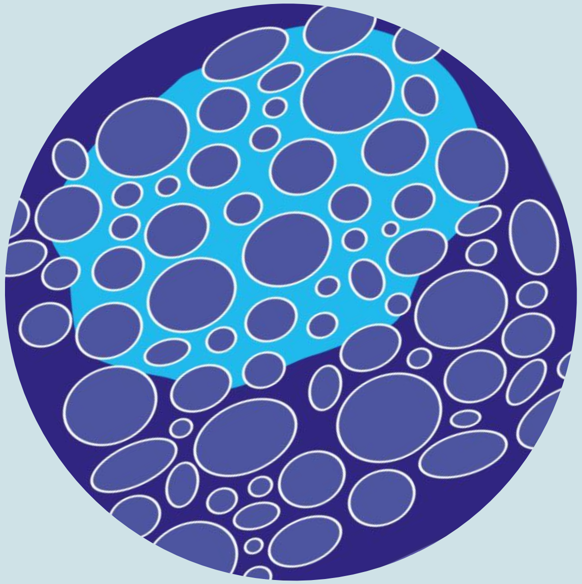

多孔介质污染迁移动力学

Contaminant Transport in Porous Media

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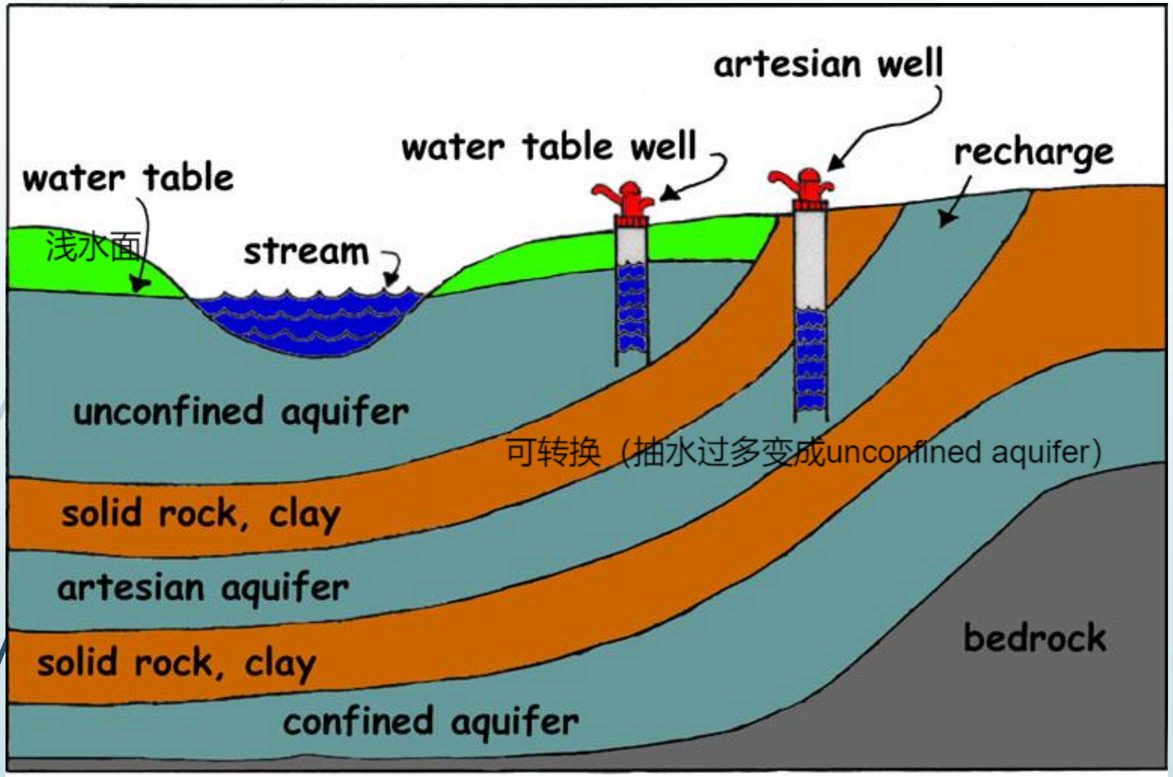
Lecture 2

- 1 Subsurface Hydrology
- 2 Review of Mathematics and Flow Equation
- 3 Mass Transport in Saturated Media

Subsurface Hydrology



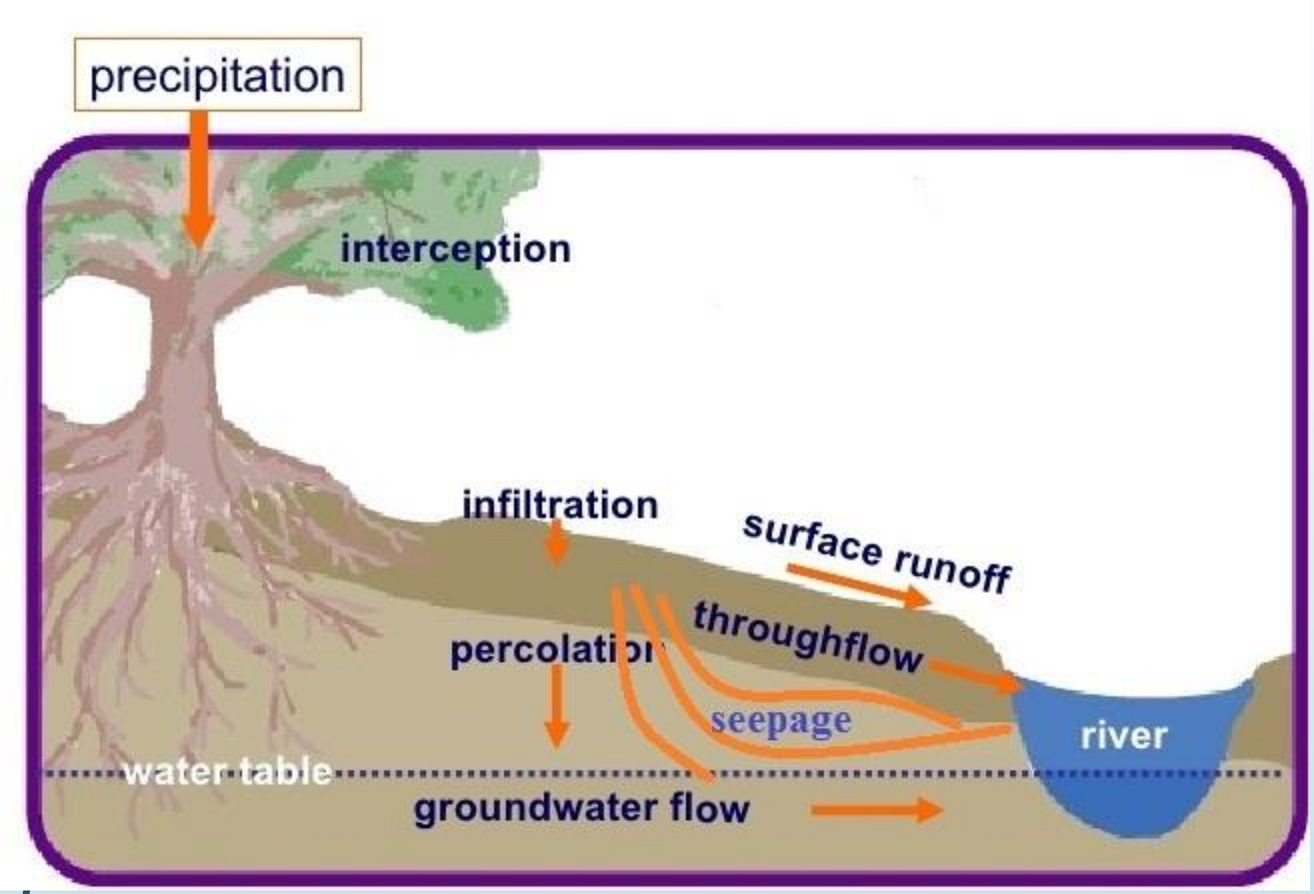
In a **sedimentary basin**, the saturated zone forms a **multiaquifer systems** containing relatively permeable **aquifers** separated by less permeable **confining layers** called **aquitards** or (if having very low permeability) **aquicludes**.

Water table aquifers (or portions thereof) are called **unconfined**.

Aquifers (or portions thereof) enclosed between less permeable strata are called **confined** or **artesian** (the latter term being sometimes reserved for aquifers at sufficiently high pressure for wells to flow spontaneously).

Though **confining beds** and the underlying **bedrock** are sometimes assumed to be impermeable, they are not. Both are sufficiently porous and/or fractured to allow through flow of water, albeit sometimes only locally and at low rates.

Subsurface Hydrology



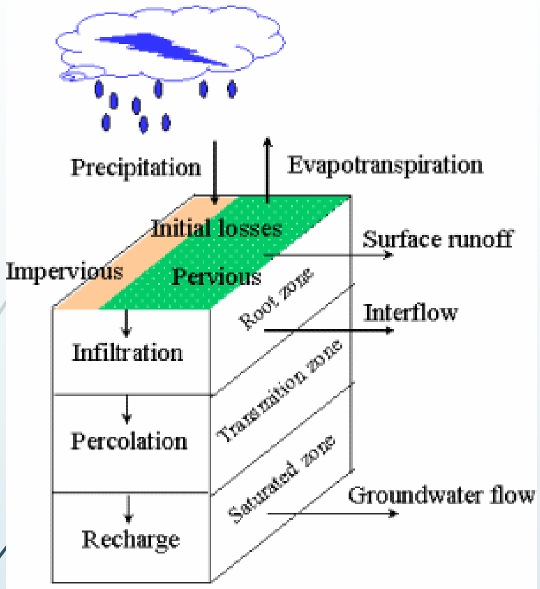
Infiltration = Rate of flow into unsaturated zone across **soil surface**

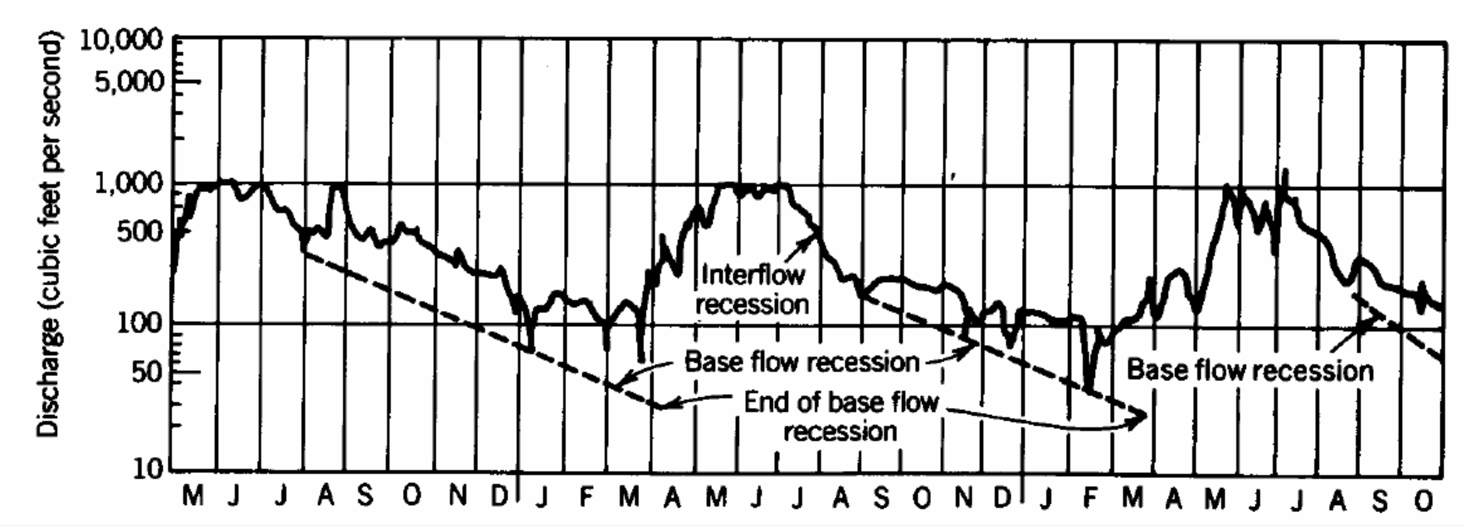
Deep percolation (**net infiltration**) = Rate of downward flow across **bottom of root zone**

Recharge = Rate of flow into saturated zone across **water table**

The three generally **differ** due to
- **Evapotranspiration** (ET) from root zone
- **Change** in water **storage** within unsaturated zone
- **Lateral flow** through unsaturated zone (due to sloping topography and layering) that may cause **interflow**

Subsurface Hydrology





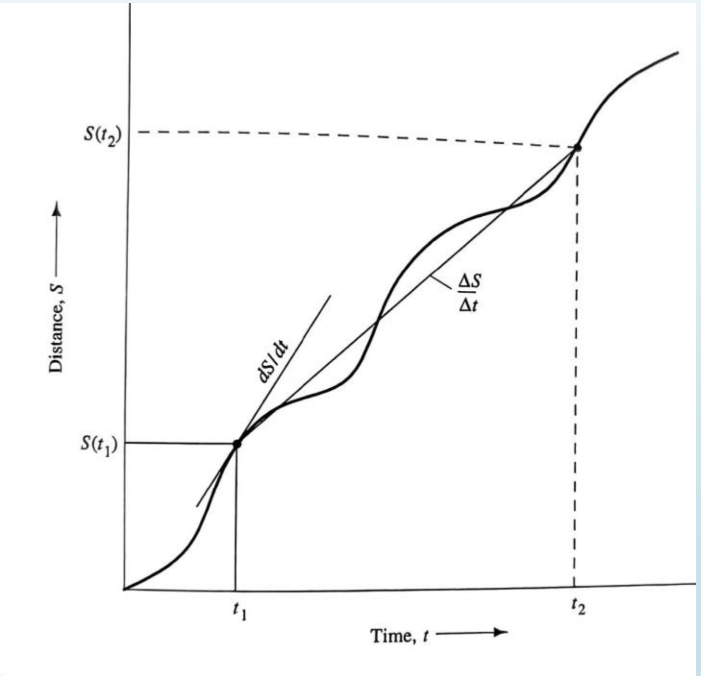
Interflow = component of stream hydrograph contributed by saturated and/or unsaturated flow of **infiltrating water** through the vadose zone.
Baseflow = component of a stream hydrograph contributed by **groundwater inflow** (the third component being **overland flow**)
Baseflow Recession = Decline in stream hydrograph associated with baseflow due to decline in baseflow following an episodic recharge event.

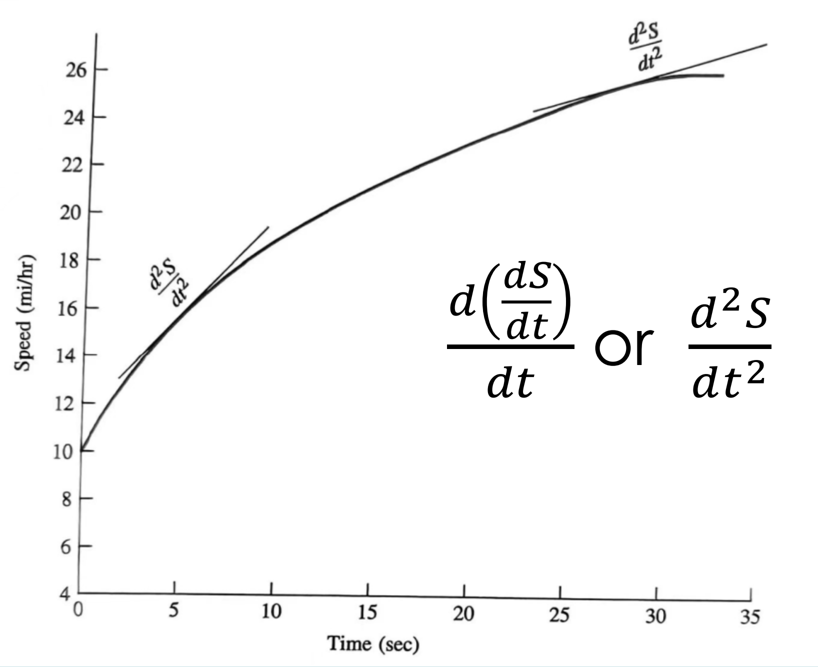
Typically **recession** is near **exponential**, so if a hydrograph is entirely due to baseflow (or interflow), it can be used to estimate the total recharge (or net infiltration) volume.

Review of Mathematics and Flow Equation

- Derivatives

Soil-moisture movement, groundwater flow, transport can be described by means of partial differential equations.





$$\frac{d\left(\frac{dS}{dt}\right)}{dt} \text{ or } \frac{d^2S}{dt^2}$$

$$\frac{\Delta S}{\Delta t} = \frac{S(t_2) - S(t_1)}{t_2 - t_1} \qquad \frac{dS(t_1)}{dt} = \lim_{t \to t_1} \frac{S(t) - S(t_1)}{t - t_1}$$

Review of Mathematics and Flow Equation

- Derivatives

In hydrogeology, h=h(x,y,z).

Partial Derivatives: differential head with respect to one of space variables while holding the other two variables constant.

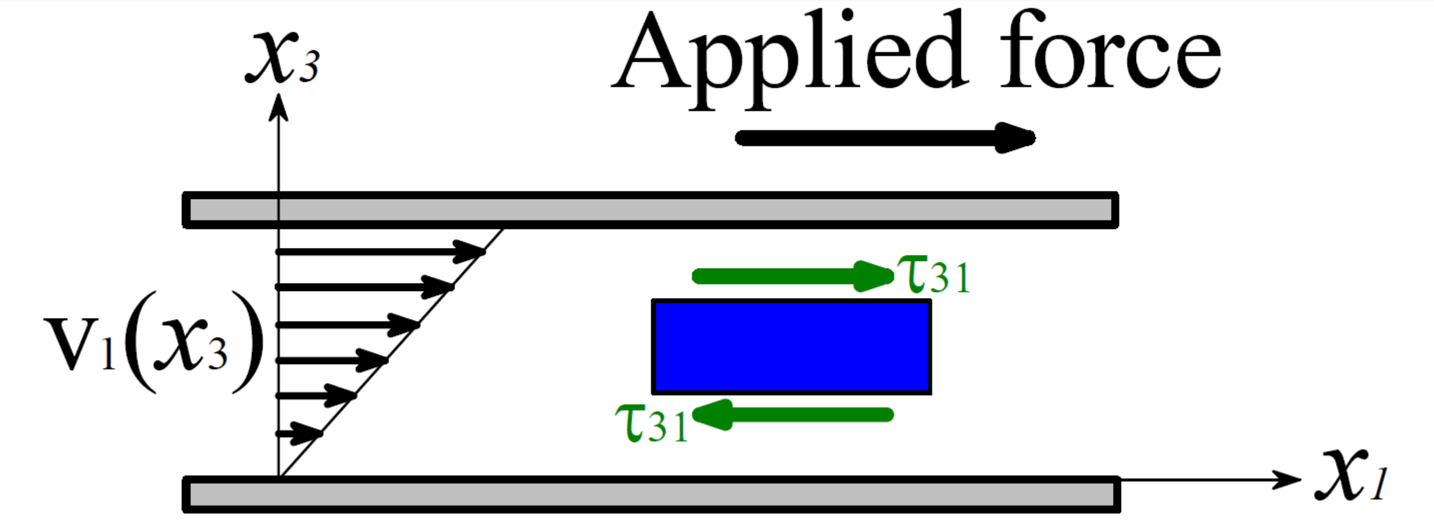
The second derivative of hydraulic head to the space variables:

$$\frac{d^2h}{dx^2} + \frac{d^2h}{dy^2} + \frac{d^2h}{dz^2}$$

Review of Mathematics and Flow Equation

Water as a Newtonian Fluid

- **Water** commonly behaves as a **Newtonian** fluid in that under **laminar flow**



$$\boxed{\tau_{31} = \mu \frac{d\mathrm{v}_1}{dx_3}}$$

μ = **dynamic viscosity**

Constitutive relation (**law**)

$$[\mu] = \frac{[\tau]}{[dv/dx]} = \frac{FL^{-2}}{LT^{-1}L^{-1}} = FTL^{-2} = MT^{-1}L^{-1}$$

剪应力

shear stresses τ acting in the planes of the lamina are **linearly proportional** to the **rate** of **velocity variation (strain rate)** normal to the lamina

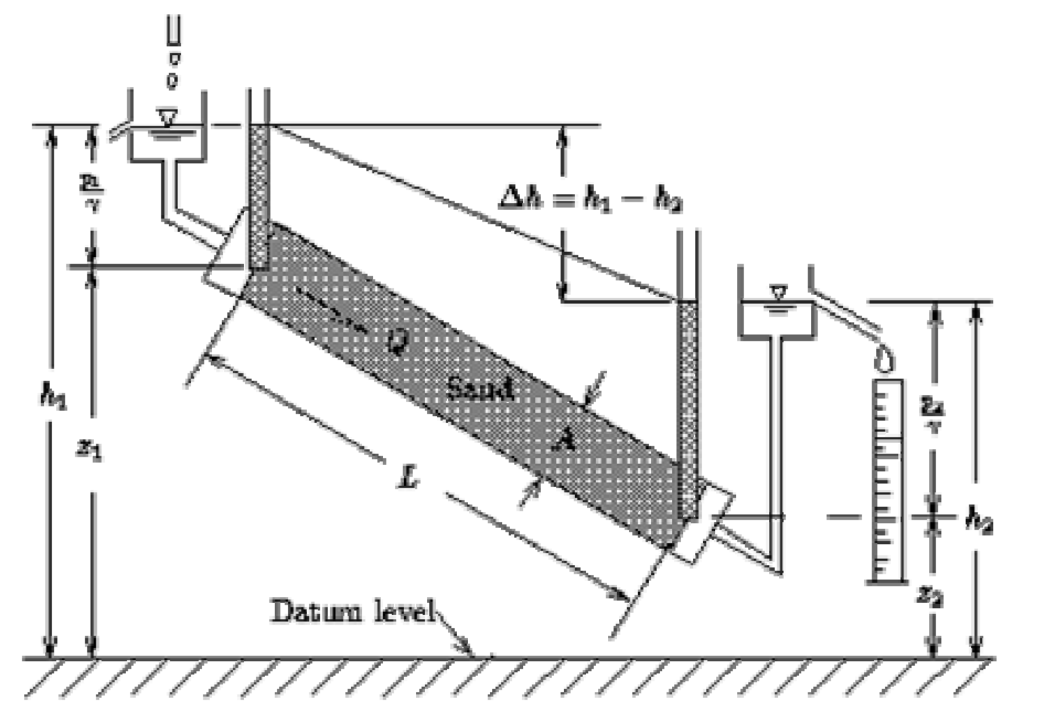
Review of Mathematics and Flow Equation

Review of Mathematics and Flow Equation

Darcy's Law

达西定律

Experiments (starting with ***Henry Darcy*** 1856) suggest that when a Newtonian fluid fully **permeates** and **flows slowly** and **steadily** through a **porous medium** under **isothermal** conditions it satisfies the **constitutive relation** (**<u>Darcy's law</u>**)



Review of Mathematics and Flow Equation

- Darcy's Law

$$Q = -KA\frac{dh}{dl}$$

Q = volumetric discharge
K = proportionality constant known as hydraulic conductivity
A = cross-sectional area
dh/dl =gradient of hydraulic head

K is a measure of ability of the fractured or porous media to transmit water

specific discharge or **Darcy flux**

$$q = -K\frac{dh}{dl}$$

q：达西流速

$$K = \frac{\gamma}{\mu}k$$

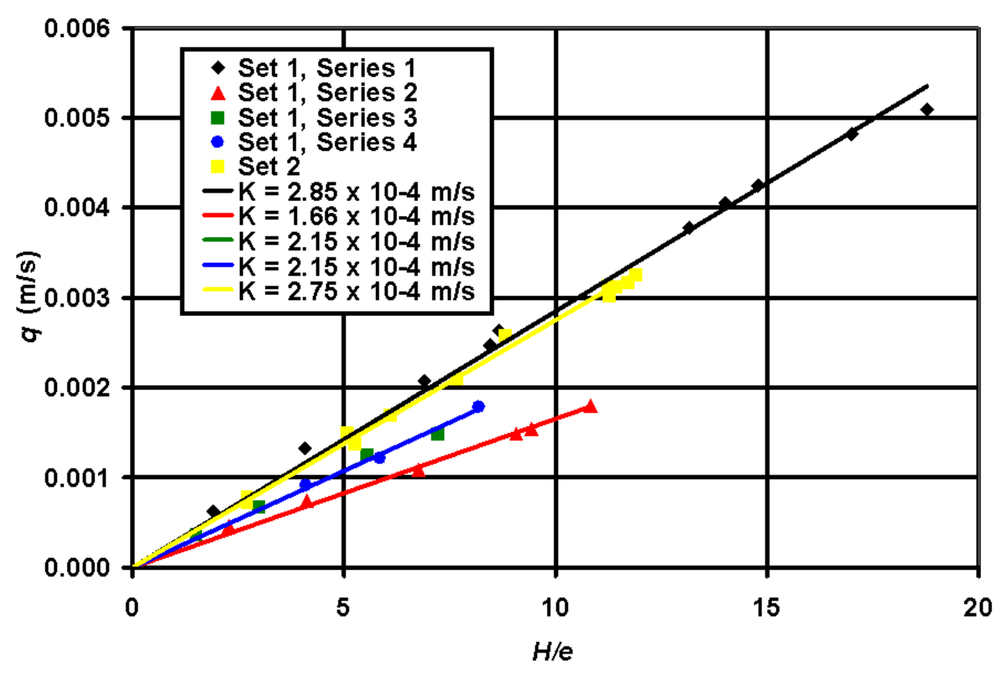
γ= ρ*g*= **unit weight** of fluid [$MT^{-2}L^2$]
ρ =fluid mass **density** [M^3/L]
g = acceleration due to **gravity**[L/T^2]
k = **intrinsic permeability** of medium[L^2]
k与介质相关

Darcy's law was obtained for one-dimensional flow. However, head is a function of all three dimensions: $h=h(x,y,x)$

Review of Mathematics and Flow Equation

Darcy’s Law

Darcy’s own experimental results look like this:



In other words, for a **given fluid** at a **given pressure and temperature** (given μ, ρ) flowing **slowly** through a **given porous medium** (given *k*) the **flux** is **linearly proportional to** the **hydraulic gradient** $\Delta h/\Delta L$.

Darcy’s law is thus equivalent to

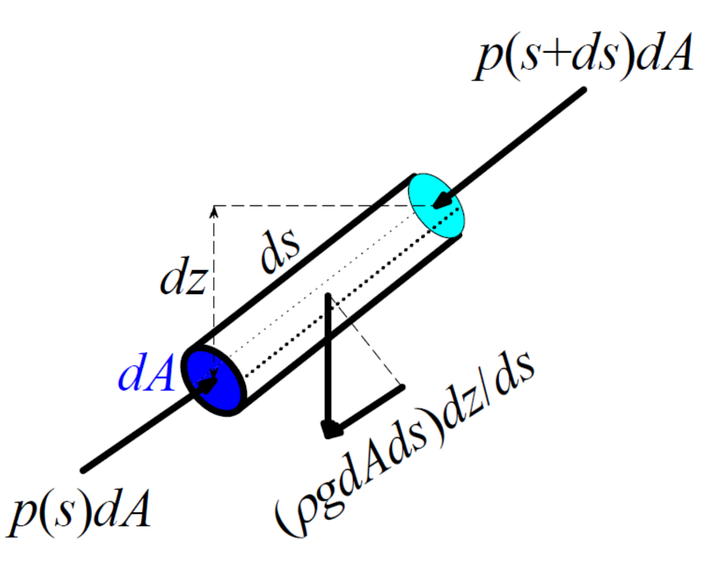
- **Fourier’s law** of heat conduction in solids
- **Fick’s 1st law** of diffusion
- **Ohm’s law** for electrical current.

Darcy’s law **does not** apply to non-Newtonian (pseudoplastic, dilatant) fluids and surfactants.

Review of Mathematics and Flow Equation

- **Hydraulic Gradient as Force**
- Consider a **stream tube** having **infinitesimal** cross-sectional area *dA* and length *ds*. The fluid is propelled in its motion by the **driving force**

$$\underbrace{\left[p(s)-p(s+ds)\right]dA}_{\text{differential pressure force}}-\underbrace{\rho g dA ds\frac{dz}{ds}}_{\text{gravity force}}$$



Expanding $p\ (s+ds)$ in **Taylor series** about *s* and discarding all but the **two leading terms**,

$$p(s+ds)=p(s)+\frac{dp}{ds}ds$$

$$\underbrace{-\frac{dp}{ds}dAds}_{\text{differential pressure force}}\quad\underbrace{-\rho g dA ds\frac{dz}{ds}}_{\text{gravity force}}$$

The **driving force per unit volume**

$$-\frac{dp}{ds}-\rho g\frac{dz}{ds}$$

Review of Mathematics and Flow Equation

- **Defining hydraulic head**

$$h = \underbrace{\int_{p_0}^{p} \frac{dp}{\rho g}}_{\text{pressure head}} + \underbrace{(z - z_0)}_{\substack{\text{elevation} \\ \text{or} \\ \text{gravity head}}}$$

implies that it represents **incremental work** performed by moving a **unit weight** of fluid up-gradient (against the driving force) from a lower to a higher state of **potential energy**. This is why surfaces or curves of equal *h* are called **equipotentials**.

$$-\frac{dh}{ds} = -\frac{1}{\rho g}\frac{dp}{ds} - \frac{dz}{ds} = \frac{\text{driving force}}{\gamma}$$

in vector form

$$-\operatorname{grad} h = -\begin{pmatrix} \partial h/\partial x \\ \partial h/\partial y \\ \partial h/\partial z \end{pmatrix} = -\frac{1}{\gamma}\begin{pmatrix} \partial p/\partial x \\ \partial p/\partial y \\ \partial p/\partial z \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

In other words, **Darcy's law** states that fluid **flux** is linearly **proportional to** the **driving force per unit weight**, the hydraulic **conductivity** acting as the constant of proportionality, representing **flux per unit gradient**.

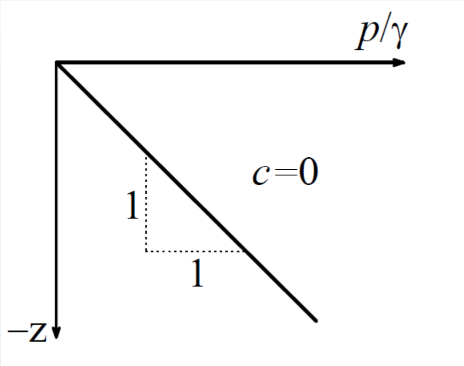
Treating water as an **incompressible** and **homogeneous liquid** under **isothermal conditions** implies $\gamma=\rho g$=constant. Setting $p_0=0$ at atmospheric conditions (*p* thus becoming **gauge pressure**) and $z_0=0$ implies

$$h = \frac{p}{\gamma} + z$$

Review of Mathematics and Flow Equation

Defining hydraulic head

- Flow does not depend on head, only on its gradient. One can therefore set an **arbitrary reference** value for h; we set $h = 0$at z=0.
- If $h \equiv c$ (**constant**) then grad$h \equiv \mathbf{0}$ and so $\mathbf{q} \equiv \mathbf{0}$, i.e., the fluid is **static** (does not flow).
- Under **static** conditions **pressure** increases **linearly** with depth: $p = \gamma\,(c - z)$

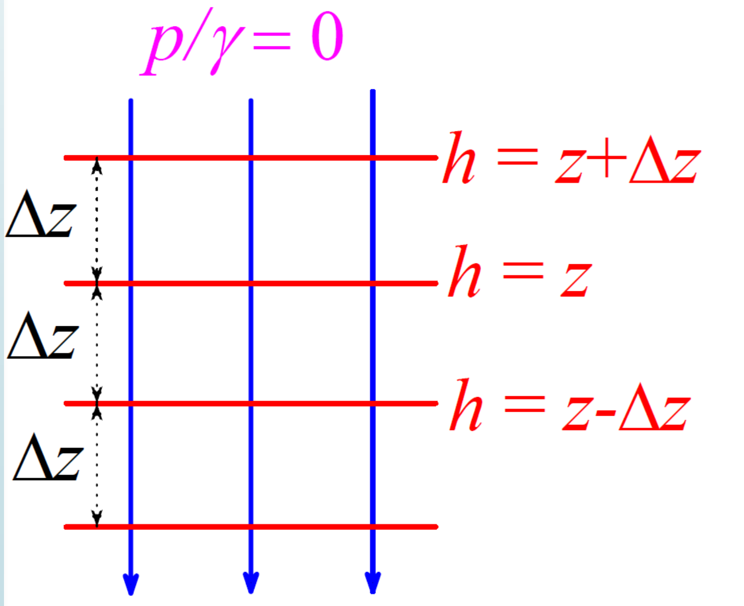


Review of Mathematics and Flow Equation

- **Defining hydraulic head**

• Under horizontal flow (say in an aquifer) the equipotentials are vertical. Setting h=c yields p =γ $(c - z)$ along any equipotential, i.e., pressure increases linearly with depth, as in the static case:

• In a domain of equal pressure (say p = 0) there is no pressure force and flow is gravitational under a unit downward force (per unit weight of fluid):



Review of Mathematics and Flow Equation

- Terms relating to tensors:

  Scalar: a zero-order tensor, a quantity characterized by its size or magnitude. (e.g., h, C, T)

  Vector: a first-order tensor, a quantity has both a magnitude and a direction. (e.g., Discharge, flux)

  Tensor: the product of two vectors, requiring nine components to account for all possible products of the three components of each vector.(e.g., hydraulic conductivity, hydrodynamic dispersion)

$$grad\ h = \mathbf{i}\frac{\partial h}{\partial x} + \mathbf{j}\frac{\partial h}{\partial y} + \mathbf{k}\frac{\partial h}{\partial z}$$

i, j, k are unit vector in x,y,z direction.

h is a scalar, but grad *h* is a vector

$$\boldsymbol{\nabla} = \mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z}$$

vector differential operator

Specific discharge **q** is a vector, three components, q_x,q_y, and q_z

Magnitude of the vector **q**, $q = |\boldsymbol{q}|$

Review of Mathematics and Flow Equation

- Terms relating to tensors:

$$\mathbf{K} = \begin{bmatrix} K_{\mathrm{xx}} & K_{\mathrm{xy}} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix}$$

- Three components of the specific discharge vector **q** :

$$q_x = -K_{\mathrm{xx}} \frac{\partial h}{\partial x} - K_{\mathrm{xy}} \frac{\partial h}{\partial y} - K_{\mathrm{xz}} \frac{\partial h}{\partial z}$$

$$q_y = -K_{y\mathrm{x}} \frac{\partial h}{\partial x} - K_{yy} \frac{\partial h}{\partial y} - K_{yz} \frac{\partial h}{\partial z}$$

$$q_z = -K_{zx} \frac{\partial h}{\partial x} - K_{zy} \frac{\partial h}{\partial y} - K_{zz} \frac{\partial h}{\partial z}$$

- Dot product/inner product: multiply two vectors together, a scalar.
- Second derivative:

$$\nabla \cdot \mathrm{grad}\ h = \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2}$$

Review of Mathematics and Flow Equation

- Terms relating to tensors:

$$\mathbf{K} = \begin{bmatrix} K_{\mathrm{xx}} & K_{\mathrm{xy}} & K_{\mathrm{x}z} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix}$$

均质：k处处相等
非均质：k不同位置不同

- Three components of the specific discharge vector **q** :

$$q_x = -K_{\mathrm{xx}}\frac{\partial h}{\partial x} - K_{\mathrm{xy}}\frac{\partial h}{\partial y} - K_{\mathrm{xz}}\frac{\partial h}{\partial z}$$

$$q_y = -K_{y\mathrm{x}}\frac{\partial h}{\partial x} - K_{yy}\frac{\partial h}{\partial y} - K_{yz}\frac{\partial h}{\partial z}$$

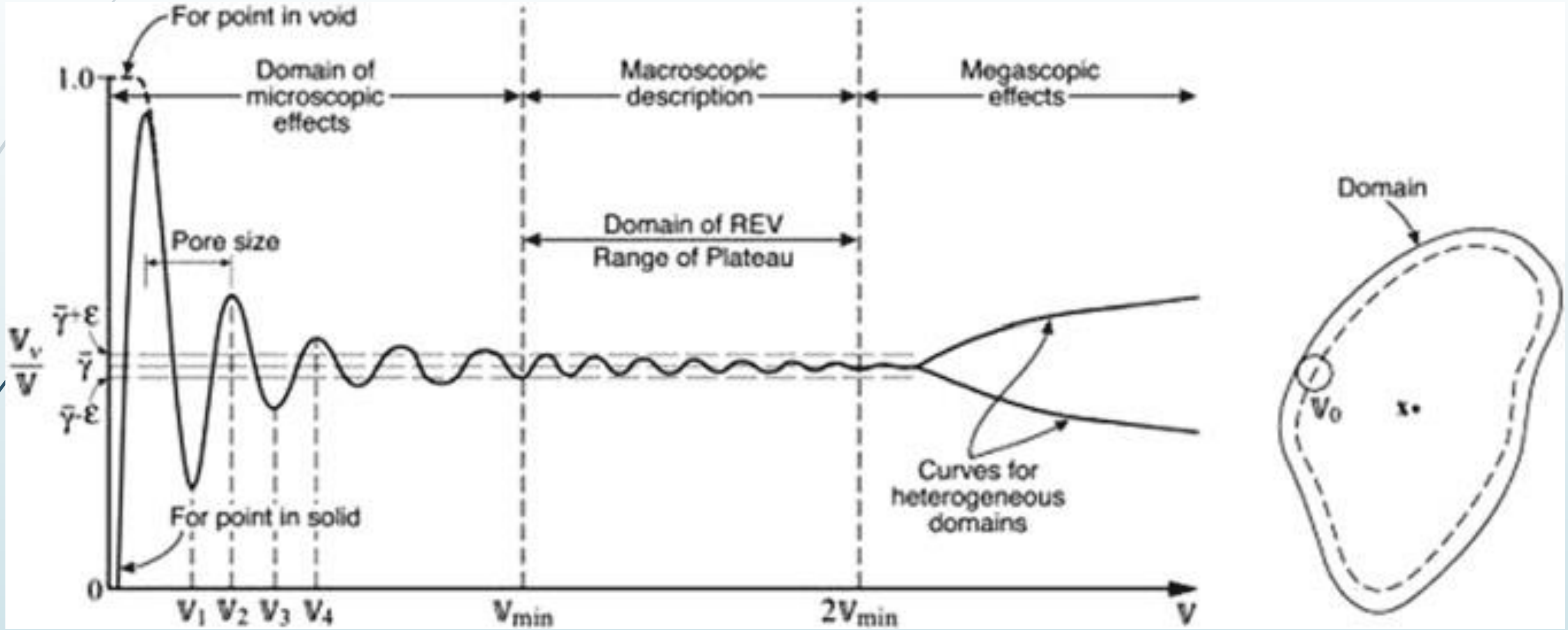
$$q_z = -K_{z\mathrm{x}}\frac{\partial h}{\partial x} - K_{zy}\frac{\partial h}{\partial y} - K_{zz}\frac{\partial h}{\partial z}$$

- Dot product/inner product: multiply two vectors together, a scalar.
- Second derivative:

$$\nabla \cdot \mathrm{grad}\, h = \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2}$$

Review of Mathematics and Flow Equation

- Representative elementary volume (REV)



For a considered porous medium, the size of the REV is selected such that:

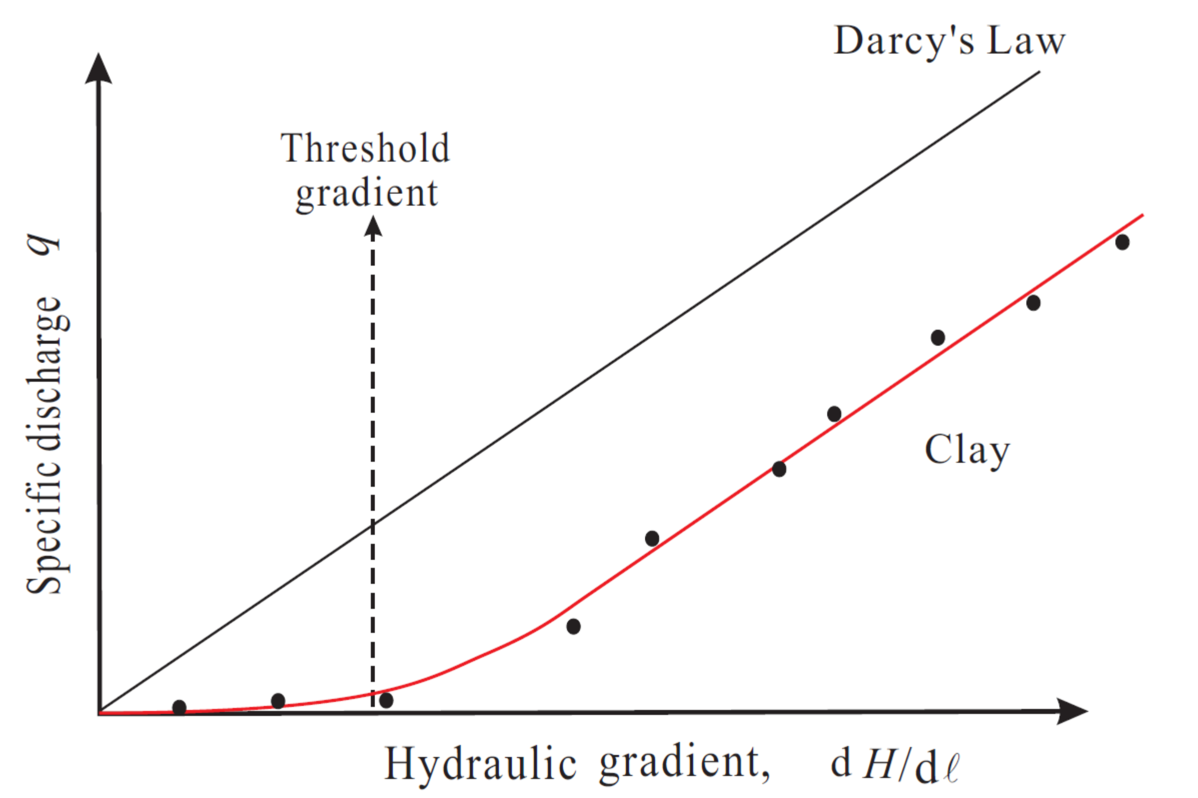
• The average value of *any relevant geometrical characteristic of the microstructure of the void space*, at any point in a porous medium, will be *a unique function of the location of that point only*.

• The measured averaged value should be *independent of small variations in the size of the* REV.

Review of Mathematics and Flow Equation

- **VALIDITY OF DARCY'S LAW**

Lower Limit



According to Darcy's law, any hydraulic head gradient, no matter how small, will cause water movement. On the contrary, many experiments have shown that the hydraulic head gradient must exceed some threshold value *dh/dl*, in order to cause water movement in clayey soils. The failure of Darcy's law in this case can be attributed to the fact that important electrostatic forces exist in the clayey soils, due to electrical charge imbalances within the mineral structure of the soil. At low hydraulic head gradients, these electrostatic forces (or internal energies) cannot be neglected in the derivation of Poiseuille's law.

Review of Mathematics and Flow Equation

- **VALIDITY OF DARCY'S LAW**

The Reynolds Number for Groundwater Flow

How slowly must a Newtonian fluid flow for Darcy's law to hold? Experiments done on unconsolidated **granular media** (glass beads, sand, silt) provide the answer in terms of a **dimensionless group** called the **Reynolds number**, generally defined as

$$Re = \frac{dq}{\nu}$$

d = **mean** grain **diameter** or **diameter** of **10th percentile** of grains by weight

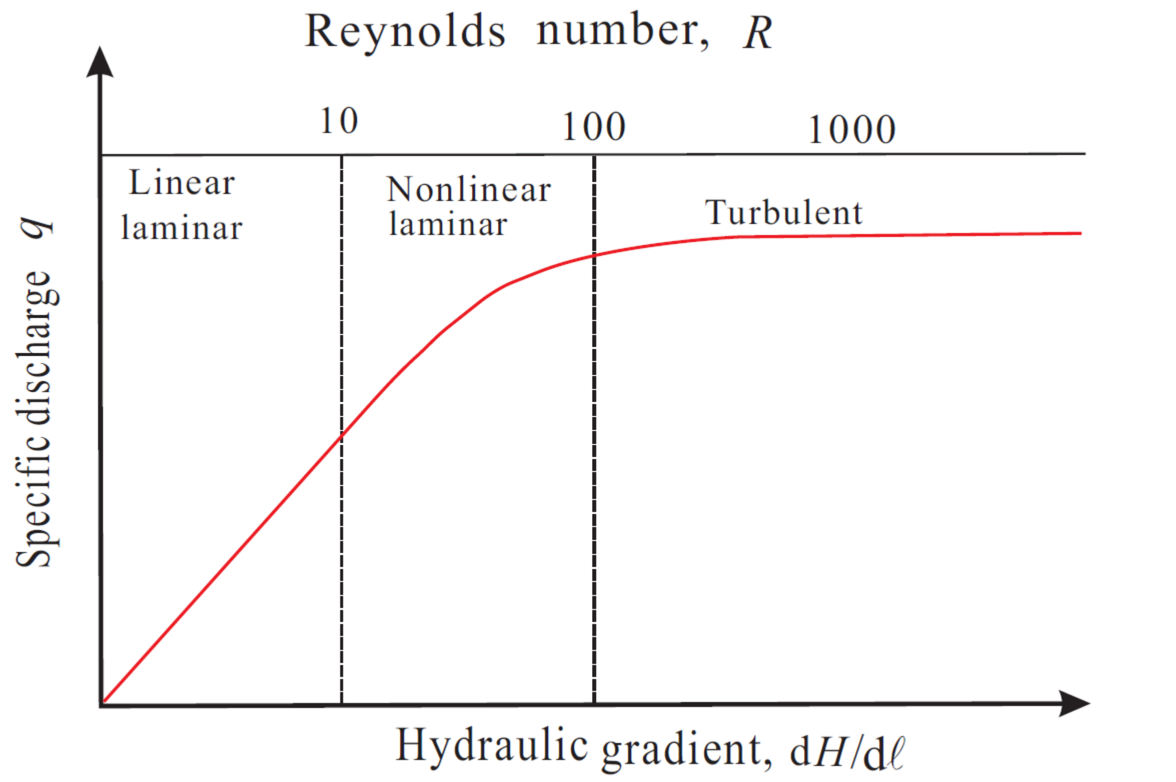
$\nu = \mu / \rho$ = **kinematic viscosity** [L^2/T]

The experiments suggest that the **Darcy regime** (known in fluid mechanics as **Stokes regime**) is valid for Re not exceeding 1 – 10; beyond that, the flow regime becomes **nonlinear** and (at still higher Re) **turbulent** (otherwise it is **laminar**):

Review of Mathematics and Flow Equation

- **VALIDITY OF DARCY'S LAW**

The Upper Limit

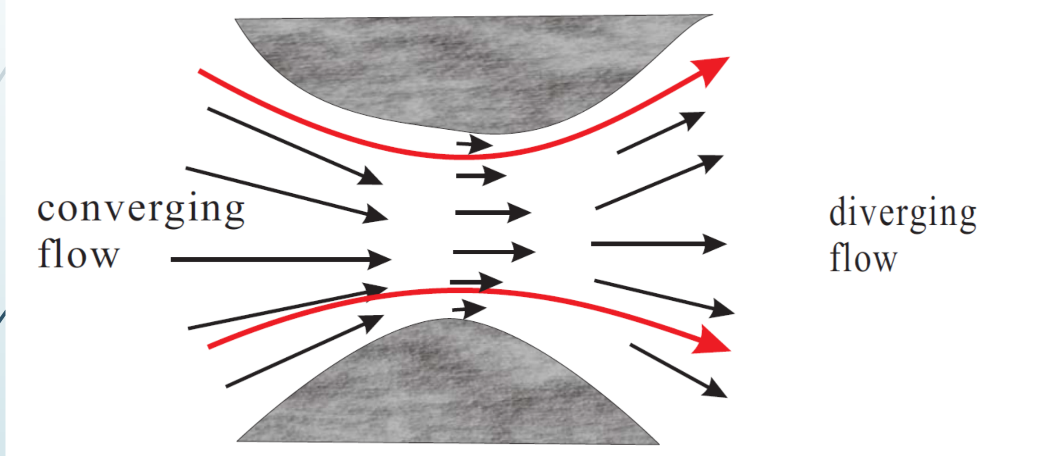


The linear relationship only exists when the hydraulic gradient is relatively small or the Reynolds number is smaller than 10. Flow behaviors deviating from the linear relationship (i.e., Darcian behavior) however have been observed at large *dh*/*dl* values (i.e., at $10 < R_e < 100$). Under these conditions, the relation between *q* and *dh*/*dl* is no longer linear, although the flow can still be in the laminar flow regime (or in a transition regime). At $R_e >> 100$, turbulent flow with streamlines crossing each other takes place. Under the turbulent flow regime, *q* is no longer correlated with *dh*/*dl* and flow exhibits chaotic behavior (random motion). Under this scenario, describing flow behavior quantitatively becomes difficult.

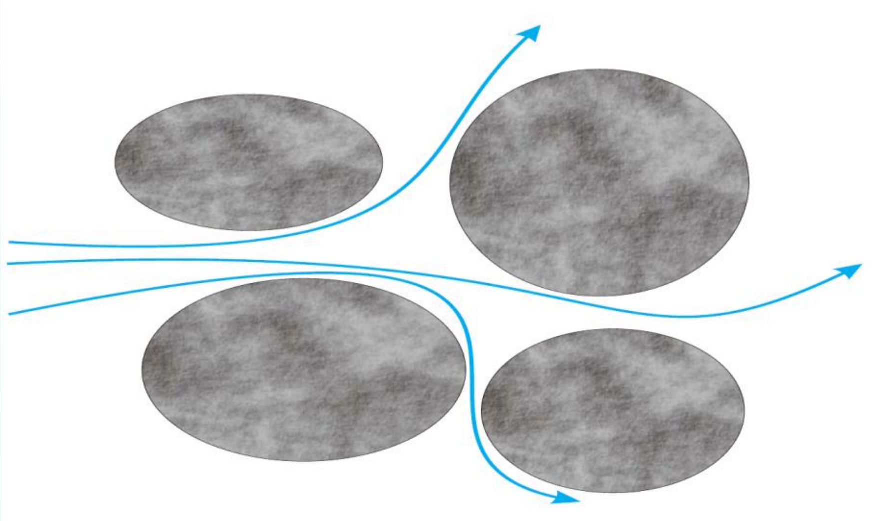
Review of Mathematics and Flow Equation

- **VALIDITY OF DARCY'S LAW**

The Upper Limit



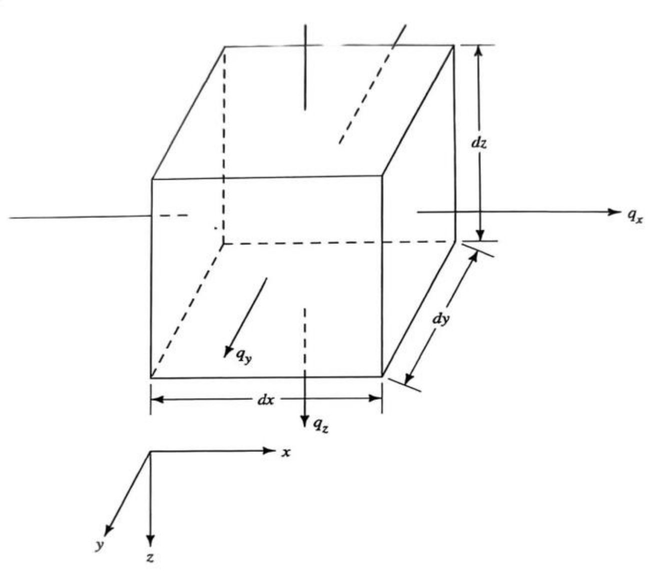
Velocity variation within a pore and converging and diverging flow



Variations in flow velocity among different pores

Review of Mathematics and Flow Equation

- **Derivation of the flow equation in a deforming medium**



The law of mass conservation states that there can be no net change in the mass of fluid in a small REV of a porous medium. In other words, the mass entering the REV less the mass leaving the REV is equal to the change in mass storage with time.

The component of mass flux into the REV parallel to the x axis is the fluid density times the flux rate:

$$\text{Mass influx along x axis} = \rho_w q_x dydz$$

$$\text{Mass outflow rate parallel to x axis} = \left[\rho_w q_x + \frac{\partial(\rho_w q_x)dx}{\partial x}\right] dydz$$

$$\text{Net mass accumulation} = \text{mass inflow- mass outflow}$$

$$= - \frac{\partial(\rho_w q_x)dxdy\,dz}{\partial x}$$

ρ_w = fluid density (M/L^3)
q_x = specific discharge or volume of flow per cross-sectional area(L/T)
$dydz$ = cross-sectional area(L^2)

Review of Mathematics and Flow Equation

- **Derivation of the flow equation in a deforming medium**

Net mass accumulation due to the flow component parallel to

the x axis $-\dfrac{\partial(\rho_w q_x)dxdy\,dz}{\partial x}$

the y axis $-\dfrac{\partial(\rho_w q_y)dydx\,dz}{\partial y}$

the z axis $-\dfrac{\partial(\rho_w q_z)dzdx\,dy}{\partial z}$

Total net mass accumulation within REV = $-\left(\dfrac{\partial}{\partial x}(\rho_w q_x) + \dfrac{\partial}{\partial y}(\rho_w q_y) + \dfrac{\partial}{\partial z}(\rho_w q_z)\right) dxdydz$

The change in mass of water to time : $\dfrac{\partial M}{\partial t} = \dfrac{\partial}{\partial t}(\rho_w n\, dxdydz)$; n: porosity

The law of conservation of mass:

$$-\left(\frac{\partial}{\partial x}(\rho_w q_x) + \frac{\partial}{\partial y}(\rho_w q_y) + \frac{\partial}{\partial z}(\rho_w q_z)\right) dxdydz = \frac{\partial}{\partial t}(\rho_w n)\, dxdydz$$

Assume: density is same in REV → $-\left(\dfrac{\partial q_x}{\partial x} + \dfrac{\partial q_y}{\partial y} + \dfrac{\partial q_z}{\partial z}\right) = \dfrac{1}{\rho_w}\dfrac{\partial}{\partial t}(\rho_w n)$

Review of Mathematics and Flow Equation

- **Derivation of the flow equation in a deforming medium**

Substitute Darcy's law for the specific discharge components:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)$$

The change in mass within REV is due to changes in porosity and the density of water as the head changes with time. The change in the volume of water in storage is proportional to the change in head with time :

$$\frac{1}{\rho_w}\frac{\partial}{\partial t}(\rho_w n) = S_s\frac{\partial h}{\partial t}$$

Combine:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) = S_s\frac{\partial h}{\partial t}$$

Review of Mathematics and Flow Equation

- **Derivation of the flow equation in a deforming medium**

In del and tensor notation:

$$\nabla \cdot \mathbf{K} \cdot \nabla \mathbf{h} = S_s \frac{\partial h}{\partial t}$$

Einstein's summation notation :

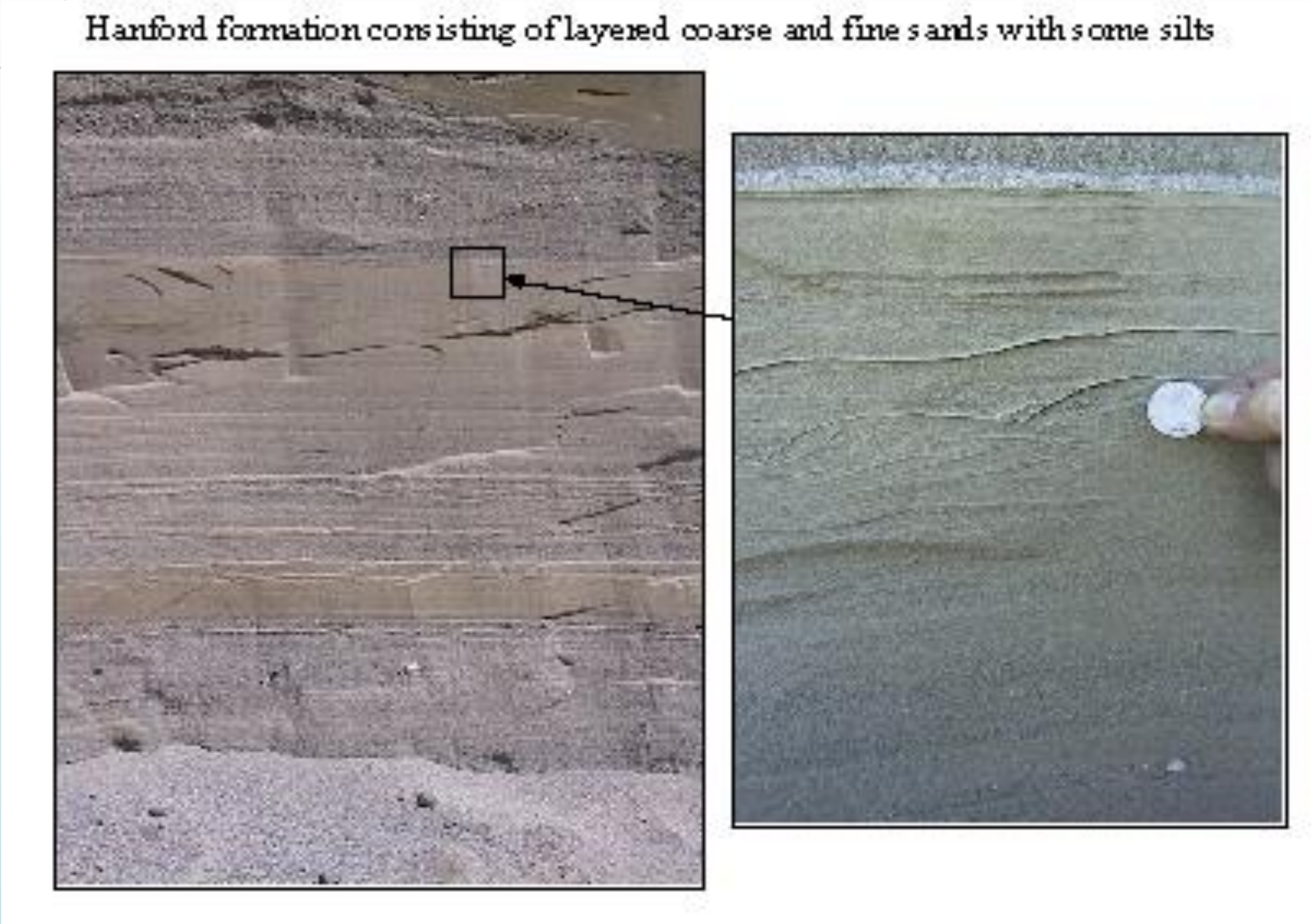
$$q = -\mathbf{K}\frac{dh}{dl}$$

$$q_i = K_{ij} h_j$$

$in\ vector\ notation:$ $\mathbf{q} = \mathbf{K} \cdot \text{grad}\, h$ $\mathbf{q} = \mathbf{K} \cdot \mathbf{h}$

$in\ del\ notation:$ $\mathbf{q} = \mathbf{K} \cdot \nabla\, \mathbf{h}$

Variation in different scale



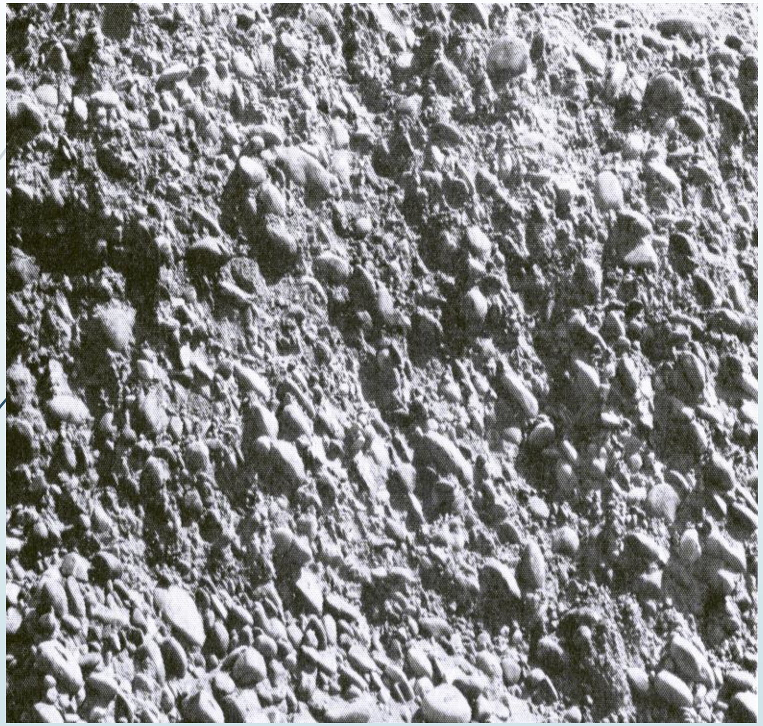
Multi-scale heterogeneity: stratifications (layers) and lamination

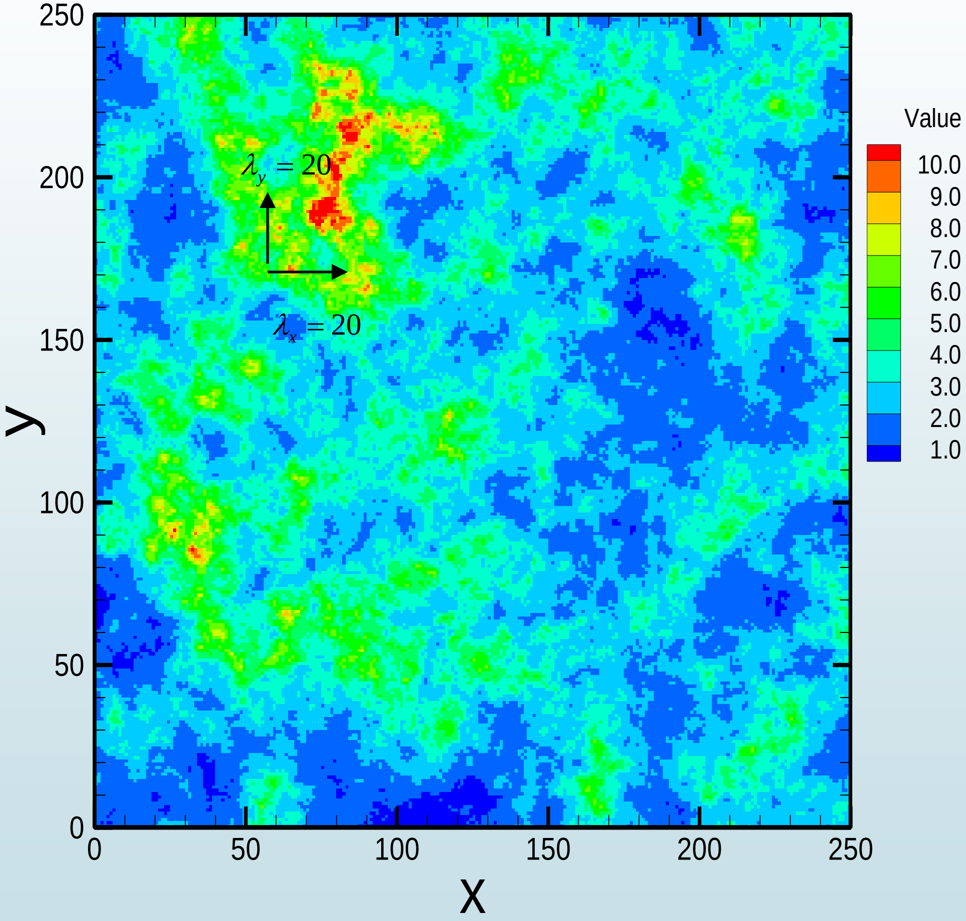
Variation in different scale

Field-scale heterogeneity
meters to hundreds of meters

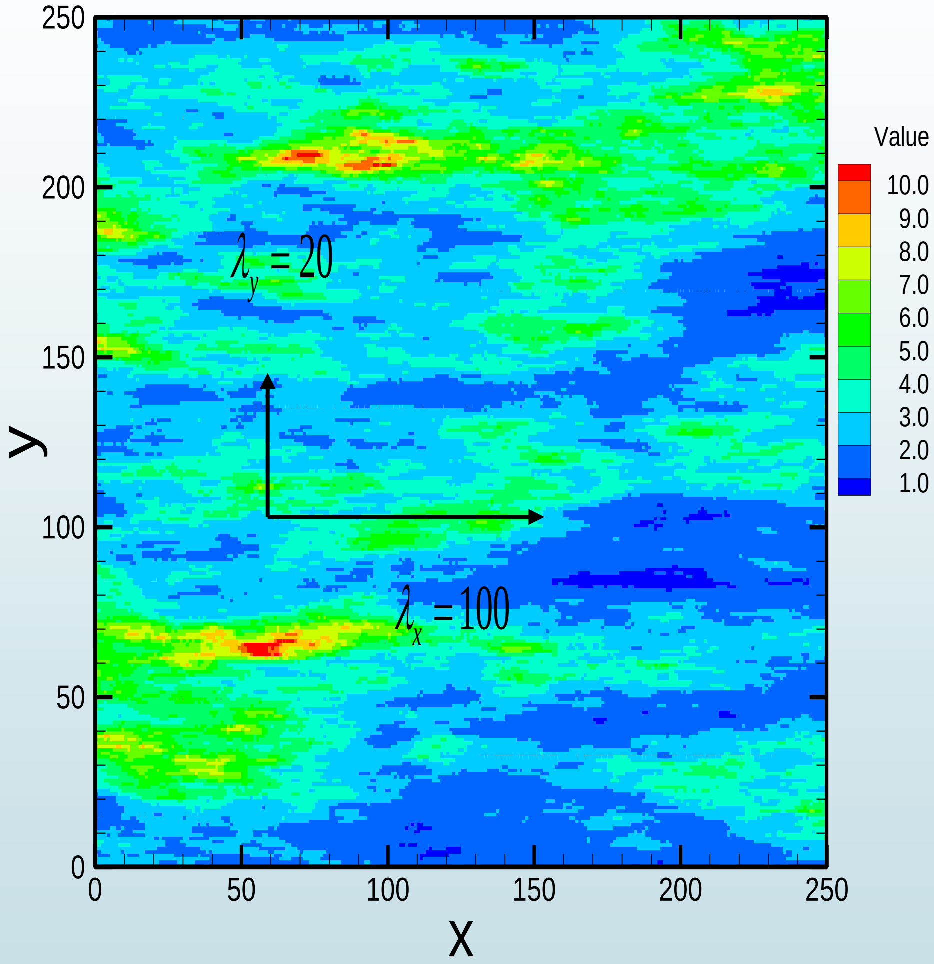
Laboratory-scale heterogeneity
Centimeters to meters

Statistically Isotropic Media





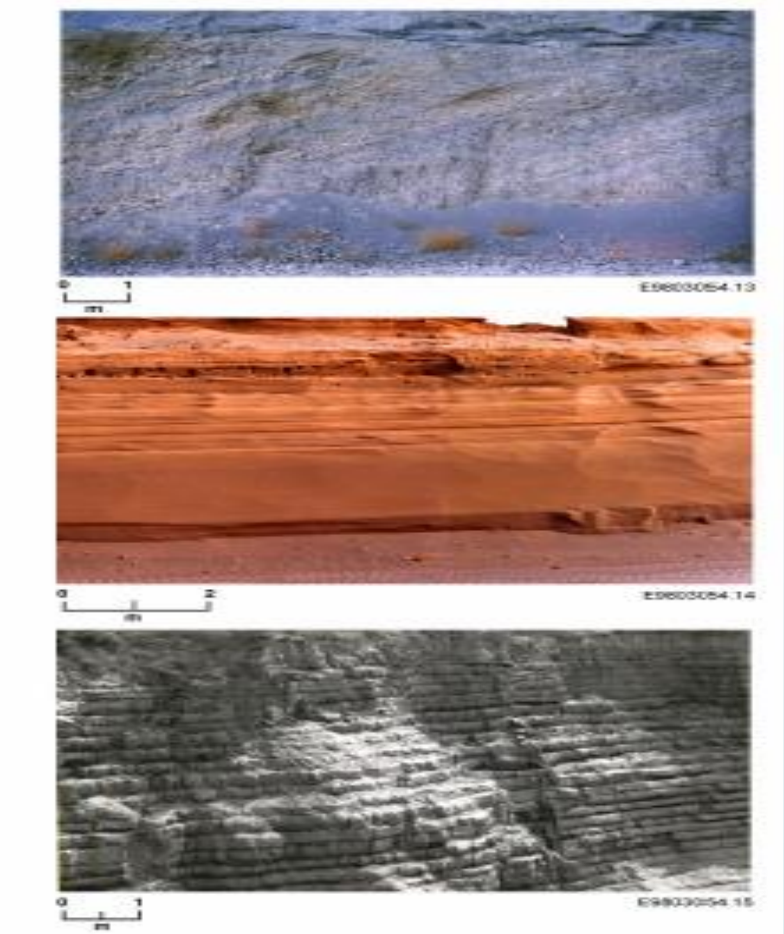
Statistically anisotropic media

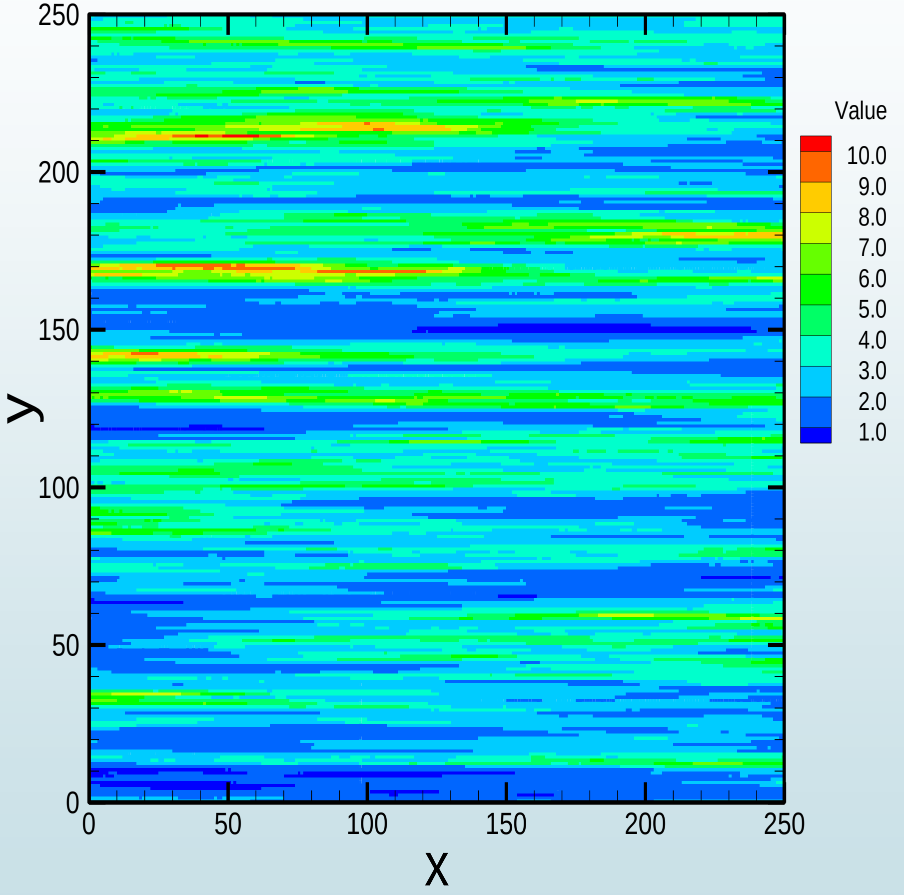


Perfectly stratified media

$$\lambda_y = 20$$

$$\lambda_x = 1000$$





Multi-scale Heterogeneity

- Pore-scale (<<centimeters)
- Laboratory scale (cm to meters)
- Field scale (tens of meters to hundreds of meters)
- Basin scale (tens and hundreds of kilometers) 流域尺度
- Regional scale
- Continental scale