

How and why do crustal fluids flow? Diffusion and the transport of water, heat and solutes in the subsurface



M.Geo.239
6 nov 2019
Elco Luijendijk

eluijen@gwdg.de

Today's menu

- Part 1: Diffusion laws, heat conduction, solute transport
- Part 2: Fluid flow & diffusion: Darcy's law

2

Diffusion

- Many physical processes are the result of diffusion or can be described by diffusion laws: heat conduction, electrical currents, solute diffusion, and groundwater flow
- Diffusion can be described by a very simple equation:
 - $q = K \frac{\partial u}{\partial x}$
- in words, the flux of a particular quantity (q) is proportional to the gradient of a particular quantity ($\frac{\partial u}{\partial x}$) times some type of constant (K)

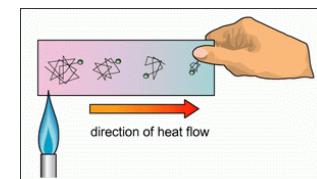
3

Heat diffusion

- The first diffusion law was discovered by the French scientist Fourier in 1811
- The work earned him the mathematics prize at the Paris Institute, but with reservations: "the manner in which the author arrives at these equations is not exempt of difficulties and his analysis to integrate them still leaves something to be desired on the score of generality and even rigour"



Fourier



Heat conduction in a metal plate

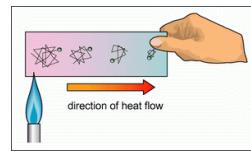
4

Heat diffusion

- The diffusion of heat in a medium can be described by Fourier's law: $q = K \frac{\partial T}{\partial x}$
- in words: the heat flux (W m^{-2}) is equal to the thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$) multiplied by the temperature gradient (K m^{-1})
- Thermal conductivity: the ease with which heat can be transported through a medium
- Examples: metals have a very high thermal conductivity (~20 $\text{W m}^{-1} \text{K}^{-1}$), water has a moderate conductivity (0.6 $\text{W m}^{-1} \text{K}^{-1}$), and air has a very low conductivity (0.025 $\text{W m}^{-1} \text{K}^{-1}$)



Fourier



Heat conduction in a metal plate

5

Next diffusion law: solute diffusion

- The next relevant diffusion law is Fick's law, which was discovered by the physician Adolf Fick in 1855

- Fick's law governs the movement of solutes in a liquid

$$q_d = -D \frac{\partial C}{\partial x}$$



- in words: solute mass flux = diffusion coefficient x concentration gradient

- Diffusion coefficient (D): governs how easy it is for solutes to move through a liquid

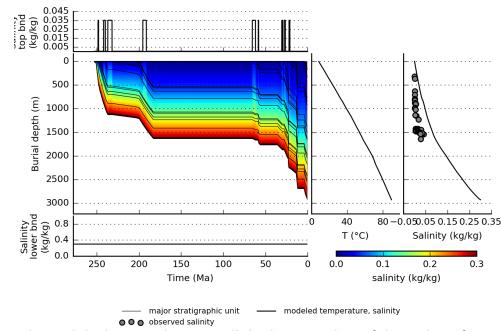
- Typical values for solute diffusion coefficients are 10^{-10} to $10^{-11} \text{ m}^2 \text{s}^{-1}$

- Note that this is orders of magnitude slower than the thermal diffusion coefficient: solute diffusion is very slow compared to the diffusion of heat

6

Solute diffusion: examples

- Model example of long-term (250 My) diffusion of solutes out of the a deep evaporite layer (Zechstein formation) in a sedimentary basin:



7

Heat diffusion and Brownian motion

- Fourier's law is a macroscopic law: i.e. it does not describe heat flow accurately at a molecular scale, but if we zoom out to a larger scale it describes heat flow perfectly well
- Diffusion in gas or a liquid is the result of the random Brownian motion of molecules
- Proof that this is the case was supplied by Albert Einstein in 1905, where he explained observations made by Brown in 1827 on the random motion of pollen grains
- This was also the final proof of the existence of atoms and molecules

Moving pollen due to Brownian motion, Pearle et al. (2010), Am. J. Phys.

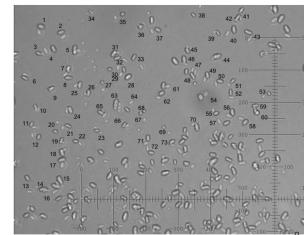


Fig. 3. *Clarkia pulchella* pollen contents before dehiscence, two superimposed photos taken 1 min apart. The scale is 2 μm per division.

8

Diffusion & brownian motion

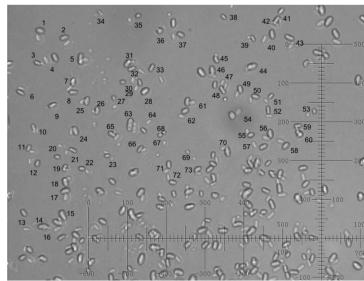


Fig. 3. *Clarkia pulchella* pollen contents before dehiscence, two superimposed photos taken 1 min apart. The scale is 2 μm per division.

Moving pollen due to Brownian motion, Pearle et al. (2010), Am. J. Phys.

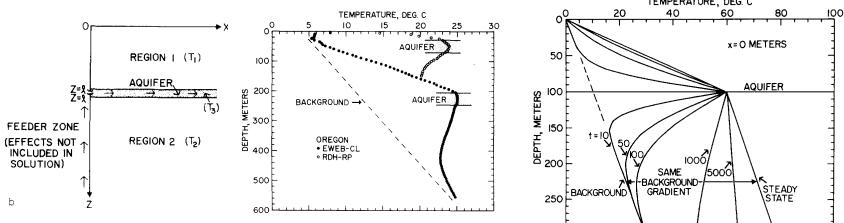


$$D = \frac{RT}{N} \frac{x}{6\pi kP}$$

equation relating diffusion and size of suspended particles
(Einstein, A (1905): Über die von der molekularkinetischen
Theorie der Wärme geforderte Bewegung von in ruhenden
Flüssigkeiten suspendierten Teilchen. Annalen der Physik 17 (8)

Examples of heat conduction in the crust

- Example of much smaller scale conduction, the reduction of a hydrothermal temperature signal over time
- Initial temperatures driven by the upward flow of hot fluids show a strong gradient, but this gradient gets lower and lower over time due to diffusion



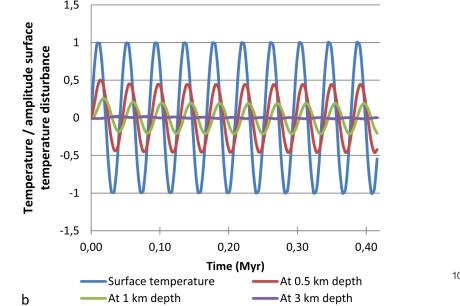
Inverted T-depth profiles, Oregon Cascades, Ziegler Blackwell(1986).
Left: conceptual model of the flow of a deep hot fluid into an aquifer. Middle:
measured temperature profiles that show a hydrothermal anomaly. Right:
modelled reduction of the temperature anomaly over time due to conduction

Heat diffusion / conduction

- According to Fourier's law heat flow is proportional to the temperature gradient
- > This means that high temperature gradients result in high heat flow
- Heat flow reduces temperature gradients, because heat gets transported from high to low temperatures. And lower temperature gradients result in low heat flows
- Result: Diffusion results in 'smearing out' of temperature differences both in space and in time

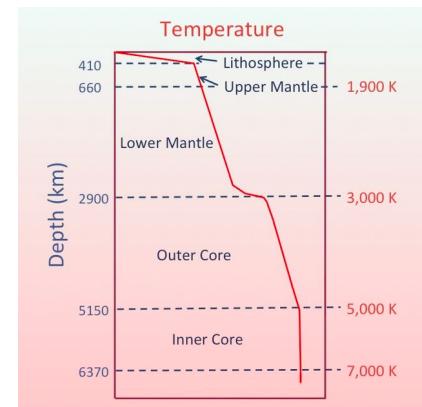
$$q = K \frac{\partial T}{\partial x}$$

Propagation of long-term climate fluctuations in the subsurface
Ter Voorde et al., (2014) NJG 93



Examples of heat conduction in the crust

- We can find the signature of heat conduction at many different scales
- Question: Can you name other heat flow mechanisms in the subsurface, for instance in the mantle?
- And in which part of the subsurface is heat conduction the dominant mechanism of heat transport?



Geothermal gradient in the earth

Other examples of diffusion processes in the earth sciences

https://twitter.com/caldera_curator/status/1191877287869702144

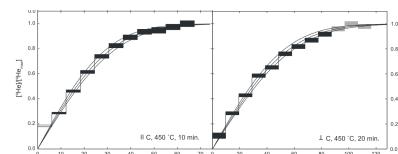


Fig. 7. LADF profiles for all Durango fluorapatite diffusion experiments. After ϕ correction, the data for each depth step have been normalized to the maximum non-uniform data point in the profile. The boxes reflect 2σ uncertainties in the normalized helium signal and the last four data points in each depth step. The first four data points are considered reliable due to the lack of noise, while the last four data points are less reliable due to the lack of data from unheated profiles at depths greater than 90 μm . Best-fit diffusion curves and 95% uncertainty bounds are shown for each experiment.

Diffusion profiles of helium in apatites (van Soest et al., GCA, 2002)

Hillslope diffusion in erosion experiments (Sweeney et al., Science, 2015)

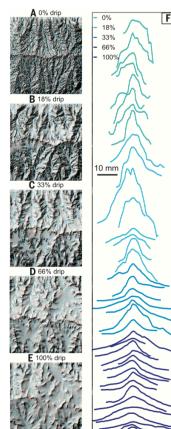


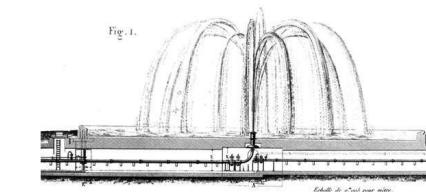
Fig. 3. Steady-state topography and hillslope morphology. (A to E) Hillslopes of experimental topography for (A) 0% drip, (B) 18% drip, (C) 33%, (D) 60%, and (E) 100% drip. Red lines mark channel networks (blue) and locations of hillslope profiles (red). Topography is 475.5 mm wide in plan view. (F) Elevation profiles of hillslopes marked by red lines in (A) to (E). Vertical and horizontal length scales are equal.

Part 2: flow through porous media: Darcy's experiments

- Henri Darcy (1803-1858): founder of quantitative hydrogeology
- Darcy was commissioned to provide clean drinking water to the town of Dijon, by using sand filters
- Darcy tried to answer the question: Can we predict the flow of groundwater through sand filters?



Henri Darcy

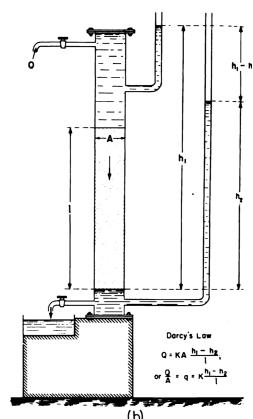


Fountains of Dijon, designed by Darcy

14

Darcy's experiments

- Goal: measure how water discharge through a sand filter varies with hydraulic gradient (ie. the difference in water level on either side)
- Experimental setup:



15

Darcy's experiments

- Result of experiments:
 - 1- Discharge is proportional to the cross-sectional area of the sand filter (A):
 - 2- Discharge is proportional to the difference in water level on either side divided by the length of the sand filter:

$$Q \propto A$$

$$Q \propto (h_2 - h_1)/L$$

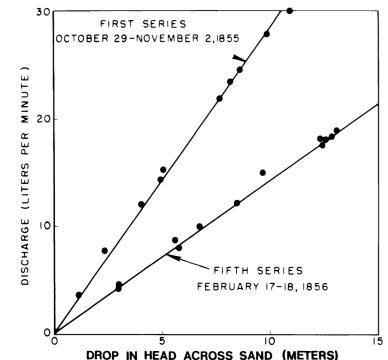


Fig. 2. Graphs compiled from Darcy's tabular data on his experiments of Oct. 29 to Nov. 2, 1855, and of Feb. 17-18, 1856, showing linear relation between flow rate and differences in heights of equivalent water manometers. [Hubbert, 1956, Figure 2.]

16

Darcy's law

- Reworking of results yields Darcy's equation for discharge Q (m³/s)

$$Q = -KA \frac{\Delta h}{\Delta x}$$

- K is a proportionally constant termed hydraulic conductivity -> K controls how easy it is for groundwater to flow through a porous material

- h is hydraulic head (m), x is distance (m)

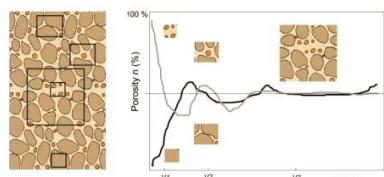
- Divide by cross sectional area (A) to get the specific discharge, also termed the Darcy flux, q (m/s)

17

$$q = -K \frac{\Delta h}{\Delta x}$$

Darcy's law and diffusion

- Like other diffusion laws, Darcy's law is macroscopic law
 - ie, flow at very small scale through individual pores does not follow Darcy's law
- Darcy's law is only valid for larger volumes
- In hydrogeology the lowest volume for which Darcy's law is valid is often termed the "representative elementary volume"



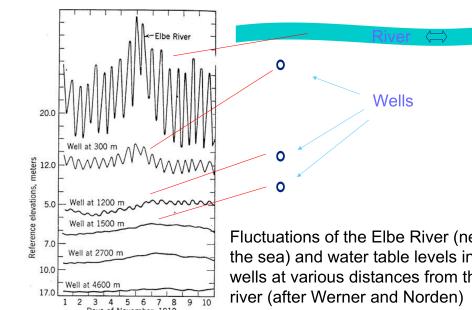
19

Darcy's law & diffusion

- Darcy's law has the same shape as all diffusion equations

$$q = -K \frac{\Delta h}{\Delta x}$$

- Results in typical reduction in contrasts in over time and space as seen in heat and solute diffusion laws:



18

Darcy's law and Navier-Stokes eq.

- Flow at the pore scale is governed by different set of equations, the so called Navier-Stokes equation:

$$\frac{\partial u}{\partial t} + (u \nabla u) - \frac{\mu}{\rho} \nabla^2 u = -\nabla \left(\frac{p}{\rho} \right) + g$$

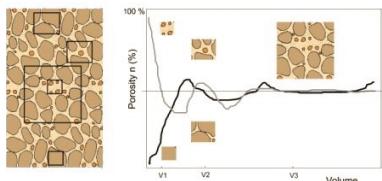
- The use of the Navier-Stokes eq. in subsurface fluid flow is limited, because:

- These equations are very hard to solve for larger systems
- And even if you could solve them, you would need information on the size and shape of all pore spaces in a rock volume

20

Discharge and flow velocity

- Note that Darcy flux / specific discharge (q) has the same units as velocity (m/s)
- However, flow velocity and Darcy flux are not the same (!)
- Example: A ‘packet’ of water moves a distance of 1 m in 1 second. The porosity is 0.5 and the cross sectional area is 1 m^2 . How much water (m^3) has moved in 1 second?



21

When does flow become turbulent? Reynolds experiments

- The conditions under which water flows transition from laminar to turbulent was studied by the English scientist Reynolds in 1883
- Reynolds experiments used dye to trace water flow in small tubes
- Temperature was varied, which results in differences in viscosity and density

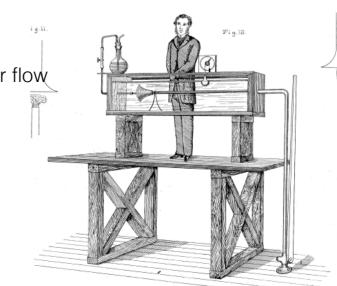
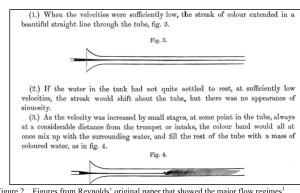
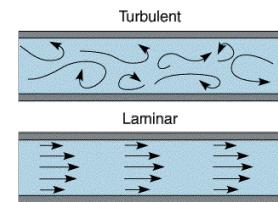


Figure 1. Drawing of one of Reynolds' original apparatus¹

23

When is Darcy's law valid?

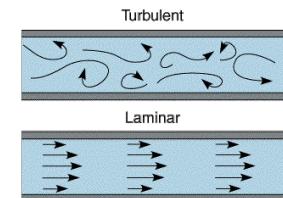
- Darcy's law is only valid for larger scales (ie several pore spaces)
- and Darcy's law is only valid for laminar flow, and not for turbulent flow:



22

Reynolds experiments: transition from laminar to turbulent flow

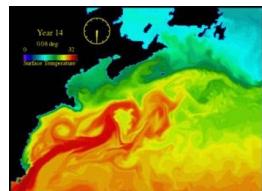
- Results: the onset of turbulent flow is governed by the dimensionless Reynolds number:
 - Reynolds number is the ratio between inertial forces / viscous forces = forces that want to keep moving divided by the friction
 - For fluids in porous media (ie., sediments or rocks):
- $$Re = \frac{\rho v D}{\mu}$$
- ρ = density (kg m^{-3}), v = flow velocity (m s^{-1}), D is particle diameter (of sediments, m), μ is viscosity (Pa s)
 - laminar flow up to $Re = 10$, fully turbulent flow at $Re = 2000$. $Re = 10$ at $v \sim 0.04 \text{ m s}^{-1}$, which is much higher than typical flow velocities of groundwater that go up to $\sim 100 \text{ m yr}^{-1}$ or $3 \times 10^{-6} \text{ m s}^{-1}$



24

Turbulent flow, examples

- Turbulent flow important in the atmosphere, oceans and rivers:



25

Turbulent flow, examples

- Turbulent flow only rarely important subsurface fluid flow
- Question: Can you think of any exceptions?

26

Turbulent flow, examples

- Turbulent flow only rarely important subsurface fluid flow
- Question: Can you think of any exceptions?
 - Flow through coarse gravels
 - Open fractures
 - Karst
 - Flow in wells



27

Hydraulic conductivity

- Hydraulic conductivity: specific discharge (q) for a 1 m difference in hydraulic head through a 1 m length of porous material (sand, clay, etc...)
- units: (m/s)

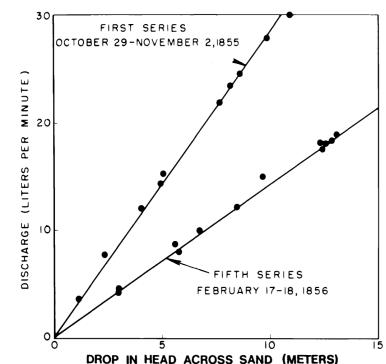
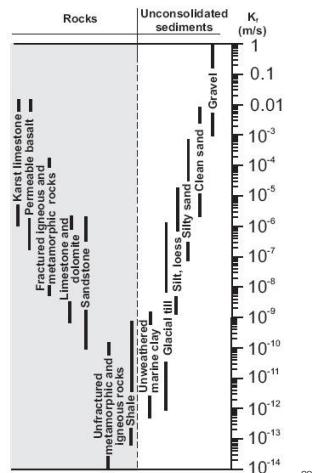


Fig. 2. Graphs compiled from Darcy's tabular data on his experiments of Oct. 29 to Nov. 2, 1855, and of Feb. 17-18, 1856, showing linear relation between flow rate and differences in heights of equivalent water manometers. [Hubbert, 1956, Figure 2.]

28

Hydraulic conductivity and porous material

- Hydraulic conductivity varies over 14 orders of magnitude
- ie, discharge and flow velocity for the same hydraulic gradient vary over 14 orders of magnitude, depending on what type of material the water flows through
- highest values: coarse sediments (gravel, coarse sand), karstic carbonates, fractured and/or weathered crystalline rocks



29

Hydraulic conductivity and fluid properties

- However, hydraulic conductivity is not only a function of the type of material, but also the properties of the fluid that flows though the porous material
- Viscous fluids (oil, honey, peanut butter) result in a much lower hydraulic conductivity than fluids with a low viscosity (water)
- The relation between hydraulic conductivity (K) and viscosity (μ) and density (ρ) of fluids was first formulated in the 1940s by M.K. Hubbert:
- ρ is density (kg/m^3), g is gravitational acceleration (m^2/s), μ is viscosity (Pa s), and k is a new material constant, permeability (m^2)



$$K = \frac{\rho g k}{\mu}$$

30

Darcy's law, update

- New form of Darcy's law using permeability instead of hydraulic conductivity:

$$q = -\frac{\rho g k}{\mu} \frac{\Delta h}{\Delta x}$$
- Darcy's law in 3D for infinitely small volumes

$$q = -\frac{\rho g k}{\mu} \nabla h$$
- Recall that ∇h is short for: $\nabla h = \partial h / \partial x + \partial h / \partial y + \partial h / \partial z$
- = the hydraulic gradient in 3 dimensions (x, y, z)

31

Permeability vs hydraulic conductivity

- Hydraulic conductivity still most frequently used parameter in shallow hydrogeology
- This is mostly ok, because density and viscosity of (fresh) water do not vary much in the upper ~100 m of the crust
- However, viscosity depends strongly on temperature and to a lesser degree on salinity
- Therefore the use of permeability instead of hydraulic conductivity is preferable, especially for deep fluid flow (high temperature) or systems containing saline water (coastal groundwater flow, or anything involving evaporites)

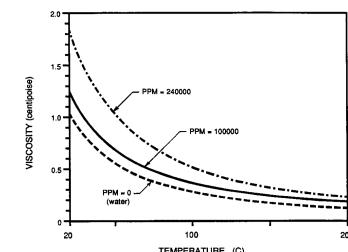


FIG. 15. Brine viscosity as a function of pressure, temperature, and salinity using the relationships of Kestin et al. (1981) are extrapolated using the curves of Matthews and Russel (1967). Above 100°C, the values are at saturation pressure (vapor and liquid are in equilibrium). The pressure dependence is small and not shown for clarity.

Batzle & Wang (1992) JGR

32

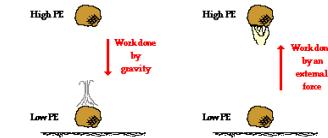
What drives fluid flow?

- Question: What forces drive fluid flow? Is fluid flow a function of pressure only?

33

What drives fluid flow?

- Fluid flow in the subsurface is driven by gravitational force and pressure force
- The easiest way to define the driving force is to define a potential energy
- The concept of potential energy was derived first by Joseph Luis Lagrange in 1788. It made Newtonian mechanics a lot easier to solve
- A mechanical system is in a state of equilibrium when the potential energy is at a minimum
- If not in equilibrium a force will act on the system to drive it to a minimum



34

Energy potential of a fluid

- Energy potential = ability to exert force
- Energy potential of a fluid = the work required to bring a mass of fluid from a reference state to a new elevation, pressure and velocity
- Work = force x displacement, units of energy (J)
- Fluid potential = gravitational potential + elastic energy + kinetic energy



35

Energy potential of a fluid

- Fluid potential = **gravitational potential** + elastic energy + kinetic energy
- Gravitational potential = the energy require to raise a mass of fluid from a reference elevation (z_1) to a new elevation (z_2)
- In mathematical terms:

$$E_g = \int_{z_1}^{z_2} mg \, dz$$

$$z_1 = 0 \rightarrow E_g = mgz$$

Note that the integral sums the difference in velocity along the way from z_1 to z_2

36

Energy potential of a fluid

- Fluid potential = gravitational potential + **elastic energy** + kinetic energy
- Elastic energy = the energy require to increase the pressure of a mass of fluid from a reference pressure (p_1) to a new pressure (p_2)
- To change pressure of a fluid we need to compress or decompress the fluid by changing its volume (V), or when looking at a fixed volume, by changing its density (ρ)

$$E_e = \int_{p_1}^{p_2} V dp = \int_{p_1}^{p_2} \frac{m}{\rho} dp$$

$$p_1 = 0 \rightarrow E_e = \frac{mp}{\rho}$$

37

Energy potential of a fluid

- Fluid potential = gravitational potential + elastic energy + kinetic energy: $E_t = \frac{1}{2}mv^2 + mgz + \frac{mp}{\rho}$
- Fluid energy potential per unit mass ($m=1$): $E_t = \frac{1}{2}v^2 + gz + \frac{p}{\rho}$
- Kinetic energy can be ignored: approximately 10 orders of magnitude smaller than gravitational or elastic potential $E_t = gz + \frac{p}{\rho}$
- Alternatively, fluid energy potential per unit volume is also often used to quantify fluid flow (note mass/volume = density (ρ)): $E_t = \rho gz + p$

39

Energy potential of a fluid

- Fluid potential = gravitational potential + elastic energy + **kinetic energy**
- Kinetic energy = the energy require to accelerate a mass of fluid from velocity v_1 to velocity v_2
- In mathematical terms:

$$E_k = m \int_{v_1}^{v_2} v dv$$

$$v_1 = 0 \rightarrow E_k = \frac{1}{2}mv^2$$

38

Energy potential of a fluid

- Fluid potential = gravitational potential + elastic energy + kinetic energy
- Potential per unit weight (instead of mass, weight = $m \times g$):

$$\frac{E_t}{g} = z + \frac{p}{\rho g} = h$$

- h = hydraulic head (m)
- = the mechanical energy of a fluid
- h = elevation + pressure head



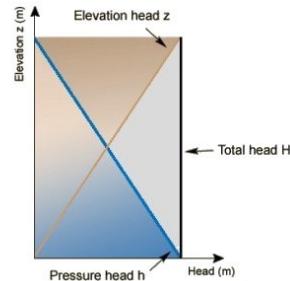
M.K. Hubbert produced the first rigorous derivation of hydraulic head and the groundwater flow equation in 1940

40

Hydraulic head & fluid flow

- When a fluid does not move, the elevation and pressure head cancel each other out and the hydraulic head is constant everywhere:

$$h = z + \frac{p}{\rho g}$$

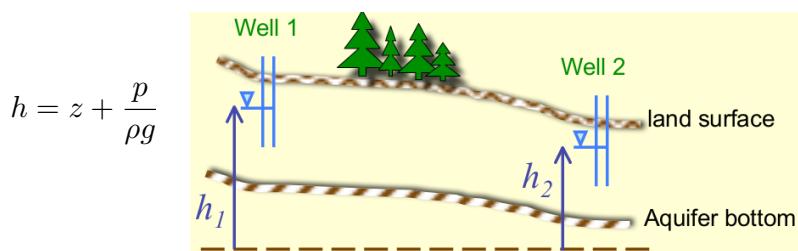


source: C. Harvey, MIT

41

Hydraulic head & fluid flow

- We can also use hydraulic head measurements in boreholes to map the direction of groundwater flow in the subsurface.
- Which way does the water flow in the figure below?



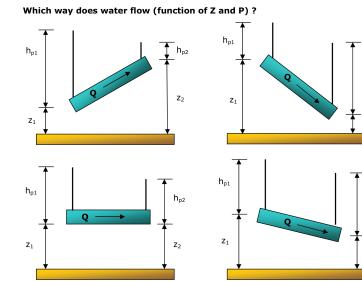
Hydraulic head in an aquifer, source: J.L. Wilson, NMT

43

Hydraulic head & fluid flow

- Try to guess which way water flows through the systems shown below:

$$h = z + \frac{p}{\rho g}$$



source: C. Harvey, MIT

42

Summary

- Heat flow, solute flow and groundwater flow are all governed by diffusion equations
- Diffusion equations follow the shape: $q = K \frac{\partial u}{\partial x}$
- Or in words, flux is a linear function of the gradient of a particular quantity u (temperature, solute concentration, hydraulic head...) and a constant K (thermal conductivity, solute diffusivity, hydraulic conductivity)
- Diffusion laws are macroscopic laws, they describe the large scale behaviour of smaller scale random walk of molecules or the quasi random flow of water in pores
- Hydraulic conductivity is a function of permeability and fluid properties (density and viscosity)
- Darcy's law: $q = -\frac{\rho g k}{\mu} \nabla h$
- Darcy's law is valid for laminar flow, i.e. flow with low Reynolds numbers
- Groundwater flow is driven by the gravitational potential energy and the elastic potential energy. These are summarised in a term called hydraulic head, which is a combination of elevation and pressure head

$$h = z + \frac{p}{\rho g}$$

44