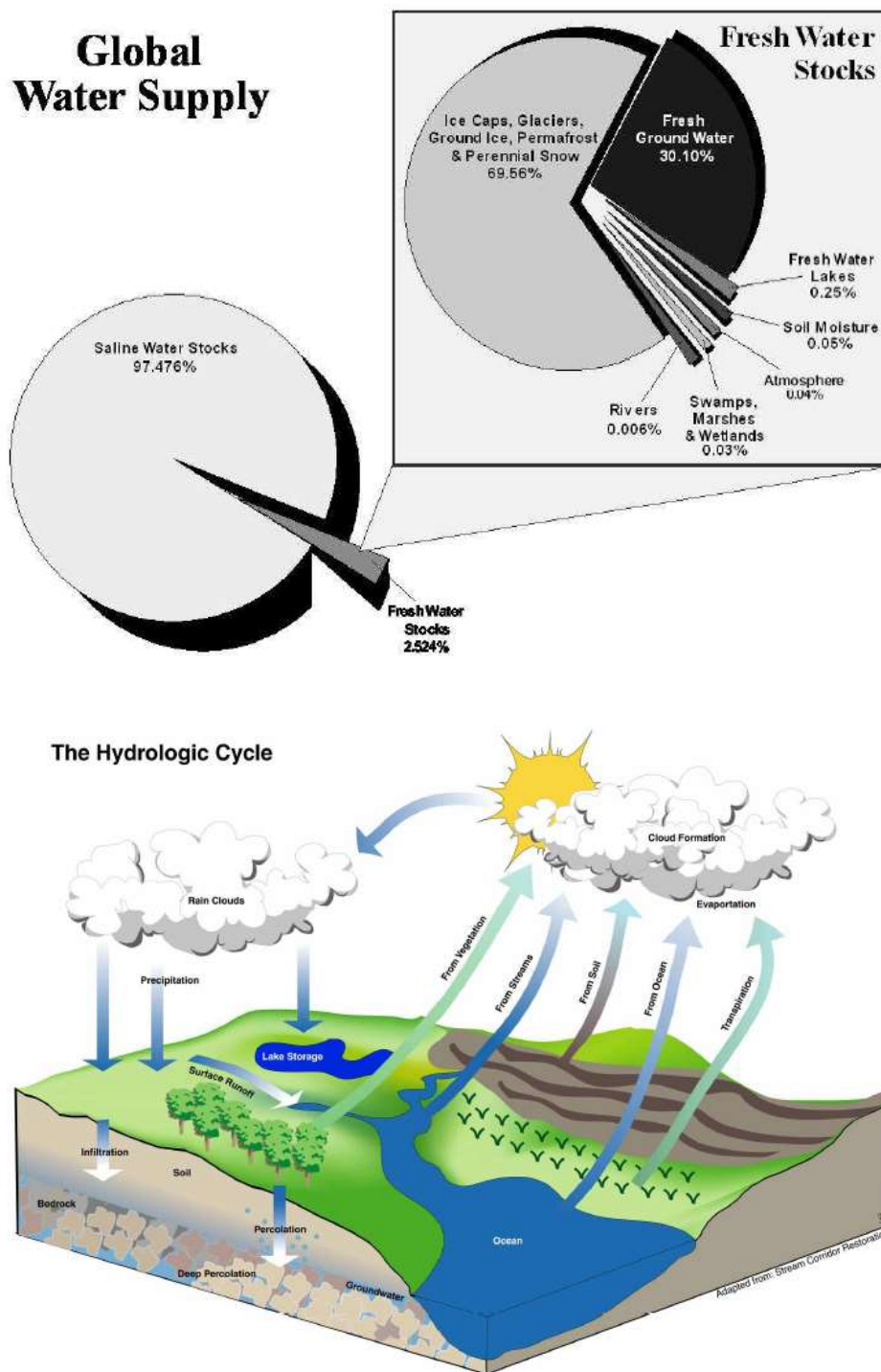


Figure 1: The distribution of global water supply and the hydrologic cycle.

1) Definitions

A **porous medium** is a body composed of a persistent solid part, called solid matrix, and the remaining void space (or pore space) that can be filled with one or more fluids (e.g. water, oil and gas). Typical examples of a porous medium are soil, sand, rubber etc.

A **phase** is defined in (Bear and Bachmat 1991) as a chemically homogeneous portion of a system under consideration that is separated from other such portions by a definite physical boundary. In the case of a **single-phase** system the void space of the porous medium is filled by a single fluid (e.g. water) or by several fluids completely miscible with each other (e.g. fresh water and salt water). In a **multiphase** system the void space is filled by two or more fluids that are **immiscible** with each other, i.e. they maintain a distinct boundary between them (e.g. water and oil). There may only be one gaseous phase since gases are always completely miscible. Formally the solid matrix of the porous medium can also be considered as a phase called the solid phase. Fig. 2 shows a two-dimensional cross section of a porous medium filled with water (single-phase system) or filled with water and oil or air (two-phase system).

Bear and Bachmat (1991) define a **component** to be part of a phase that is composed of an identifiable homogeneous chemical species or of an assembly of species (ions, molecules). The number of components needed to describe a phase is given by the conceptual model, i.e. it depends on the physical processes to be modeled. The example of fresh and salt water given above is described by a single-phase two component system.

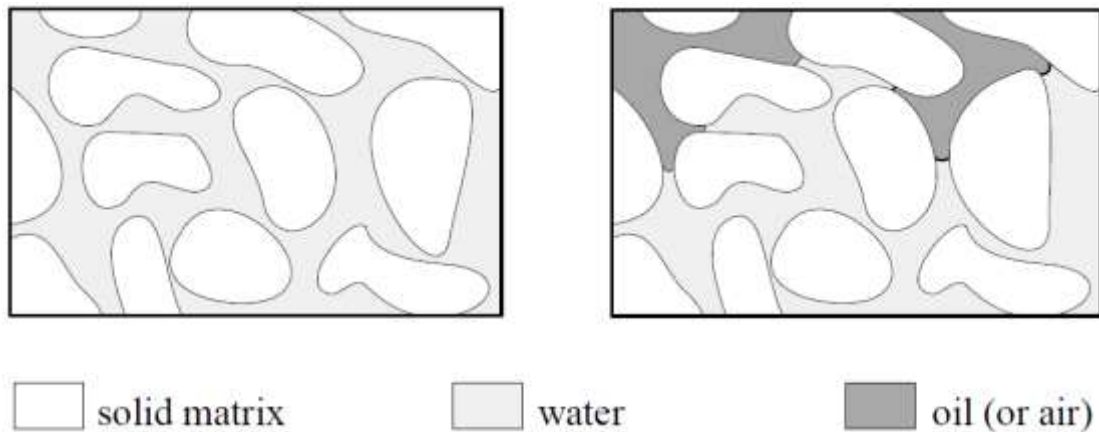


Figure 2: Schematic drawing of a porous medium filled with one or two fluids.

In order to derive mathematical models for fluid flow in porous media some restrictions are placed upon the geometry of the porous medium:

- 1) The void space of the porous medium is interconnected. Since no flow can take place in a disconnected void space.
- 2) The dimensions of the void space must be large compared to the mean free path length of the fluid molecules.
- 3) The dimensions of the void space must be small enough so that the fluid flow is controlled by adhesive forces at fluid–solid interfaces and cohesive forces at fluid–fluid interfaces (multiphase systems).

2) Microscopic and Macroscopic Models

The important feature in modeling porous media flow is the consideration of different length scales. Fig. 3 shows a cross section through a porous medium consisting of different types of sands on three length scales.

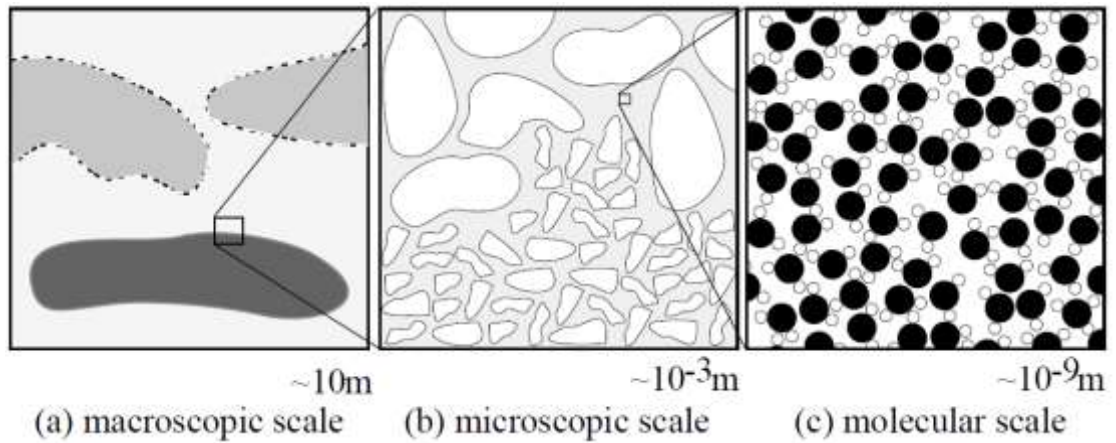


Figure 3: Different scales in a porous medium.

In Fig. 3a the cross section is on the order of 10 meters wide. This scale is called the **macroscopic scale**. A larger scale than the macroscopic scale is often called **regional scale** but is not considered here.

If we zoom in to a scale of about 10^{-3} m as shown in Fig. 3b we arrive at the **microscopic scale** where individual sand grains and pore channels are visible.

Magnifying further into the water-filled void space one would finally see individual water molecules as shown in Fig. 3c. The larger black circles are oxygen atoms, the smaller white circles are the hydrogen atoms. This scale of about 10^{-9} m will be referred to as the **molecular scale**.

It is important to note that the behavior of the flow is influenced by effects on all these different length scales. Fluid properties like viscosity, density, binary diffusion coefficient and miscibility are determined on the molecular scale by the individual properties of the molecules. On the microscopic scale the configuration of the void space influences the flow behavior through properties like the tortuosity of the flow channels or the pore size distribution; whereas on the macroscopic scale the large scale

inhomogeneities play a role. The following macroscopic properties of porous media are of interest.

$$\text{Total porosity } (\omega) = \frac{\text{volume of the voids}}{\text{total volume of the medium}}$$

$$\text{Void ratio } (\epsilon) = \frac{\text{volume of the voids}}{\text{volume of the solid}}$$

$$\text{Surface porosity } (\omega_s) = \frac{\text{surface area of the voids in a cross-section}}{\text{total surface area of a cross-section}}$$

$$\text{Specific surface area } (S_{sp}) = \frac{\text{total surface area of the voids}}{\text{total volume of the medium}}$$

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 Fig. 4. Since these parameters are used as coefficients in differential equations, they are treated mathematically as point values. This is accomplished by revoking a concept of the **Representative Elementary Volume (REV)**, according to which macroscopic parameters at a point x are representative of a volume $V_T(x)$ surrounding this point. The REV is then defined as a volume that is both:

- (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.

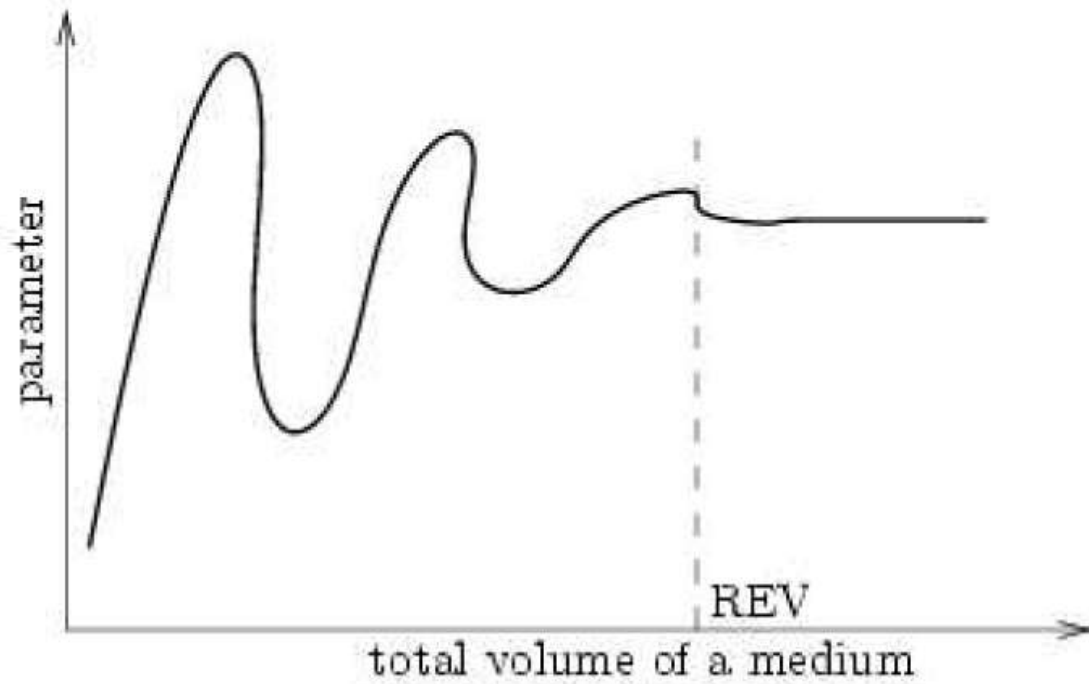


Figure 4: Parameter's variability with the volume of a sample. In homogeneous porous media, this variability diminishes when the sample becomes large enough. The smallest volume at which this occurs is called the Representative Elementary Volume (REV).

3) 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 \underline{A} filled with a porous material, say sand (Fig. 5). The tube is equipped with two piezometers located at elevations Z_1 and Z_2 , a distance ΔL apart. A fluid is introduced through the inlet at a constant rate \underline{Q} . The medium is allowed to saturate, at which point the outflow rate equals the inflow rate \underline{Q} and the elevations of the fluid levels in the piezometers are h_1 and h_2 , respectively. Consider a quantity:

$$q = \frac{Q}{A} \quad (1)$$

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

$$q = -K \frac{\Delta h}{\Delta L} \quad (q \propto \frac{\Delta h}{\Delta L}) \quad K = \frac{cd^2 \rho g}{\mu} \quad (2)$$

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 from a point where the fluid elevation is higher to a point where it is lower. The experimental relation (2) can be written in differential form as

$$q = -K \frac{dh}{dl} \quad (3)$$

and further generalized to flow in two and three dimensions as

$$q = -K \nabla h \quad (4)$$

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

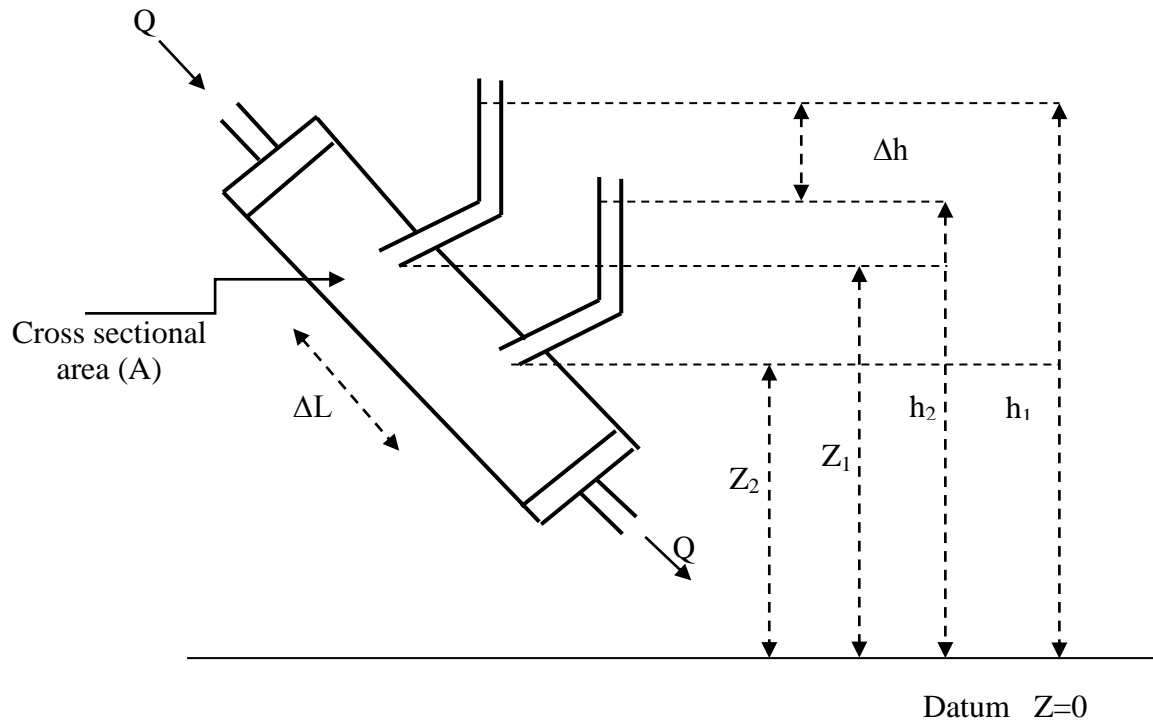


Figure 5: A schematic representation of Darcy's experiment.

4) Hydraulic and Piezometric Head

The physical meaning of the quantity h in Darcy's law (Eq.4) must be examined. Following the standard practice in fluid mechanics, the mechanical energy balance during the flow process will be as follows:

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

$$W_1 = mgz \quad (5)$$

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

$$W_2 = \frac{mu^2}{2} \quad (6)$$

(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 $p = p_o$ at the datum to p at point **M** is

$$W_3 = m \int_{p_o}^p \frac{dp}{\rho(p)} \quad (7)$$

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 equation

$$W = gz + \frac{u^2}{2} + m \int_{p_o}^p \frac{dp}{\rho(p)} \quad (8)$$

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

$$h = z + \frac{u^2}{2g} + m \int_{p_o}^p \frac{dp}{g\rho(p)} \quad (9)$$

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 (Eq.4) predicts.

In porous media, the real fluid velocities u are exceedingly small, so that the dynamic head, the second term in (Eq.9), can be neglected. This reduces the hydraulic head to the static or piezometric head,

$$h = z + m \int_{p_o}^p \frac{dp}{g\rho(p)} \quad (10)$$

In applications of porous-media flow to subsurface phenomena, it is common to select atmospheric pressure as a reference pressure, $p_o \equiv p_{\text{atm}}$, and to express hydraulic heads in relation to the mean sea level. Finally, for incompressible fluids, such as water, (Eq.10) further simplifies to yield

$$h = z + \psi, \quad \psi = \frac{p}{g\rho} \quad (11)$$

where, in accordance with Darcy's experiment (Fig. 5), z and ψ are called *elevation* and *pressure heads*, respectively.

5) Hydraulic Conductivity and Permeability

- Experiments have been carried out with ideal porous media consisting of uniform glass beads of diameter (d).
- When various fluids of density ρ and dynamic viscosity μ are run through the cylinder under constant $\frac{dh}{dl}$, the following relationships are observed

$$q \propto d^2, \quad q \propto \rho g, \quad q \propto \frac{1}{\mu}, \quad (12)$$

$$q = -\frac{cd^2\rho g}{\mu} \frac{dh}{dl} \quad (13)$$

Where c = constant of proportionality (depends on media properties) such as:

1. Distribution of grain sizes
2. The sphericity and roundness of the grain
3. The nature of packing

- Comparison of Eq.13 with the original Darcy's law (Eq.4) shows

$$K = \frac{cd^2\rho g}{\mu} = \frac{k\rho g}{\mu} \quad (14)$$

Hence, Darcy's law (Eq.4) can be written as

$$q = -\frac{k\rho g}{\mu} \nabla h \quad (15)$$

It now becomes apparent that K is indeed a property of both the porous medium (through its intrinsic permeability (k , L^2)) and the fluid (through its density and viscosity).

6) Single-Phase Flow in Porous Media

Equations of groundwater flow are derived by combining Darcy's law (Eq.15) with mass conservation law, i.e., with continuity equations. Mass conservation is represented schematically in Fig.6. It is expressed mathematically as follows.

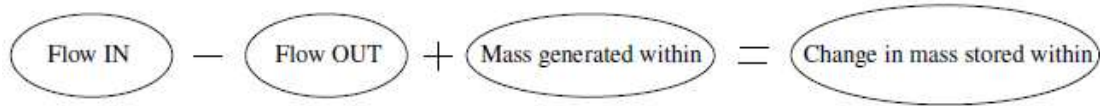


Figure 6: Mass conservation.

Inside a fully saturated porous medium, we select a small cube (Fig.7), whose dimensions are Δx_1 , Δx_2 and Δx_3 , and whose volume is $\Delta V = \Delta x_1 \Delta x_2 \Delta x_3$. The rate of fluid mass flow into the cube through the side $x_1 + \Delta x_1$ during the time interval $[t, t + \Delta t]$ is $Q_1(x_1 + \Delta x_1) = \rho q(x_1 + \Delta x_1) \Delta x_2 \Delta x_3 \Delta t$. According to Darcy's law (Eq.4) this gives:

$$Q_1(x_1 + \Delta x_1) = \rho K \frac{\partial h}{\partial x_1} (x_1 + \Delta x_1) \Delta x_2 \Delta x_3 \Delta t \quad (16)$$

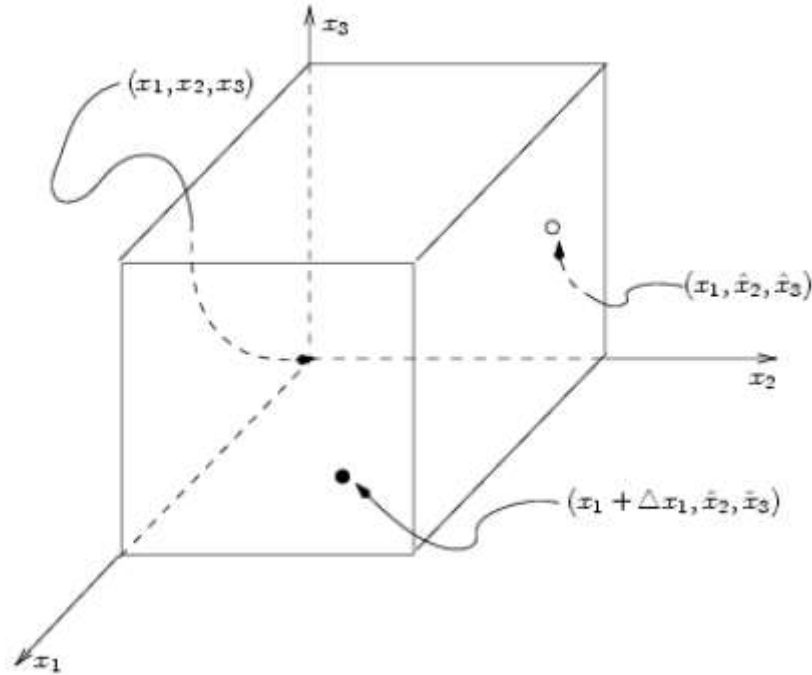


Figure 7: An elementary volume used to derive equations of groundwater flow.

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

$$Q_1(x_1) = \rho K \frac{\partial h}{\partial x_1}(x_1) \Delta x_2 \Delta x_3 \Delta t \quad (17)$$

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

$$\Delta Q_1 = \left[\rho K \frac{\partial h}{\partial x_1}(x_1 + \Delta x_1) - \rho K \frac{\partial h}{\partial x_1}(x_1) \right] \Delta x_2 \Delta x_3 \Delta t \quad (18)$$

In a similar manner, one can derive expressions for ΔQ_2 and ΔQ_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 $f(x, t)$ 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 $[t, t + \Delta t]$ is $Q_a = \rho f \Delta x_1 \Delta x_2 \Delta x_3 \Delta t$.

Finally, the change in fluid mass during the time interval $[t, t + \Delta t]$ is $\Delta m = m(x, t + \Delta t) - m(x, t) = [\rho \omega(t + \Delta t) - \rho \omega(t)] \Delta x_1 \Delta x_2 \Delta x_3$ (19)

The conservation of energy in Fig. 6 can now be written as:

$$\begin{aligned} \frac{\rho \omega(t + \Delta t) - \rho \omega(t)}{\Delta t} = & \frac{1}{\Delta x_1} \left[\rho K \frac{\partial h}{\partial x_1} (x_1 + \Delta x_1) - \rho K \frac{\partial h}{\partial x_1} (x_1) \right] \\ & + \frac{1}{\Delta x_2} \left[\rho K \frac{\partial h}{\partial x_2} (x_2 + \Delta x_2) - \rho K \frac{\partial h}{\partial x_2} (x_2) \right] \\ & + \frac{1}{\Delta x_3} \left[\rho K \frac{\partial h}{\partial x_3} (x_3 + \Delta x_3) - \rho K \frac{\partial h}{\partial x_3} (x_3) \right] + \rho f \end{aligned} \quad (20)$$

Taking the limit as $\Delta x_i \rightarrow 0$ ($i = 1, 2, 3$) and $\Delta t \rightarrow 0$ yields

$$\frac{\partial(\rho \omega)}{\partial t} = \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(\rho K \frac{\partial h}{\partial x_i} \right) + \rho f \quad (21)$$

The left hand side of Eq.21

$$\frac{\partial(\rho \omega)}{\partial t} = \omega \frac{\partial \rho}{\partial t} + \rho \frac{\partial \omega}{\partial t} \quad (22)$$

reflects both the compressibility of a fluid (the first term on the right hand side of (Eq.22)) and the compressibility of a porous medium (the second term on the right hand side of (Eq.22)). However, this term can be written as:

$$\frac{\partial \rho}{\partial t} = \beta_f \rho \frac{\partial p}{\partial t} \quad (23)$$

where β_f is the compressibility coefficient of the fluid [$M^{-1}LT^2$].

The compressibility of porous media consists of two phenomena: (i) the compressibility of the solid grains and (ii) the compressibility of the solid matrix. Understanding of these processes requires some familiarity with solid mechanics. Assuming that, in analogy with (Eq.23), the density of the solids ρ_s can be written as,

$$\frac{\partial \rho_s}{\partial t} = \beta_s \rho_s \frac{\partial p}{\partial t} \quad (24)$$

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

$$\frac{\partial(\rho_s V_s)}{\partial t} = 0 \quad \rightarrow \quad V_s \frac{\partial \rho_s}{\partial t} = -\rho_s \frac{\partial V_s}{\partial t} \quad (25)$$

Combining Eq.24 and Eq.25, result in

$$\frac{\partial V_s}{\partial t} = -\beta_s V_s \frac{\partial p}{\partial t} \quad (26)$$

The total volume of a porous medium ($V_t = V_s + V_v$) consists of the volumes occupied by solids (V_s) and by pores (V_p or V_v), so that $V_s = (1 - \omega) V_t$. Hence

$$V_t \frac{\partial \omega}{\partial t} = \beta_s V_s \frac{\partial p}{\partial t} \quad \rightarrow \quad \frac{\partial \omega}{\partial t} = (1 - \omega) \beta_s \frac{\partial p}{\partial t} \quad (27)$$

The quantity $\alpha = (1 - \omega) \beta_s$ is called the compressibility of a porous medium [$\text{L}^2 \text{F}^{-1}$]. Substitution of Eqs.23 and 27 into Eq.22 yields,

$$\frac{\partial(\rho \omega)}{\partial t} = \rho (\alpha + \omega \beta_f) \frac{\partial p}{\partial t} \quad (28)$$

Combining Eq.28 with Eq.21 and multiplying both sides of the resulting equation with g gives

$$S_s \frac{\partial p}{\partial t} = g \nabla(\rho K \nabla h) + \rho g f \quad (29)$$

Where the coefficient

$$S_s \equiv \rho g (\alpha + \omega \beta_f) \quad (30)$$

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

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 yields

$$\frac{S_s}{\rho g} \frac{\partial p}{\partial t} = \nabla(K \nabla h) + f \quad (31)$$

Finally, recall the definition of hydraulic head (Eq.11) to observe that $p = \rho g(h - z)$ and

$$\frac{\partial p}{\partial t} = g(h - z) \frac{\partial \rho}{\partial t} + \rho g \frac{\partial h}{\partial t} \quad (32)$$

Accounting for Eq.23

$$\frac{\partial p}{\partial t} [1 - g(h - z)\beta_f \rho] = \rho g \frac{\partial h}{\partial t} \quad (33)$$

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

$$\frac{1}{\rho g} \frac{\partial p}{\partial t} \approx \frac{\partial h}{\partial t} \quad (34)$$

Substituting this expression into (Eq.31) yields the final form of the groundwater flow equation,

$$S_s \frac{\partial h}{\partial t} = \nabla(K \nabla h) + f \quad (35)$$

This equation forms the foundation of modern groundwater modeling.

7) 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 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.

Groundwater, is water found beneath the surface of the ground and seeped down from the surface by migrating through the soil matrix and spaces in geologic formations, it is generally more reliable for use than surface water (Bear 1979).

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 (Fig. 8).

A well drilled into a confined aquifer will be filled with water to the depth $h_0 > b$ which is the depth of the upper limit of the aquifer (Fig.8). If the piezometric 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 piezometric surface coincides with the free (or phreatic) surface, also known as water table (Fig.8). 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.

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- The diagram illustrates the hydrological cycle in a subsurface cross-section. At the top, a green hill represents the land surface. On the left, a 'PUMPED WELL' is shown with a circular symbol and arrows indicating water being drawn up. On the right, a 'Stream' flows over the surface. The subsurface is divided into several layers: a top 'Unconfined aquifer' (light blue) with a dashed line representing the 'Water table'; a 'Confining bed' (orange); a 'Confined aquifer' (light blue); another 'Confining bed' (orange); and a deeper 'Confined aquifer' (light blue). Arrows show water flowing from the 'RECHARGE AREA' (left) through the unconfined and confined aquifers towards the 'DISCHARGE AREA' (right). Time scales are indicated along the flow paths: 'Days' and 'Years' for the unconfined aquifer, 'Centuries' for the first confined aquifer, and 'Millennia' for the second confined aquifer. Trees are shown on the surface, and blue arrows indicate the direction of groundwater flow.



Since the same (or almost the same) groundwater flow (Eq.35) 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 (Eq.35). 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

$$h(x, t) = H(x, t) \quad x \in \Gamma_D$$

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 $n \nabla h$ (or, equivalently the normal Darcy's flux $n q$) is determined by external forces rather than the processes occurring in the aquifer. Boundary conditions

$$-Kn \nabla h(x, t) = Q(x, t) \quad x \in \Gamma_N$$

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

$$h(x, t) = x_3, -Kn \nabla h(x, t) = V_n$$

The first boundary condition implies that on the free surface where the pressure $p = p_{\text{atm}} = 0$. 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 or recharge.

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

$$h(x, 0) = H_{in}(x) \quad x \in \Omega$$

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

8) Parameter Identification

Having derived the governing equations and boundary conditions, the only remaining thing is to parameterize 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 (Table 1) from one aquifer to another and within each aquifer. This section is devoted to the question of how to measure K .

Table 1: Saturated hydraulic conductivity K values found in nature. Values represent typical fresh groundwater conditions (http://en.wikipedia.org/wiki/Hydraulic_conductivity)

K (cm/s)	10^4	10	10^3	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		

8.1) Laboratory determination of hydraulic conductivity

Permeameters are used for laboratory determination of hydraulic conductivity K from Darcy's law (Fig. 9):

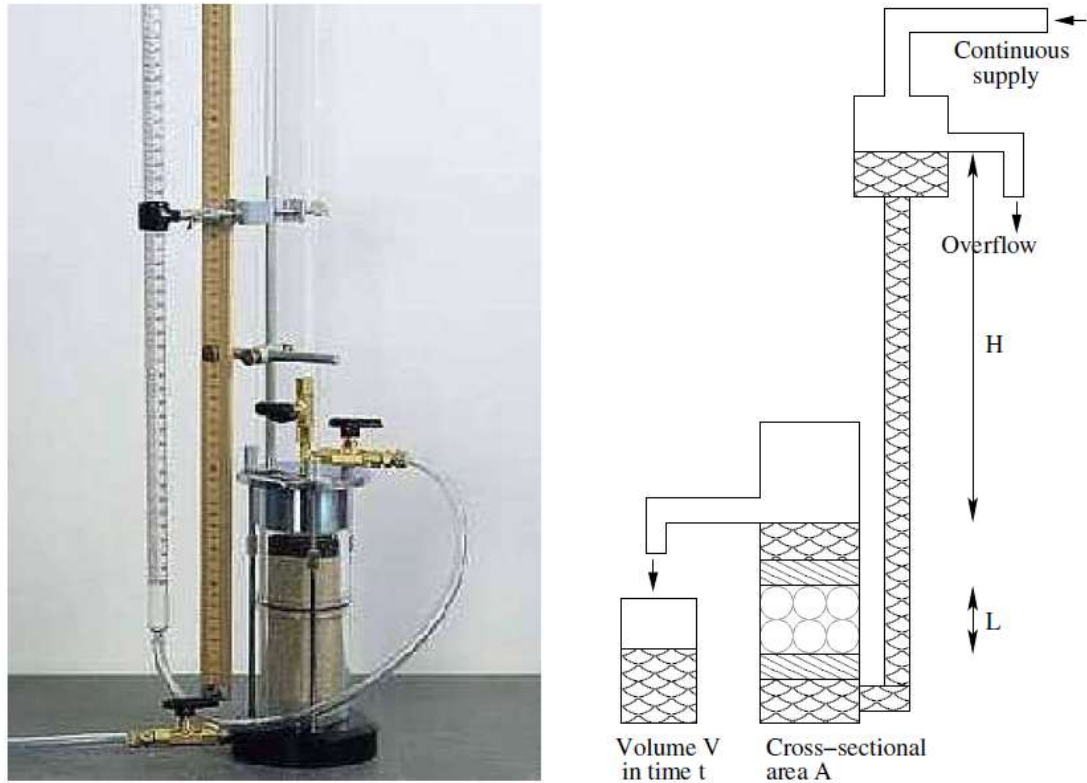


Figure 9: Permeameters are used to measure the hydraulic conductivity of a sample in the laboratory.

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

$$K = \frac{QL}{AH} \quad (36)$$

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 calculate the hydraulic conductivity,

$$-K \frac{H}{L} A = Q(t) \quad (37)$$

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

$$v(t) = -\frac{dh}{dt} \quad (38)$$

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

$$K \frac{H}{L} A = a \frac{dh}{dt} \rightarrow K = \frac{aL}{At} \ln \left(\frac{H_1}{H_0} \right) \quad (39)$$

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

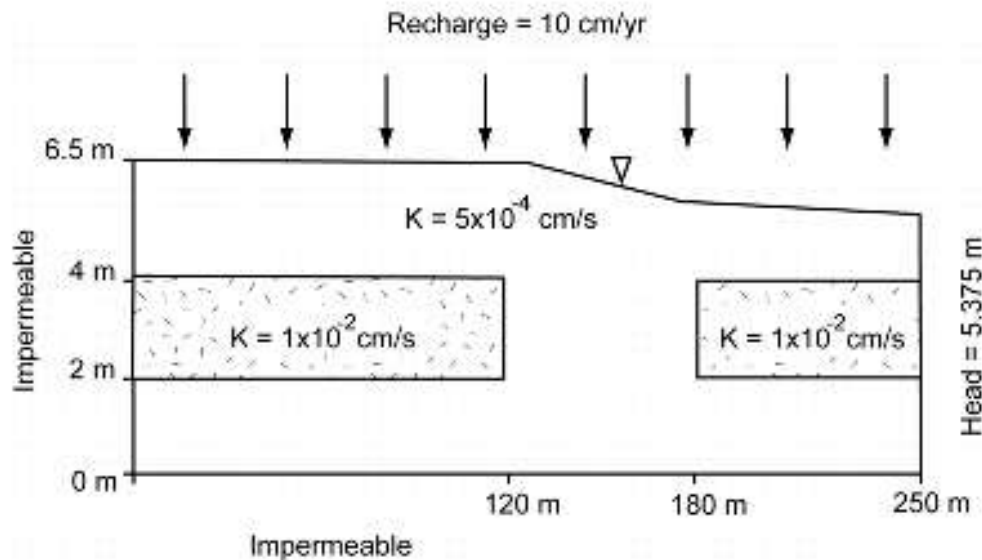
8.2) Field-scale experiments: Pumping tests

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

Q1/ Derive an expression for calculating the discharge from a) unconfined aquifer and b) confined aquifer.

Q2/ Fig. 10 illustrates the hydrologic setting (Ref. 2) for groundwater flow at steady state. The aquifer is composed largely of fine-grained silty sand of hydraulic conductivity $K_1 = 5 \times 10^{-4} \text{ cm/s}$ (equivalent to $K_1 = 5 \times 10^{-6} \text{ m/s}$) with lenses of relatively coarse material of hydraulic conductivity $K_2 = 1 \times 10^{-2} \text{ cm/s}$ (equivalent to $K_2 = 1 \times 10^{-4} \text{ m/s}$).

Groundwater generally moves from the upper surface of the saturated zone, the water table, to the outlet at $x = 250$ m. The water table is a free surface: the exact location is unknown when you set up the model. Instead you solve for it knowing that the fluid pressure equals zero on the water table, and it receives recharge, R , of 10 cm/yr (equivalent to 3.215×10^{-9} m/s). The groundwater divide, a line of symmetry, occurs at $x = 0$. The base of the aquifer is impermeable. Find the hydraulic heads and velocity distributions.



9) Multi-Phase Flow in Porous Media

Previously, we considered flow in porous media that are fully saturated with one fluid. There are many situations where several fluids coexist in the pores, e.g., air and water in soils; oil, gas and water in oil reservoirs; and water and non-aqueous phase liquids (NAPLs; LNAPLs and DNAPLs) in contaminated aquifers.

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

- **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.

9.1) Basic definitions

While the presentation below is applicable to any number of phases and any fluids, we will use only two fluids, air and water, to be concrete (Fig. 11). In addition to averaged quantities defined over the REV, we define the following:

$$S_w = \frac{\text{volume of water}}{\text{volume of voids}} = \text{water saturation} \quad (40)$$

And

$$S_a = \frac{\text{volume of air}}{\text{volume of voids}} = \text{air saturation} \quad (41)$$

Of course,

$$S_a + S_w = 1 \quad (42)$$

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

$$P_c = P_a - P_w \quad (43)$$

is called *capillary pressure*. It is given by

$$P_c = \frac{2\sigma_{aw}}{r} \quad (44)$$

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, $P_c < 0$.

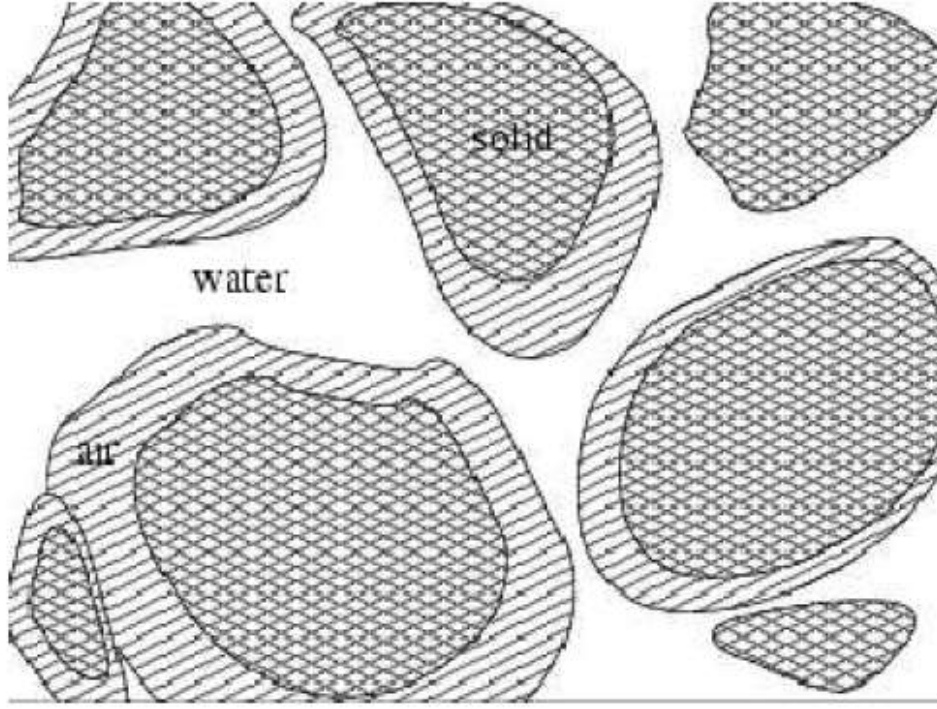


Figure 11: REV of a porous medium containing air and water.

9.2) Generalized Darcy's Law

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

$$h_w = \frac{p_w}{\rho_w g} + z \quad \text{and} \quad h_a = \int_{p_0}^{p_a} \frac{dp_a}{\rho_a g} \quad (45)$$

Here both the compressibility of water and the weight of air are disregarded. In analogy to (Eq.15), we postulate the generalized Darcy's law for water and air

$$q_w = -\frac{\rho_w g}{\mu_w} k_w \nabla h_w \quad \text{and} \quad q_a = -\frac{\rho_a g}{\mu_a} k_a \nabla h_a = -\frac{k_a}{\mu_a} \nabla P_a \quad (46)$$

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 water saturation S_w , the larger portion of the pores is available for flow of water, and the larger permeability for water k_w . Likewise, the higher water saturation S_w , the smaller portion of the pores is available for flow of air, and the smaller permeability for air k_a . This behavior is demonstrated schematically by Fig. 12, which shows the dependence of *relative permeabilities for water* ($k_{rw} = k_w/k$) and *air* ($k_{ra} = k_a/k$) 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.

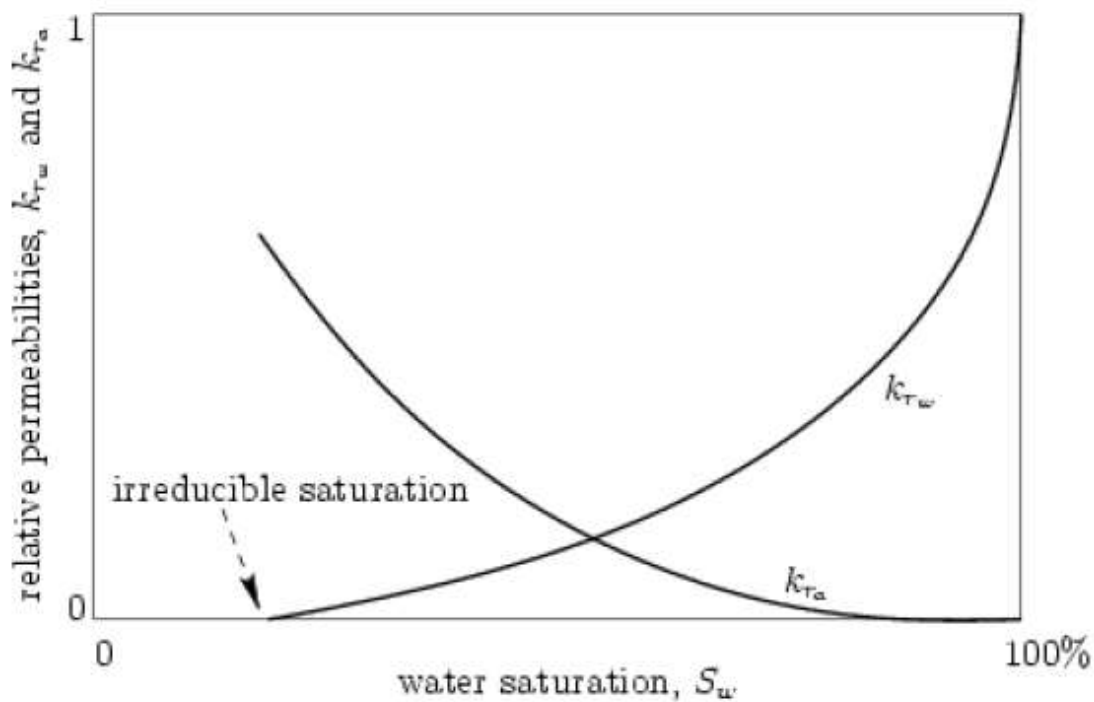


Figure 12: Dependence of relative permeabilities for water (k_{rw}) and air (k_{ra}) on water saturation S_w .

9.3) 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, continuity (mass conservation) equations for water and air phases read

$$\begin{aligned} -\nabla(\rho_w q_w) + f_w &= \omega \frac{\partial S_w \rho_w}{\partial t} \\ -\nabla(\rho_a q_a) + f_a &= \omega \frac{\partial S_a \rho_a}{\partial t} \end{aligned} \quad (47)$$

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 (Eq.47) 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 (Eq.47) 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 $\nabla q = 0$, with the transient effects, caused by source and boundary fluctuations, propagating instantaneously through the system.

Combining generalized Darcy's law (Eq.46) with continuity equations (Eq.47), we obtain the multi-phase flow equations

$$\begin{aligned} \omega \frac{\partial S_w \rho_w}{\partial t} &= \nabla(\rho_w K_w \nabla h_w) + f_w \\ \omega \frac{\partial S_a \rho_a}{\partial t} &= \nabla(\rho_a K_a \nabla h_a) + f_a \end{aligned} \quad (48)$$

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

$$K_w = \frac{\rho_w g}{\mu_w} k_w \quad \text{and} \quad K_a = -\frac{\rho_a g}{\mu_a} k_a \quad (49)$$

It is important to remember that these two equations are coupled through the relationships (Eq.42) and (Eq.43),

This system of equations 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:

$$\rho = AP^m e^{cp} \quad c > 0 \quad (50)$$

- For liquids, $m = 0$ (and incompressible liquids; $c=0$).
- For gases, $c = 0$

-Ideal isotherm gases; $m=1$

$$\rho = \frac{p M}{R T} \quad (51)$$

where $R = 8.3145\text{J}/(\text{mol.K})$ is the universal gas constant, T is the absolute temperature, and M is the molecular weight (mass of 1mole).

-Real gases;

$$\rho = \frac{p M}{Z R T} \quad (52)$$

where Z is the super-compressibility factor (Van der Waals corrections).

10) 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., $p_a = \text{constant}$. 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., $\rho_w = \text{constant}$.

The first assumption implies that flow in unsaturated soils (vadose zone) can be completely described by the first equation in (Eq.48),

$$\frac{\partial \theta \rho_w}{\partial t} = \nabla(\rho_w K_w \nabla h_w) + f_w \quad (53)$$

where

$$\theta \equiv \omega S_w = \frac{\text{volume of water in pores}}{\text{total volume of the medium}} \quad (54)$$

is called the volumetric water content.

The second assumption implies that the capillary pressure in (Eq.43) and the hydraulic head of water in (Eq.45) become,

$$p_c = -p_w \quad (55)$$

and

$$h_w = \psi + z, \quad \psi \equiv \frac{p_w}{\rho_w g} = \frac{-p_c}{\rho_w g}, \quad (56)$$

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

The third assumption, combined with (Eq.56), allows one to rewrite (Eq.53) as

$$\frac{\partial \theta}{\partial t} = \nabla(K_w \nabla \psi) + \frac{\partial K_w}{\partial x_3} + F \quad (57)$$

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

Eq. 57, 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 Fig.13, are determined experimentally (more on this later) and allow one to write Richards equation (Eq.58) in one of the following forms.

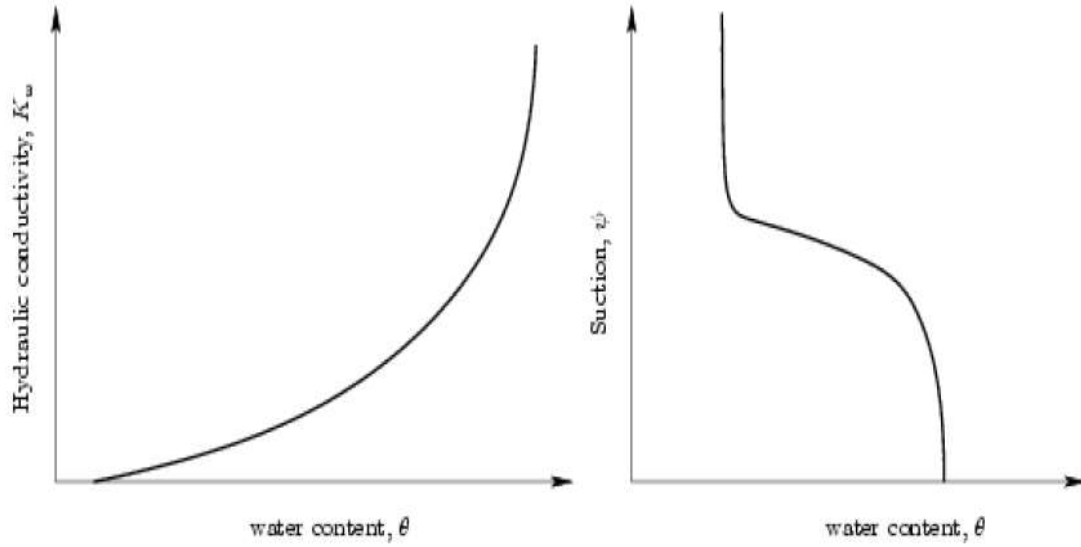


Figure 13: Dependence of hydraulic conductivity K_w and suction ψ on volumetric water content θ .

The ψ -based form. Since

$$\frac{\partial \theta}{\partial t} = C(\psi) \frac{\partial \psi}{\partial t}, \quad C(\psi) \equiv \frac{\partial \theta}{\partial \psi} \quad (58)$$

Richards' equation (Eq.58) can be expressed in the ψ -based form

$$C(\psi) \frac{\partial \psi}{\partial t} = \nabla(K_w(\psi) \nabla \psi) + \frac{\partial K_w}{\partial x_3} + F \quad (59)$$

The function $C(\psi)$ is called the *specific moisture capacity*. It is a property of the medium, whose general behavior is shown in Fig.14.

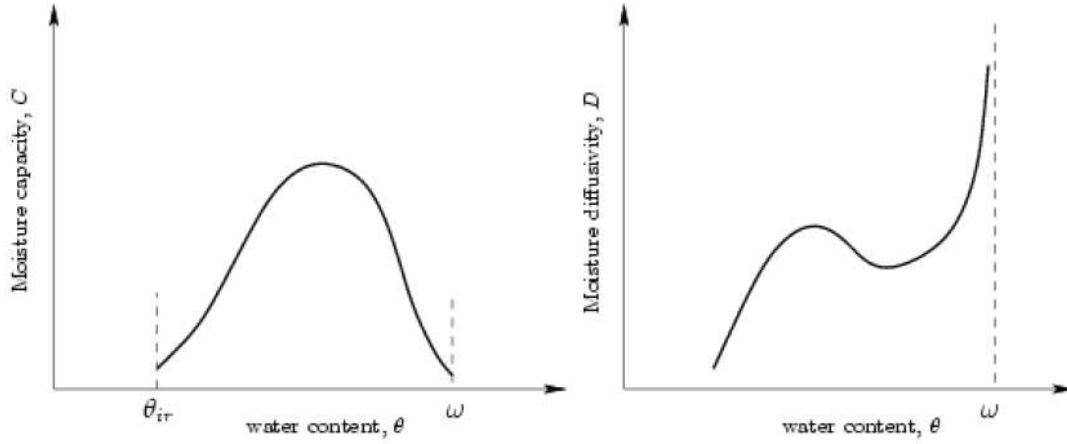


Figure 14: A schematic representation of the functional dependences of the specific moisture capacity $C(\theta)$ and moisture diffusivity $D(\theta)$.

The θ -based form. Since

$$\nabla\psi = \frac{\partial\psi}{\partial\theta} \nabla\theta \quad (60)$$

Richards' equation (Eq.57) can be expressed in the θ -based form

$$\frac{\partial\theta}{\partial t} = \nabla(D(\theta)\nabla\theta) + \frac{\partial K_w}{\partial x_3} + F \quad (61)$$

The function $D(\theta)$ is called the *moisture diffusivity*. It is a property of the medium, whose general behavior is shown in Fig.14.

The advantages of the ψ -based form of the Richards' equation

- Since equation (Eq.59) 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 (Eq.59).

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 advantages of the θ -based form of the Richards' equation

Its left hand side is linear. This fact facilitates numerical solutions of (Eq.61) for infiltration into dry soils.

The disadvantages of the θ -based form of the Richards' equation

- One can see from Fig.14 that $D(\theta) \rightarrow \infty$ as $\theta \rightarrow \omega$. This invalidates Eq.61 for regions close to saturation.
- Since θ is discontinuous across material interfaces, solving Eq.61 for layered media is problematic.

11) Characterization of Vadose Zone

A brief overview of some of the approaches used to measure various parameters describing flow in unsaturated regions (vadose zone) presented below:

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

$$w = \frac{\text{wet weight} - \text{dry weight}}{\text{dry weight}} \quad (62)$$

$$\text{Finally, use } \theta = \frac{\rho_b}{\rho_w} w \quad (63)$$

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 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 equilibrates with the surrounding. 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 $\psi = \psi(\theta)$.

2. Measurement of Suction

Tensiometers are often used for in situ measurements of hydraulic head and suction. A tensiometer consists of a porous cup that is connected to a tube fully filled with water and equipped with a vacuum gauge (Fig.15). 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 reading on the vacuum gauge.



Figure 15: Tensiometers are often used to measure suction in unsaturated soils.

11) Constitutive relationships

There are several unknowns for equation governed the multiphase fluid flow in porous medium (Eq.48). Constitutive relationships that relate these unknowns must be specified. These relationships can be written in a variety of ways that result in different variables becoming the dependent variables for the system. The most common choices for dependent variables are the individual phase pressures and the phase saturations.

For three-phase systems, the relative permeability-saturation-capillary pressure ($K_r - S - P_c$) relationships are typically determined experimentally and fitted with some empirical mathematical functions originally derived by soil physicists for air-water systems (e.g. Brooks and Corey in 1966 and Van Genuchten in 1980) as follows:

• Brooks and Corey (1964) as cited by Kueper and Frind (1991b)

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}} \quad 0 \leq S_e \leq 1 \quad (B1)$$

$$S_e = \left(\frac{h_{ow}}{h_d} \right)^{-\lambda} \quad h_{ow} \geq h_d \quad (B2)$$

$$S_{te} = \left(\frac{h_{ao}}{h_d} \right)^{-\lambda} \quad (B3)$$

$$K_{rw} = S_e^{\left[\frac{(2+3\lambda)}{\lambda} \right]} \quad (B4)$$

$$K_{ro} = (1 - S_e)^2 \left(1 - S_e^{\left[\frac{(2+3\lambda)}{\lambda} \right]} \right) \quad (B5)$$

where h_{ow} oil-water capillary pressure head ($=h_o-h_w$); h_{ao} air-oil capillary pressure head ($=h_a-h_o$); h_a the water height-equivalent pressure head of air; S_e effective water saturation; S_w water saturation; S_{wr} residual water saturation; S_{te} effective total liquid saturation and oil saturation $S_o=S_t-S_w$; h_d the displacement pressure head; λ a pore size distribution index. Phase conductivities are assumed to be described by:

$$K_w = K_{ws} K_{rw}$$

$$K_o = \frac{K_{ws} K_{ro}}{\mu_{ro}} \quad (B6)$$

where K_{rw} and K_{ro} are relative permeabilities of water and oil respectively, μ_{ro} is the ratio of oil to water viscosity, and K_{ws} is the saturated conductivity for water.

For non-wetting fluid (oil), there is a certain minimum pressure needed to displace the wetting fluid (water). This minimum capillary pressure is referred to as the displacement pressure (or as entry pressure or as threshold pressure) and is related to the largest pores of the porous medium. Also, the residual water saturation is defined as the limiting saturation of the water, where the water loses its capacity to move as a linked phase.

• **Parker et al. (1987) based on Van Genuchten's model (1980)**

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}} \quad (V1)$$

$$S_{te} = \frac{S_t - S_{wr}}{1 - S_{wr}} \quad (V2)$$

$$S_e = \left[1 + (\alpha \cdot \beta_{ow} \cdot h_{ow})^n \right]^{-m} \quad h_o > h_o^{cr.} \quad (V3)$$

$$S_e = \left[1 + (\alpha \cdot h_{aw})^n \right]^{-m} \quad h_o \leq h_o^{cr.} \quad (V4)$$

$$h_o^{cr.} = \beta_{ow} h_w / (\beta_{ao} + \beta_{ow}) \quad (V5)$$

$$S_{te} = \left[1 + (\alpha \cdot \beta_{ao} \cdot h_{ao})^n \right]^{-m} \quad (V6)$$

$$k_{rw} = S_e^{1/2} \left[1 - \left(1 - S_e^{1/m} \right)^m \right]^2 \quad (V7)$$

$$k_{ro} = (S_t - S_w)^{1/2} \left[\left(1 - S_w^{1/m} \right)^m - \left(1 - S_t^{1/m} \right)^m \right]^2 \quad (V8)$$

Where h_o^{cr} critical oil pressure head, [L], h_{aw} air-water capillary pressure head ($=h_a-h_w$), [L], S_w water saturation, S_t total liquid saturation, S_e effective water saturation, S_{te} effective total liquid saturation. The α , n and $m(=1-1/n)$ are Van Genuchten's soil parameters, β_{ao} & β_{ow} are fluid-dependent scaling coefficients. Lenhard and Parker in 1987 as cited by (Kechavarzi, 2005) proposed the scaling factor could be estimated from ratio of interfacial tension γ_{ij} (i.e. $\beta_{ij} = \gamma_{aw} / \gamma_{ij}$).

12) Measurement of capillary pressure-saturation curve

12.1 Equipment

The experimental apparatus represents a modification of one used by Demond and Roberts (1991). This apparatus is consisted of pressure cell, effluent collection bottle, and tubes with specified lengths. The pressure cell is made-up of stainless steel with Teflon core. While effluent collection bottle and tubes of the apparatus are made-up of Perspex which they are able to bear values of pressure and temperature arrived to 3.0 bars and 600 °C respectively.

The pressure cell (Fig.16) represents a middle part of the apparatus. This cell has inner diameter (ID) equal to 5.5 cm and total height equal to 7.0 cm. The net inner height of the cell is equal to 4.0 cm. This cell is the location of the tested sand sample. The upper and lower parts of the cell are supplied with a short tube which has inner diameter equal to 15 mm. Kerosene enter the cell by the upper tube and it will be in contact with sand sample. On the other hand, the lower tube is used to; supply the sand sample with CO₂, saturate the sample with wetting phase (water) and transport the discharged water from the sample under specified oil pressure head to effluent collection bottle. In the bottom of the pressure cell there is a ceramic plate as shown in Fig.17. This plate (Fig.18) is the

filter disk with a certain pressure and mesh size fraction which is able to separate between oil and water.

The effluent collection bottle represents the lower part of experimental apparatus with a capacity of 500 mL. It was sealed with a viton stopper, with a 1 mm inner diameter of tube inserted in the stopper to allow pressure equilibration between the ambient atmosphere and the head space in the bottle while minimizing evaporation.

Tubes represent the upper part of the experimental apparatus. They consist of a number of pieces with inner diameter equal to 15 mm and each piece has a length equal to 0.25 m with a number of side vents. These vents are located at different spaces. The upper part of one of these pieces has a funnel shape which is located at top of other pieces. Combination of these pieces of tubes with others will lead to a different heads of organic liquid. The specified constant pressure head of organic liquid was achieved by reservoir(1), reservoir(2) and any side vent. Fig.19 is schematic diagram of the experimental apparatus.



Figure 16: Front view for pressure cell.



Figure 17: Location of ceramic plate.



Figure 18: Top view for ceramic plate.

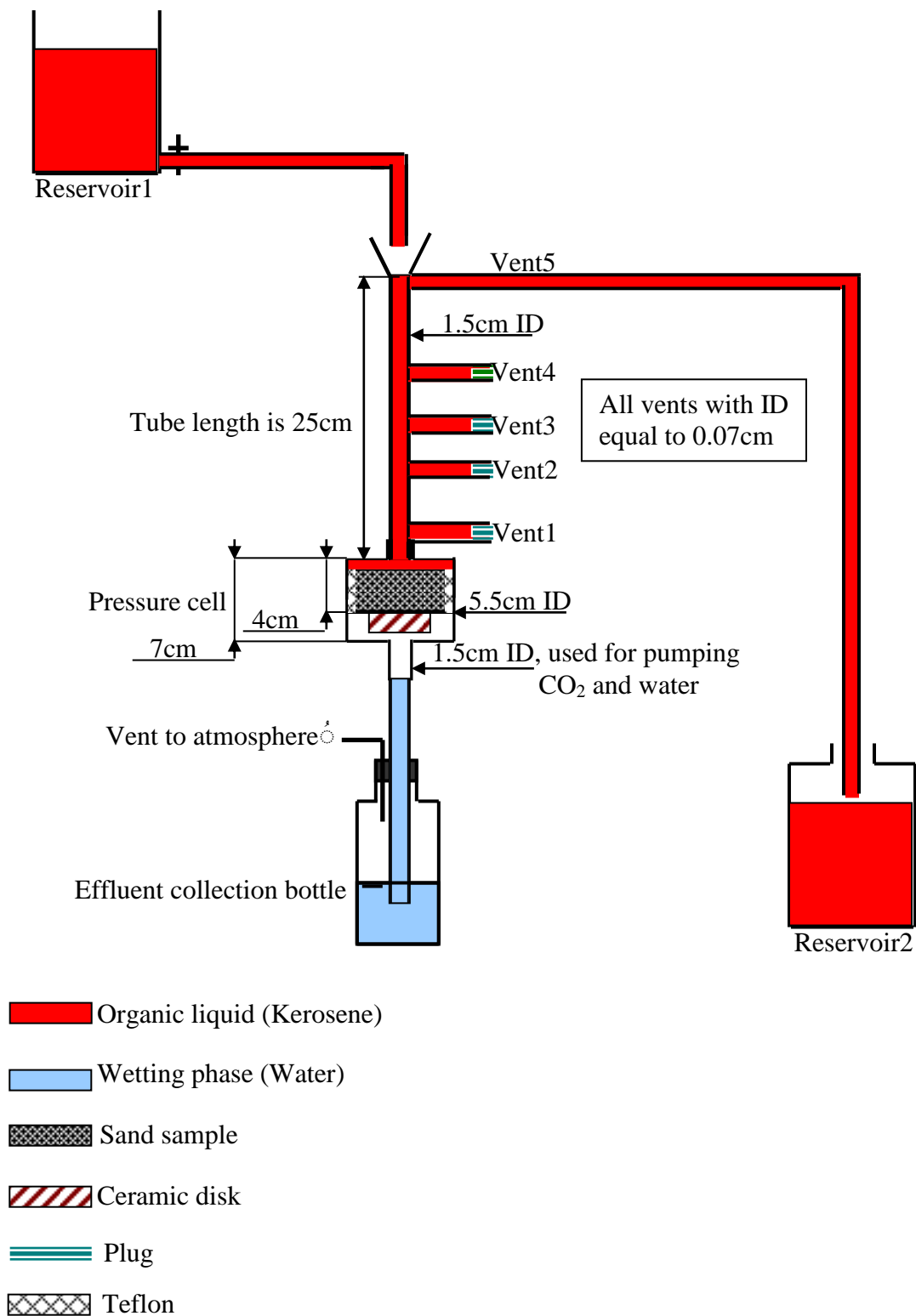


Figure 19: Schematic diagram of the experimental apparatus.

12.2 Experimental procedure

A slightly moist sand sample was placed inside the pressure cell directly on the ceramic disk. Sand was packed with height equal to 3 cm and diameter equal to 5.5 cm. Initially, the sample was saturated with carbon dioxide at 15 psi to displace the air in the pore space of the sand. After that, the sample was wetted completely with deionized water through slowly flooded upward with a degassed aqueous phase at a rate of 2.5 mL/min in order to displace or dissolve as much gas as possible. After the water (or aqueous) phase appeared at the top of the sample, the flow rate was increased 5 times to displace the CO₂-saturated water and to dissolve any residual gas. The system was allowed to equilibrate overnight at about 3 cm of capillary pressure, measured using the bottom of the sand sample as the reference point. This pressure was below displacement pressure of the system studied and, thus, was considered satisfactory as the starting point of the measurements. All measurements were made in a constant room temperature ($20 \pm 1^\circ \text{C}$).

The capillary pressure was increased by increasing the elevation of organic liquid (kerosene) in the upper tube which connected with pressure cell by a suitable fitting. A powdered, nonvolatile red dye (Suden III) was added to the kerosene at a concentration of 1 mg/l of kerosene in order to enable visual observations. Upon achieving equilibrium after a step increase in capillary pressure, the amount of water discharged from the sample was measured by the weight gain of the effluent collection bottle. Evaporation was negligible. Ten hours was allowed to elapse between a change in pressure and the determination of the weight change for that step. The weight stabilization was assumed to indicate the achievement of equilibrium, although it is recognized that this apparent equilibrium is for the bulk liquid only and that discontinuous portions of liquid may take orders of magnitude longer to equilibrate (Demond and Roberts, 1991).

The above procedure was used to measure the primary drainage capillary pressure-saturation curve. The above procedure was repeated until a negligible amount of efflux for an increment in capillary pressure was achieved, suggesting that the aqueous phase had lost its ability to move in response to a hydraulic gradient and that a residual saturation had been achieved (Luchner et al., 1989).

In the primary drainage measurements, the aqueous phase content of the porous medium was expressed as S_w , the saturation of the aqueous phase. S_w was determined by subtracting the cumulative effluent volume from the total pore volume and dividing that quantity by the total pore volume.

The primary drainage relationship for kerosene-water system is shown in Fig.20. This relationship was measured firstly as described previously and, then, it is fitted with Van Genuchten's relationship in order to determine the Van Genuchten's parameters (i.e. α and n). These values together with Eq.V7, drainage relative permeability-saturation curve can be drawn as in Fig.21.

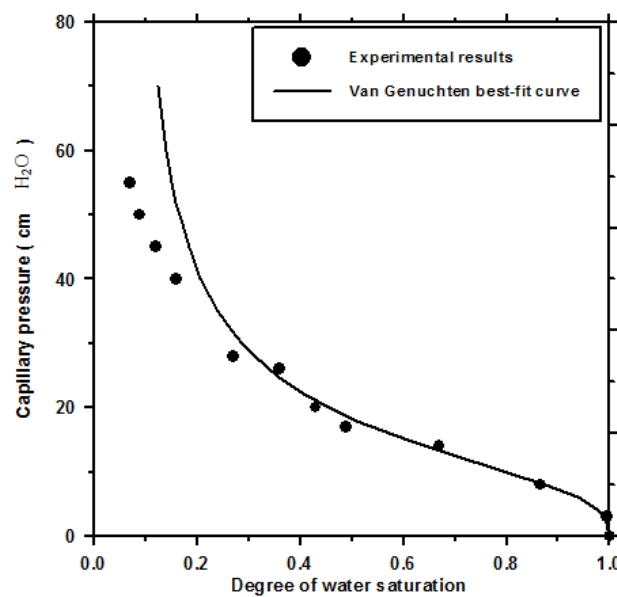


Figure 20: Capillary pressure-water saturation curve for sand.

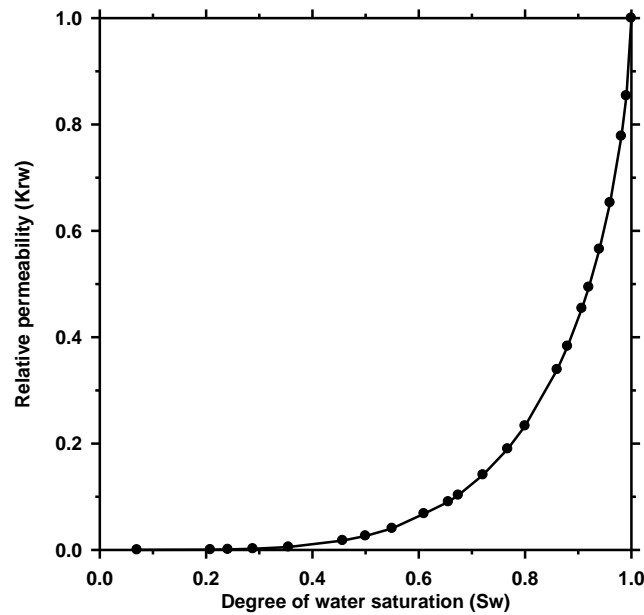


Figure 21: Relative permeability-water saturation curve of sand for kerosene-water system.

Hysteresis: The relationship between ψ and θ can be measured in two ways: (i) in desorption or drainage, 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 or imbibition, by gradually wetting up an initially dry sample while reducing the suction. Unfortunately, these two alternatives often result in two different water retention curves (Fig.22). This phenomenon is called hysteresis.

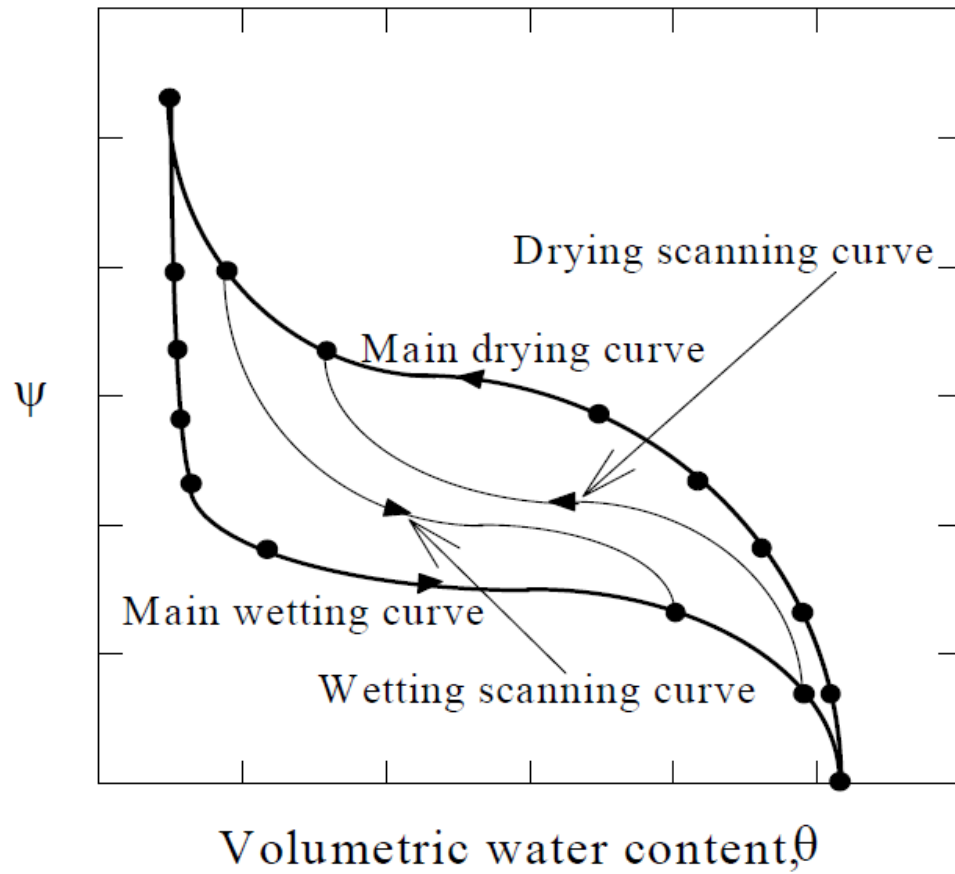


Figure 22: Hysteresis in the water retention curves $\psi = \psi(\theta)$.

13) 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 $x = L$. The 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 Eq.61:

$$0 = \frac{d}{dx} \left[D(\theta) \frac{d\theta}{dx} \right] \quad (62)$$

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

$$\theta(x = 0) = \omega \quad \theta(x = L) = \theta_r \quad (63)$$

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 Fig.14. For simplicity, we assume that the moisture diffusivity increases exponentially with water content, i.e, that $D = \exp(\theta)$. These results in

$$\theta = \ln(cx + e^\omega) \quad (64)$$

where c is a constant of integration. Using the boundary condition at $x = L$ to determine c , we obtain the final expression for the moisture profile,

$$\theta(x) = \ln \left[(e^{\theta_r} - e^\omega) \frac{x}{L} + e^\omega \right] \quad (65)$$

Use $\omega=0.4$, $\theta_r=0.05$, $L=100$ cm and **draw $\theta(x)$** .

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 $x = 0$. The 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 Eq.61:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left[D(\theta) \frac{\partial \theta}{\partial x} \right] \quad (66)$$

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

$$\theta(x, 0) = \theta_r, \quad \theta(0, t) = \omega, \quad \theta(\infty, t) = \theta_r \quad (67)$$

Boltzmann's transformation

$$\xi = \frac{x}{\sqrt{t}} \quad (68)$$

transforms the partial differential equation (66) into an ordinary differential equation

$$-\frac{\xi}{2} \frac{d\theta}{d\xi} = \frac{d}{d\xi} \left[D(\theta) \frac{d\theta}{d\xi} \right] \quad (69)$$

The three initial and boundary conditions (Eq.67) are transformed into two boundary conditions

$$\theta(\xi = 0) = \omega, \quad \theta(\xi = \infty) = \theta_r \quad (70)$$

For general functional relations of moisture diffusivity $D(\theta)$, the boundary value problem (Eqs. 69 and 70) has to be solved numerically. The advantages of using Boltzmann's transformation are twofold. First, the ordinary differential equation (69) is easier and computationally less expensive to solve numerically than the partial differential equation (66). Second, it shows that water content θ depends on space x and time t only in combination $\xi = \frac{x}{\sqrt{t}}$, rather than separately. This implies that the

wetting front moves through the column in a self-similar manner, i.e., without changing its shape (Fig.23).

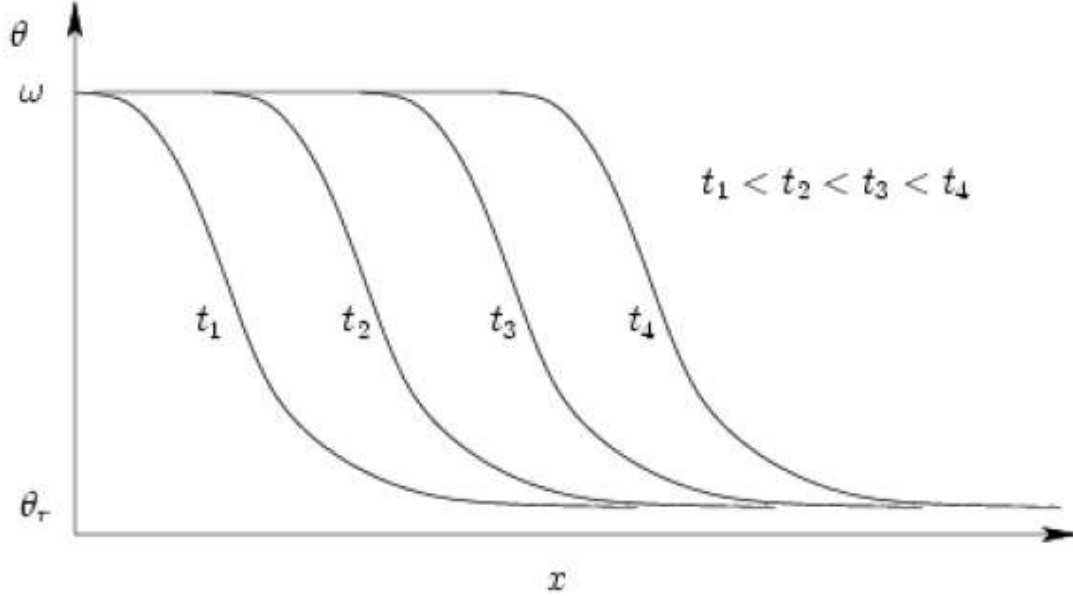


Figure 23: Propagation of a self-similar wetting front.

14) 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 (Eq.57):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K \frac{\partial \psi}{\partial z} \right] + \frac{\partial K}{\partial z} \quad (71)$$

subject to the initial and boundary conditions

$$\theta(z, 0) = \theta_r, \quad \theta(0, t) = \omega, \quad \theta(\infty, t) = \theta_r \quad (72)$$

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 several cases. Here we consider one such a case, which employs the following exponential relations:

$$K(\psi) = K_s e^{\alpha \psi}, \quad \theta = e^{\alpha \psi} \quad (73)$$

Substituting (Eq.73) into (Eq.71) and introducing a new dependent variable

$$\Phi = e^{\alpha\psi} \quad (74)$$

We obtain,

$$\frac{\partial \Phi}{\partial t} = \frac{K_s}{\alpha} \frac{\partial^2 \Phi}{\partial z^2} + \frac{\partial \Phi}{\partial z} \quad (75)$$

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.

Q1// Toluene is used in the manufacture of model airplane glue. A small amount is spilled when an above ground storage tank outside a glue factory is being filled from a tanker truck. A volume of 1.3 L of toluene is spilled and soaks into a dry sand soil with a porosity of 0.33. If the vapors fill a volume of soil that occupies a volume of 2.5 m³ (a) what is the concentration of toluene in the soil atmosphere, (b) how much toluene remains in the soil as a LNAPL and (c) what is the concentration of toluene in the soil phase? Assume that no toluene is evaporated to the atmosphere. The soil at a temperature of 20°C (293 K) and the vapor pressure of toluene is 22 mm of mercury at 20°C and formula weight is 92.14 gm/mol.

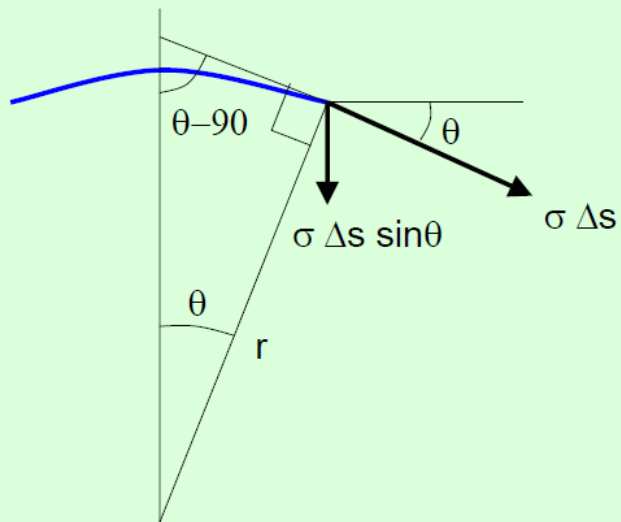
Q2// “Given a spill on the land surface, how long will it take for the NAPL to penetrate to the water table?” residual saturation.

Q3// Specify the factors affecting NAPL movement.

Q4// How can NAPL and water exist together in soil at two different pressures?

Q5// An undisturbed cylindrical core sample of soil 10 cm high and 5 cm in diameter weights 350gm. The density of solids is $\rho_s = 2.65\text{g/cm}^3$. Calculate the total porosity.

Relationship between P_c and σ



Force balance:

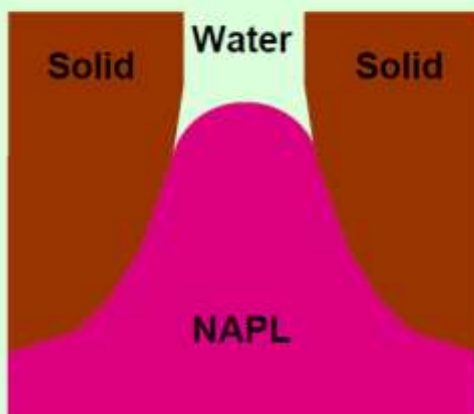
$$P_c (\Delta s)^2 = -4\sigma \Delta s \sin \theta$$

$$\sin \theta \approx \theta \approx (\frac{1}{2}\Delta s)/r$$

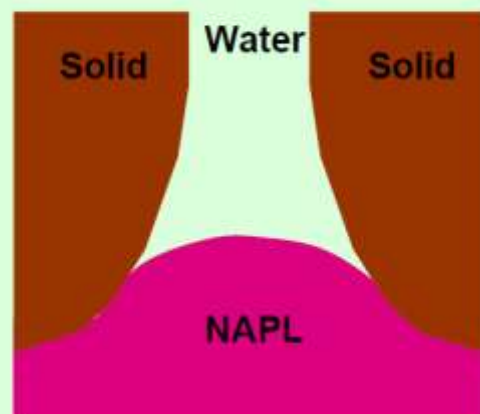
$$P_c (\Delta s)^2 = -4\sigma \Delta s \Delta s/2r$$

$$P_c = -2\sigma / r$$

P_c depends on NAPL and porous medium



Large P_c (small r or large σ)
 → small water content,
 large NAPL residual



Small P_c (large r or small σ)
 → large water content,
 small NAPL residual

Questions

1. How is the saturated zone defined
2. What is an aquifer?
3. What is an aquitard?
4. What is an unconfined aquifer?
5. What is a confined aquifer?
6. What is a conceptual model?
7. How is specific storage defined?
8. How is specific yield defined?
9. How is storage coefficient defined?
10. What is hydraulic conductivity?
11. What is the difference between hydraulic conductivity and permeability?
12. What is transmissivity?
13. What is the typical range for hydraulic conductivity for sand?
14. What is the typical range for hydraulic conductivity for clay?
15. How is hydraulic head defined?
16. What is the Darcy velocity?
17. What is the pore water velocity?
18. Which two equations are joined in the governing equation for groundwater flow?

15) Mathematical basis for groundwater flow

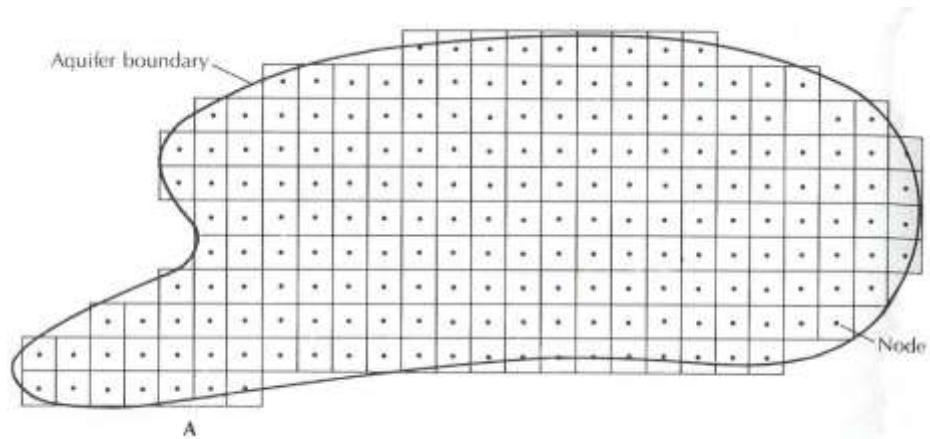
Eq.35 (continuity equation combined with the Darcy's law) can be written as follows:

$$K_x \frac{\partial^2 h}{\partial x^2} + K_y \frac{\partial^2 h}{\partial y^2} + K_z \frac{\partial^2 h}{\partial z^2} - f = S_s \frac{\partial h}{\partial t} \quad (76)$$

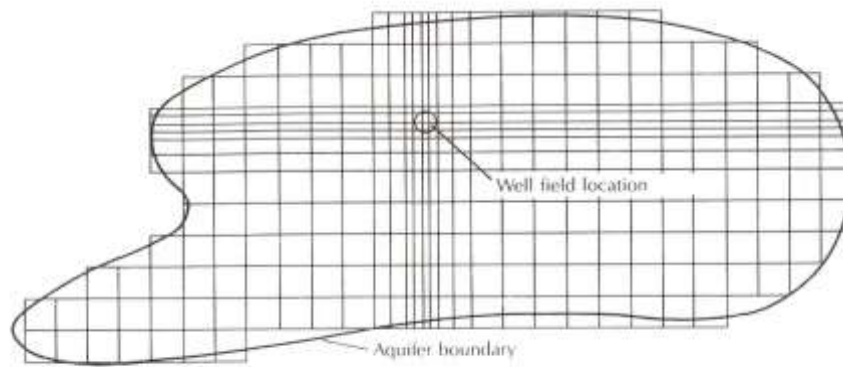
This equation can be solved numerically by: **Finite Difference method** and **Finite Element Method**.

Finite Difference method

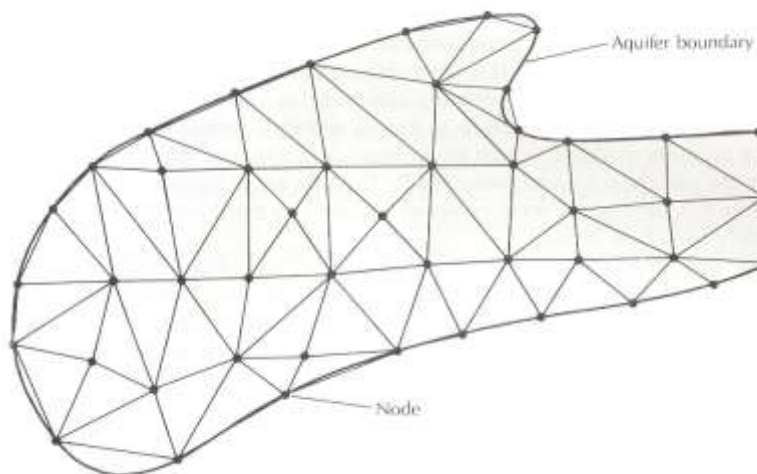
Square cells



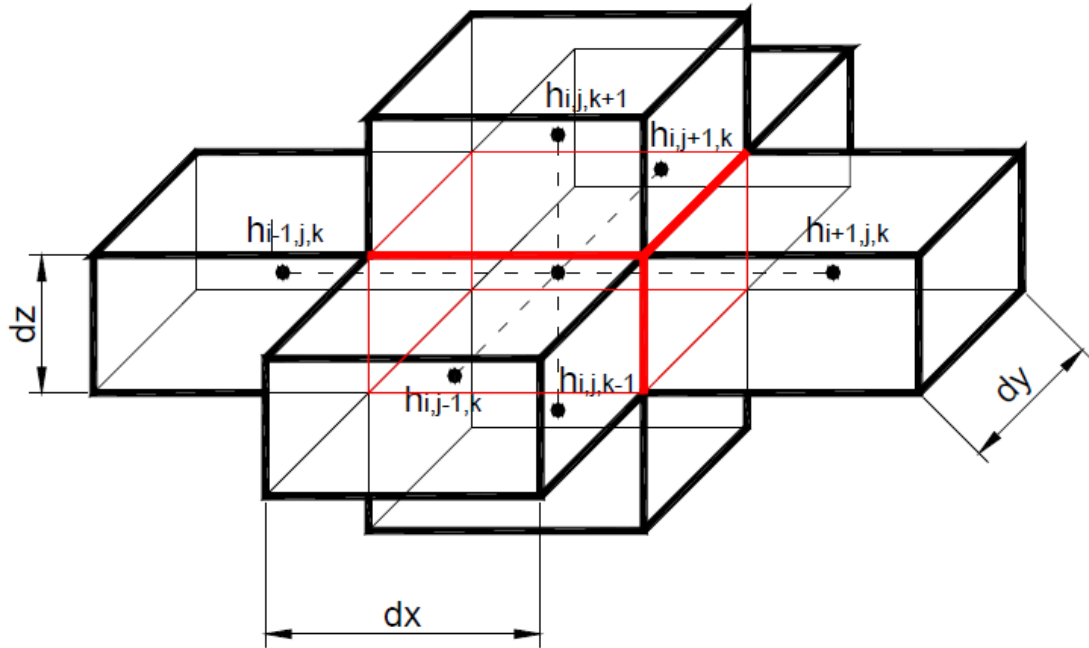
Rectangular cells



Finite Element Method



Description of Finite Difference equations for 3D groundwater flow



Continuity Equation

In-out = Δsto

$$\Delta t(Q_x^- - Q_x^+ + Q_y^- - Q_y^+ + Q_z^- - Q_z^+ - f) = \Delta sto$$

The Darcy's Law

$$Q_x^- = -\frac{h_{i,j,k}^{n+1} - h_{i-1,j,k}^{n+1}}{\Delta x} K x_{i,j,k} \Delta y \Delta z$$

$$Q_x^+ = -\frac{h_{i+1,j,k}^{n+1} - h_{i,j,k}^{n+1}}{\Delta x} K x_{i,j,k} \Delta y \Delta z$$

$$Q_y^- = -\frac{h_{i,j,k}^{n+1} - h_{i,j-1,k}^{n+1}}{\Delta y} K y_{i,j,k} \Delta x \Delta z$$

$$Q_y^+ = -\frac{h_{i,j+1,k}^{n+1} - h_{i,j,k}^{n+1}}{\Delta y} K y_{i,j,k} \Delta x \Delta z$$

$$Q_z^- = -\frac{h_{i,j,k}^{n+1} - h_{i,j,k-1}^{n+1}}{\Delta z} K z_{i,j,k} \Delta x \Delta y$$

$$Q_z^+ = -\frac{h_{i,j,k+1}^{n+1} - h_{i,j,k}^{n+1}}{\Delta z} K z_{i,j,k} \Delta x \Delta y$$

Storage


$$\Delta sto = S_s \frac{h_{i,j,k}^{n+1} - h_{i,j,k}^n}{\Delta t} \Delta x \Delta y \Delta z$$

$$\begin{aligned}
& \left(Kx_{i,j,k} \frac{\Delta y \Delta z}{\Delta x} \right) h_{i+1,j,k}^{n+1} + \left(Kx_{i,j,k} \frac{\Delta y \Delta z}{\Delta x} \right) h_{i-1,j,k}^{n+1} \\
& \left(Ky_{i,j,k} \frac{\Delta x \Delta z}{\Delta y} \right) h_{i,j+1,k}^{n+1} + \left(Ky_{i,j,k} \frac{\Delta x \Delta z}{\Delta y} \right) h_{i,j-1,k}^{n+1} \\
& \left(Kz_{i,j,k} \frac{\Delta x \Delta y}{\Delta z} \right) h_{i,j,k+1}^{n+1} + \left(Kz_{i,j,k} \frac{\Delta x \Delta y}{\Delta z} \right) h_{i,j,k-1}^{n+1} \\
& \left(-2Kx_{i,j,k} \frac{\Delta y \Delta z}{\Delta x} - 2Ky_{i,j,k} \frac{\Delta x \Delta z}{\Delta y} - 2Kz_{i,j,k} \frac{\Delta x \Delta y}{\Delta z} - \frac{S_s \Delta x \Delta y \Delta z}{\Delta t} \right) h_{i,j,k}^{n+1} \\
& = f - \frac{S_s \Delta x \Delta y \Delta z}{\Delta t} h_{i,j,k}^n \\
& Ah_{i+1,j,k}^{n+1} + Bh_{i-1,j,k}^{n+1} + Ch_{i,j+1,k}^{n+1} + Dh_{i,j-1,k}^{n+1} + Eh_{i,j,k+1}^{n+1} + Fh_{i,j,k-1}^{n+1} + Gh_{i,j,k}^{n+1} = H
\end{aligned}$$

Description of Finite Difference equations for 1D groundwater flow

$$\begin{aligned}
& (Kx_i)h_{i+1}^{n+1} + (Kx_i)h_{i-1}^{n+1} \\
& \left(-2Kx_{i,j,k} - \frac{S_s \Delta x \Delta x}{\Delta t} \right) h_i^{n+1} \\
& = f \frac{\Delta x}{\Delta y \Delta z} - \frac{S_s \Delta x \Delta x}{\Delta t} h_{i,j,k}^n \\
& A_i h_{i-1}^{n+1} + B_i h_i^{n+1} + C_i h_{i+1}^{n+1} = D_i
\end{aligned}$$

$$\begin{array}{c}
\left| \begin{array}{cccc}
B_1 & C_1 & & \dots \\
A_2 & B_2 & C_2 & \\
\vdots & & \ddots & \\
& A_{n-1} & B_{n-1} & C_{n-1} \\
& & A_n & B_n
\end{array} \right| \left\| \begin{array}{c}
h_1 \\
h_2 \\
\vdots \\
h_{n-1} \\
h_n
\end{array} \right\| = \left| \begin{array}{c}
D_1 \\
D_2 \\
\vdots \\
D_{n-1} \\
D_n
\end{array} \right|
\end{array}$$



For each node (i), there is a one linear equation in three variables h_{i-1}^{n+1} , h_i^{n+1} & h_{i+1}^{n+1} . The collection of equations for each solution node leads to have a global tri-diagonal coefficient matrix (its bandwidth equal to three) to whole solution domain. For example, a ten noded domain, the soil

column is divided into ten vertical grids; there are ten equations that form the whole grids.

Implementation of B.Cs

1) Dirichlet condition (prescribed head)

$$\begin{aligned} & (Kx_i)h_{i+1}^{n+1} + (Kx_i)h_{i-1}^{n+1} \\ & \left(-2Kx_{i,j,k} - \frac{S_s \Delta x \Delta x}{\Delta t} \right) h_i^{n+1} \\ & = f \frac{\Delta x}{\Delta y \Delta z} - \frac{S_s \Delta x \Delta x}{\Delta t} h_{i,j,k}^n \end{aligned}$$

In this case h_{i-1}^{n+1} is known

$$A_i h_{i-1}^{n+1} + C_i h_{i+1}^{n+1} = D_i - B_i h_i^{n+1}$$

The right hand side is known

2) Neumann's condition (prescribed flux)

$$Q_x^- + \frac{h_{i+1,j,k}^{n+1} - h_{i,j,k}^{n+1}}{\Delta x} Kx_{i,j,k} \Delta y \Delta z - f = S_s \frac{h_{i,j,k}^{n+1} - h_{i,j,k}^n}{\Delta t} \Delta x \Delta y \Delta z \quad \text{the first term is known}$$

$$\left(Kx_{i,j,k} \frac{\Delta y \Delta z}{\Delta x} \right) h_{i+1,j,k}^{n+1} - \left(Kx_{i,j,k} \frac{\Delta y \Delta z}{\Delta x} \right) h_{i,j,k}^{n+1} = f \frac{\Delta x}{\Delta y \Delta z} - S_s \frac{h_{i,j,k}^n}{\Delta t} \Delta x \Delta x - Q_x^-$$

$$A_i h_{i-1}^{n+1} + C_i h_{i+1}^{n+1} = D_i - Q_x^-$$

The right hand side is known

Fluid Flow: Domain Equations and Boundary Conditions

Steady groundwater flow is generally expressed by a conservation equation built with Darcy's law for velocity:

$$\nabla \cdot (K\nabla H) + R = 0$$

where K is hydraulic conductivity; R the volumetric rate of recharge to water table per unit volume of aquifer, and the dependent variable h is total hydraulic head. Total hydraulic head, the driving force for flow, is

$$H = H_p + y$$

where H_p is the pressure head; and y the elevation. With the base of the model at $y = 0$, the total hydraulic head H at any point in the aquifer equals the height of the water column H_p above it plus the point's elevation y along the vertical axis.

The equation for groundwater flow and solute transport link through the Darcy velocity, \mathbf{u} :

$$\mathbf{u} = -K\nabla H$$

The velocity vector \mathbf{u} consists of x - and y -directed components denoted u and v .

Figure of the problem gives the boundary conditions for the groundwater flow problem. A zero flux Neumann condition corresponds to both the symmetry boundary at $x = 0$ m and the impermeable boundary at $y = 0$ m:

$$\mathbf{n} \cdot K\nabla H = 0$$

The hydraulic head at $x = 250$ m is the simple Dirichlet condition

$$H(x, t) = H_0$$

At the water table the recharge is R ; the pressure head H_p is zero since there is no water above it; still its height y is unknown. We first use a Neumann boundary to model the known recharge

$$\mathbf{n} \cdot K\nabla H = R$$

Next we implicitly specify the pressure head H_p at the water table to zero and explicitly determine its height y