Course: Groundwater Flow and Cont Transp. Modeling
(for HG, EE, PGE students)
2019

Basics of GW flow modeling

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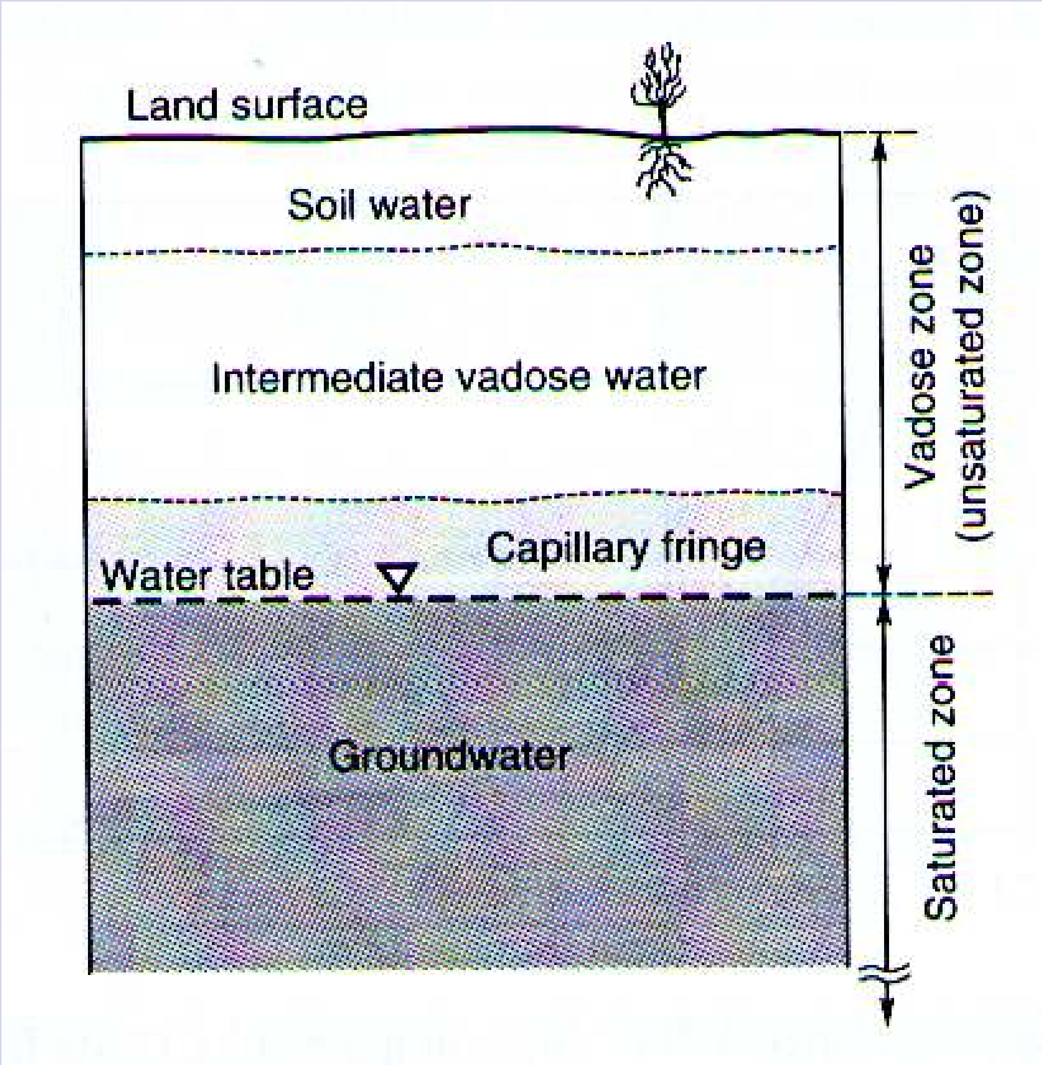
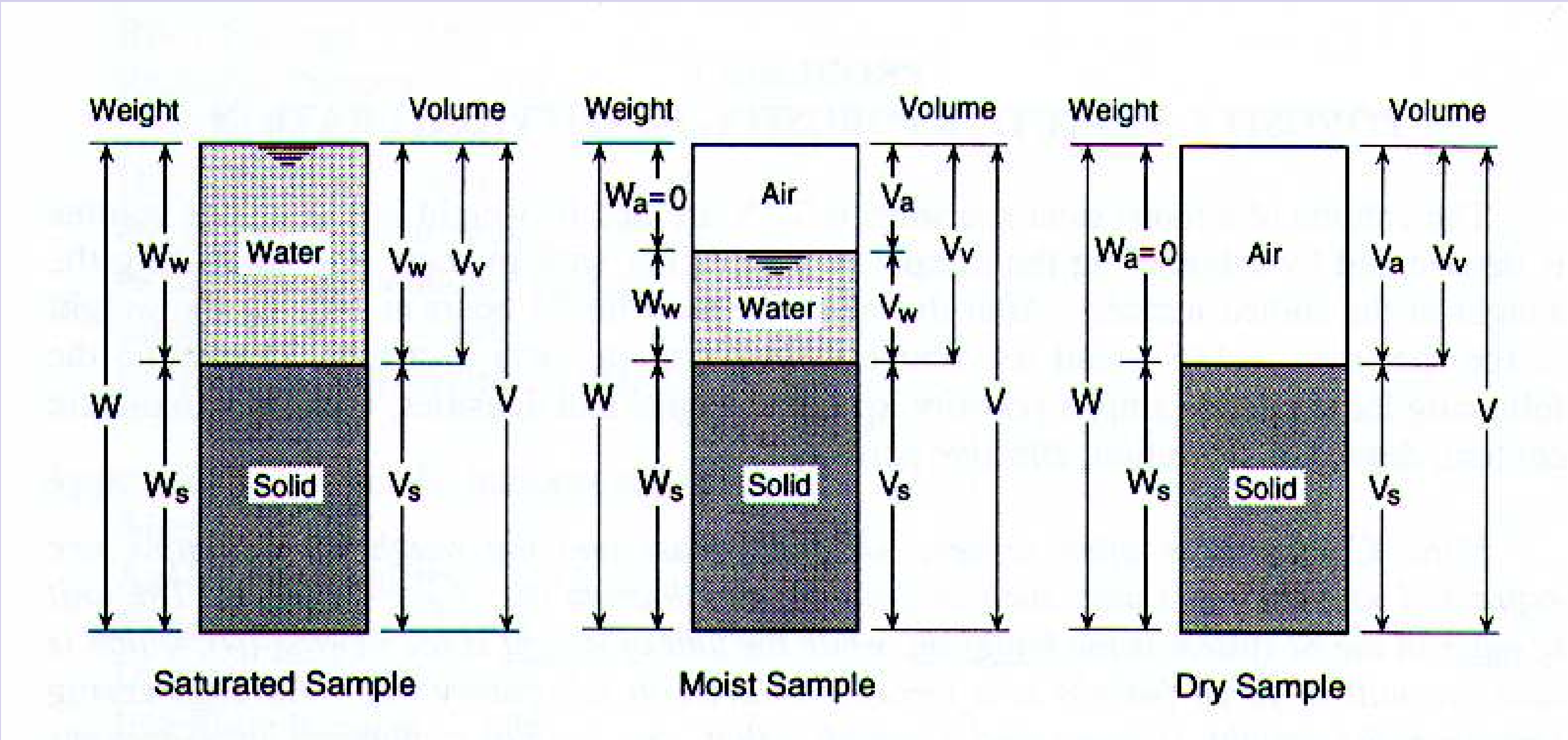
Elements of basic hydrogeology to understand modeling issues

Types of water in the subsurface



(Kresic 2008, after Meinzer)

Porosity



$$e=\frac{V_a+V_w}{V_s}=\frac{V_v}{V_s}$$

$$n=\frac{V_a+V_w}{V}=\frac{V_a+V_w}{V_a+V_w+V_s}=\frac{V_v}{V}$$

$$v=1+e$$

Kresic, 1997

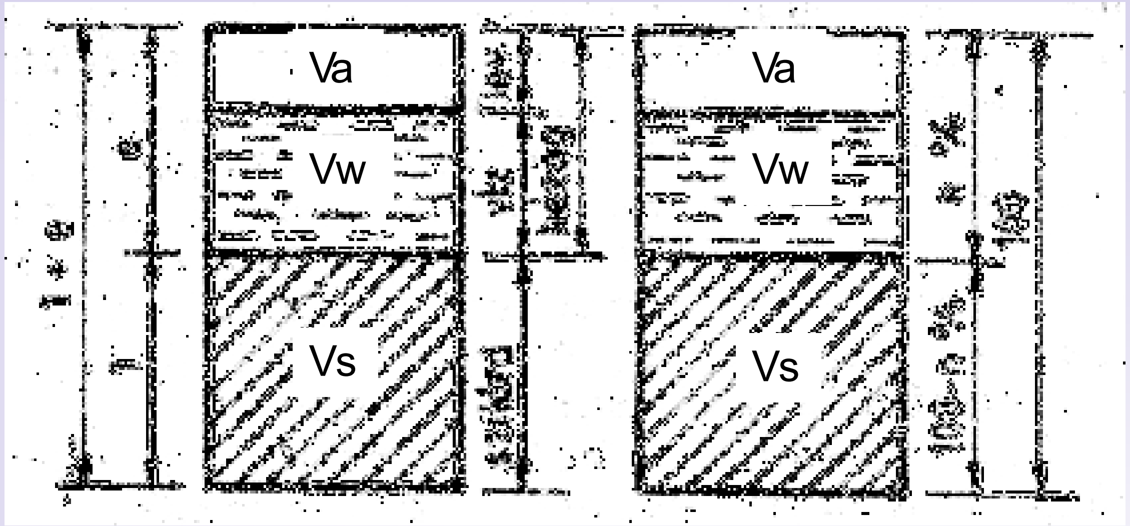
Porosity and void ratio

Porosity

$$n = \frac{V_v}{V_v + V_s} = \frac{V_v}{V}$$

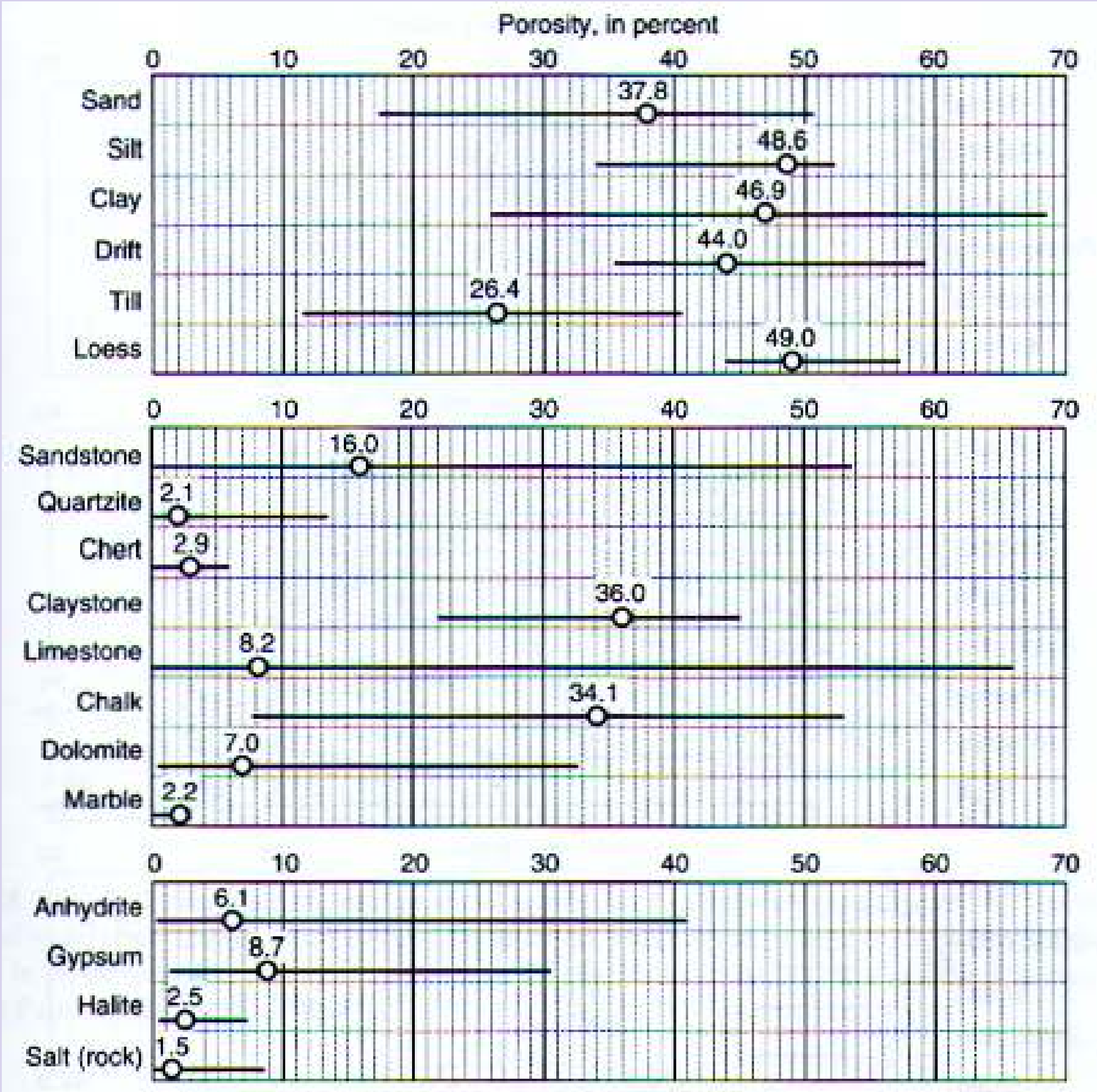
Void ratio

$$e = \frac{V_v}{V_s}$$



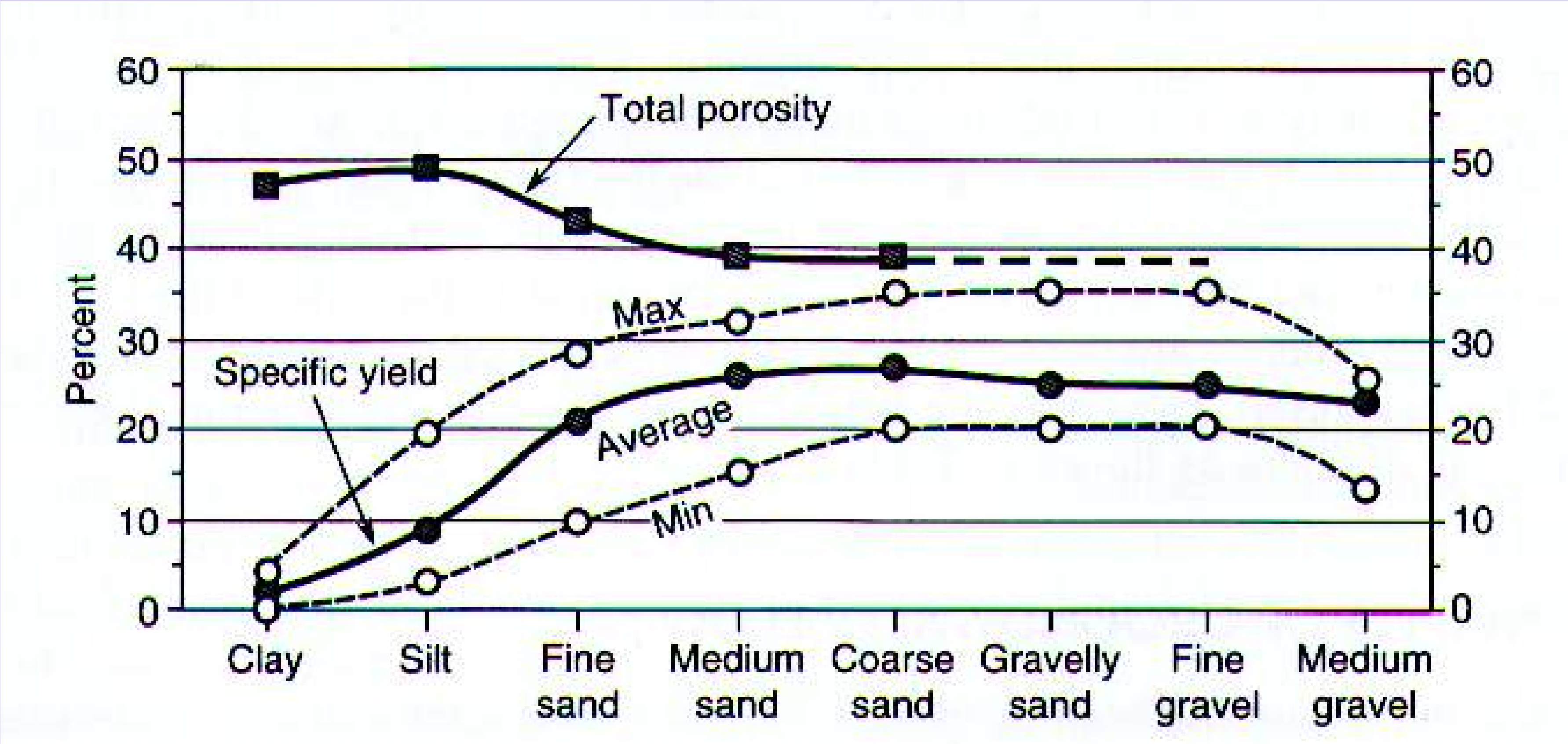
$$e = \frac{n}{1-n}; \quad n = \frac{e}{1+e}.$$

Porosity



Kresic, 2006

Total, effective porosity and specific yield



Kresic, 2006

Hydraulic conductivity

- velocity dimension [L/T], refers to the seepage velocity at unit hydraulic gradient
- refers both to the fluid and the medium
- the „fluid"part is proportional to the specific weight of the liquid (ρ) and inverse proportional to the viscosity (μ) of the fluid
- the „medium" part is proportional to the square of the grainsize (d^2) and the shape of the grains (c), called intrinsic permeability ($K_i = cd^2$)
- the permeability is widely used in petroleum engineering, and has an areal dimension (m^2)
- the connection between hydaulic conductivity and intrinsic permeability is as follows:

$$K = \frac{K_i \cdot \rho g}{\mu}$$

Darcy law

$$Q = K\,A\,(h_1 - h_2)/dl$$

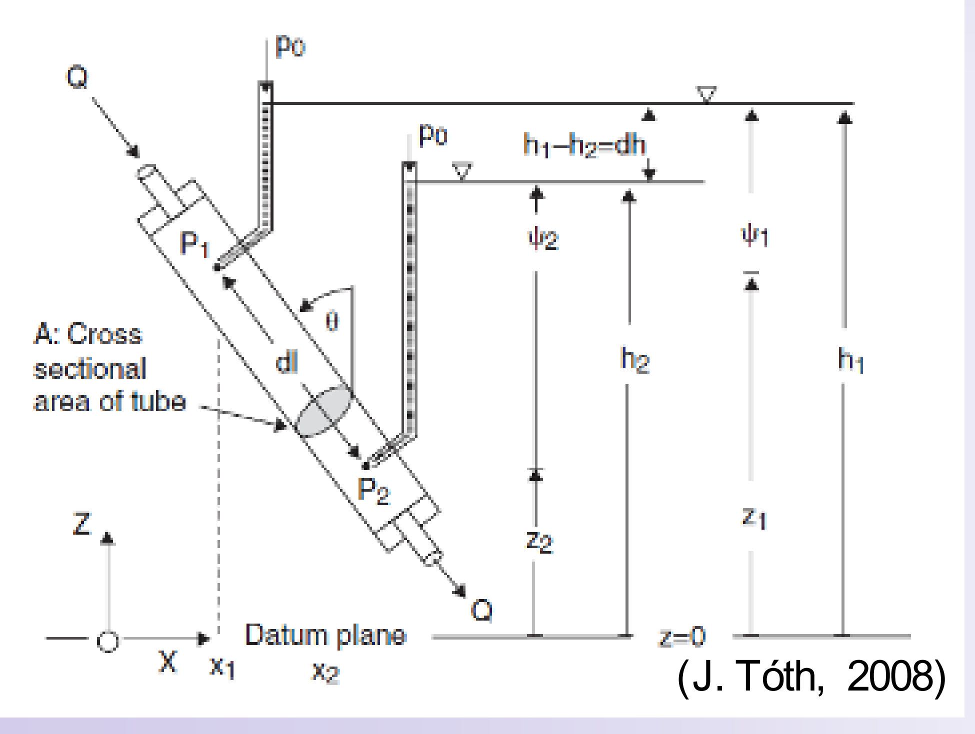
where

Q : flux [L^3/T];

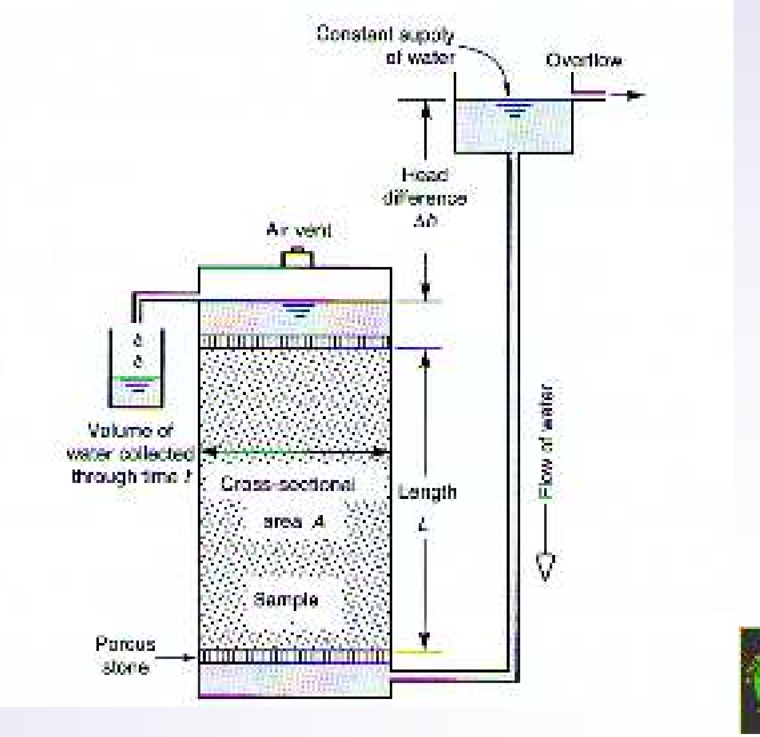
$h_A - h_B$: hydraulic head at P1, P2 points [L];

dl: distance of P1 and P2 points [L]

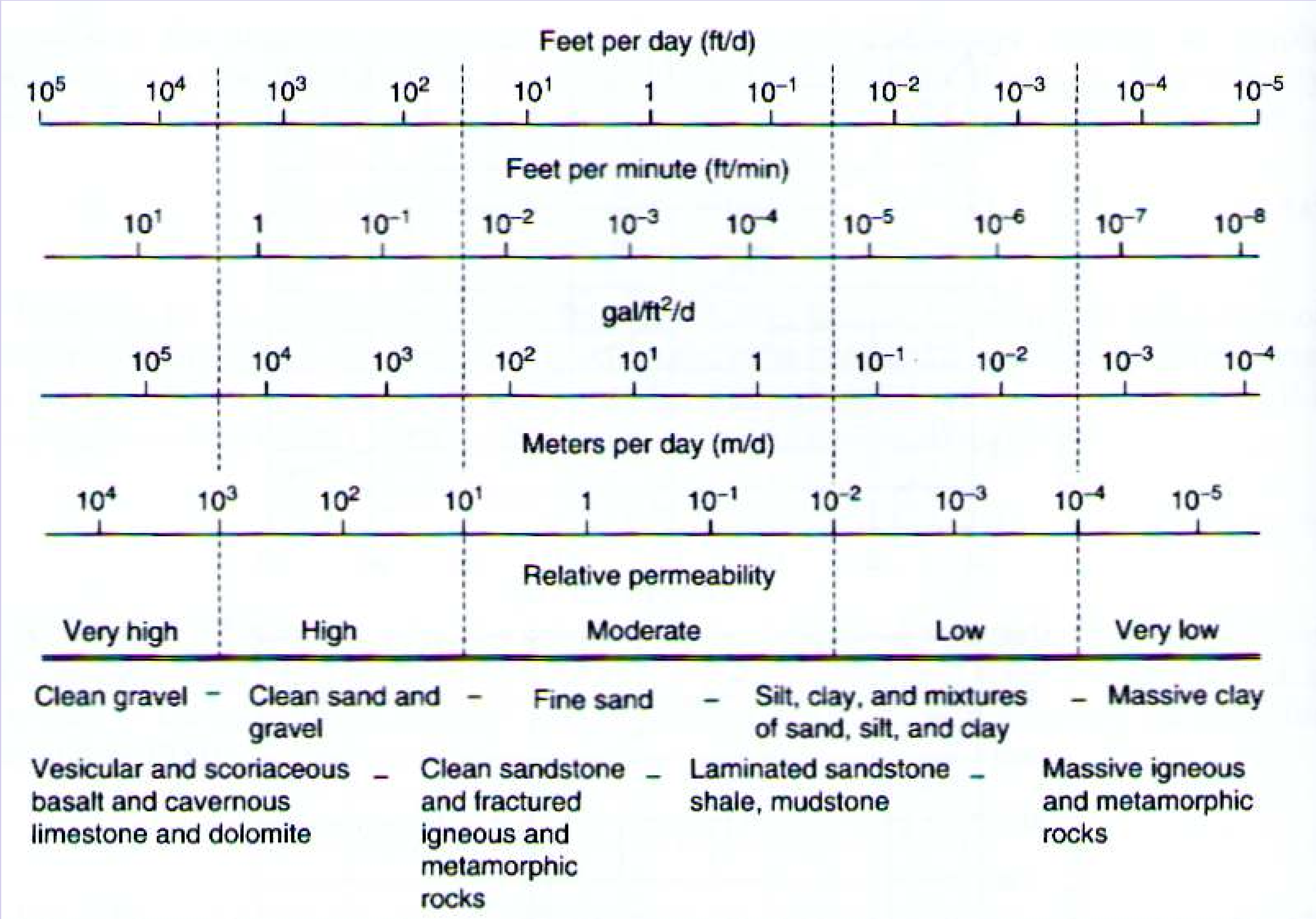
K: hydraulic conductivity [L/T]



(J. Tóth, 2008)



Hydraulic conductivity of formations



Darcy vs. real seepage velocity

Darcy seepage velocity is linear, assuming full cross-sectional flow:

$$v(v_D) = K \cdot i = K \cdot \frac{dh}{dl}$$

Real seepage velocity is non-linear, assuming flow in the gravity affected pore volumes :

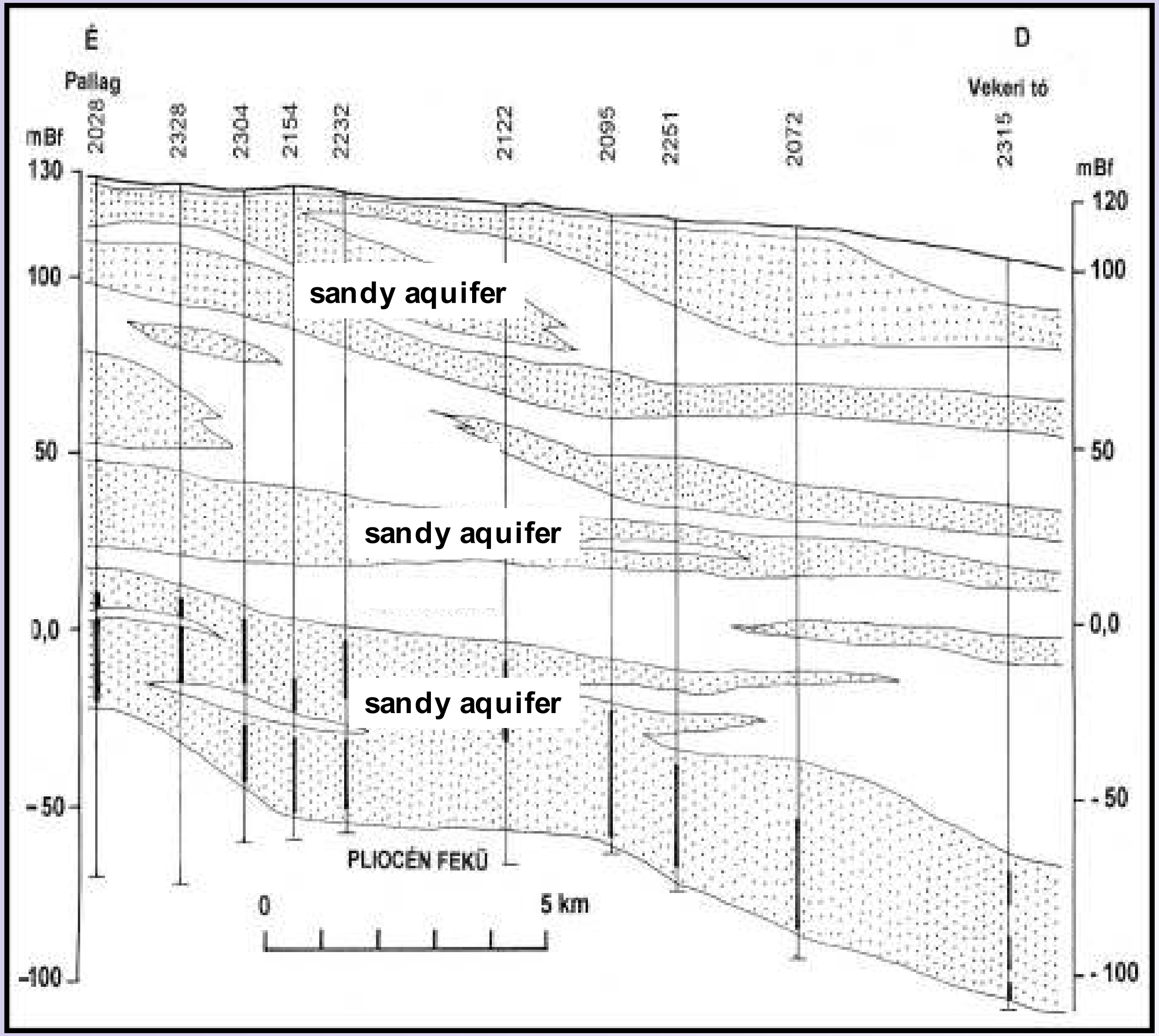
$$v_{real} = \frac{v(v_D)}{n_0} = \frac{K \cdot i}{n_0} = \frac{K}{n_0} \cdot \frac{dh}{dl}$$

Transmissivity

- transmissivity is the water supplying capacity of a given layer
- it is proportional to the hydraulic conductivity and the thickness of the layer

$$T = K \cdot m$$

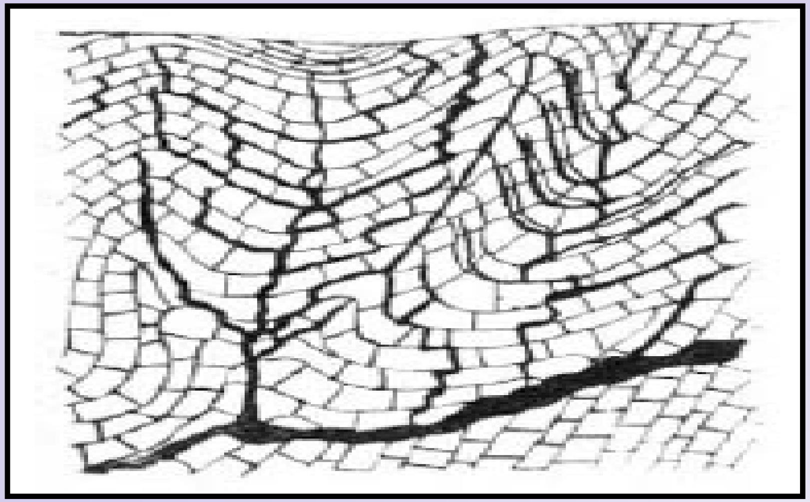
Hydrostratigraphy



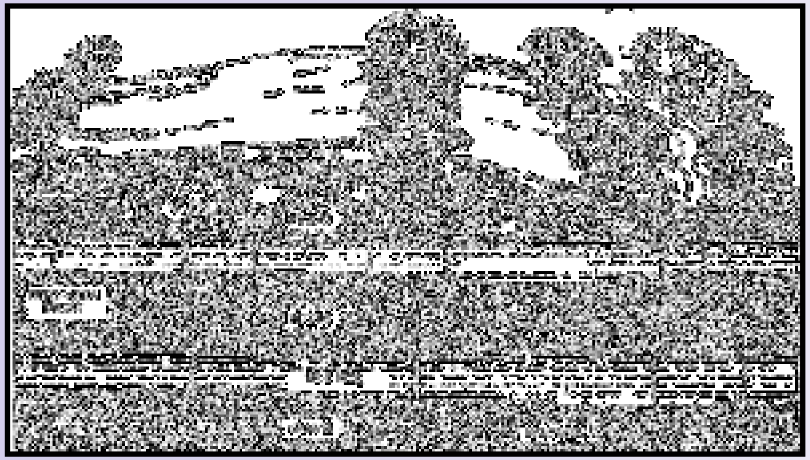
Aquifer

Aquitards or aquicludes

Aquifer classification

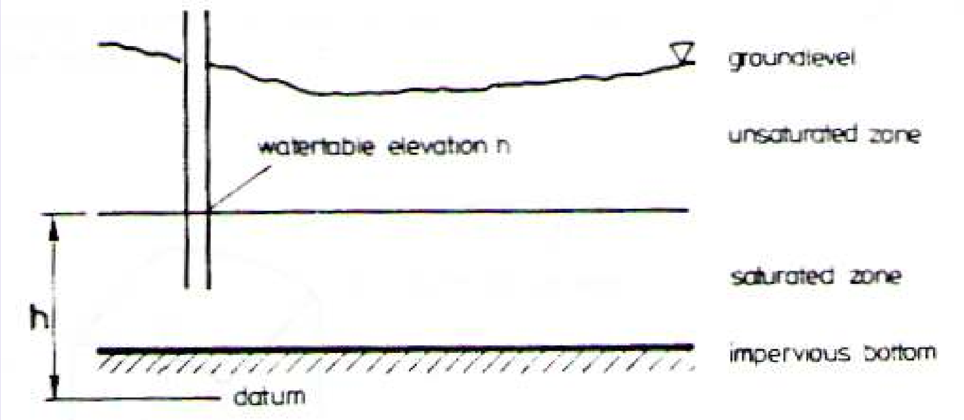


- Karstic aquifers

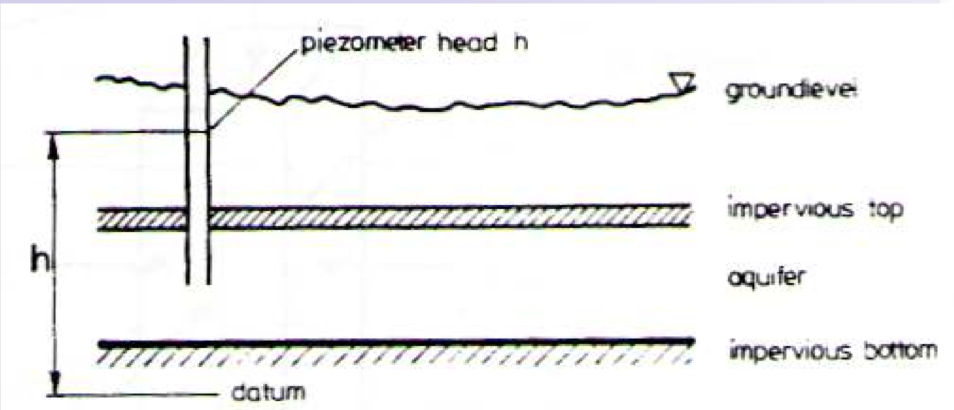


- Porous aquifers
- Double porosity aquifers

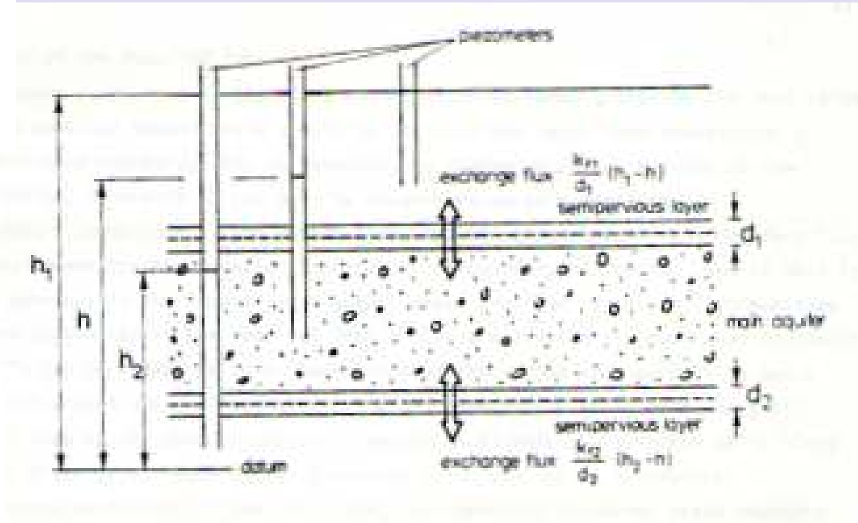
Aquifer types



Phreatic aquifer

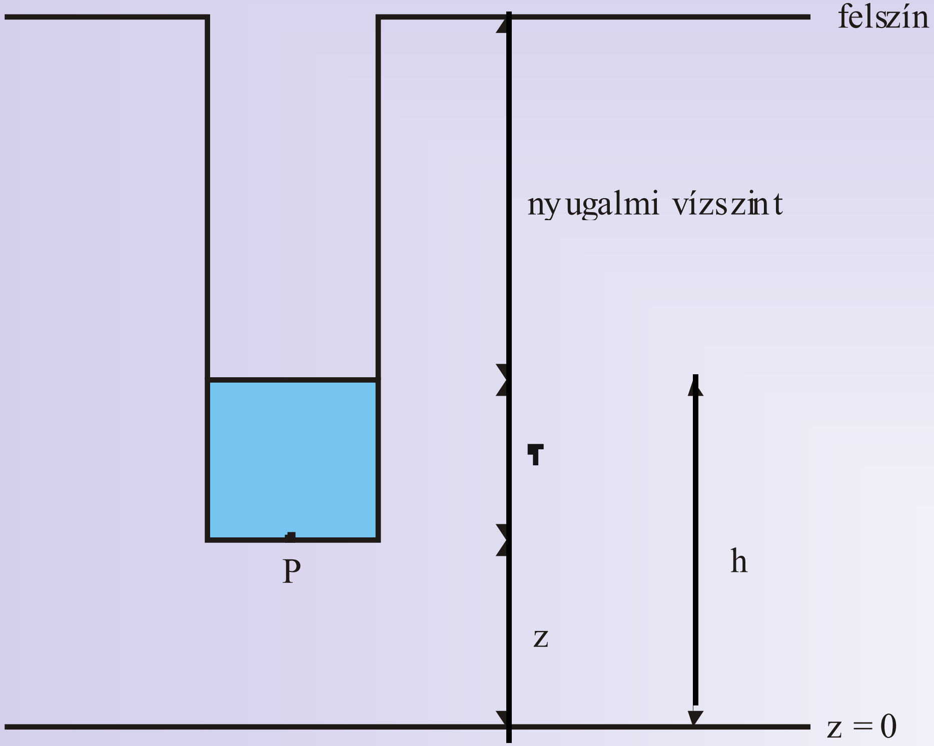


Confined aquifer



Semipermeable aquifer system

hydraulic head and pressure at point P



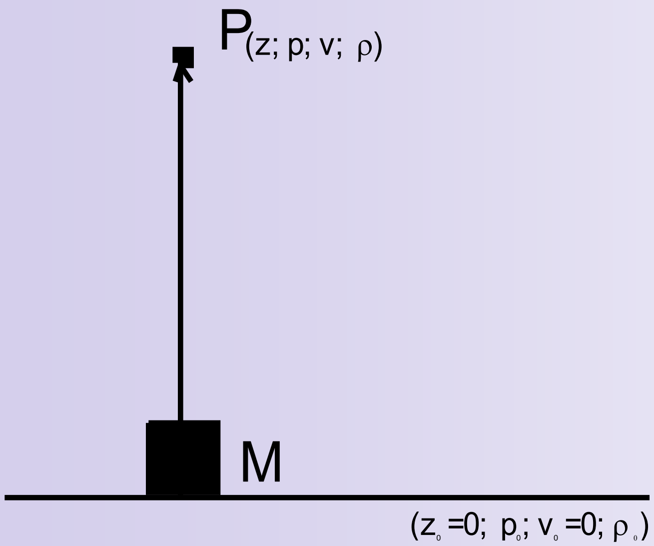
$$P = \gamma\varphi$$

$$P = \rho g \varphi$$

$$\varphi = h - z$$

GW Flow potential as energy of the unit mass

Energy need of rising an m mass to z height



- Work against gravity:

$$W_1 = mgz$$

- Work to accelerate the mass:

$$W_2 = \frac{mv^2}{2}$$

- Work due to extention due to pressure loss:

$$W_3 = m\int_{p_0}^{p} \frac{dp}{\rho}$$

GW flow potential

- Total work is the sum of the energy of the liquid of m mass:

$$W = m\Phi$$

Specific energy to unit mass:

$$\Phi = \frac{W}{m} = \frac{W_1 + W_2 + W_3}{m} = gz + \frac{v^2}{2} + \int_{p_0}^{p} \frac{dp}{\rho} \qquad \text{(Bernoulli equation)}$$

Estimation:

$$\Phi = gz + \frac{p - p_0}{\rho} \qquad \text{(Hubbert-type energy equation)}$$

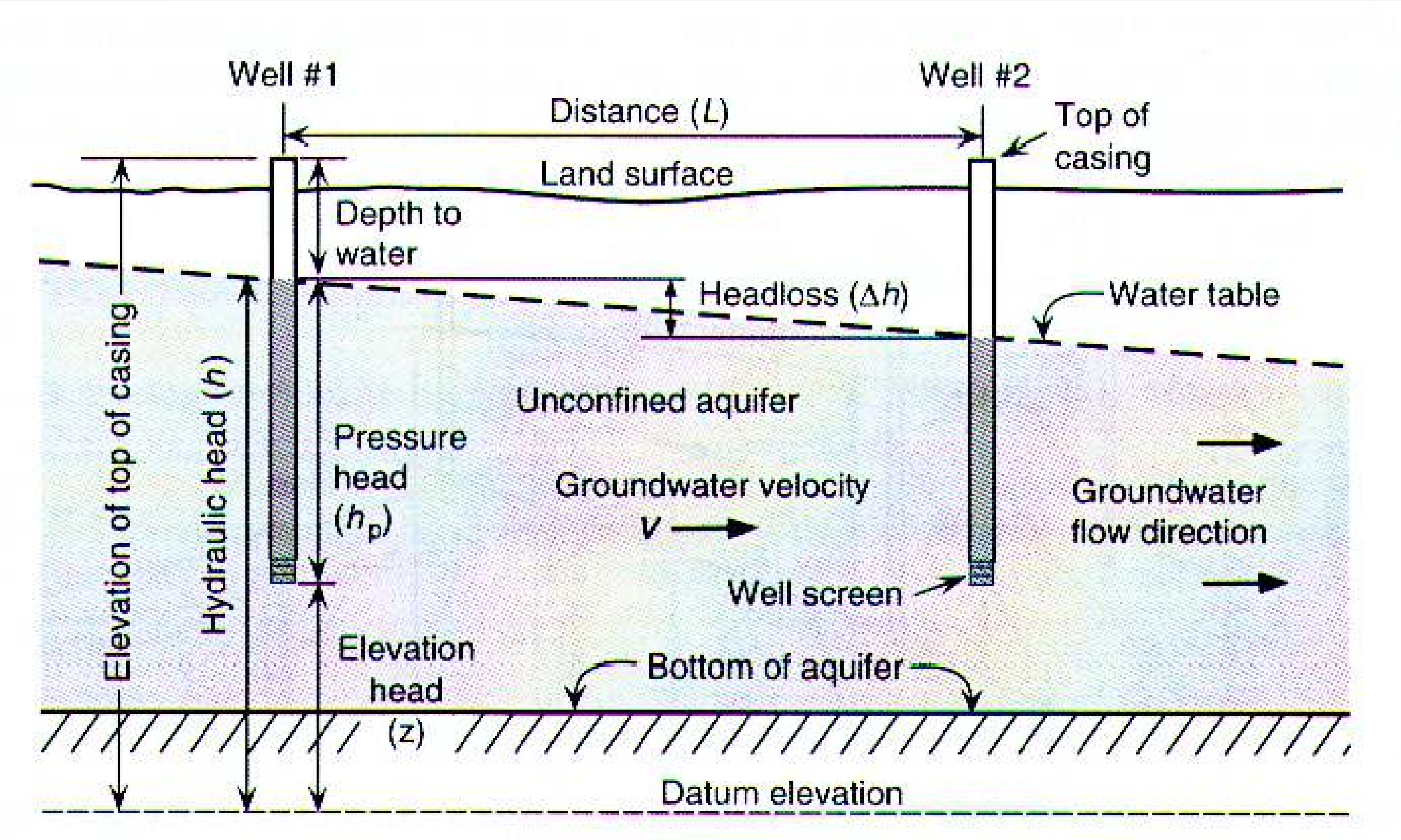
- Pressure at point P:

$$p = \rho g \varphi + p_0 \quad \text{therefore} \quad p = \rho g (h - z) + p_0$$

- Modifying the Hubbert type energy equation

$$\Phi = gz + \frac{\rho g (h - z) + p_0 - p_0}{\rho} = gh$$

Groundwater seepage scheeme



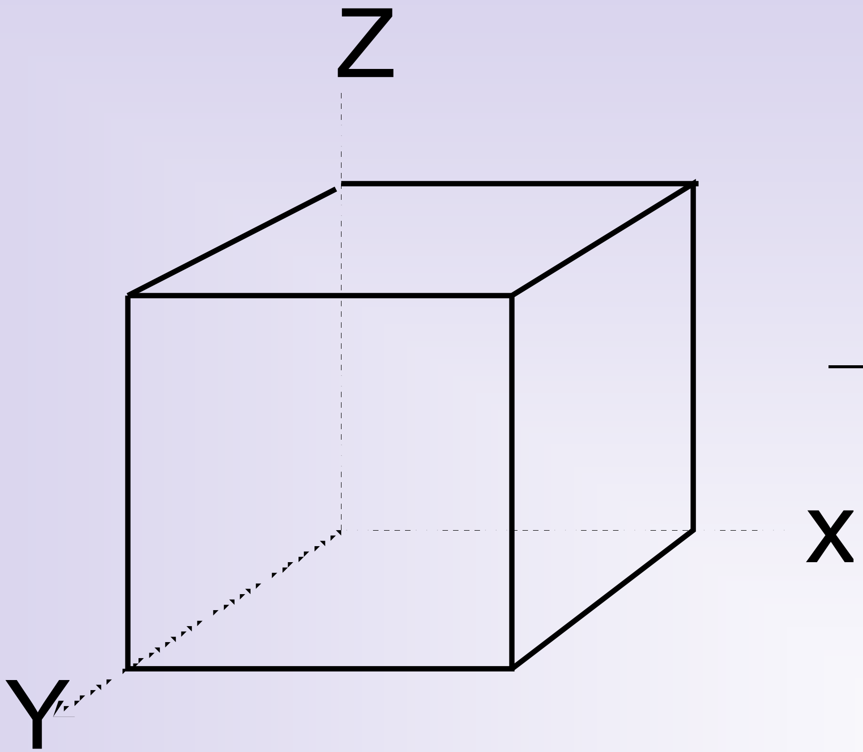
Hydraulic gradient

$$i = \frac{dh}{dl}$$

- the hydraulic gradient is the slope of the potential surface
- the hydraulic gradient is proportional to the seepage velocity, v=Ki
- dimensionless number [m/km]
- horizontal and vertical components could be investigated

Matematical description of continuity – flow equations

$$+\rho q_x \longrightarrow$$



$$\longrightarrow -\left[\rho q_x + \frac{\partial(\rho q_x)}{\partial x}\right]$$

where q_x is the flux, ρ is the density, $q_x.\rho$ is the amount of material inflowing to the domain

Steady flow

- Total sum of material inflow & outflow is zero

$$\frac{\partial(\rho q_x)}{\partial x}+\frac{\partial(\rho q_y)}{\partial y}+\frac{\partial(\rho q_z)}{\partial z}=0$$

- From Darcy law

$$q_x=-K\frac{\partial h}{\partial x}$$

- Substituation

$$\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z}\right)=0$$

- Result in isotropic case (Laplace equation) case of no sinks and sources

$$\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\frac{\partial^2 h}{\partial z^2}=0$$

Transient flow

- The result of laterary fluxes is not zero teherfore there is a storage or loss of material to or from the domain

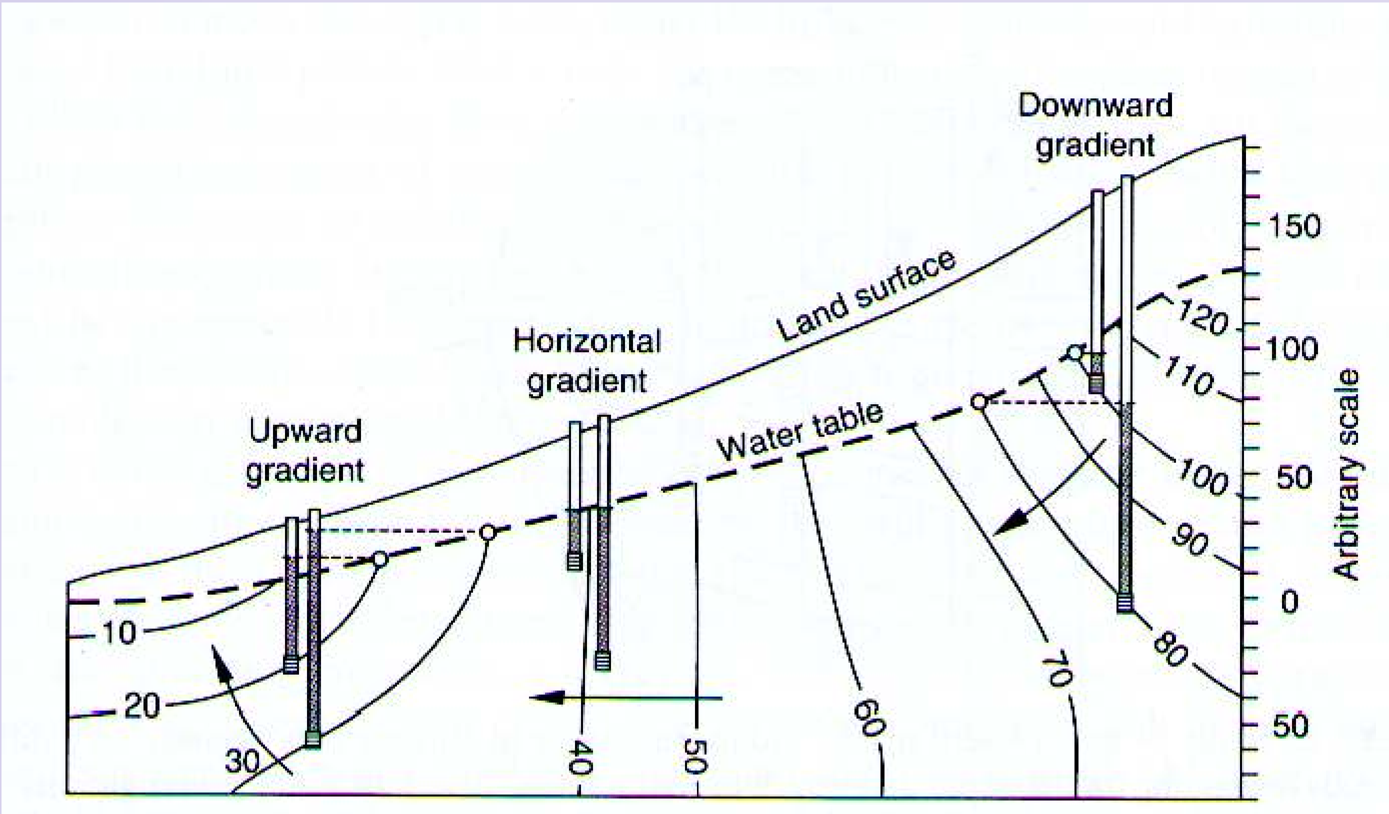
$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = \frac{S_s}{K}\frac{\partial h}{\partial t}$$

- where S_s is the specific storage
- Specific storage ($S_S[L^3/L^4]$) is the volume of stored or released water due to unit alteration of the pressure compared to unit volume of the aquifer
- Storage coefficient (S $[L^3/L^3]$) is the volume of stored or released water due to unit alteration of the pressure at each unit area of the aquifer

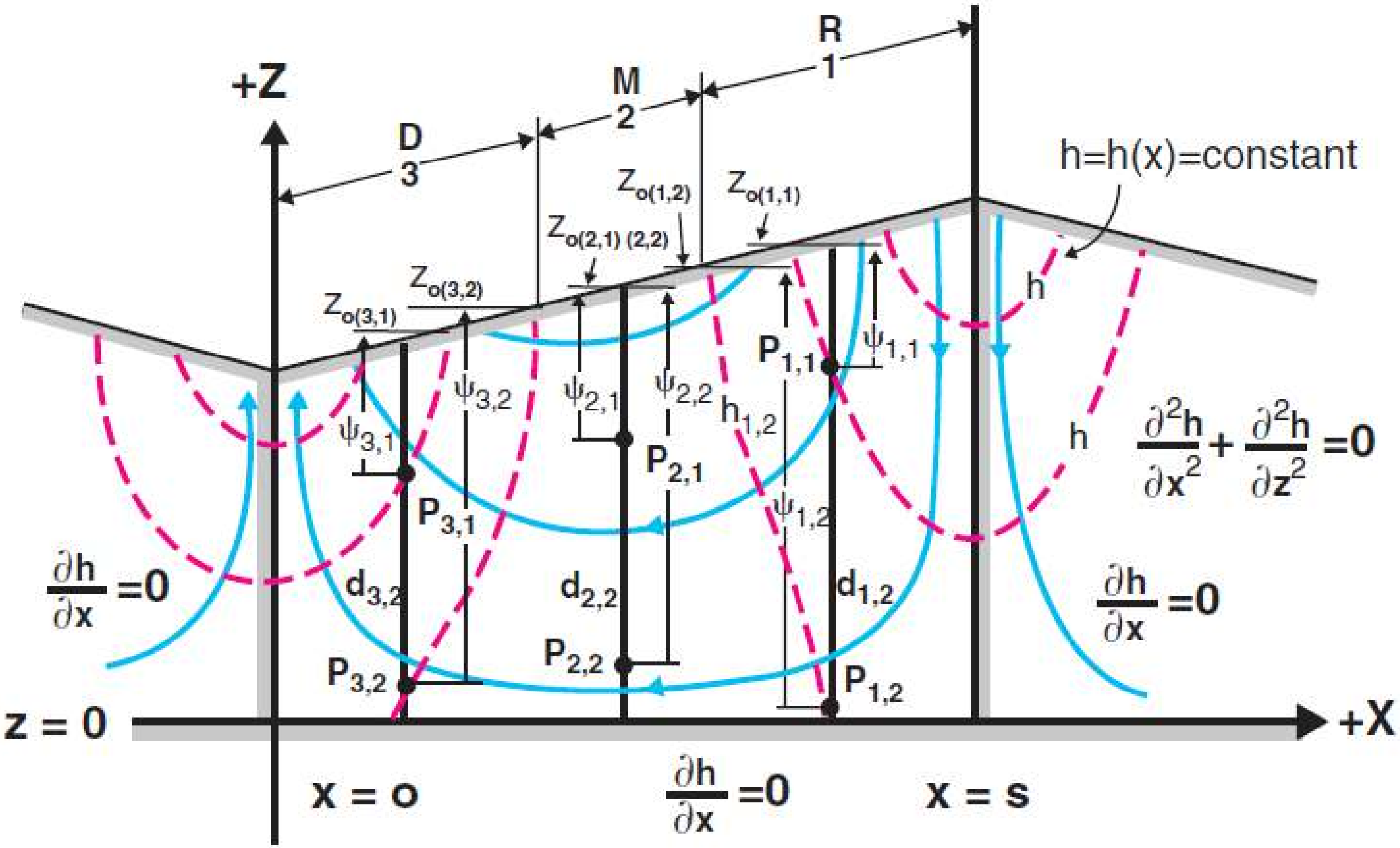
$$S = S_s m$$

- Specific yield (S_y $[L^3/L^3]$) is the ratio of volume of water released at water level decrease from a unit volume of the aquifer

Groundwater flow regime (unit basin)



Groundwater flow regime (unit basin)

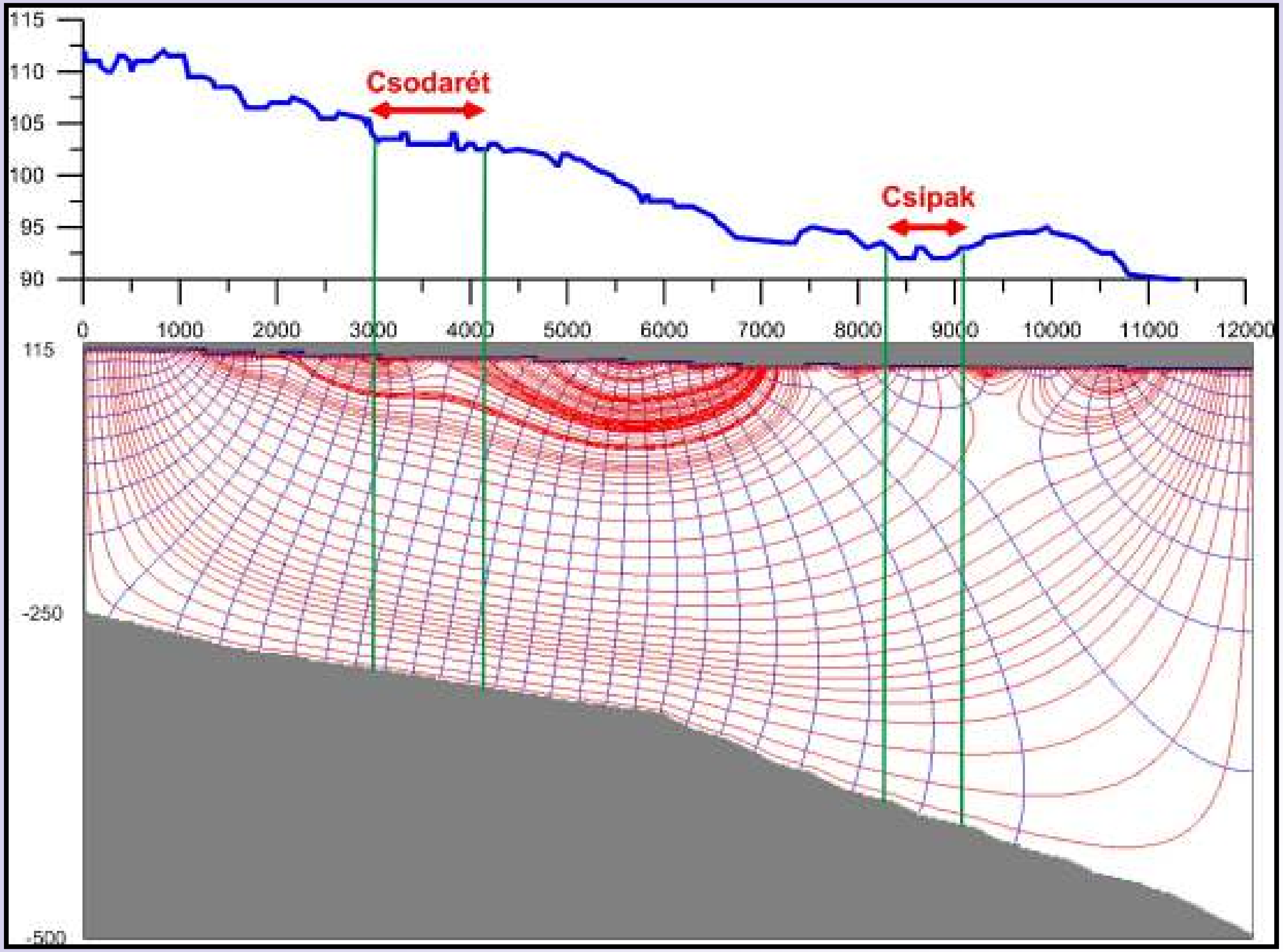


R, M, D : Area of Recharge, Midline, Discharge, respectively;

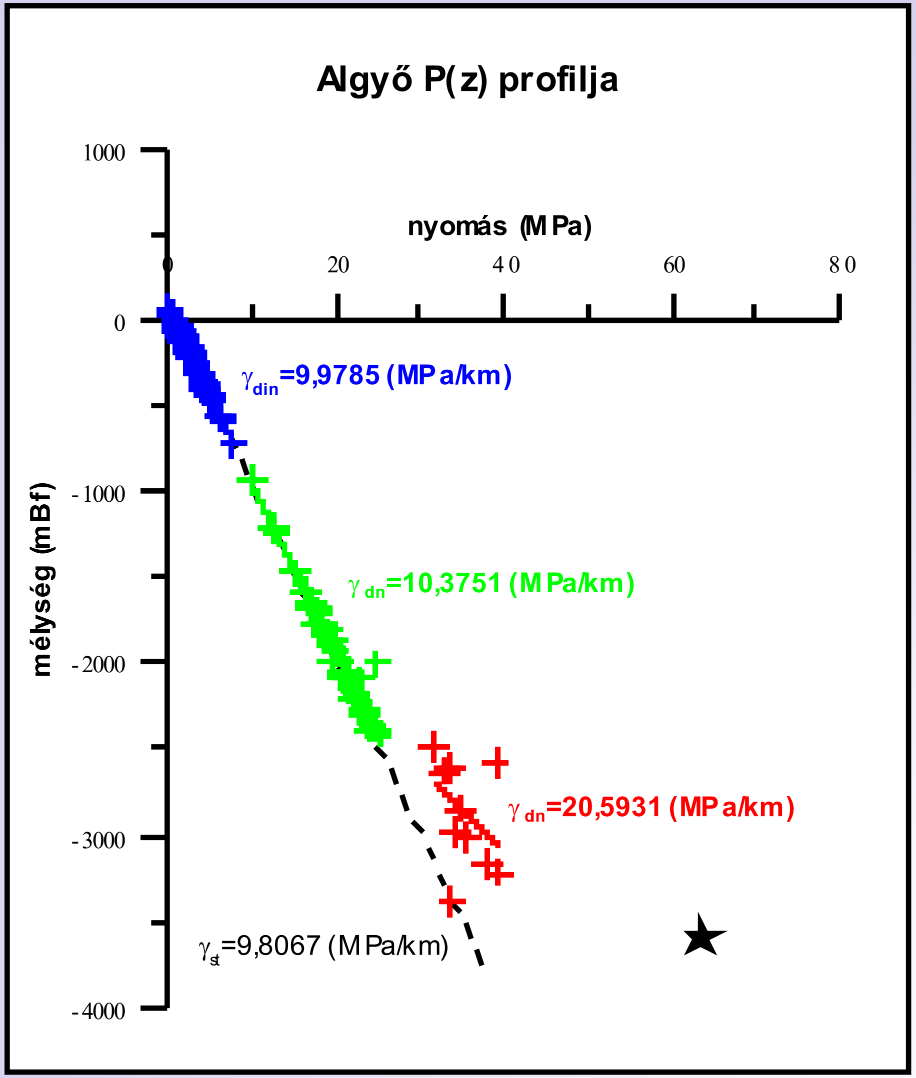
$P_{1,2}$: point of measurement in cased well; $d_{1,2}$: well depth; $\psi_{1,2}$: pressure head;

h : hydraulic head; $z_{o(1,2)}$: intersection of isopotential $h_{1,2}$ with water table.

Nested groundwater systems



Pressure vs. depth profiles



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Modeling using PMWin

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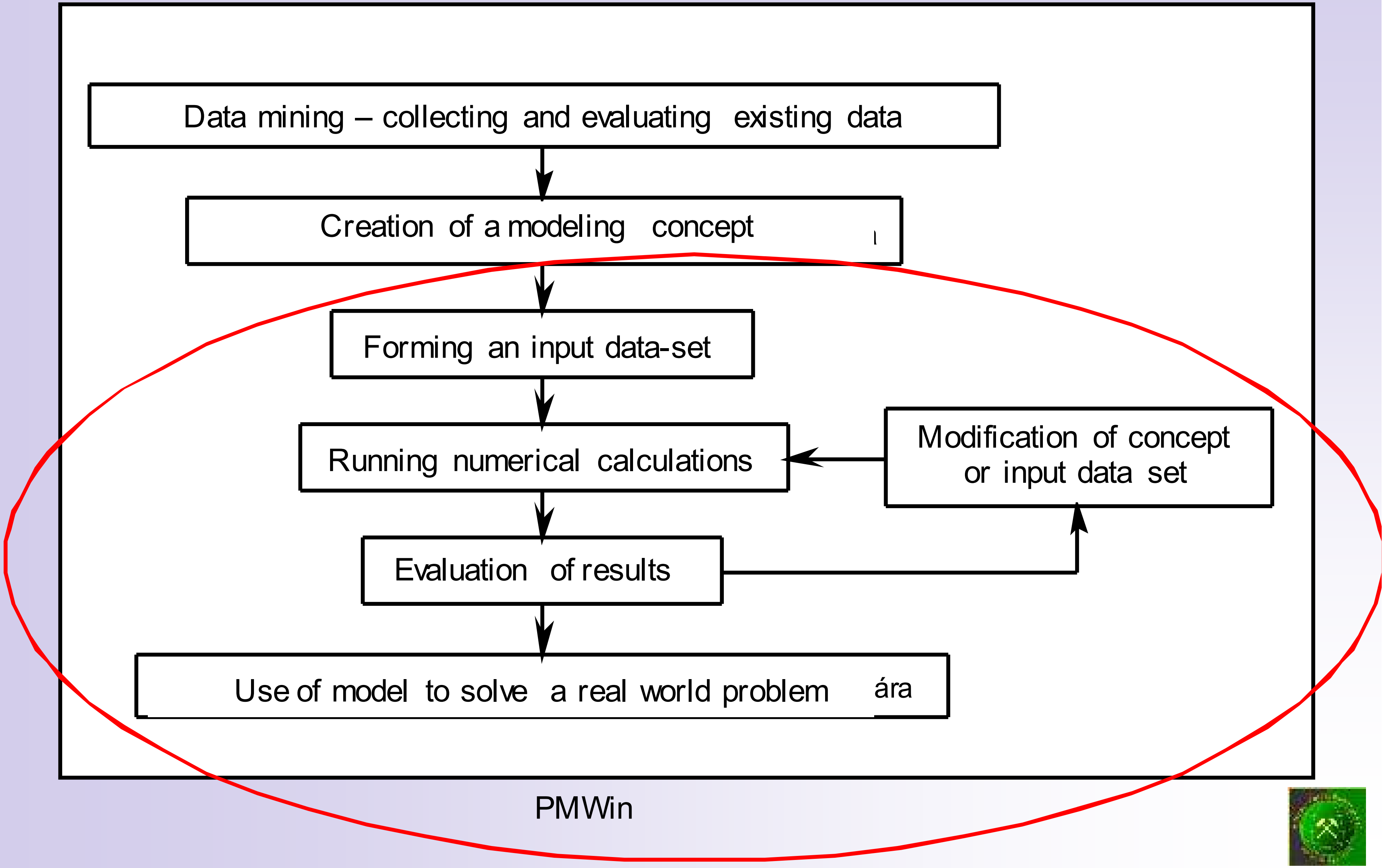
Processing Modflow for Windows

- Authors: Wen-Hsing Chiang and Wolfgang Kinzelbach
- Commercial code (v8.0 and X) but earlier version is freeware (v5.3.3)
- Uses the USGS MODFLOW computing kernel (FORTRAN) and concept
- Download from www.simcore.com
- Full documentation available for free
- Both for GW flow and contaminant (heat) transport modeling

Processing Modflow for Windows specifications

- Finite difference method is used
- Dominantly for porous formations but with some limitations it can be used also fro fractured reservoirs
- Deterministic modeling, but some stochastic features also
- GW flow modeling (MODFLOW)
- Particle tracking (PMPATH and MODPATH)
- Contaminant (heat in v8) transport modeling (MT3D, MT3DMS, MOC3D (SEAWAT in v8))

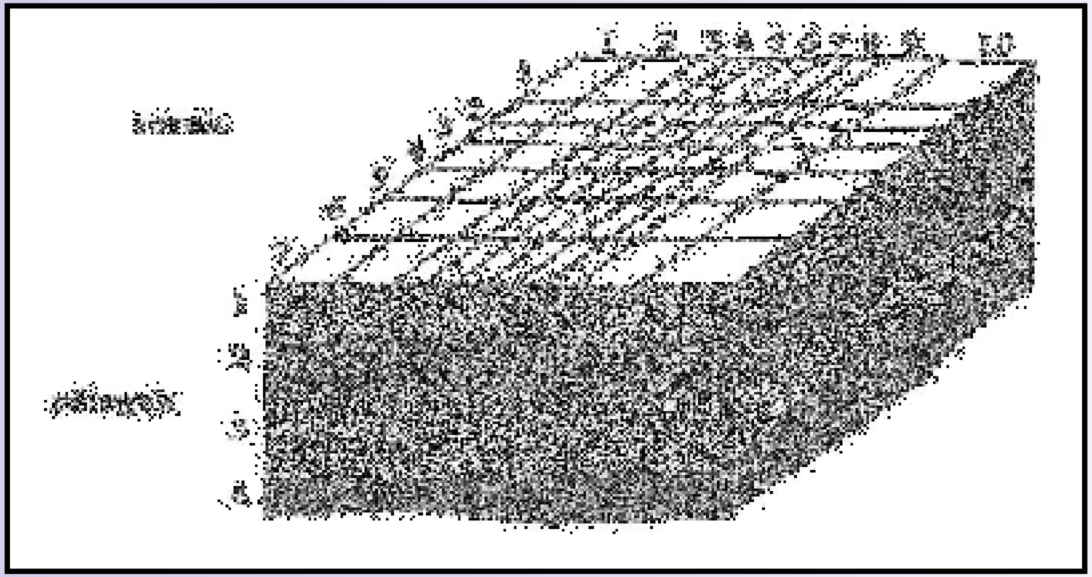
The process of numerical modeling



PMWin

Numerical methods applied in the practice

- **Finite difference method:** the modelled domain is discretized by a rectangular grid where all the neighbouring elements contacts each other by their sides. The system is desctibed by an equation system consisting of the water budget af the elements and the unknown parameter is the average hydraulic head (GW flow potential) in the element. The equation system solved iteratively using different numeric techniques
  - advantage: Ease of use, partial results has physical meaning
  - disadvantage: restrictions in shape of elements



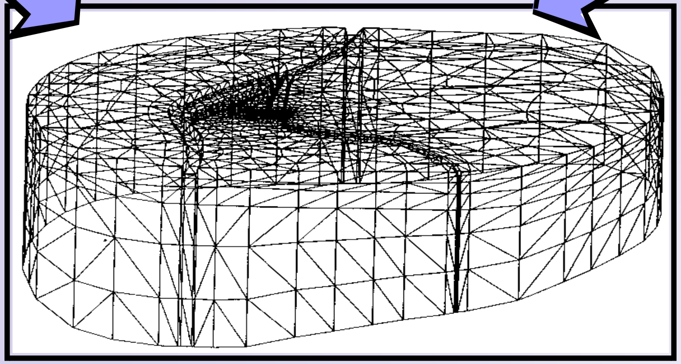
Finite difference grid of a four laayer system
(CHIANG és KINZELBACH, 1999)

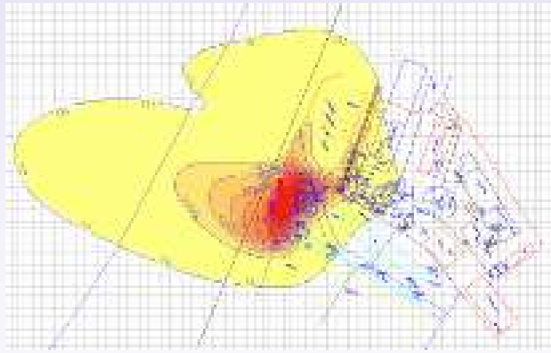
A deterministic modeling work flow

K, n, S_s, S_y, K_d, α, λ

$$\frac{\partial}{\partial x}\left(k_x \frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y \frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_z \frac{\partial h}{\partial z}\right)=\rho S_s \frac{\partial h}{\partial t}$$

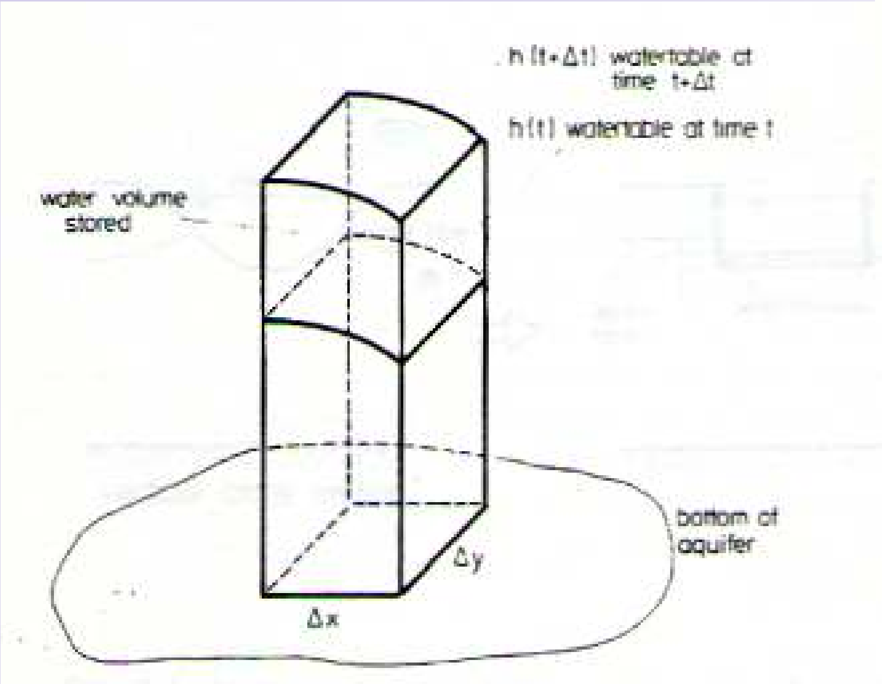
$$\frac{dM}{n\,dV\,dt} = D^*_{xx}\frac{\partial^2 C}{\partial x^2} + D^*_{xy}\frac{\partial^2 C}{\partial x \partial y} + D^*_{xz}\frac{\partial^2 C}{\partial x \partial z} + D^*_{yx}\frac{\partial^2 C}{\partial y \partial x} + D^*_{yy}\frac{\partial^2 C}{\partial y^2} + D^*_{yz}\frac{\partial^2 C}{\partial y \partial z} + D^*_{zx}\frac{\partial^2 C}{\partial z \partial x} + D^*_{zy}\frac{\partial^2 C}{\partial z \partial y} + D^*_{zz}\frac{\partial^2 C}{\partial z^2} - \frac{\partial}{\partial x}\left(\frac{v_x C}{n}\right) - \frac{\partial}{\partial y}\left(\frac{v_y C}{n}\right) - \frac{\partial}{\partial z}\left(\frac{v_z C}{n}\right) - \frac{\partial}{\partial t}\left(\frac{\rho_b K_d C}{n}\right) - \lambda\left(C + \frac{\rho_b K_d C}{n}\right)$$

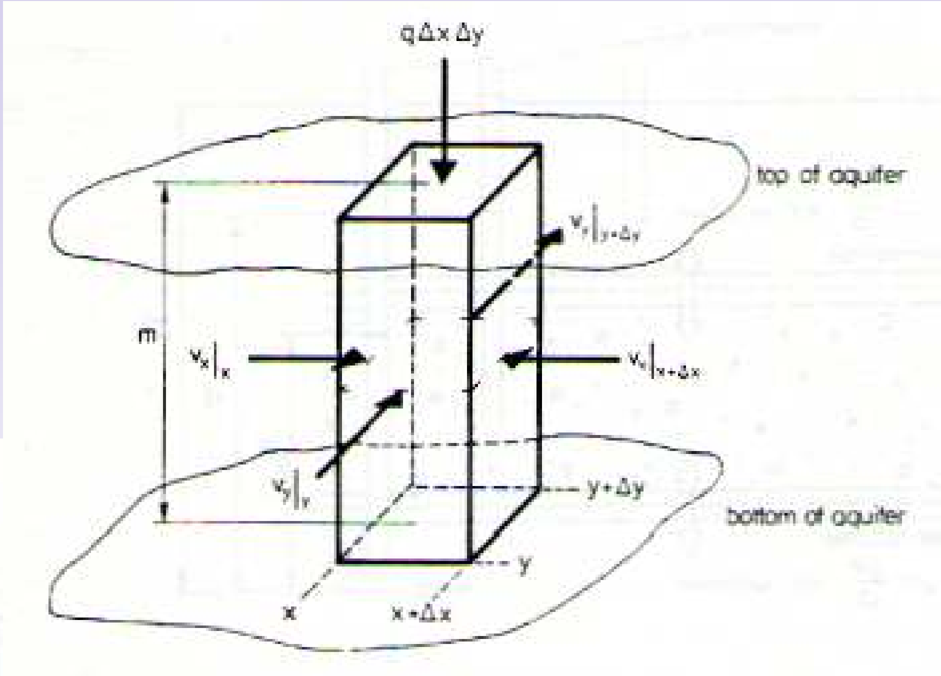




Water budget calculation of a finite difference cell

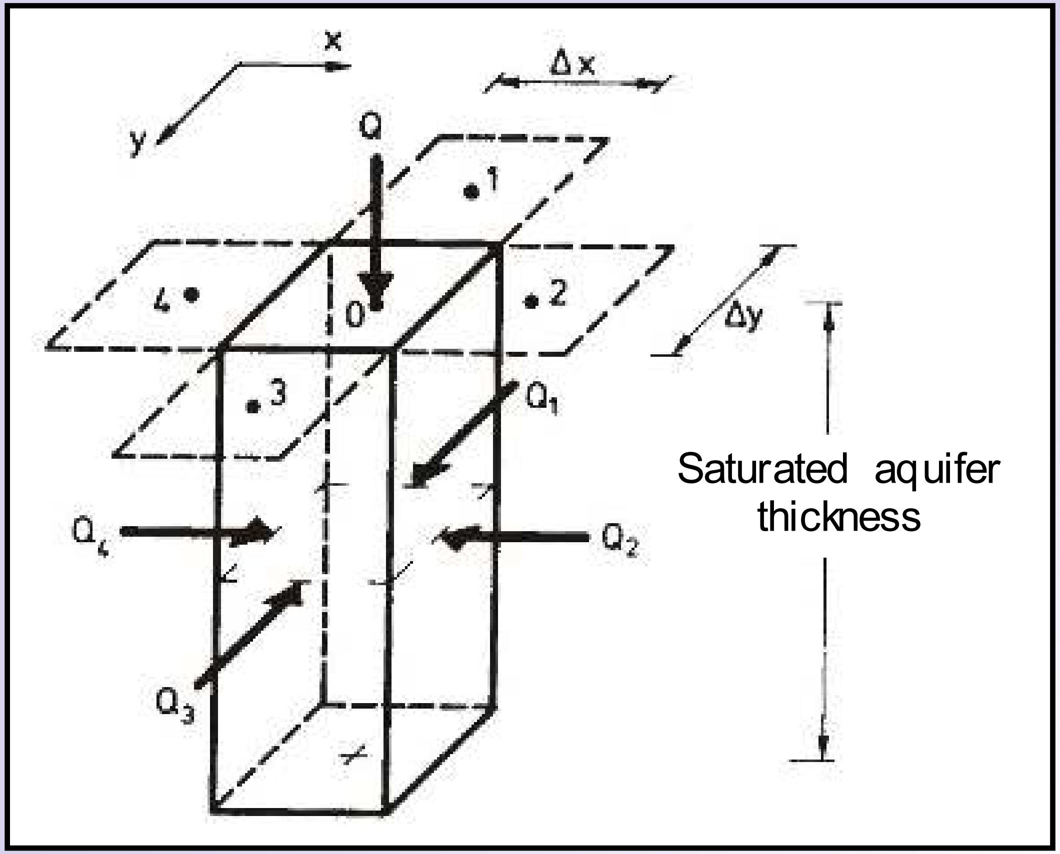
Phreatic aquifer





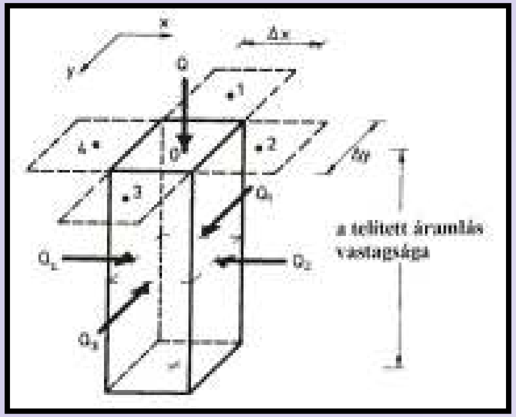
Confined aquifer

Water budget calculation of a finite difference cell



$$\Delta t(Q_0 + Q_{10} + Q_{20} + Q_{30} + Q_{40}) = \left(h_0(t + \Delta t) - h_0(t)\right) \cdot S \cdot \Delta x \Delta y$$

Water budget of a cell



$$\Delta x \cdot T_{10} \frac{h_1(t_i) - h_0(t_i)}{\Delta y} + \Delta y \cdot T_{20} \frac{h_2(t_i) - h_0(t_i)}{\Delta x} + \Delta x \cdot T_{30} \frac{h_3(t_i) - h_0(t_i)}{\Delta y} +$$

$$+ \Delta y \cdot T_{40} \frac{h_4(t_i) - h_0(t_i)}{\Delta x} = \frac{\left(h_0(t + \Delta t) - h_0(t)\right) \cdot S \cdot \Delta x \Delta y}{\Delta t}$$

Averaging:

$$T_{10} = \frac{\frac{\Delta y_0 + \Delta y_1}{2}}{\frac{\frac{\Delta y_0}{2}}{T_0} + \frac{\frac{\Delta y_1}{2}}{T_1}}; \quad T_{20} = \frac{\frac{\Delta x_0 + \Delta x_2}{2}}{\frac{\frac{\Delta x_0}{2}}{T_0} + \frac{\frac{\Delta x_2}{2}}{T_2}}; \quad \textit{and so on...}$$

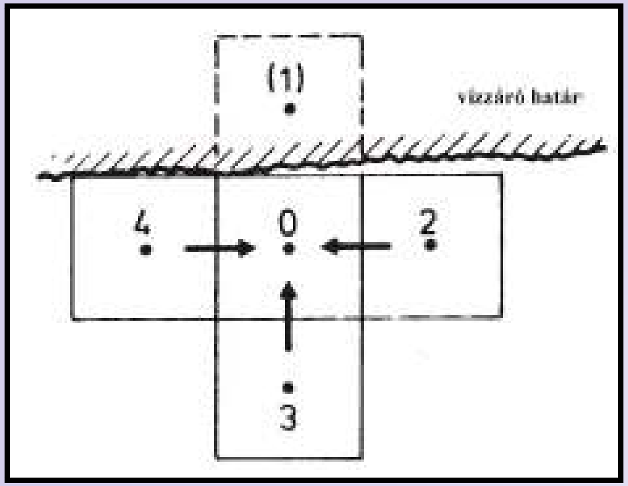
Numerical average:

$$T_{i0} = \frac{T_i + T_0}{2}$$

Geometric average:

$$T_{i0} = \frac{2 \cdot T_i \cdot T_0}{T_i + T_0}$$

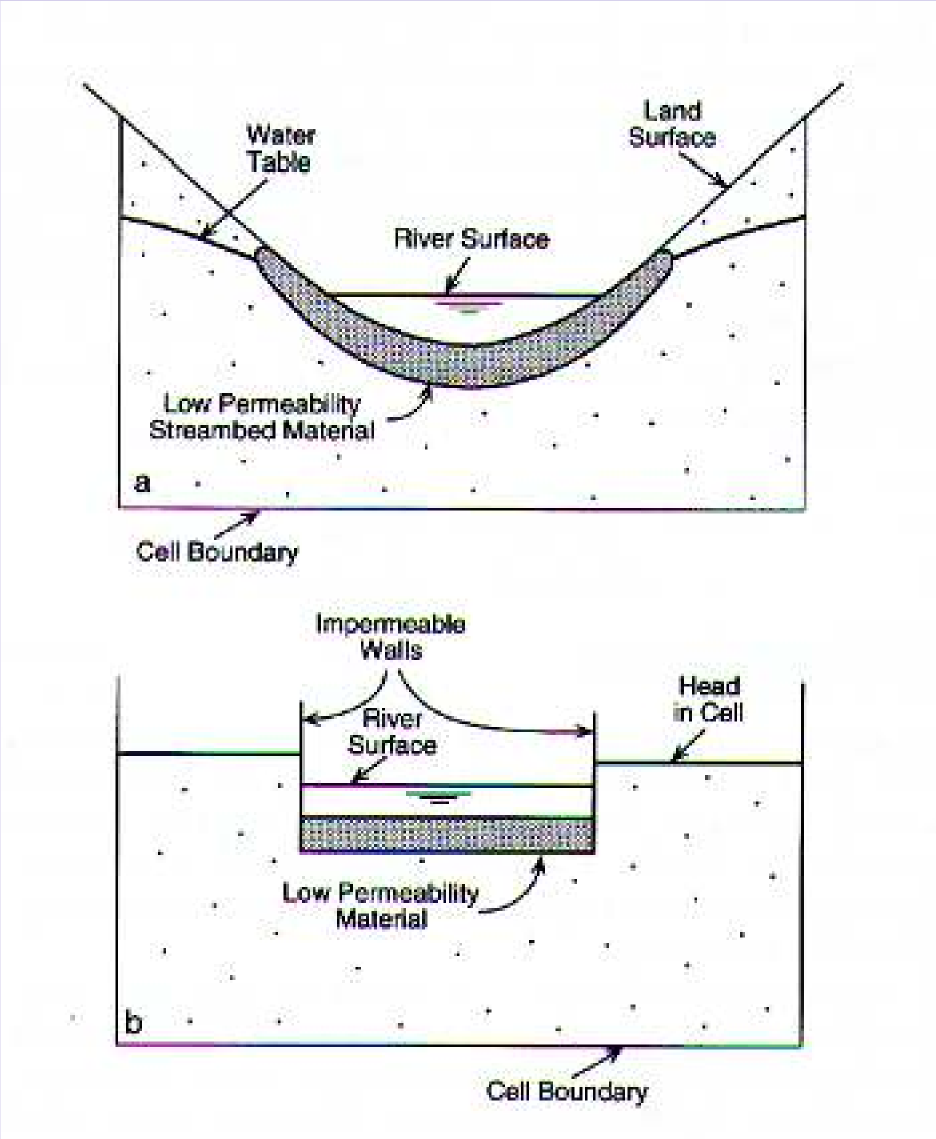
Sinks and sources

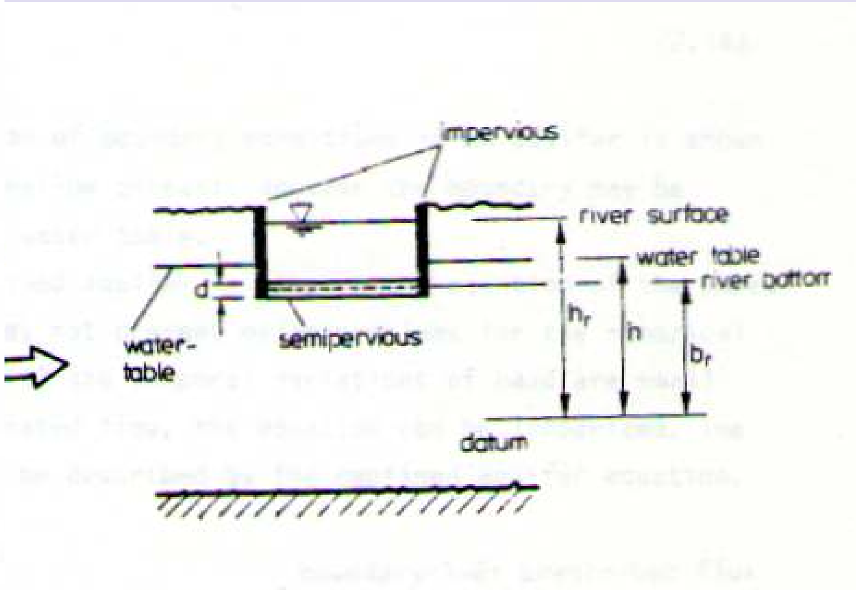


Zero flux boundary

- Rivers
- Drains
- Wells
- Recharge
- Discharge by evapotranspiration
- etc...

Finite difference modeling concept of GW-SW interactions

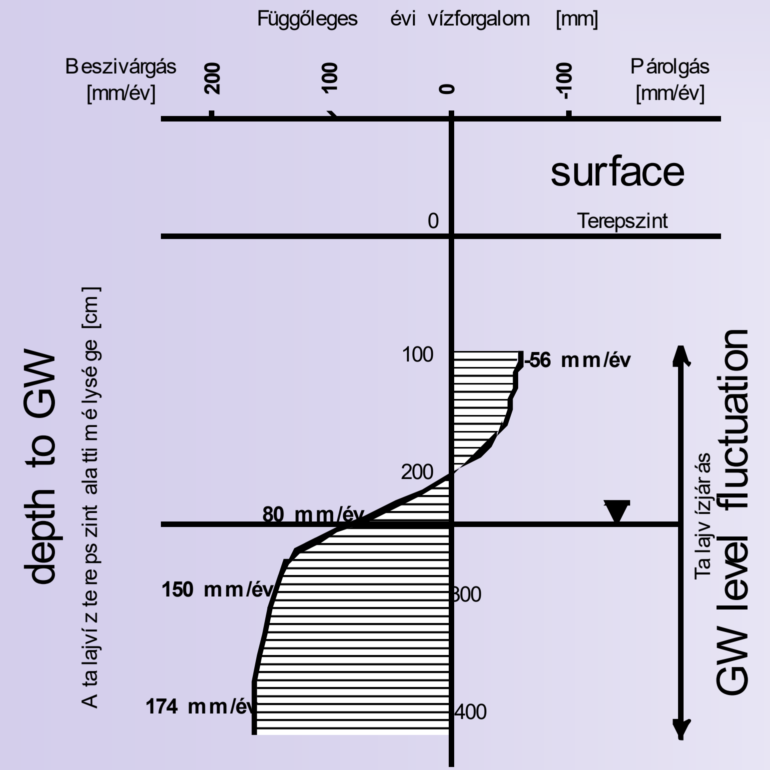




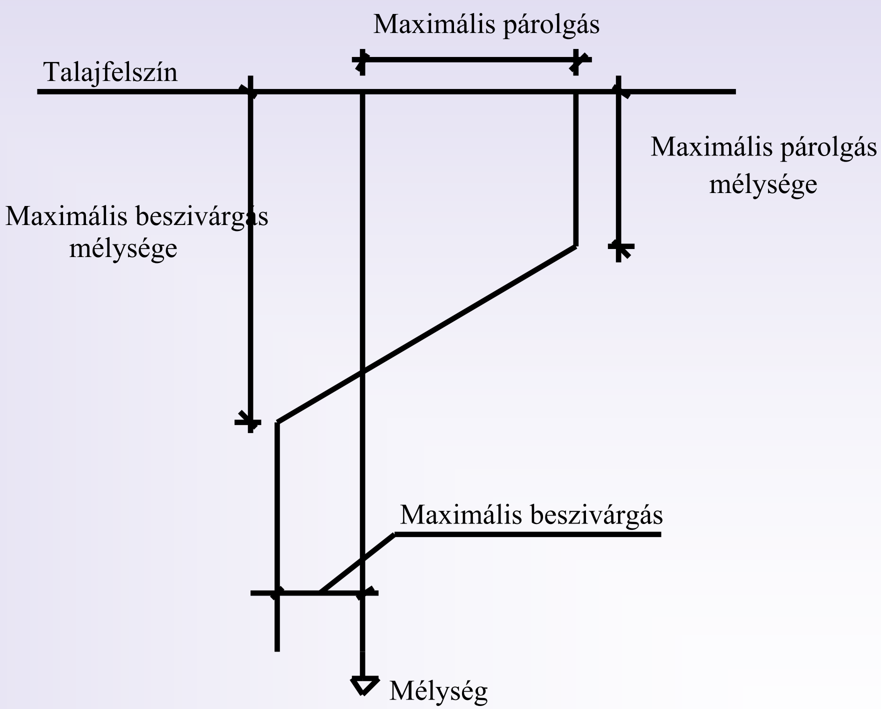
Recharge from precipitation

Recharge from precipitation = infiltration - evapotranspiration

infiltration evaporation



model of the vertical inflow budget



Boundary conditions

- Dirichlet type
  - fix head
  - fix concentration
- Neumann type
  - fix flux (inc. no-flow)
  - fixed mass flux (inc. no-flux)
- General
  - general head boundary
  - leaky or river boundary

Whether modeling or real life, never give up easily!"

(Wen-Hsing Chiang, creator of PMWIN)

Thanks for Your attention!