Presentation 4

Concepts and Equations of Variable-Density Groundwater Flow

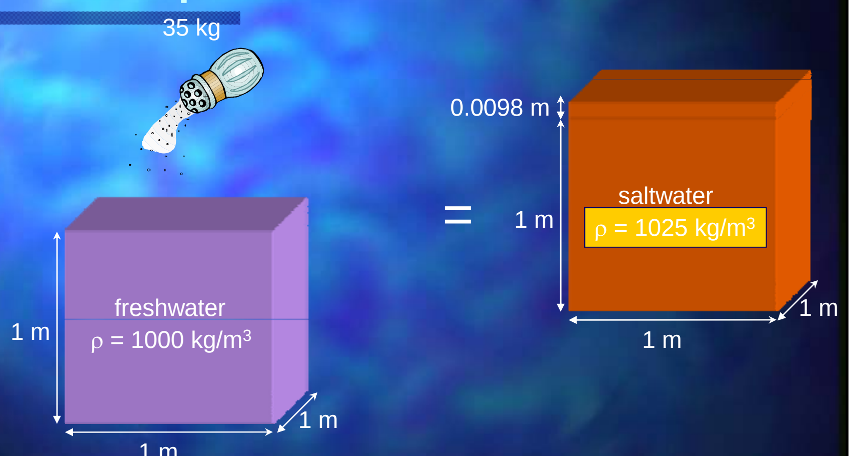
Fluid Density (ρ)

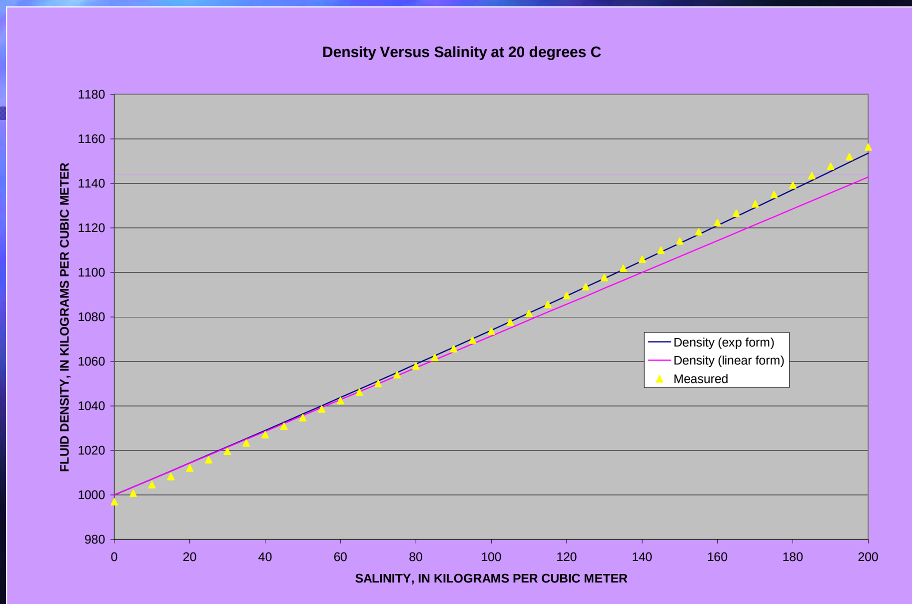
- Total Mass (fluid and salt) / Volume
- Dimensions [ML^{-3}]
- Commonly denoted with ρ
- Typical Values for Water
  - Fresh: ρ = 1000 kg/m^3; ρ = 62.43 lbs/ft^3
  - Seawater: ρ = 1025 kg/m^3; ρ = 64.00 lbs/ft^3

Solute Concentration (C)

- Solute mass fraction (ω)
  - Mass of solute / total mass of fluid
- Solute volumetric concentration (C)
  - Mass of solute / volume of fluid
- Relation: $C = \rho * \omega$

Solutal Expansion

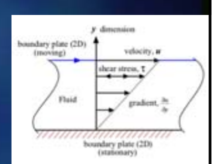


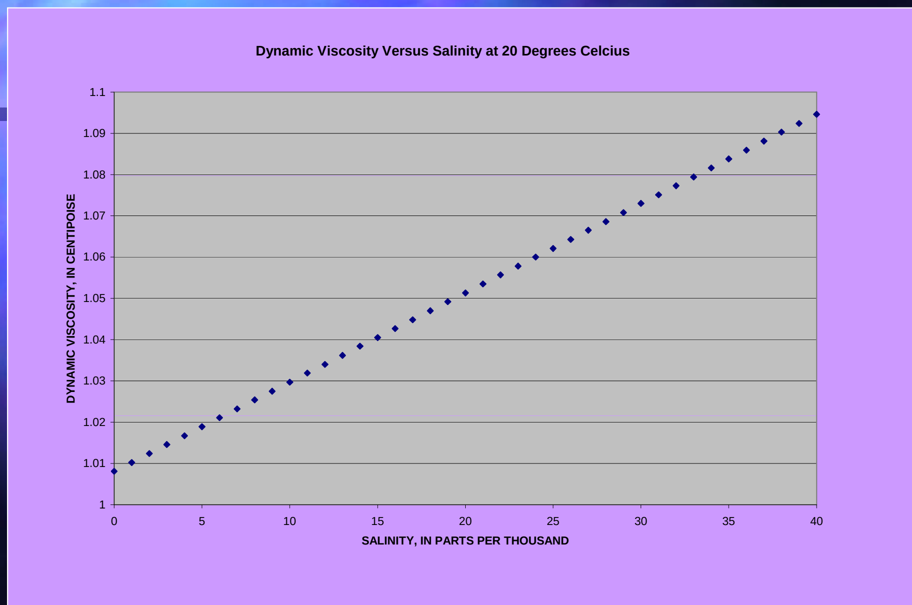


Source for measured values: http://www.unisense.com/support/pdf/gas_tables.pdf

Dynamic Viscosity (μ)

- Defined as the internal resistance of fluid to deform under shear stress
- Dimensions $[ML^{-1}T^{-1}]$
- Values:
  - Water, μ = 8.9 x 10^{-4} kg m^{-1} s^{-1}
  - Olive oil, μ = 8.1 x 10^{-2} kg m^{-1} s^{-1}
- Dynamic viscosity is related to kinematic viscosity (ν) with the following equation:
  - $\nu = \mu / \rho$





Source: http://www.unisense.com/support/pdf/gas_tables.pdf

Pressure (P)

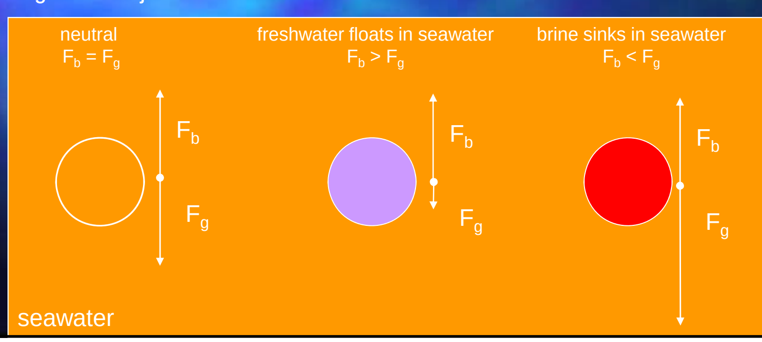
- Definition: Force per unit area
- Dimensions: $[ML^{-1}T^{-2}]$
- Typical units: N/m^2
- For a column of water of height, h, the hydrostatic pressure is:
  - $P = \rho g h$
- Absolute versus gauge pressure

Hydrostatic Conditions

- Pressure increases with depth according to the weight of the fluid
- $dP/dz = \rho g$

Buoyancy

- Upward force (F_b) on a submersed object equal to the weight of the displaced fluid
  - $F_b = \rho_{fluid} V_{object}\ g$
- Movement occurs due to differences between F_b and F_g ($F_g = m_{object}\ g$)



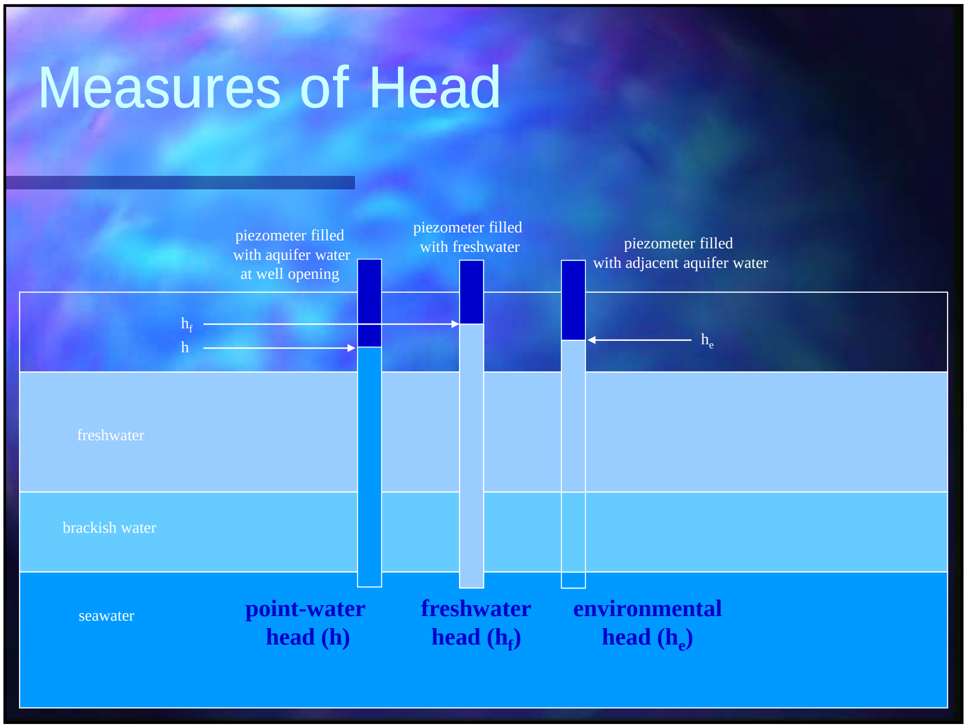
Darcy's Law

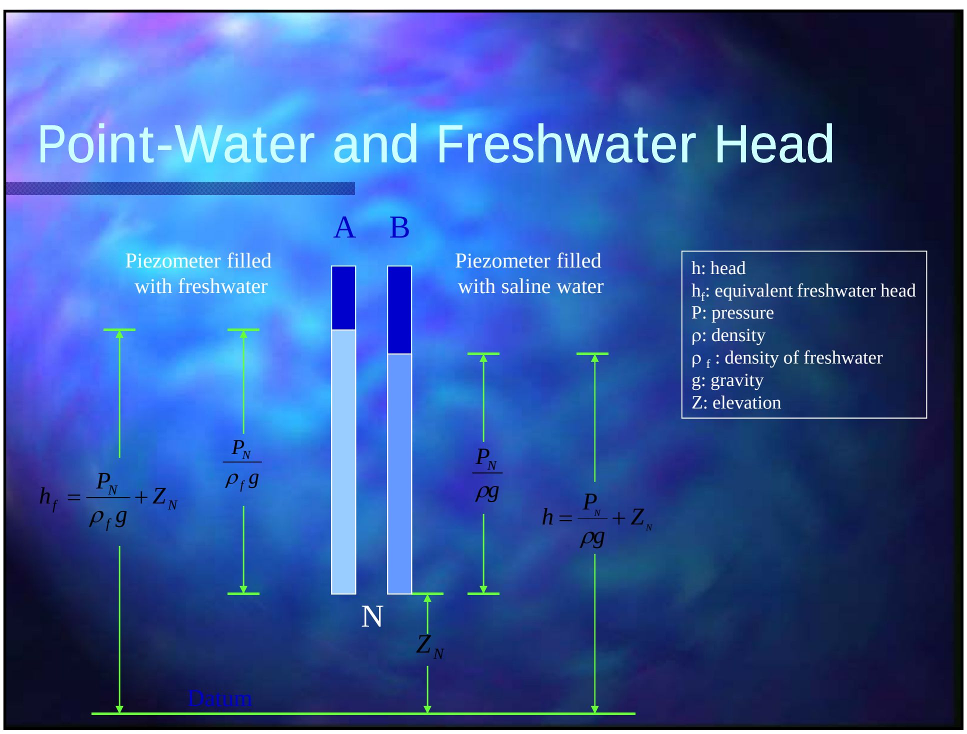
$$q_x = -\frac{k_x}{\mu}\frac{\partial P}{\partial x}$$

$$q_z = -\frac{k_z}{\mu}\left(\frac{\partial P}{\partial z} + \rho g\right)$$

Head-Based Formulation?

- Many variable-density codes solve equations in terms of pressure, but equations can also be formulated using head
- Why head instead of pressure?
  - Perhaps more intuitive
  - Use popular codes, such as MODFLOW?
- Complication: what is "head" in a variable-density system?


Measures of Head
piezometer filled with aquifer water at well opening
piezometer filled with freshwater
piezometer filled with adjacent aquifer water
h_f
h
h_e
freshwater
brackish water
seawater
point-water head (h)
freshwater head (h_f)
environmental head (h_e)


Point-Water and Freshwater Head
A
B
Piezometer filled with freshwater
Piezometer filled with saline water
h: head
h_f: equivalent freshwater head
P: pressure
ρ: density
ρ_f : density of freshwater
g: gravity
Z: elevation
$h_f = \frac{P_N}{\rho_f g} + Z_N$
$\frac{P_N}{\rho_f g}$
$\frac{P_N}{\rho g}$
$h = \frac{P_N}{\rho g} + Z_N$
N
Z_N
Datum

Converting between h_f and h

$$P_A = P_B \quad \Rightarrow \quad \begin{cases} h_f = \dfrac{\rho}{\rho_f} h - \dfrac{\rho - \rho_f}{\rho_f} Z \\[2ex] h = \dfrac{\rho_f}{\rho} h_f + \dfrac{\rho - \rho_f}{\rho} Z \end{cases}$$

Lusczynski (1961)

- Horizontal flow is proportional to the gradient of freshwater head
- Vertical flow is proportional to the gradient in environmental head
- Horizontal and vertical flow are not necessarily proportional to the gradient of point-water head

Why use h_f in SEAWAT?

- Conceptually straightforward (i.e. for freshwater system, $h_f = h$)
- Finite-difference form of governing equation can be solved by MODFLOW (with a few modifications)

Darcy's Law

pressure and permeability

$$q_x = -\frac{k_x}{\mu}\frac{\partial P}{\partial x}$$

$$q_z = -\frac{k_x}{\mu}\left(\frac{\partial P}{\partial z} + \rho g\right)$$

$$P = \rho_f g\left(h_f - z\right)$$

$$K_f = \frac{k \rho_f g}{\mu_f}$$

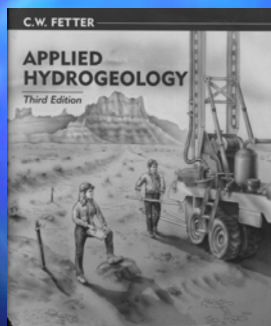
equivalent freshwater head and hydraulic conductivity

$$q_x = -K_f \frac{\mu_f}{\mu}\frac{\partial h_f}{\partial x}$$

$$q_z = -K_{fz}\frac{\mu_f}{\mu}\left(\frac{\partial h_f}{\partial x} + \frac{\rho - \rho_f}{\rho_f}\right)$$

can assume $\frac{\mu_f}{\mu} = 1$

Be Careful! Some Published Material is Incorrect

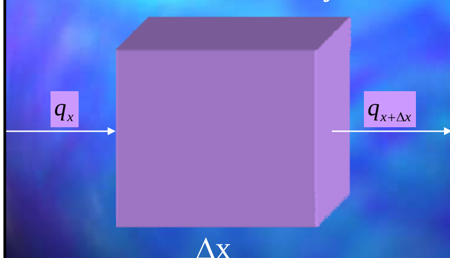


"If the density of water in aquifers varies **vertically**, all point-water heads should be converted to fresh-water pressure heads. Fresh-water heads can then be determined and used for the **determination of hydraulic gradients and flow directions**."

"For theoretical reasons equivalent **fresh-water heads cannot be used to determine the hydraulic gradient** in aquifers where there is a **lateral variation in density**."

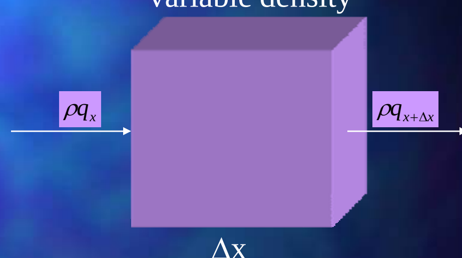
Governing Equation for Flow

constant density



$$-\nabla \cdot \vec{q} + q_s = \frac{\partial \theta}{\partial t}$$

variable density



$$-\nabla \cdot (\rho \vec{q}) + \rho_s q_s = \frac{\partial (\rho \theta)}{\partial t}$$

Storage Term

$$\frac{\partial(\rho\theta)}{\partial t} = \rho\frac{\partial\theta}{\partial t} + \theta\frac{\partial\rho}{\partial t}$$

$$\theta = f(P)$$

$$\rho = f(P,C)$$

$$\frac{\partial\theta}{\partial t} = \frac{\partial\theta}{\partial P}\frac{\partial P}{\partial t}$$

$$\frac{\partial\rho}{\partial t} = \frac{\partial\rho}{\partial P}\frac{\partial P}{\partial t} + \frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t}$$

$$\frac{\partial(\rho\theta)}{\partial t} = \rho\frac{\partial\theta}{\partial P}\frac{\partial P}{\partial t} + \theta\frac{\partial\rho}{\partial P}\frac{\partial P}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t}$$

Storage Term (cont.)

$$\frac{\partial(\rho\theta)}{\partial t} = \rho\frac{\partial\theta}{\partial P}\frac{\partial P}{\partial t} + \theta\frac{\partial\rho}{\partial P}\frac{\partial P}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t}$$

compressibility of the aquifer

compressibility of water

accumulation of mass as a result of concentration changes

$$\xi = \frac{1}{(1-\theta)}\frac{\partial\theta}{\partial P}$$

$$\zeta = \frac{1}{\rho}\frac{\partial\rho}{\partial P}$$

$$\frac{\partial(\rho\theta)}{\partial t} = \rho\left[\xi(1-\theta)+\zeta\theta\right]\frac{\partial P}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t}$$

Formulated in terms of pressure

Storage Term (cont.)

$$\frac{\partial(\rho\theta)}{\partial t} = \rho[\xi(1-\theta)+\zeta\theta]\frac{\partial P}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t}$$

$$S_P = \xi(1-\theta)+\zeta\theta$$

Bear, 1979

$$\frac{\partial(\rho\theta)}{\partial t} = \rho S_P\frac{\partial P}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t}$$

$$P = \rho_f g(h_f - Z) \qquad S_f = \rho_f g[\xi(1-\theta)+\zeta\theta]$$

$$\boxed{\frac{\partial(\rho\theta)}{\partial t} = \rho S_f\frac{\partial h_f}{\partial t} + \theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t}}$$

Formulated in terms of h_f; Used in SEAWAT

Governing Equation for Variable-Density Flow

$$\frac{\partial}{\partial x}\left[\rho K_{fx}\left(\frac{\partial h_f}{\partial x}+\frac{\rho-\rho_f}{\rho_f}\frac{\partial z}{\partial x}\right)\right]+\frac{\partial}{\partial y}\left[\rho K_{fy}\left(\frac{\partial h_f}{\partial y}+\frac{\rho-\rho_f}{\rho_f}\frac{\partial z}{\partial y}\right)\right]+\frac{\partial}{\partial z}\left[\rho K_{fz}\left(\frac{\partial h_f}{\partial z}+\frac{\rho-\rho_f}{\rho_f}\right)\right]=\rho S_f\frac{\partial h_f}{\partial t}+\theta\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t}-\rho_s q_s$$

or

$$\nabla\cdot\rho K_f\left(\nabla h_f+\frac{(\rho-\rho_f)}{\rho_f}\nabla z\right)=\rho S_f\frac{\partial h_f}{\partial t}+n\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t}-\rho_s q_s$$

Governing Equation for Solute Transport

$$\frac{\partial C}{\partial t} = \underbrace{-\nabla \cdot \left(\vec{v} C\right)}_{\text{ADV}} + \underbrace{\nabla \cdot \left(D \cdot \nabla C\right)}_{\text{DSP}} \underbrace{- \frac{q_s}{\theta} C_s}_{\text{SSM}} + \underbrace{\sum_{k=1}^{N} R_k}_{\text{RCT}}$$

Equation of State

- Equation of state is used to relate fluid density to pressure, temperature, and concentration
- Most rigorous form:
  - $\rho = \rho_0 \exp[B_P(P-P_0) + B_T(T-T_0) + B_C(C-C_0)]$
  - $B_P = 1/\rho * \delta\rho/\delta P|_{T,C}$ (fluid compressibility)
  - $B_T = 1/\rho * \delta\rho/\delta T|_{P,C}$ (fluid coefficient of thermal expansion)
  - $B_C = 1/\rho * \delta\rho/\delta C|_{P,T}$ (slope of fluid density as a function of solute concentration, divided by reference density)
- A linear approximation is often used, which can be written as:
  - $\rho = \rho_0[1 + B_P(P-P_0) + B_T(T-T_0) + B_C(C-C_0)]$, or
  - $\rho = \rho_0 + d\rho/dP * (P-P_0) + d\rho/dT * (T-T_0) + d\rho/dC * (C-C_0)]$
- In SEAWAT, we assume that density is not affected by pressure or temperature, and that the reference density is freshwater with a concentration of zero
  - $\rho = \rho_f + d\rho/dC * C$
  - `DENSE = DENSEREF + DENSESLP * CONC`
- Value for $d\rho/dC$ is about 0.7143 (25/35) for a freshwater-seawater mixture, if density and concentration are expressed in equivalent units

Note: parts of this taken from Kipp (1987), Kolditz et al. (1998) and Diersch and Kolditz (2002)

Coupled Flow and Transport

- Groundwater flow is affected by fluid density
  - $q = f(\rho,...)$
- Concentration is affected by flow velocity (advection and dispersion)
  - $C = f(q,...)$
- Fluid density is function of solute concentration
  - $\rho = f(C)$

Major Constituents in Seawater