Contaminant Transport

How would one determine contaminant transport:

- Long term monitoring
- Modeling

What are environmental systems?

What is modeling?

Simplification and representation of the environmental system by a set of equations which can be used to explain and predict the behaviour of any system.

Why do we need to model?

- for a better understanding of the fate and transport of pollutants
- to determine exposure conc. to humans and organisms in the past, present and future
- to predict future conditions under different loading situations

Transport – movement/migration of pollutants from one point to another

Fate – transformation of a pollutant

<u>Impact</u>

- air
- water (ground water and surface water)
- land

<u>Concerns</u>

- Inorganics such as heavy metals – Hg, Pb, Cd, Cr, etc.
- Organics such as pesticides, hydrocarbons etc.

For a better understanding of biological responses degradation, uptake, toxicity, pharmacokinetics, etc. have to be known.

Environmental toxicology

- study of fate and effects of chemicals in the environment
- can be subdivided into
  - human health toxicology
  - ecological health toxicology

Chemicals pose an environmental threat due to

- toxicity
- environmental persistence
- bio accumulation

Environmental Persistence
- resist degradation e.g. DDT, PCB, TCDD, etc.
- e.g. mirex in Lake Ontario
- e.g. DDT in Lake Apopka, Florida

Abiotic Degradation
- Photolysis — light
  UV-potential to break chemical bonds e.g. PAH
- Hydrolysis — water
  Water with light or heat can break chemical bonds e.g. parathion

Biotic Degradation
- action of microorganisms

Nondegradative Elimination Processes
- by altering distribution e.g. lindane

Bioaccumulation
- process by which organisms accumulate chemicals from abiotic and dietary sources
- lungs, gills, gastrointestinal, dermal
- aquatic animals can bioaccumulate chemicals several orders of magnitude greater than that existing in the environment.

Bioaccumulation of some environmental contaminants in fish.

Chemical	Bioaccumulation factor
DDT	127,000
TCDD	39,000
Endrin	6,800
Pentachlorobenzene	5,000

Bioaccumulation factor (BCF) is the concentration of a chemical in the tissue of a target organism divided by the concentration in the diet.

Chemicals transfer along the food chain from prey organisms to predator

Factors Influencing Bioaccumulation
- environmental persistence
- lipophilicity
- biotransformability

Hydro Fobic → contaminant particles hates water

Acute Toxicity Immidiat effect

- toxicity as a result of short term exposure to a toxicant
- quantified by LD50 or LC50

Chronic Toxicity consetiration

Causes Cancer

- toxicity as a result of long term exposure to a toxicant
- carcinogenicity, mutagenicity, teratogenicity
- can cause death by bio-accumulation
- measured by end points
  NOEL, LOEL and others

changes DNA

effects next Generation but not DNA Example: Alcohol

observed Effect level

Law of conservation of Mass (or Energy)

The rate of change or accumulation of mass in a system is equal to the difference between the rate of mass input and mass output.

Accumulation = Input - output ± generation/Consumption

Key Elements
- clearly defined control volume
- knowledge of inputs and outputs
- knowledge of transport characteristics within the control volume
- knowledge of reaction kinetics in control volume

Accumulation in control volume = Mass input – Mass output ± generation/consumption

Flow Balance in surface waters

Δ storage = Σ inflow - Σ outflow + Precipitation – Evaporation

$$\Delta V = \left(\sum Q_{in} + Q_{gw_{in}} - \sum Q_{out} - Q_{gw_{seep}} + IA - EA\right)\Delta t$$

where

Q = flow rate
E = evaporation rate
A = surface area of water body
I = precipitation rate
Δt = time increments

ΔV = change in storage volume

Practice Example:
The inflow to a small reservoir is given as

$Q = 1000\,(1 - e^{-kt})$
k = runoff rate = 1.0/hr
t = time in hr
Q = flow in cfs
outflow = 800 cfs
Initial Vol. of the reservoir = 10×10^6 cu. ft.

Question 1: Write the differential equation describing the rate of change in reservoir vol. with time.
Question 2: Determine vol. of the reservoir after each hr for 4 hrs.

$$\frac{dV}{dt} = Q_{in} - Q_{out}$$

$$Q_{in} = 1000\,[1 - e^{-kt}] = 3600 \times 1000\,[1 - e^{-kt}]\ ft^3/h$$

$$Q_{out} = 800\ fps = 800 \times 3600\ ft^3/h$$

$$\frac{dV}{dt} = 3.6 \times 10^6\,[1 - e^{-kt}] - 2.88 \times 10^6$$

$$\int_{V_1}^{V_2} dV = \int_0^t [0.72 \times 10^6 - 3.6 \times 10^6\, e^{-kt}]\, dt$$

$$\text{or}\quad V_2 - V_1 = \left[0.72 \times 10^6\, t + \frac{3.6 \times 10^6}{k}\, e^{-kt}\right]_0^t$$

Up until now only water was considered.
Now consider that there is a solute that is moving with the flow, e.g. NaCl (brine solution).
Then the questions which arise are:
How much solute is being transported?
How much solute is being treated, etc.?

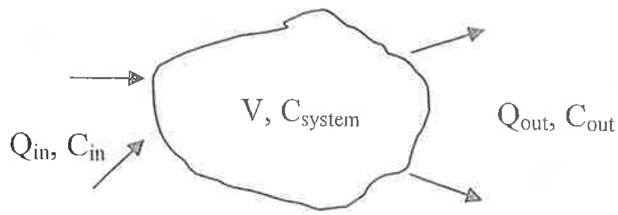
$$\text{Input} = Q_{in}\, C_{in}$$

$$= \frac{m^3}{s} \cdot \frac{mg}{m^3} = \frac{mg}{s}$$

Two things to consider:

- flow (Q)
- concentration (C)

Thus, if Q_m is mass of solute entering a system then
$Q_m = Q_{in} \cdot C_{in}$
where Q_{in} is the inflow and
C_{in} is the conc. in the inflow



$$\frac{d}{dt}\left[VC_{system}\right]=\sum_{i=1}^{N}Q_{in,i}C_{in,i}-\sum_{j=1}^{M}Q_{out,j}C_{out,j}$$

since, V = constant

$$\frac{dC_{system}}{dt}=\frac{1}{V}\left[\sum_{i=1}^{N}Q_{in,i}C_{in,i}-\sum_{j=1}^{M}Q_{out,j}C_{out,j}\right]$$

Under steady state conditions

$$\frac{dC_{system}}{dt}=0$$

Practice Examples:

A processing plant gives out contaminants at a rate of 150 mg/L. The flow rate is 3 l/s. We want to treat the waste stream to get a contaminant conc. of 15 mg/L and a flow rate of 2.5 l/s. What should be the concentration of the sludge generated as a result of treatment?

$\boxed{\text{Process:}} \xrightarrow[3\ L/s]{150\ mg/L}$ $\boxed{\text{Treatment}} \xrightarrow{}$ 15 mg/L, 2.5 L/s

↓ 0.5 L/s ↓ C

Input = out put $\Rightarrow$ $150\ \frac{mg}{L} \times 3\ L/s = (15\ \frac{mg}{L} \times 2.5\ L/s) + (0.5\ \frac{L}{s} \times C)$

$C = 825\ mg/L$

A river has a volumetric discharge of 40 m^3/s from a stretch of agricultural area. Runoff (500l/s) from an agricultural area, which carries 0.2 mg/l of a pesticide endrin (used in the past to control rodents and used as an insecticide in rice, cotton and maize crops) mixes with the river flow. Determine the concentration of endrin in the river water, downstream from the agricultural area (assume no degradation) $1\ m^3 = 1000\ L$

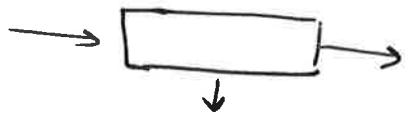
Acc = input - output ± reaction

$0 = (40)(0) - (500\ \frac{L}{s})(0.2\ \frac{mg}{L}) = (40.5)\ C$

$C = \frac{100}{40.5} = 2.469 \times 10^{?}\ mg/l$

Q_{in}

C_{in}



$Q_{w\,out} = 300$ kg/h

$C_{w\,out} = 0$ (pure)

$Q_{b\,out} =$

$C_{in} = \frac{3}{97}$

$C_{b\,out} = \frac{10}{90}$

A continuous and steady state freezing process is used to purify seawater (3% NaCl and 97% water, by weight). The liquid brine concentration existing the process is 10% NaCl. Determine the mass rate of sea water required to produce 300kg/h of pure water in the form of ice.

Mass balance of water

$Q_{in} = Q_{b\,out} + 300$ --(1)

Mass Balance of Salt

$Q_{in}\left(\frac{3}{97}\right) = Q_{b\,out}\left(\frac{10}{90}\right) + Q_{w\,out}(0)$

Substituting from (1)

$[Q_{b\,out} + 300]\left(\frac{3}{97}\right) = Q_{b\,out}\left(\frac{1}{9}\right)$

$Q_{b\,out} = 415.7$ kg/h

A certain pesticide is fatal to fish at 0.5 ppm. A leaking metal can containing 5 kg of the pesticide is dumped into a stream with a flow of 10 lts/sec. The CS area of the stream = 10 m^2. The pesticide is leaking at a constant rate of 5 mg/sec.
For what distance downstream is the water contaminated by pesticide by the time the container is empty? Assume no degradation.

Velocity of flow $= \frac{Q}{A} = \frac{10 \times 10^{-3}\ m^3/s}{10\ m^2} = 10^{-3}$ m/s

Time to empty $= \frac{5 \times 10^6\ mg}{5\ mg/s} = 10^6$ sec $= 278$ h

Distance to which water is contaminated $= 10^{-3}\ \frac{m}{s} \times 10^6\ s = 10^3\ m = 1$ km

The volumetric discharge in a river, upstream of an agricultural land is 54 m^3/s. It carries a pesticide concentration of 0.0006 mg/L. Runoff from a nearby agricultural land has a flow of 0.12 m^3/s and carries the same pesticide with a concentration of 1.2 ppm. Determine the concentration of the pesticide in the river water, assuming fully mixed conditions and no degradation.

$\boxed{mg/L = ppm}$

Input = output

$Q_1 \times C_1 + Q_2 \times C_2 = (Q_1 + Q_2)\, C_{out} \rightarrow$

$54\ \frac{m^3}{s} \times 0.0006\ mg/L + 0.12\ \frac{m^3}{s} \times 1.2\ \frac{m^3}{s} = 54.12\ m^3/s \times C_{out}$

$C_{out} = 0.00326$ mg/L

The ventilation rate in a house is 80 m^3/hr. A heater used in the house constantly emits 900 g/hr of CO_2. Calculate the steady state conc. of CO_2 in the house. (The conc. of CO_2 at 20 °C and 1 atm press. is 0.031% by volume).

1 Litre of Air has 0.031×10^{-2} L of CO_2

44 g of CO_2 ($=12+32$) occupies 24.05 L at 20°C (Avogadro's law)
or 22.4 L at 0°C

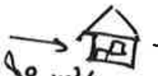
1 L of CO_2 weighs $\frac{44}{24.05}$ g at 20°C

0.00031 L of CO_2 weighs $\frac{44}{24.05} \times 0.0031 = 5.67 \times 10^{-4}$ g at 20°C

$\therefore$ Conc. of CO_2 $= 5.67 \times 10^{-4}$ g/L of air

Mass balance

~~$\sum Q_{in} C_{in} = \sum Q_{out} C_{out}$ - generation~~



$Q_{in} = 80$ m³/h $\longrightarrow$ $Q_{out} = 80$ m³/h

$C_{CO_2\,in} =$ $\quad C_{CO_2\,out} = ?$

Transport Phenomena

A chemical in the environment can have 3 possible (or a combination of these) outcomes:
- be stationary
- be transported
- be transformed

A chemical can enter a human system through:
- dermal (through skin)
- oral
- inhalation

It can redistribute from their point of entry by:
- fluid dynamics
- intermedia transport processes
- complexation

An environmental source can be:
- a point source
- non-point sources

Chemicals can be transported by 2 phenomena:
- advection
- dispersion

Advection – refers to movement of chemicals due to velocity

Acc = Input − Output ∓ gen/cons

$0 = \sum Q_{in} C_{in} - \sum Q_{out} C_{out} + 900$

$80 \times C_{out} = (80)(5.67 \times 10^{-4}) + 900$

$C_{out} = 11.017$ g/m³

Avogadro's law

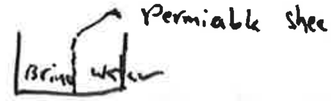
$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

$$\frac{22.4}{273} = \frac{V_2}{293}$$

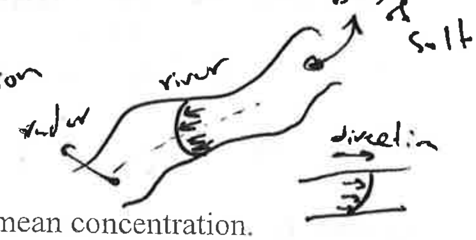
$V_2 = 24.04$

Brine = salti water

Dispersion – refers to contaminant transport due to deviations in velocity and heterogeneity leading to mixing and dilution



- Molecular diffusion → brownian motion of Particles
- Turbulent diffusion
- Dispersion



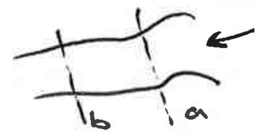
Advection

Advective transport is the product of the volumetric flow rate and mean concentration.

$\therefore J = QC$ or $\qquad$ J is mass transport per unit time

$\therefore J = \bar{u}AC$

If flow occurs from point a to point b, in say, a river:



Change in mass from a to b

Δm = (mass inflow rate – mass outflow rate) x time

Δm = $(Q_aC_a - Q_bC_b))\Delta t$

$C.Q = \frac{m^3}{s} . \frac{mg}{m^3}$

again, $\Delta m = \Delta(VC)$; $\quad V$ = volume, m^3

$\quad C$ = conc. g/m^3

$$\therefore \frac{\Delta(VC)}{\Delta t} = Q_aC_a - Q_bC_b$$

if V is constant

$$V. \frac{\Delta C}{\Delta t} = \Delta(QC)$$

$$V = A . \Delta x$$

Again, $V = A\Delta x$; A = area

$$\frac{\Delta C}{\Delta t} = \frac{-\Delta(QC)}{A\Delta x}$$

or

$$\frac{\partial C}{\partial t} = -\frac{1}{A}\frac{\partial(QC)}{\partial x}$$

$$\frac{\partial C}{\partial t} = -\frac{Q}{A}\frac{\partial C}{\Delta x}$$

$-v$

$\boxed{\frac{\partial C}{\partial t} = -u_x \frac{\partial C}{\partial x}}$ if Q does not change with x and as $Q/A = u_x$ (velocity in x direction)

In three dimension, this equation can be written as

$v = u =$ velocity

$$\frac{\partial C}{\partial t} = -u.\nabla C$$

$$\text{or} \quad \boxed{\frac{\partial C}{\partial t} = -\left[u_x \frac{\partial C}{\partial x} + u_y \frac{\partial C}{\partial y} + u_z \frac{\partial C}{\partial z} \right]}$$

Practice Example

A river carries a pesticide, alachlor, with an average concentration of 1.5 mg/l. The mean flow in the river is 125 m^3/s. Determine the average mass flux of alachlor passing a point in the river.

$= 1.5$ mg/L $\times 125$ m^3/s $=$ average max flux

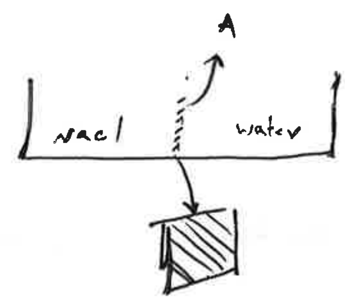
Watch for units

Dispersion

Fick's 1st Law

for steady state

$J \propto \frac{dC}{dx}$



1st Law: $J \propto A \frac{dC}{dx}$

$$\boxed{J = -DA \frac{dC}{dx}}$$

D is diffusion coefficient

Free solution diffussion Coefficient
effective diffussion coefficient
use it for a river

Molecular diffusion, turbulent diffusion and dispersion all use Fick's Law

Mass Flux due to turbulent diffusion, J_t

$$J_t = -\in_m A \frac{dC}{dx}$$

$$J_t = -EA \frac{dC}{dx}$$

$$\boxed{E >> \in_m >> D}$$

because of mixing and dillution

$\in_m$ is turbulent diffusion coefficient; E is dispersion coefficient; D is molecular diffusion coefficient

Practice Examples

The molecular diffusivity of a chloride ion is $2x10^{-5}$ cm^2/s. Calculate the mass flux (mg/s) through a membrane of thickness 100 μm. The area of the membrane is $1m^2$ and the concentrations on the two sides are 5mg/l and 1mg/l.

$$J = -DA \frac{dc}{dx}$$

$$J = (2\times10^{-9} \frac{m^3}{s})(1m^2)\left(\frac{(5-1)10^3 \quad mg/m^3}{100\times10^{-6} \quad m}\right)$$

$$= 0.08 \ mg/s$$

The molecular diffusivity of caffeine in water is $0.63x10^{-3}cm^2/s$. Assuming the coffee to have a caffeine concentration of 2 mg/l, determine the mass flux through the walls of the intestine, over an area of $0.075\ m^2$. Assume caffeine concentration in the blood to be 0. How long will it take for 1 mg of caffeine to get in the blood stream?

thickness = 60 μm (given)

$$J = DA \frac{dc}{dx}$$

$$= (0.63\times10^{-7} \ m^2/s)(0.075 \ m^2)\left[\frac{(2000-0) \ mg/m^3}{60\times10^{-6}}\right]$$

$$= 0.1575 \ mg/s$$

$$J.t = w$$

$$(0.1575 \frac{mg}{s})(t) = 1 \ mg \longrightarrow t = 6.35 \ sec$$

Fick's 2nd Law

- For transient state

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$, if D is a constant

Otherwise

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[D\frac{\partial C}{\partial x}\right]$$

We need one initial condition and two boundary conditions to solve this equation. Under steady state conditions, $\frac{\partial C}{\partial t}=0$. The solution of the Fick's second law for steady state and for the following boundary conditions:
$C=C_1$ when x =0 and $C=C_2$ when x=L is:

$C = C_1$ when $x = 0$
$C = C_2$ when $x = L$

Integrating the equation $D\frac{\partial^2 C}{\partial x^2} = 0$ twice → we need 2 boundary conditions
C=a+bx where a and b are integration constants. Upon substituting the boundary conditions:

$$C = C_1 + \frac{C_2 - C_1}{l}x$$

The mass flux is $J = -DA\frac{dC}{dx} = \frac{DA(C_1 - C_2)}{l}$

$\frac{dc}{dx} = B$

$C = Bx + A$

when $x = 0$, $C_1 = A$ --- ①

when $x = L$, $C_2 = BL + A$ --- ②

Substituting from ① to ②

$C_2 = BL + C_1$

or $B = \frac{C_2 - C_1}{L}$

$C = \frac{C_2 - C_1}{L} . x + C_1$

if

$C = C_1$ when $x = 0$

$\frac{dc}{dx} = K$ when $x = L$

what is the solution ?

$C = Bx + A$

$B = K$

$A = C_1$

$C_1 = A$ --- ①

$\frac{dc}{dx} = B = K$

$C = Kx + C_1$

A reservoir has a capacity of 10,000 m^3 and it is half full
The ~~inside~~ initial concentration of salt in the reservoir is 50 mg/L
Run off from near by deicing salt storage place brings in water at a concentration of 20,000 mg/L. The runoff is 5 m^3/day and assuming the seapage losses from the reservoir to be the same, determine the change in salt conc. with time

$$\cancel{\frac{\partial Q}{\partial t}} = \frac{d(C \cdot V)}{dt} = Q_{in} C_{in} - Q_{out} C$$

V does not change with time

$$\frac{dc}{dt} = \frac{Q_{in} C_{in}}{V} - \frac{Q_{out} C}{V}$$

$$\frac{dc}{dt} = \left(\frac{5 \; m^3/d}{5000 \; m^3} \; 20000 \; \frac{mg}{L} \right) - \left(\frac{5 \; m^3/d}{5000 \; m^3} \; C \right)$$

$$\frac{dc}{dt} = 10^{-3} [20{,}000 - C]$$

$$\int_{C_0}^{C} \frac{dC}{20{,}000 - C} = \int_0^t 10^{-3} \, dt$$

$$\ln \frac{20\,000 - C_0}{20{,}000 - C} = 10^{-3} t$$

$$\frac{20\,000 - C_0}{20{,}000 - C} = e^{0.001 t} \quad \text{or} \quad C = 20\,000 - 19950 \, e^{-0.001 t}$$

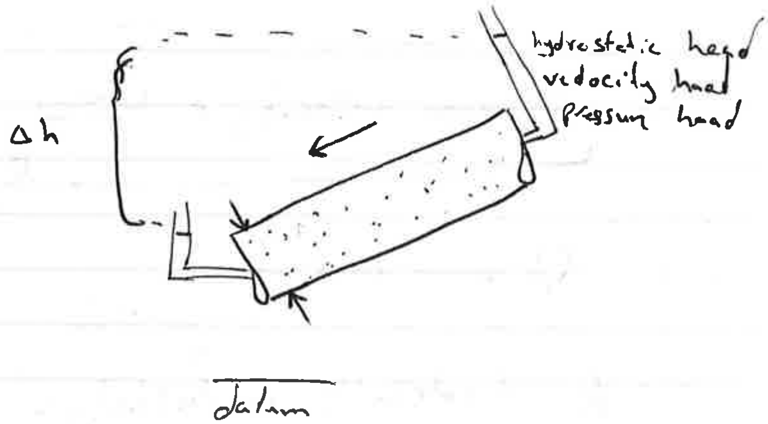
after 1 day, C = 69.94 mg/L

5 days, C = 149.5 mg/L

100 days, C = 1948.5 m/L

$$\boxed{\int \frac{dx}{(1-x)} = -\ln |1-x|}$$

Darcy's law



$$Q \propto A$$
$$\propto \frac{\Delta h}{L} \; (= i)$$

$$Q = -k(i)A$$
$$= -k\left(\frac{\Delta h}{L}\right)A$$

k is hydrolic conductivity

$Q = \frac{m^3}{s}$ $\quad A = m^2 \quad$ i , dimensionless

So, $k = m/s$ $\qquad \frac{m^3}{s} = (k) \cdot (m^2)$

$$Q = -k i A$$

$$\frac{Q}{A} = -k i$$

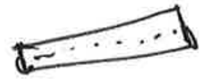
Darcy velocity, q

time to flow through poruse media t_p

$$t_p = \frac{V}{Q} = \frac{(A.L)\theta}{Q}$$ θ → porosity

$$t_p = \frac{\theta AL}{Q}$$

$t_p = \frac{L}{\text{Velocity}}$ for 1 particle of water



$t_p = \frac{\theta A\cancel{L}}{Q} = \frac{\cancel{L}}{\text{Velocity of water particle}}$

seapage velocity
= Velocity of water partce $= \frac{Q}{A\theta}$

$$\boxed{\text{Seapage velocity} = \frac{\text{Darcy Velocity } (q)}{\theta}}$$

$$Q = -k\,i\,A$$

k, hydraulic conductivity = f (Porous media, fluid characteristics) ← -m/s

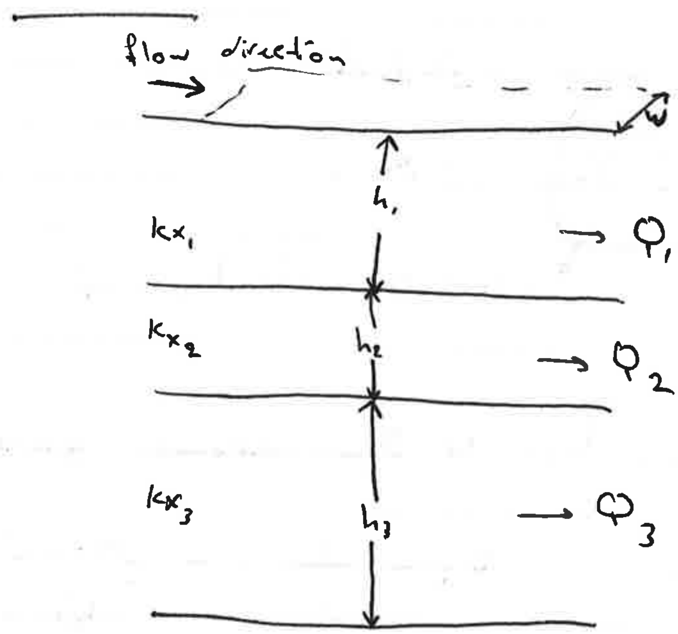
$$k = k\,\boxed{\frac{\rho g}{\mu}}$$

ρ → density; μ → viscosity → fluid characteristics

k → Permeability → Porous media Characteristics

Permeability → Darcies, m^2, cm^2,

Equivalent hydrulic Conductivity



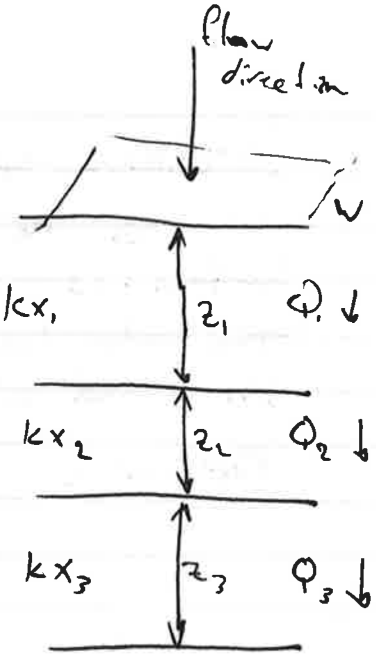
$$(h_1+h_2+h_3) = k_1 h_1 + k_2 h_2 + k_3 h_3$$

$$k_{eq} = \frac{k_1 h_1 + k_2 h_2 + k_3 h_3}{\Sigma h}$$

$$Q = Q_1 + Q_2 + Q_3$$

$$\hookrightarrow k_{eq} \cdot \frac{\Delta h}{L} (h_1+h_2+h_3)\,w$$

$$= k_1 \frac{\Delta h}{L} (h_1)\,w + k_2 \frac{\Delta h}{L} (h_2)\,w + k_3 \frac{\Delta h}{L} (h_3)\,w$$



$$Q = Q_1 + Q_2 + Q_3$$

$$\Delta h = \Delta h_1 + \Delta h_2 + \Delta h_3 \quad \text{—} (1)$$

$$i_1 = \frac{\Delta h_1}{z_1}, \quad i_2 = \frac{\Delta h_2}{z_2}, \quad i_3 = \frac{\Delta h_3}{z_3}$$

$$i = \frac{\Delta h}{(z_1 + z_2 + z_3)}$$

$$Q = k_{eq} \frac{\Delta h}{z_1 + z_2 + z_3} \cdot A$$

$$= k_{eq} \frac{\Delta h_1 + \Delta h_2 + \Delta h_3}{z_1 + z_2 + z_3} \cdot A = k_1 \frac{\Delta h_1}{z_1} \cdot A = k_2 \frac{\Delta h_2}{z_2} \cdot A = k_3 \frac{\Delta h_3}{z_3} \cdot A$$

$$\Delta h_1 = \frac{Q \, z_1}{k_1 \, A}$$

$$\Delta h_2 = \frac{Q \, z_2}{k_2 \, A}, \quad \Delta h_3 = \frac{Q \, z_3}{k_3 \, A}$$

$$\Delta h = \frac{Q \, (z_1 + z_2 + z_3)}{k_{eq} \cdot A} \quad \text{—} (2)$$

$$\frac{(z_1 + z_2 + z_3)}{k_{eq}} = \frac{z_1}{k_1} + \frac{z_2}{k_2} + \frac{z_3}{k_3}$$

$$k_{eq} = \frac{z_1 + z_2 + z_3}{\frac{z_1}{k_1} + \frac{z_2}{k_2} + \frac{z_3}{k_3}}$$

A chlorine spill occurs in the sub surface and quickly makes its way to the gw (ground water). The saturated k of the surface is 1×10^{-3} m/s and an effective porosity = 0.3
The water level at a well near the spill is at an altitude of 310 m and at another well 1.6 km down stream is at 295 m

Determine
- Darcy velocity
- Seapage velocity
- time for the plume to reach the down gradient well

$$i = \frac{15}{1600}$$

$$q = -ki = (1 \times 10^{-3})\left(\frac{15}{1600}\right) = 9.375 \times 10^{-6} \text{ m/s (darcy's velocity)}$$

$$v_{\text{seepage}} = \frac{q}{\theta} = \frac{9.375 \times 10^{-6}}{0.3} = 3.125 \times 10^{-5} \text{ m/s}$$

$$\text{time to travel} = \frac{1600 \text{ m}}{3.125 \times 10^{-5}} = 592.6 \text{ days}$$

$$= 1.6 \text{ years}$$

$k = 1 \times 10^{-2}$ m/s

$\rho = 1000$ kg/m^3

$g = 9.81$ m^2/s

$\mu = 1.3097 \times 10^{-3} \frac{N.S}{m^2}$

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

$$R = \frac{k \mu}{\rho g} = \frac{(1 \times 10^{-2})(1.3097 \times 10^{-3})}{(1000)(9.81} = 1.335 \times 10^{-14} \ m^2$$

Fick's 2nd law

$$\frac{\partial C}{\partial t} = D \frac{d C^2}{d x^2}$$

Example for illustration
no need to write down

BC:

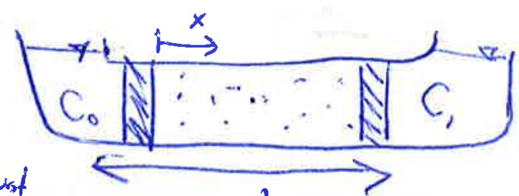
$C = C_0$ $x = 0$ at all t

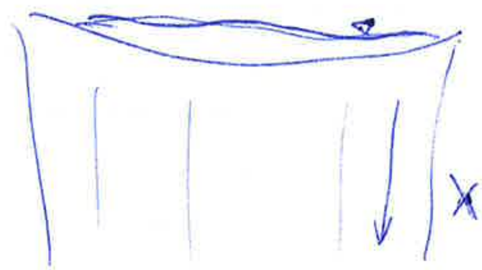
$C = C_1$ $x = \cancel{\ } L$ " " "

$C = 0$ at all x when $t = 0$

2 types of solutions

- Analytical sol. (Exact sol not easy to solve)
- Numerical Sol.

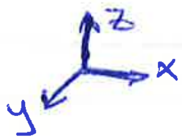




$C = 0$

$X = \infty$

Mass Transport Equation of water



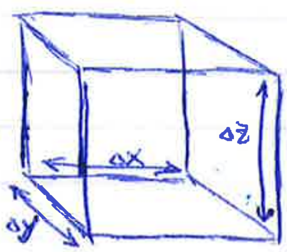
$$\text{Accumulation} = \cancel{\rho V_x} - \left[\rho V_x + \frac{\partial}{\partial x}(\rho V_x)\Delta x\right]$$
$$= -\frac{\partial}{\partial x}(\rho V_x)\Delta x$$

mass flow rate → $M_i = \rho V_x$ (raw: ρ; darcy's velocity: V_x)

$= \rho v$

$= J \cdot A$ (J: mass flux)

$$\left(\frac{kg}{m^3}\cdot\frac{m}{sec}\right) = \frac{kg}{m^3 \cdot sec}$$



$$M_o = \rho V_x + \frac{\partial}{\partial x}(\rho V_x)\Delta x$$

if we consider the area

$$\text{Accumulation} = -\frac{\partial}{\partial x}(\rho V_x)\underbrace{\Delta x \Delta y \Delta z}_{V}$$

$$= -\frac{\partial}{\partial x}(\rho V_x) \cdot V$$

if we consider all three directions

$$\text{Accumulation} = -\left[\frac{\partial}{\partial x}(\rho V_x) + \frac{\partial}{\partial y}(\rho V_y) + \frac{\partial}{\partial z}(\rho V_z)\right] \cdot V$$

Over a time period, Δt,

$$\text{Accumulation} = -\left[\frac{\partial}{\partial x}(\rho V_x) + \frac{\partial}{\partial y}(\rho V_y) + \frac{\partial}{\partial z}(\rho V_z)\right] V \cdot \Delta t$$

$$\frac{1}{m}\cdot\frac{kg}{m^3}\cdot\frac{m}{s}\cdot m^3\cdot s$$

Mass of water in the Cube = $\rho \theta V$
volume (m^3)
Porosity
density (kg/m^3)

Mass of water in the Cube after a time, Δt

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

Accumulation $= \frac{\partial}{\partial t}(\rho . \theta . V)\Delta t$ --- ②

$$\frac{1}{s} \cdot \frac{kg}{m^3} \cdot 1 \cdot m^3 \cdot s$$

Substitute

$$\frac{\partial}{\partial t}(\rho . \theta . V)\Delta t = -\left[\frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial y}(\rho v_y) + \frac{\partial}{\partial z}(\rho v_z)\right] V . \Delta t$$

if V does not change with time ⇒

$$\frac{\partial}{\partial t}(\rho . \theta) = -\left[\frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial y}(\rho v_y) + \frac{\partial}{\partial z}(\rho v_z)\right]$$

$$\rho \frac{\partial \theta}{\partial t} + \theta \frac{\partial \rho}{\partial t} = \rho S_s \frac{\partial h}{\partial t}$$

Specific Storage "S_s" - Volume of water released from a unit volume of aquifer per unit decline in head

$$\rho S_s \frac{\partial \overset{\text{head}}{h}}{\partial t} = -\left[\frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial y}(\rho v_y) + \frac{\partial}{\partial z}(\rho v_z) \right]$$

if ρ does not change with direction

$$S_s \frac{\partial h}{\partial t} = -\left[\frac{\partial}{\partial x}(v_x) + \frac{\partial}{\partial y}(v_y) + \frac{\partial}{\partial z}(v_z) \right]$$

$$v_x = -k_x z = -K_x \frac{\partial h}{\partial x} \quad \Big| \quad v_y = -k_y \frac{dh}{dy} \quad \Big| \quad v_z = -k_z \frac{\partial h}{\partial z}$$

Substituting these,

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

In steady state, $S_s \frac{\partial h}{\partial t} = 0 = \frac{\partial}{\partial x}\left(k_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{dh}{dy}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial h}{\partial z}\right)$

if k_x, k_y & k_z do not change with x

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

For Isotropic or homogeneous Conditions, $k_x = k_y = k_z$

For Isotropic homogeneous Conditions in steady state,

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

Laplace equation

Including a source / sink term

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

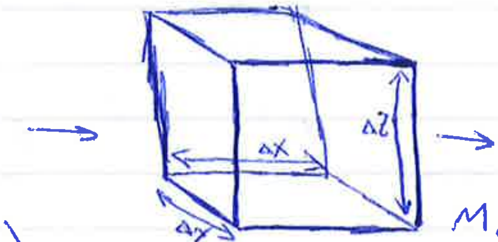
Source / sink

Development of an advective transport equation

M

M_i

$(q.C)$



$$M_o = M + \frac{\partial M}{\partial x}(\Delta x)$$

$$\text{Accumulation} = M - \left\{ M + \frac{\partial M}{\partial x} \cdot \Delta x \right\}$$

$$M = q\,C$$

$$\frac{m^3}{s.m^2} \cdot \frac{mg}{m^3} \quad \frac{mg}{s.m^2}$$

No regeneration / Consumption

$$Acc. = \text{input} - \text{output} = -\frac{\partial}{\partial x}(qC) \cdot \Delta x$$

Including area, $Acc. = -\dfrac{\partial (qc)}{\partial x} \cdot \Delta x \cdot \Delta y \cdot \Delta z$

Amount of Contaminant in the Cube $= \theta \cdot V \cdot C$ mg/m³

Volume of Pores

$$Acc. = \frac{\partial(\theta . V . C)}{\partial t} \cdot \Delta t$$

$$\frac{\partial}{\partial t}(\theta . V . C)\cancel{\Delta t} = -\frac{\partial (qc)}{\partial x} \Delta x \; \Delta y \; \Delta z \cdot \cancel{\Delta t}$$

$$\frac{\partial(\theta . C)}{\partial t} = -\frac{\partial (q\,c)}{\partial x}$$

if porosity does not change with time,

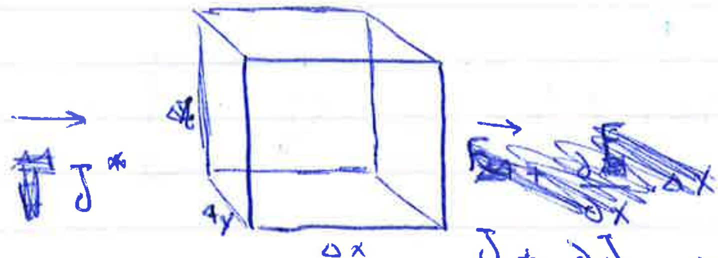
$$\theta \frac{\partial c}{\partial t} = - \frac{\partial (qc)}{\partial x}$$

$$\frac{\partial c}{\partial t} = - \frac{\partial (q/\theta \cdot c)}{\partial x}$$

$$q/\theta = v_{seepage}$$

$$\boxed{\frac{\partial c}{\partial t} = - v_{seepage} \frac{\partial c}{\partial x}}$$ (assuming q does not vary with x)

Dispersive Transport Equation



$J + \frac{\partial J}{\partial x} \cdot \Delta x$

*J instead of μ (same thing)

Acc. = input − output ± regeneration / consumption

Accumulation = $\frac{\partial}{\partial t}(\theta \cdot V \cdot C) \cdot \Delta t$

$$= -\frac{\partial J}{\partial x} \overbrace{\Delta x \cdot \Delta y \cdot \Delta z}^{V} \cdot \Delta t$$

$$\frac{\partial}{\partial t}(\theta \cdot c) = -\frac{\partial J}{\partial x}$$

if we substitute, Fick's 1st law here

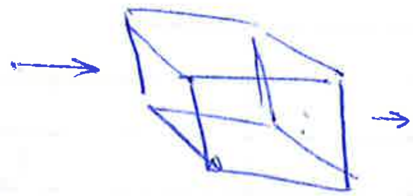
$$J = -D\theta \frac{\partial c}{\partial x}$$

$$\theta \cdot \frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x}$$

$$\theta \cdot \frac{\partial c}{\partial t} = \theta \frac{\partial}{\partial x}\left(D \frac{\partial c}{\partial x}\right) \text{ or } \boxed{\frac{dc}{\partial t} = D \frac{\partial^2 c}{\partial x^2}}$$

if D is not dependent on x

Advective - Dispersive Transport equation

$[qc + J]$  $J + \frac{\partial J}{\partial x} \cdot \Delta x$

$qc + \frac{\partial}{\partial x}(qc)\,\Delta x$

$$acc. = \left[-\frac{\partial J}{\partial x} \cdot \Delta x - \frac{\partial (qc)}{\partial x} \cdot \Delta x \right] \Delta t \cdot \Delta y \cdot \Delta z$$

$$acc = -\frac{\partial J}{\partial x} V \cdot \Delta t - \frac{\partial (qc)}{\partial x} V \cdot \Delta t \quad \text{— (1)}$$

$$acc = \frac{\partial (c \cdot V \cdot \theta)}{\partial t} \quad \text{— (2)}$$

$$\cancel{\frac{\partial (c.V.\theta)}{\partial t} \cdot \Delta t = \frac{\partial (c.V.\theta)}{\partial t}}$$

$$\frac{\partial (c \cdot V \cdot \theta)}{\partial t} \cdot \Delta t = -\frac{\partial J}{\partial x} V \cdot \Delta t - \frac{\partial (qc)}{\partial x} V \cdot \Delta t$$

V is constant

Fick's 1st law

$$J = -D \frac{\partial c}{\partial x} \theta \rightarrow \frac{\partial c\,\theta}{\partial t} \cdot \cancel{\Delta t} = -\frac{\partial qc}{\partial x} \cancel{\Delta t} - \frac{\partial}{\partial x}\left(-D_x \frac{\partial c}{\partial x}\right) \cdot \Delta t\, \theta$$

θ constant

divide by θ $\rightarrow$

$$\boxed{\frac{\partial c}{\partial t} = -\nu_x \frac{\partial c}{\partial x} + D_x \frac{\partial^2 c}{\partial x^2}}$$

ν_x ↳ seepage velocity

$$\frac{\partial c}{\partial t} = -\nu_x \frac{\partial c}{\partial x} + D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + D_z \frac{\partial^2 c}{\partial z^2}$$

3 direction

Adding a Source / sink term

$$\frac{\partial c}{\partial t} = -V_x \frac{\partial c}{\partial x} + \frac{\partial}{\partial x}\left(D_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial c}{\partial z}\right) \pm \frac{q_s C_s}{\theta}$$

Source / Sink

q_s is the volumetric flow rate per unit aquifer volume

$$, \; q_s = \frac{Q}{\Delta x \Delta y \Delta z}$$

Adsorption

2 theories

monolayer

→ langmuir's adsorption Isotherm ~~principle~~

– Freundlichi

multilayer

$$S = k_d C^n$$

adsorption

langmuir constant

$$S = \frac{k_\ell \cdot \bar{S} C}{1 + k_\ell C}$$

max. amount that can be adsorbed

$$\frac{ds}{dc} = \frac{k_1 \bar{S} (1 + \cancel{k_\ell C}) - \cancel{k_\ell (k_1 \bar{S} C)}}{(1 + k_\ell C)^2} = \frac{k_\ell \bar{S}}{(1 + k_\ell c)^2}$$

when $C \to \infty$, $\frac{ds}{dc} \to 0$

$$S = \frac{k_\ell \bar{S} C}{1 + k_\ell C}$$

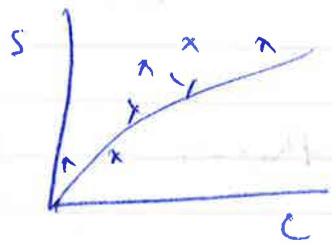
$$\frac{1}{S} = \frac{1}{k_\ell \bar{S} C} + \cancel{\frac{k_\ell C}{k_\ell \bar{S} C}}$$

$$\frac{1}{S} = \frac{1}{k_\ell \bar{S} C} + \frac{1}{\bar{S}}$$

when $C \to \infty$ $\quad \frac{1}{S} = \frac{1}{\bar{S}}$ or $S \to \bar{S}$

GMS Software

To compare which theory is better



For Langmuir

Plot $\frac{1}{S}$ vs. $\frac{1}{C}$

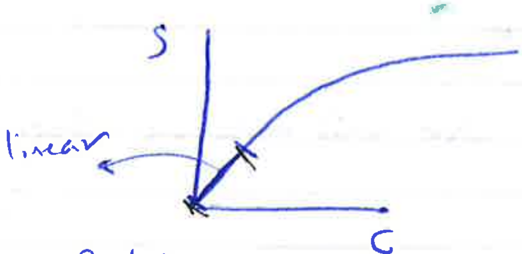
for Freundlich: $S = k_d C^n$

plot

$\ln S = \ln k_d + n \ln C$

$\ln S$ v. $\ln C$

the one that ~~has~~ closer to a perfect straight line is better



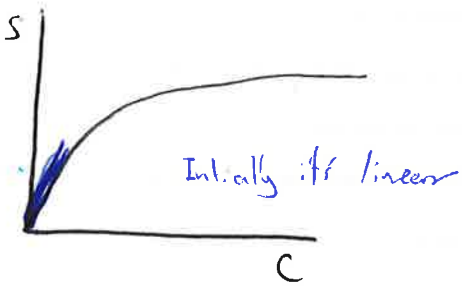
if taking only this part $S = k_d C$

29-Sep-2014

Adsorbtion & Absobtion if you are confused call it <u>Sorbtion</u>

Freundlich's Isotherm $S = K_F C^n$

Langmuir's Isotherm $S = \dfrac{K_L \bar{X} C}{1 + K_L C}$



if you take the first part

$S = K_d \cdot C$

mass / Vol

distribution coefficient

1 / mass

$\underline{S}$ is amount adsorbed per unit mass of soil

$$S = K_d \cdot C$$

$$\frac{dS}{dt} = K_d \cdot \frac{dC}{dt}$$

if adsorbtion is happening in the control volume, $\Delta x \Delta y \Delta z$, then the rate of adsorbtion $= \rho_b \cdot (\Delta x \Delta y \Delta z) \dfrac{dS}{dt}$

bulk density, or dry density

$$\frac{\text{kg of soil}}{\text{Vol. of soil}} \times \text{Vol. of soil} \left[\frac{\text{amount adsorbed}}{\text{mass of soil}}\right] \frac{1}{\text{time}}$$

$$\rho_b \cdot (\Delta x \Delta y \Delta z) \frac{dS}{dt} = \rho_b \cdot V \cdot \frac{dS}{dt} = \rho_b \cdot V \cdot K_d \frac{dC}{dt}$$

, if Contaminant is disolved in water and the water is moving with speed of v the the Contaminant is moving in a velocity of $v \cdot R$

if sorbing happens → contaminant is slower than non-sorbing

$$\theta \frac{dc}{\partial t} = -\frac{\partial (qc)}{\partial x} + \theta \left[\left(\frac{\partial}{\partial x} D_x \frac{\partial c}{\partial x} \right) + \left(\frac{\partial}{\partial y} D_y \frac{\partial c}{\partial y} \right) + \left(\frac{\partial}{\partial z} D_z \frac{dc}{dz} \right) \right] + q_s C_s - \rho_b k_d \frac{\partial c}{\partial t}$$

$$\frac{\partial c}{\partial t} = -\frac{\partial \left(\frac{q}{\theta} c \right)}{\partial x} + \left[\left(\frac{\partial}{\partial x} D_x \frac{\partial c}{\partial x} \right) + \left(\frac{\partial}{\partial y} D_y \frac{\partial c}{\partial y} \right) + \left(\frac{\partial}{\partial z} D_z \frac{\partial c}{\partial z} \right) \right] + \frac{q_s C_s}{\theta} - \frac{\rho_b k_d}{\theta} \frac{\partial c}{\partial t}$$

R

$$\boxed{\left(1 + \frac{\rho_b k_d}{\theta} \right)} \frac{\partial c}{\partial t} = -\frac{\partial (vc)}{\partial x} + \left[\left(\frac{\partial}{\partial x} D_x \frac{\partial c}{\partial x} \right) + \left(\frac{\partial}{\partial y} D_y \frac{dc}{\partial y} \right) + \left(\frac{\partial}{\partial z} D_z \frac{\partial c}{\partial z} \right) \right] + \frac{q_s C_s}{\theta}$$

$$\frac{\partial c}{\partial t} = -\frac{1}{R} \frac{d (vc)}{dx} + \frac{1}{R} \left[\left(\frac{\partial}{\partial x} D_x \frac{\partial c}{\partial x} \right) + \left(\frac{\partial}{\partial y} D_y \frac{\partial c}{\partial y} \right) + \left(\frac{\partial}{\partial z} D_z \frac{\partial c}{\partial z} \right) \right]$$

$$R = 1 + \frac{k_d \rho_b}{\theta} \geq 1$$

if contaminant is non-adsorbing, then $k_d \simeq 0$, $R = 1$

" " " adsorbing, then $k_d > 0$, $R > 1$

adsorbtion make contaminent velocity slower

Dispersim

Mechanical dispersion

Diffusion

A combination of mechanical dispersion & molecular diffusion is termed as **hydrodynamic dispersion**

Coefficient of longitudinal mechanical dispersion = $\alpha_i \, v_i$

seapage velocity

longitudinal dispersivity

Coefficent of tranverse mechanical dispersion = $\alpha_j \, v_i$

transverse dispersivity

ynamic
n
al)

longitudinal mechanical dispersion

$$D_L = \alpha_L v_i + D^*$$

diffusion Coefficent

$$D_T = \alpha_j v_i + D^*$$

when velocity is zero $(v_i = 0) \Rightarrow D_L = D^*$

$D_T = D^*$

Peclet Number

dimenssionless

- ratio between advective transport versus dispersive transport

$$P_e = \frac{v_i L}{D_L} = \frac{(m/s)(m)}{(m^2/s)} = \text{dimensionless}$$

$P_e > 10$ ignore dispersive transport

An underground storage tank leaks benzene into subsurface. The hydrolic conductivity of the aquifer is 0.03 cm/s. It has a porosity of 0.3 and temperature of 20°C. The longitudinal dispersivity is 2 m. Determine the relative importance of mechanical disperssion compared to diffusion when the hydrolic gradient is 0.001

assumed factor

Mol. diffusion ~~coef~~ f. of benzene is $1 * 10^{-6}$ cm²/s

Sol

Effective diffusion Coeff = (0.65) (1×10^{-6} cm²/s)

$$v_i = \frac{q}{\theta} = \frac{ki}{\theta} = \frac{0.03 \text{ cm/s} \times 0.001}{0.3}$$

$$= \frac{\cancel{3} \times 10^{-2} \times 10^{-3}}{\cancel{3} \times 10^{-1}} = 10^{-4}$$

$$\text{Ratio} = \frac{v_i * \alpha_i}{D} = \frac{10^{-4} \text{ (cm/s)} \times 2 \text{ m}}{0.65 \times 10^{-6} \text{ cm}^2/\text{s}} \times \frac{100 \text{ cm}}{1 \text{ m}}$$

$$= \frac{10^{-4} * 2 * 10^{2}}{0.65 \times 10^{-6}} = \frac{2}{0.65} \times 10^{4}$$

A Continuous leak of a degradable Solute occurs from an UG (under ground) storage tank. Assuming 1 D (dimension) no dispersion mass transport equation derive the equation for Concentration gradient in steady state (assume 1st order decay)

$A + B \rightarrow D$

$\frac{dA}{dt} = k[A][B]$

$\frac{dc}{dt} = -k$ (0 order)

$\frac{dc}{dt} = -kc$ (1 order)

Sol

$$\frac{\partial c}{\partial t} = -v \frac{dc}{\partial x} + D \frac{d^2 c}{\partial x^2} - kc$$

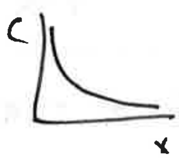
$$\frac{\partial c}{\partial t} = 0 \quad ; \quad D \approx 0$$

$$v \frac{dc}{\partial x} = -kc$$

$$\int_{C_0}^{C} \frac{dc}{c} = -\int_0^x \frac{k}{v}\, dx$$

$$\ln C - \ln C_0 = -\frac{kx}{v}$$

or $\boxed{C = C_0 e^{-\frac{kx}{v}}}$



$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - kc$$ standard Dispersive - advective eq.

in steady state, $\frac{\partial c}{\partial t} = 0$

~~BC are~~

BC are : $C = C_0$ when $x = 0$

$\frac{\partial c}{\partial x} = 0$ when : $x \to \infty$

$$D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - kC = 0$$

Assume a Solution, $C = Ae^{mx}$

then $\frac{\partial c}{\partial x} = Ame^{mx}$

$\frac{\partial^2 c}{\partial x^2} = Am^2 e^{mx}$

Substitute in the equation

$$D\{Am^2 e^{mx}\} - v\{Ame^{mx}\} - kAe^{mx} = 0$$

$$Ae^{mx}\{Dm^2 - vm - k\} = 0$$

As $Ae^{mx} \neq 0$, therfore $Dm^2 - vm - k = 0$

$$m_{1,2} = \frac{v \pm \sqrt{v^2 + 4kD}}{2D}$$

if we write $\sqrt{v^2 + 4kD} = P$ $\Rightarrow$ $m_{1,2} = \frac{v \pm P}{2D}$

We know that $P \geq v$

$$m_1 = \frac{v - P}{2D} \quad ; \quad m_1 < 0$$

$$m_2 = \frac{v + P}{2D} \quad ; \quad m_2 > 0$$

$$C = C_1 A e^{m_1 x} + C_2 A e^{m_2 x} \quad *$$

$C_1 \qquad C_2$

C_1, C_2 are constants

* Differensial equations general solution

Implementing the BC

$$\boxed{C_0 = C_1 + C_2} \text{ — } ①$$

very small — very large

$$\frac{dc}{dx} = C_1 m_1 e^{m_1 x} + C_2 m_2 e^{m_2 x}$$

when $x \to \infty$

Ignore the V. small number

$$0 = C_2 m_2 e^{m_2 x}$$

$$\therefore \boxed{C_2 = 0} \text{ — } ②$$

$$C_0 = C_1$$

Substituting

$$C = C_1 e^{m_1 x} + C_2 e^{m_2 x}$$

$$C = C_0 e^{\left[\frac{v-P}{2D}\right]}$$

Practice Problem

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - kC$$

In steady state, $\frac{\partial C}{\partial t} = 0$

BC are $C = 0$ when $x = 0$

$\frac{\partial C}{\partial x} = 0$ when $x \rightarrow \infty$

Sol

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - kC$$

$$0 = D \frac{\partial^2 C}{\partial x^2} - kC$$

assume a solution, $C = Ae^{mx}$

$$\frac{\partial C}{\partial x} = Ame^{mx}$$

$$\frac{\partial^2 C}{\partial x^2} = Am^2 e^{mx}$$

$$DAm^2 e^{mx} - kAe^{mx} = 0$$

$$Ae^{mx}\left[Dm^2 - k\right] = 0$$

$Ae^{mx} \neq 0$ so $Dm^2 - k = 0$

$$m = \mp\sqrt{\frac{k}{D}}$$

$m_1 = -\sqrt{\frac{k}{D}}$ $m_1 < 0$

$m_2 = \sqrt{\frac{k}{D}}$ $m_2 > 0$

$$C = C_1 e^{m_1 x} + C_2 e^{m_2 x}$$

Implement BC1 $x = 0,\ C = C_0$

$$C_0 = C_1 + C_2$$

BC2 $x \to \infty,\ \frac{dC}{dx} = 0$

$$\frac{dc}{dx} = C_1 m_1 e^{m_1 x} + C_2 m_2 e^{m_2 x}$$

$$0 = C_2 m_2 e^{m_1 x}$$

$$C_2 = 0$$

$$C_0 = C_1$$

$$C = C_0 e^{-\sqrt{k/D}\, x}$$ [illegible]

---

flow gorned by h ملاحظة

transport governd by C

Solve for flow first to get ν

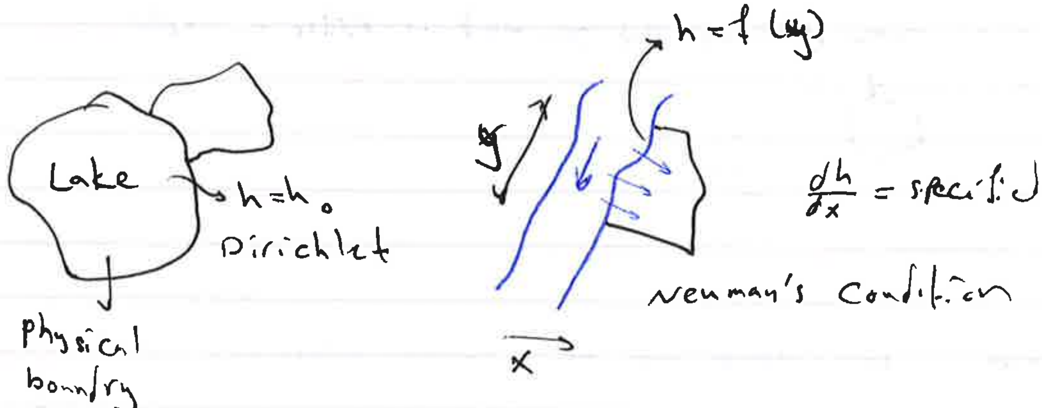
then you will be able to solve for transport

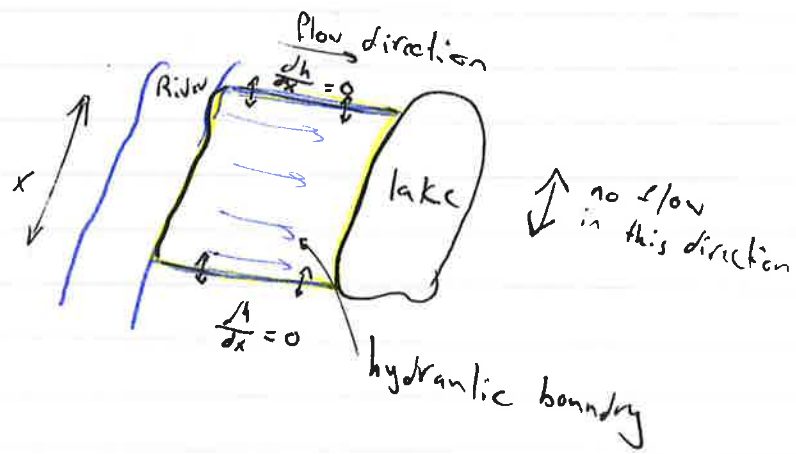
Three types of boundry Condition we Can have (for flow)

- Dirichlet's Condition $C = C_0$, $h = h_0$

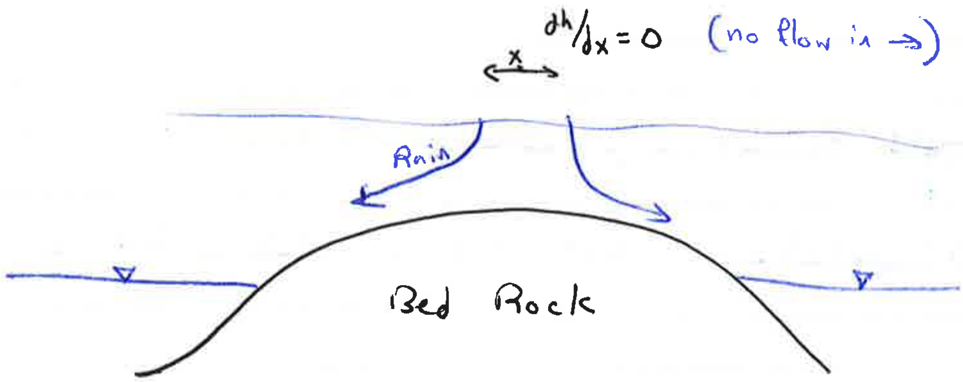
- Neuman's Condition, $\frac{dc}{dx}$ = specified, $\frac{dh}{dx}$ = specified

- Cauchy's Condition $vc + D\frac{dc}{dx}$ = specified (mixed BC)

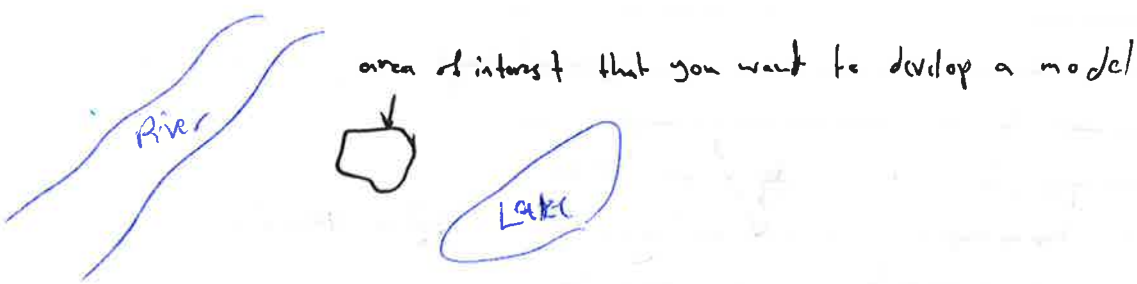




you want to avoid hydraulic boundry



ground water
divide



to solve you look at the entire physical BC and then focus on yours (telescopic method)

Back to adsorption

$$S = k_d C$$

$k_d = k_{oc} \cdot f_{oc}$ (valid if we have hydrophobic material and not high ~~content of~~ f_{oc}

f_{oc} ← organic carbon fraction

k_{oc} ← organic carbon coeff.

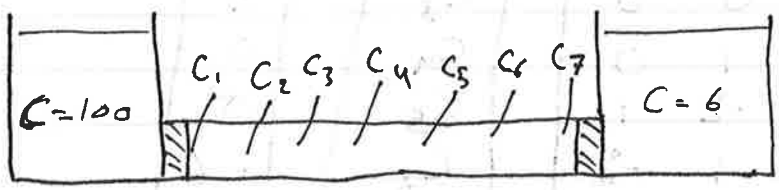
k_{oc} is a function of k_{ow} (octanol.water partition coefficient)

" " " " Solubility

if we know the relationship between

Nov 15 _ Sat

One - D diffusion problem



Fixed Concentrations in the containers

diffusion equation

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

in steady state , $\frac{\partial C}{\partial t} = 0$

$$D \frac{\partial^2 C}{\partial x^2} = 0$$

$$\frac{C_{i+1} - 2C_i + C_{i-1}}{(\Delta x)^2} = 0$$

$i = 2$

$$C_3 - 2C_2 + C_1 = 0 \rightarrow C_3 - 2C_2 + 100 = 0$$

$i = 3$

$$C_4 - 2C_3 + C_2 = 0 \rightarrow C_4 - 2C_3 + C_2 = 0$$

$i = 4$

$$C_5 - 2C_4 + C_3 = 0 \rightarrow C_5 - 2C_4 + C_3 = 0$$

$i = 5$

$$C_6 - 2C_5 + C_4 = 0 \rightarrow C_6 - 2C_5 + C_4 = 0$$

$i = 6$

$$C_7 - 2C_6 + C_5 = 0 \rightarrow \cancel{C_7}\,6 - 2C_6 + C_5 = 0$$

In matrix form

$$\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \end{bmatrix} \begin{bmatrix} -100 \\ 0 \\ 0 \\ 0 \\ -6 \end{bmatrix}$$

$$[a_{ij}][X] = [b]$$

we have 2 families of solutions

- direct methods
  - matrex invertion
  - Gos: elemention
- Indirect method
  - Jacobi
  - Gauss Seidal
  - SOR

$R_1 = -100 - C_3 + 2C_2$

$R_2 = 2C_3 - C_2 - C_4$

$R_3 = 2C_4 - C_3 - C_5$

$R_4 = -C_4 + 2C_5 - C_6$

$R_5 = -C_5 + 2C_6 - 6$

$$X_i^{(k+1)} = X_i^{(k)} + \frac{R_i^{(k)}}{a_{ij}}$$

$$R_i^{(k)} = b_i - \sum_{j=1}^{n} a_{ij} \, x_j^{(k)}$$

Book by Holman
for indirect methods

Linear variation

$$\begin{cases} C_1 = 100 \\ C_2 = 85 \\ C_3 = 70 \\ C_4 = 55 \\ C_5 = 40 \\ C_6 = 25 \\ C_7 = 6 \end{cases}$$

$$C_2^{(2)} = C_2^{(1)} + \left(\frac{1}{-2}\right)\left\{-100 - 70 + (85)2\right\} = 85$$

$$C_3^{(2)} = C_3^{(1)} + \left(-\frac{1}{2}\right)\left\{2(70) - 85 - 55\right\} = 70$$

$$C_4^{(2)} = 55$$

$$C_5^{(2)} = 40$$

$$C_6^{(1)} + \left(\frac{-1}{a_{ii} \to 2}\right)\left[\overbrace{-6 - C_5^{(1)} + 2C_6^{(1)}}^{-6-40+2(25)}\right]$$

$$C_6^{(2)} = 25 + \left(\frac{-1}{2}\right)(40) = 23$$

Next iteration

* Jacobi method does not update the values for variables within the same iteration

$$C_2^{(3)} = 85$$

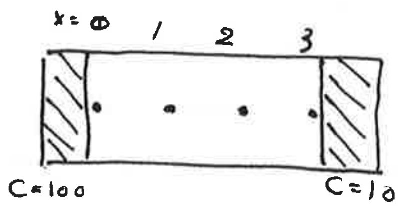
$$C_3^{(3)} = 70$$

$$C_4^{(3)} = 55$$

$$C_5^{(3)} = 40 + \left(\frac{-1}{2}\right)\left\{2(40) - 55 - 13\right\} = 39$$

$$C_6^{(3)} = 25 + \left(-\frac{1}{2}\right)\left\{2(23) - 40 - 6\right\} = 25$$

this is Jacobi method



$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

unsteady state diffusion equation

$$\frac{\partial^2 c}{\partial x^2} = \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2}$$

time dimension

$$\frac{C_i^{n+1} - C_i^{n}}{\Delta t} = \frac{D}{\Delta x^2}\left\{ C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n} \right\}$$

bc
$$\begin{cases} C(0,t) = 100 \\ C(L,t) = 10 \\ C(x,0) = 0 \end{cases}$$

when $x=0$ and $t=t$, $C=100$
when $x=L$ and $t=t$, $C=10$
when $x=x$ and $t=0$, $C=0$ (initial condition)

A way to develop your initial condition, you can ~~run~~ solve for steady state first to get the initial condition and then move to transient state..

$$C_i^{n+1} = \frac{D\Delta t}{\Delta x^2}\left\{ C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n} \right\} + C_i^{n}$$

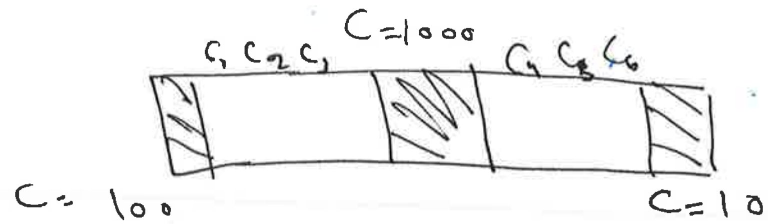
if
$$\frac{D\Delta t}{(\Delta x)^2} = \alpha$$

$$C_i^{n+1} = \alpha C_{i+1}^{n} - (2\alpha - 1) C_i^{n} + \alpha C_{i-1}^{n}$$

$i = 1$

$$C_1^{2} = \alpha C_2^{1} - (2\alpha - 1) C_1^{1} + \alpha C_0^{1}$$

Explicit Method



← Final Exam question

if $\alpha = 0.25$

$$C_1^2 = 0.25\ C_2^1 + 0.5\ C_1^1 + 0.25\ C_0^1$$

$$= (0.25)(0) + 0 + (0.25)(100) = 25$$

$$C_1^2 = 25$$

$$C_2^2 = 0.25\ C_3^1 + 0.5\ C_2^1 + 0.25\ C_1^1$$

$$= 0.25(10) + 0 + 0$$
$$= 2.5$$

Explicit method is stable & Convergent if $\Delta t \leq \frac{\Delta x}{2D}$

or $\lambda = \frac{D\Delta t}{\Delta x^2} \leq 1/2$

if $\lambda \leq 1/4$, then solution does not oscillate

D for cl $= 2\times10^{-6}$ cm^2/s

$\Delta x = 0.01$ m (recomended)

$$\Delta t \leq \frac{(0.01)^2}{2\times2\times10^{-6}}$$

$$\leq \frac{1}{4}\times10^{-2}$$

$$\leq 25 \text{ sec}$$

Δx will determine Δt when you assume it

Implicit method (for the same Problem)

$$\frac{C_i^{(n+1)} - C_i^{n}}{\Delta t} = \frac{D}{\Delta x^2}\left[C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}\right]$$

$$C_i^{n+1} - C_i^{n} = \left[\alpha C_{i+1}^{n+1} - 2\alpha C_i^{n+1} + 2 C_{i-1}^{n+1}\right]$$

$$\boxed{-\alpha C_{i+1}^{n+1} + (1+2\alpha) C_i^{n+1} - \alpha C_{i-1}^{n+1} = C_i^{n}}$$

the only known

$n=0$, $i=1$, $\alpha = 0.25$

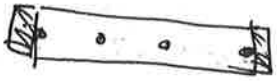
$$-0.25\, C_2^1 + 1.5\, C_1^1 - \underbrace{0.25\, C_0^1}_{=25} = \underbrace{C_1^0}_{=0}$$

$n=0$, $i=2$

$$\underbrace{-0.25\, C_3^1}_{=-2.5} + 1.5\, C_2^1 - 0.25\, C_1^1 = \underbrace{C_2^0}_{=0}$$

$$\begin{pmatrix} 1.5 & -0.25 \\ -0.25 & 1.5 \end{pmatrix}\begin{pmatrix} C_1^1 \\ C_2^1 \end{pmatrix} = \begin{pmatrix} 25 \\ 2.5 \end{pmatrix}$$

Solve for C_1^1 & C_2^1



after solving for C_1^1 & C_2^1 we can repeat for the next

Crank - Nicolson Method (more accurate than Implicit & Explicit)

$$\frac{\partial C}{\partial t} = \left.\frac{C_i^{n+1} - C_i^{n}}{\Delta t}\right|_{n+\frac{1}{2}}$$

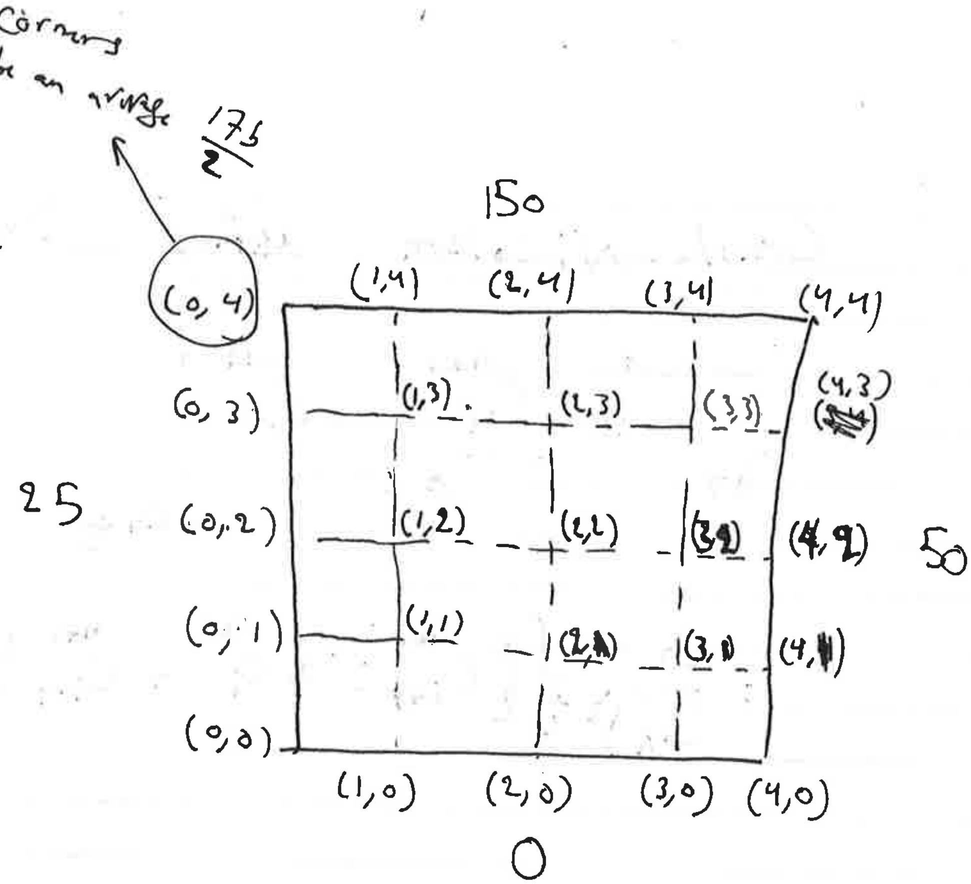
$$= \frac{D}{(\Delta x)^2}\frac{1}{2}\left[\left\{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}\right\} + \left\{C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n}\right\}\right]$$

$$C_i^{n+1} - C_i^{n} = \frac{\alpha}{2}\left[\left\{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}\right\} + \left\{C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n}\right\}\right]$$

$$\alpha = \frac{D\Delta t}{(\Delta x)^2}$$

You can solve it using the same techniques from the implicit method)

2-D steady state



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

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} = 0$$

if $\Delta x = \Delta y$

$$T_{i+1,j} - 4T_{ij} + T_{i-1,j} + \cancel{T_{i-1,j}} + T_{i,j+1} + T_{i,j-1} = 0$$

For node (1,1)

$$T_{2,1} - 4T_{1,1} + T_{0,1} + T_{1,2} + T_{1,0} = 0$$

For node (1,2)

$$T_{2,2} - 4T_{1,2} + T_{0,2} + T_{1,3} + T_{1,1} = 0$$

* you can only do the 9 middle node because if you take the outsid one you get th. $j+1 = 5$ outside the boundry

For node (1, 3)

$$T_{2,3} - 4T_{1,3} + T_{0,3} + T_{1,4} + T_{1,2} = 0$$

for node (2,1)

$$T_{3,1} - 4T_{2,1} + T_{1,1} + T_{2,2} + T_{2,0} = 0$$

Revision with Class

$\frac{dc}{dx} = 5 \frac{mg}{L} \cdot \frac{1}{m}$

$$\frac{C_i^{n+1} - C_i^{n}}{\Delta t} = \frac{D}{\Delta X^2}\left[C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}\right] - k\, C_i^{n+1}$$

$$0 = C_i^{n} - 10.43\, C_i^{n+1} + 3.456\, C_{i+1}^{n+1} + 3.456\, C_{i-1}^{n+1}$$

node 1:

$$1428 = 10.43\, C_1^1 - 3.456\, C_2^1$$

node 2:

$$100 = 10.43\, C_2^1 - 3.456\, C_3^1 - 3.456\, C_1^1$$

node 3:

$$100 = 10.43\, C_3^1 - 3.456\left(C_4^1\right) - 3.456\, C_2^1$$

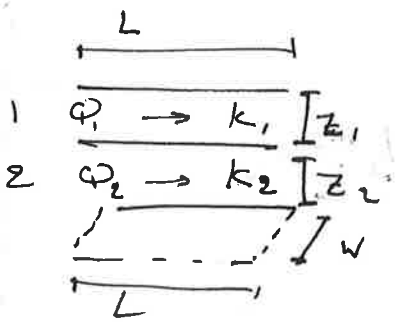
$$3.456\left(10\, C_2^1\right) = -34.56 - 3.456\, C_2^1$$

$$134.56 = 10.43\, C_3^1 - 6.912\, C_2^1$$

@ node 3 know dc/dx

by finite (central) difference

$$\frac{\partial C}{\partial x} = \frac{C_{i+1} - C_{i-1}}{2\Delta X} = 5 = \frac{C_4^1 - C_2^1}{2} \Rightarrow \underbrace{C_4^1 = 10 + C_2^1}_{\text{all times}}$$



find k_{eq} $\quad Q_T = Q_1 + Q_2$

$$Q = K\,i\,A \qquad i = \frac{h}{L}$$

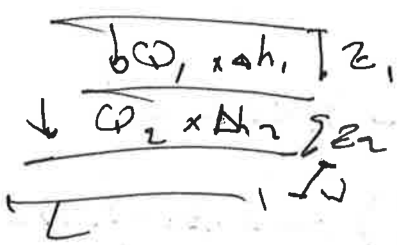
$$Q_1 = k_1 \frac{\Delta h}{L} \cdot w \cdot z_1$$

$$Q_2 = k_2 \frac{\Delta h}{L} \cdot w \cdot z_2$$

$$Q_T = k_{eq} \frac{\Delta h}{L} \cdot w \cdot (z_1 + z_2)$$

$$Q_T = Q_1 + Q_2$$

$$k_{eq} \frac{\Delta h}{L} w (z_1 + z_2)$$



$$Q_T = Q_1 = Q_2$$

$$\Delta h_T = \Delta h_1 + \Delta h_2$$

$$Q_T = k_{eq} \frac{\Delta h_T}{L} w (z_1 + z_2) \Rightarrow$$

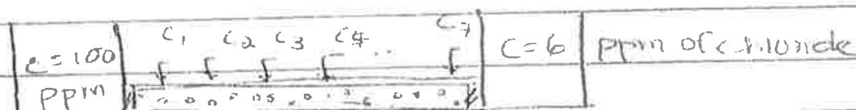
$$\Delta h_T = \frac{Q}{k_{eq}(z_1 + z_2)}$$

$$Q_1 = k_1 \frac{\Delta h_1}{L} w (z_1) \Rightarrow \Delta h_1 = \frac{Q}{k_1 z_1}$$

$$Q_2 = k_2 \frac{\Delta h_2}{L} w (z_2) \Rightarrow \Delta h_2 = \frac{Q}{k_2 z_2}$$

How to apply such Concepts to our Mass Transport problems :

(x) One-D diffusion problem.



of chloride

Steady state Conditions - how does chloride move from the Constant C of 100 to Constant C of 6 :

$$\frac{\partial c}{\partial t} = -D\frac{\partial^2 c}{\partial x^2} \xrightarrow[\text{Steady-State}]{} \frac{\partial c}{\partial t} = 0 \Rightarrow D\frac{\partial^2 c}{\partial x^2} = 0$$

$$\frac{C_{i+1} - 2C_i + C_{i-1}}{(\Delta x)^2} = 0$$

(if we put i=1, we have a C_{i-1} term, that's why we would need C_0, and C_0 should be defined)

$i = 2$: $C_3 - 2C_2 + C_1 = 0 \Rightarrow C_3 - 2C_2 + 100 = 0$

$i = 3$: $C_4 - 2C_3 + C_2 = 0 \Rightarrow C_4 - 2C_3 + C_2 = 0$

$i = 4$: $C_5 - 2C_4 + C_3 = 0 \Rightarrow C_5 - 2C_4 + C_3 = 0$

$i = 5$: $C_6 - 2C_5 + C_4 = 0 \Rightarrow C_6 - 2C_5 + C_4 = 0$

$i = 6$: $C_7 - 2C_6 + C_5 = 0 \Rightarrow 6 - 2C_6 + C_5 = 0$

(5 equations, 5 unknowns)

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \end{pmatrix} = \begin{pmatrix} -100 \\ 0 \\ 0 \\ 0 \\ -6 \end{pmatrix}$$

How to solve the matrix?

- Direct methods → Gaussian Elimination
  - → Matrix Inversion
- Indirect methods → Jacobian
  - → Gauss Seidel
  - → SOR

Direct methods are very cumbersome you can solve 2/3 equations by hand, ~~By~~ you can push your computer to solving 7, 8 But they're generally more computationally intensive.

So, it you have the precise value, you plug it into ~~the~~ each of the eq. you'll get zero but indirect methods work in a way that you assume a value and it's not precise, so you'll get a remainder and then they work in such a way that the remainder (error) is zero (minimized)

① Jacobian.

$R_1 = -100 - C_3 + 2C_2$
$R_2 = 2C_2 - C_2 + C_4$
$R_3 = 2C_4 - C_3 + C_5$
$R_4 = -C_4 + 2C_5 - C_6$
$R_5 = -C_5 + 2C_6 - 6$
$R_6 = -6 + C_5 + 2C_6$

you make the whole calc and once you're done, you start from the top for the second iteration.

② Gauss Seidel

Make an assumption for x, find out R (error):
Advantage is you can correct your assumption in each step, Don't have to go thru the whole calc

$$x_i^{(k+1)} = x_i^{(k)} + R_i^{(k)} / a_{ii}$$
$$R_i^{(k)} = b_i - \sum_{j=1}^{n} a_{ij} \times x_j^{(k)}$$

To solve our problem:
linear variation:
Assume $\underline{\underline{C_1 = 100}}$ $C_2 = 85$ $C_3 = 70$ $C_4 = 55$ $C_5 = 40$ $C_6 = 25$ $\underline{\underline{C_7 = 6}}$

$$C_2^{(2)} = C_2^{(1)} + \left(\frac{1}{-2}\right)_{a_{ii}} \left[-100 - 70 + (85)2\right] = 85$$

$$C_3^{(2)} = C_3^{(1)} + \left(\frac{1}{-2}\right)\left[2(70) - 85 - 55\right] = 70$$

$$C_4^{(2)} = C_4^{(1)} + \left(\frac{1}{-2}\right)\left[-55 + 2(40) - 25\right] = 55$$

$$C_5^{(2)} = 40$$

$$C_6^{(2)} = 25 + (-1/2)(40) = 23$$

Next iteration.

$$C_2^{(3)} = 85$$

$$C_3^{(3)} = 70$$

$$C_4^{(3)} = 55$$

$$C_5^{(3)} = 40 + \left(\frac{-1}{2}\right)\left[-40 + 2(23) - 6\right] = 39$$

$$C_6^{(3)} = 6 + \left(\frac{1}{2}\right)\left[-6 - 40 + 2(23)\right] = 6$$

you don't use the last iteration value which is 39, you use the initial value, which is 40.

But for Gauss Seidel, we use the last value that u have.

Back to our unsteady state problem: $\frac{\partial c}{\partial t} = \frac{D\partial^2 c}{\partial x^2}$

Change in Conc. in time step (n)

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \frac{D}{\Delta x^2}\left(C_{i+1}^n - 2C_i^n + C_{i-1}^n\right)$$ using conc @ the same time step

super script (n) shows that the term is written for time (n)

subscripts indicate space dimensions

$C(x, 0) = 0$ → initial conc.

$C(0, t) = 100$ → constant conc @ all times @ point

$C(L, t) = 10$, →

you need an initial condition for time, and it is very imp to set that, cause it's the point from which you start marching in time and remember

Sometimes your problem doesn't give you an initial condition - you can solve your problem for ~~un~~steady then move to transient conditions (Nothing is going to put a stress on your system) That will be your initial condition.

$$C_i^{(n+1)} = \frac{D\Delta t}{\Delta x^2}\left\{ C_{i+1}^{(n)} - 2C_i^{(n)} + C_{i-1}^{(n)} \right\} + C_i^{n}$$

if : $\frac{D(\Delta t)}{\Delta x^2} = \alpha \Rightarrow C_i^{n+1} = \left\{ \alpha C_{i+1}^{n} - (2\alpha - 1) C_i^{n} + \alpha C_{i-1}^{n} \right.$

$i = 1$ (you have C_0 here so $i-1$ will be fine)

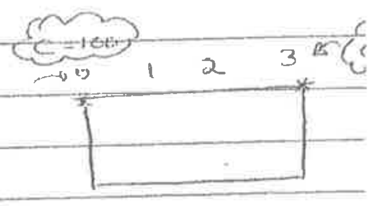
$C_1^2 = \alpha C_2^1 - (2\alpha - 1) C_1^1 + \alpha C_0^1$ if $\alpha = 0.25 \rightarrow$

$C_1^2 = 0.25 C_2^1 + 0.5 C_1^1 + 0.25 C_0^1$

at time ① ~~everything~~ is zero, remember your initial condi

$\Rightarrow C_1^2 = 0 + 0 + 0.25(100) = 25$

still @ time step ② write conc. @ spaces ②, ③, ...



$C_2^2 = \alpha C_3^1 - (2\alpha - 1) C_2^1 + \alpha C_1$

$C_2^2 = 0.25 C_3^1 + 0.5 C_2^1 + 0.25(10)$

$C_2^2 = 2.5$

$C_3^2 = 0.25 C_3^1 + 0.5 C_2^1 + 0.25 C_1^1 \Rightarrow C_3$ @ anytime

points	time ①	②	③	④
0	100	100	100	100
1	0	25		
2	0	2.5		
3	10	10	10	10

$C_1^3 = 0.25 C_2^2 + 0.5 C_1^2 + 0.25 C_0^2 = 0.25(2.5) + 0.5(25) + 0.2$

$C_1^3 = 38.125$ and so forth

α can be calculated directly from your values for D_{ce}, x^*/c

Δx (in the column defined as) = 1 cm

and Δt can be defined as:

Explicit method is stable and convergent @ $\left(\Delta t \le \frac{\Delta x^2}{2D} \right)$

~~diffusion time~~
scale remember?

or $\alpha = \frac{D \Delta t}{\Delta x^2} < 1/2$

If $\alpha < 1/4$ then your solution does not oscillate

$\rightarrow \Delta t < \frac{(10^{-2})^2}{2 \times 2 \times 10^{-6}} = \frac{1}{4} \times 100 = 25$ (s)

So this is very easy, @ each step the only unknown is the conc. @ that point for the next time step, all the rest is the same

So to reduce error we can decrease Δx and based on the $\Delta t < \frac{\Delta x^2}{2D}$, your Δt will squeeze even further

Now let's look at the implicit method for solving this problem:

$$\frac{C_i^{n+1} - C_i^{n}}{\Delta t} = \frac{D}{\Delta x^2} \left[C_{i+1}^{n+1} - 2 C_i^{n+1} + C_{i-1}^{n+1} \right]$$

Remember the implicit method, you wrote everything for the next time step:

$$C_i^{n+1} - C_i^{n} = \alpha C_{i+1}^{n+1} - 2\alpha C_i^{n+1} + \alpha C_{i-1}^{n+1}$$

$$C_i^{n} = -\alpha C_{i+1}^{n+1} + (2\alpha + 1) C_i^{n+1} - \alpha C_{i-1}^{n+1}$$

you have 3 unknowns here (anything from the next time step is unknown) so the solution is more complicate

$n = 0 \quad i = 1$

$$C_1^{0} = -0.25\, C_2^{1} + 1.5\, C_1^{1} - 0.25\, C_0^{1} = 100$$

(1) $C_1^{0} = -0.25\, C_2^{1} + 1.5\, C_1^{1} - 25 = 0$

$n=0 \quad i=2$

$-0.25\, c_3^1 + 1.5\, c_2^1 - 0.25\, c_1^1 - c_2^0 = 0$

(2) $-2.5 + 1.5\, c_2 - 0.25\, c_1 = 0$

$$\rightsquigarrow \begin{pmatrix} 1.5 & -0.25 \\ -0.25 & 1.5 \end{pmatrix} \begin{pmatrix} c_1' \\ c_2' \end{pmatrix} = \begin{pmatrix} 25 \\ 2.5 \end{pmatrix}$$

we can solve for c_1' and c_2' $\qquad c_2' = 4.75$

$\qquad c_1' = 17.42$

points	time (0)	(1)	(2)	(3)
0	100	100	100	100
1	0	x		
2	0	x		
3	10	10	10	10

solve for other "n"s

Looking at the error we can see that the method we're using here is more accurate for space than for time (central diff. for space & forward diff. for time). Now we want to bring them both to the same level. and remember 2nd order had the same level of acc. as central diff?

"Crank Nicolson" Method

$$\frac{\partial c}{\partial t} = \left.\frac{c_i^{n+1} - c_i^{n}}{\Delta t}\right|_{n+1/2} = \frac{D}{(\Delta x)^2} * \frac{1}{2}\left[\left\{c_{i+1}^{n+1} - 2c_i^{n+1} + c_{i-1}^{n+1}\right\} + \left\{c_{i+1}^{n} - 2c_i^{n} + c_{i-1}^{n}\right\}\right]$$

&

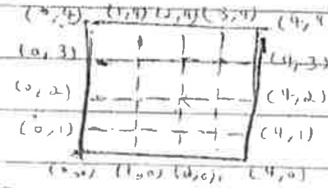
Averaging the two cone. in time (using central diff. instead of forward diff.)

$$c_i^{n+1} - c_i^{n} = \frac{\alpha}{2}\left[\left\{c_{i+1}^{n+1} - 2c_i^{n+1} + c_{i-1}^{n+1}\right\} + \left\{c_{i+1}^{n} - 2c_i^{n} + c_{i-1}^{n}\right\}\right]$$

↳ So the technique is the same, but you have more terms to work w/ (even the unknowns are the same)

* Solve the same problem using Crank Nicolson Me

2 D Steady



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

So we have two dimensions here, for each dimension we can write the same central diff. thingy:

$$\frac{(T_{i+1,j} - 2T_{i,j} + T_{i,j-1})}{\Delta x^2} + \frac{(T_{i,j+1} - 2T_{i,j} + T_{i,j-1})}{\Delta y^2} = 0$$

if $\Delta x = \Delta y$ (grids are the same, if not use ratios like $\Delta x^2 = 1/4\ \Delta y^2$, . .) either way use one variable:

$\Rightarrow T_{i+1,j} - 4T_{i,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} = 0$

For node (1,1):

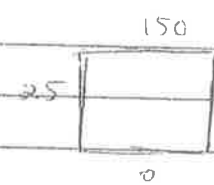
(*) $T_{2,1} - 4T_{1,1} + T_{0,1} + T_{1,2} + T_{1,0} = 0$

for node (1,2):

(*) $T_{2,2} - 4T_{1,2} + T_{0,2} + T_{1,3} + T_{1,1} = 0$

for node (1,3)

(*) $T_{2,3} - 4T_{1,3} + T_{0,3} + T_{1,4} + T_{1,2} = 0$



Boundary Condition (like S the ave @ that border)

for node (1,4) → This one is 150

(*) $T_{2,4} - 4T_{1,4} + T_{0,4} + T_{1,5} + T_{1,3} = 0$ X

Cannot write the equation for the Boundary.

Substitute values

(1) $T_{2,1} - 4T_{1,1} + 25 + T_{1,2} + 0 = 0$
(2) $T_{2,2} - 4T_{1,2} + 25 + T_{1,3} + T_{1,1} = 0$
(3) $T_{2,3} - 4T_{1,3} + 25 + \underbrace{T_{1,4}}_{150} + T_{1,2} = 0$

} for first row . . .

for node (2,1)

(*) $T_{3,1} - 4T_{2,1} + T_{1,1} + T_{2,2} + T_{2,0} = 0$

for node (2,2)

(*) $T_{3,2} - 4T_{2,2} + T_{1,2} + T_{2,3} + T_{2,1} = 0$

for node (2,3)

(*) $T_{3,3} - 4T_{2,3} + T_{1,3} + \overset{150}{T_{2,4}} + T_{2,2} = 0$

For node (3,1):

(*) $\overset{50}{T_{4,1}} - 4T_{3,1} + T_{2,1} + T_{3,2} + \overset{0}{T_{3,0}} = 0$

For node (3,2):

(*) $\overset{50}{T_{4,2}} - 4T_{3,2} + T_{2,2} + T_{3,3} + T_{3,1} = 0$

For node (3,3):

(*) $\underset{50}{T_{4,3}} - 4T_{3,3} + T_{2,3} + \underset{150}{T_{3,4}} + T_{3,2} = 0$

Develop Matrix

$$\underset{9*9}{\begin{bmatrix} -4 & & \\ & & \\ & & \end{bmatrix}} \underset{3*3\ /\ 9*1}{\begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}} = \underset{9*1}{\begin{bmatrix} \\ \\ \end{bmatrix}}$$

What if you had a Neuman's Boundary condition @ Boundary (4) "you have $\frac{\partial T}{\partial x} = -5$?

↳ solving the B.C using finite difference (central diff. preferably):

$$\frac{T_{i+1,j} - T_{i,j}}{2\Delta x} = -5 \rightarrow T_{i+1,j} - T_{i,j} = -10\Delta x$$

Now you have 12 unknowns instead of 9, the 3 nodes on boundary (4) are also unknown

(cont.

For node $(i=3, j=1)$

$$T_{4,1} - 4T_{3,1} + T_{2,1} + T_{3,2} + T_{3,0} = 0$$

on Boundary (4) so we should write the BC for this node

$$\frac{T_{i+1,j} - T_{i-1,j}}{2\Delta x} = -5$$

$$\Rightarrow T_{5,1} - T_{3,1} = -10\Delta x$$

→ False node (so it adds 3 False nodes to the unknowns)

you can't have all Neuman's conditions, (in the end Neuman's is all about the slope") you should have a starting point to put or pin on and move from there

* 2-D Transient State

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2}$$

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = D_x \left\{ \frac{C_{i+1,j}^{n} - 2C_{i,j}^{n} + C_{i-1,j}^{n}}{\Delta x^2} \right\} + D_y \left\{ \frac{C_{i,j+1}^{n} - 2C_{i,j}^{n} + C_{i,j-1}^{n}}{\Delta y^2} \right\}$$

Explicit method → Conditionally Stable → Time - Δx - Δy Condition

$$t \le \frac{1}{8D} \left\{ \Delta x^2 + \Delta y^2 \right\}$$

Using Implicit method:

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = D_x \left\{ \frac{C_{i+1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i-1,j}^{n+1}}{\Delta x^2} \right\} + D_y \left\{ \frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{\Delta y^2} \right\}$$

5 unknowns

$[\;\;][C]$ Really difficult to solve

→ penta diagonal matrix

you can break it down to [illegible] to [illegible] Solve

Mon 17-11

From last lecture

if you want to be more precise choose higher M

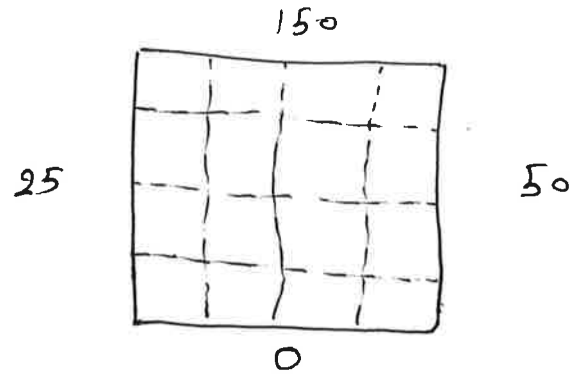
$$f(x+\Delta x) = f(x) + \Delta x\, f'(x) + \frac{\Delta x^2}{2!} f''(x) + \underline{\frac{\Delta x^3}{3!} f'''(x)}$$

if you want to start from here then $M = 3$

M is the remainder term

$$\frac{d^2y}{dx^2} = \frac{y_{i+1} - 2y_i + y_{i-1}}{(\Delta x)2}$$

back to the 2D problem from sat lecture



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

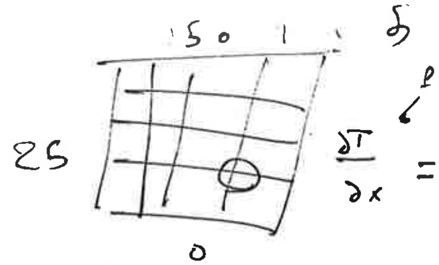
$\Delta x = \Delta y$ because it is evenly spaced

$y\, j \uparrow$

$\rightarrow x\, i$

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} = 0$$

$$T_{i-1,j} - 4T_{i,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} = 0$$



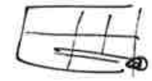
flux

$$\frac{\partial T}{\partial x} = -5 \rightarrow \text{rewrite } \frac{T_{i+1,j} - T_{i-1,j}}{2\Delta x} = -5$$

$i = 3,\ j = 1$

$$T_{4,1} - 4T_{3,1} + T_{2,1} + T_{3,2} + T_{3,0} = 0$$

$$T_{i+1,j} = -10\,\Delta x - T_{i-1,j}$$

if we take Point $i=4,\ j=1$ 

$$\cancel{10X} + T_{5,1} - 4T_{4,1} + T_{3,1} + T_{4,2} + T_{4,0}$$

$$\frac{T_{5,1} - T_{3,1}}{2\Delta x} = -5$$

$$\underbrace{T_{5,1}}_{\text{False node}} = -10X + T_{3,1}$$

for node $i=4,\ j=0$ you need to choose you value to be either 0 or $\frac{\partial y}{\partial x} = -5$

you can't take average because they are different

* you can't have four sides Neuman Condition (ex. $\frac{\partial T}{\partial x} = -5$) at least one side has to be a number

---

$$\frac{\partial c}{\partial t} = D_x \left\{ \frac{\partial^2 c}{\partial x^2} \right\} + D_y \left\{ \frac{\partial^2 c}{\partial y^2} \right\}$$

explict method

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = D_x \left\{ \frac{C_{i+1,j}^{n} - 2C_{i,j}^{n} + C_{i-1,j}^{n}}{(\Delta x)^2} \right\} + D_y \left\{ \frac{C_{i,j+1}^{n} - 2C_{i,j}^{n} + C_{i,j-1}^{n}}{(\Delta y)^2} \right\}$$

we need relationship of Δt, Δx, Δy

if we use implicit method

$$\frac{C_{i,j} - C_{i,j}}{\Delta t} = D_x \left\{ \frac{C_{i+1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i-1,j}^{n+1}}{(\Delta x)^2} \right\} + D_y \left\{ \frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{(\Delta y)^2} \right\}$$

$i=5,\ j=3$

$$C_{6,3} - 4C_{5,3} + C_{4,3} + C_{5,4} + C_{5,2} = 0$$

Penta diagram matrix

$$\begin{bmatrix} \ddots & & 0 \\ & \ddots & \\ 0 & & \ddots \end{bmatrix} [C] = [\ ]$$ to solve (Complicated)

tridiagonal matrix ← easier to solve

Thomas Algorithm

if we have 2 tridiagonal matrix instead of 1 Penta, we can solve it alot faster

Here Comes the

ADI method (Alternating direction Implicit method)

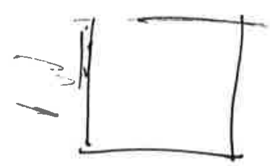
2 step Process

(1) $$\frac{C_{i,j}^{n+\frac{1}{2}} - C_{i,j}^{n}}{\Delta t/2} = \frac{D}{\Delta x^2}\left[C_{i+1,j}^{n} - 2C_{i,j}^{n} + C_{i-1,j}^{n}\right] + \frac{D}{\Delta y^2}\left[C_{i,j+1}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i,j-1}^{n+\frac{1}{2}}\right]$$

(2) $$\frac{C_{i,j}^{n+1} - C_{i,j}^{n+\frac{1}{2}}}{\Delta t/2} = \frac{D}{\Delta x^2}\left[C_{i+1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i-1,j}^{n+1}\right] + \frac{D}{\Delta y^2}\left[C_{i,j+1}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i,j-1}^{n+\frac{1}{2}}\right]$$

Modelling

water budget (how much water entering & Exsiting the system)



- define the flow system (which way, is it changing with time)

- Flow model
- transport model

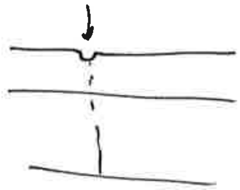
- water chimistry data

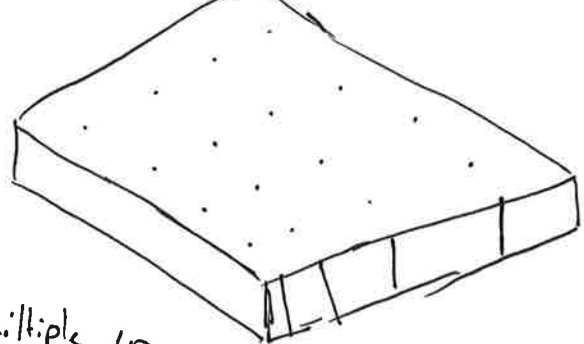
You can have 1D, 2D, 3D model

2D areal, 2D Profile

quasi 3D or a full 3D

1 D model

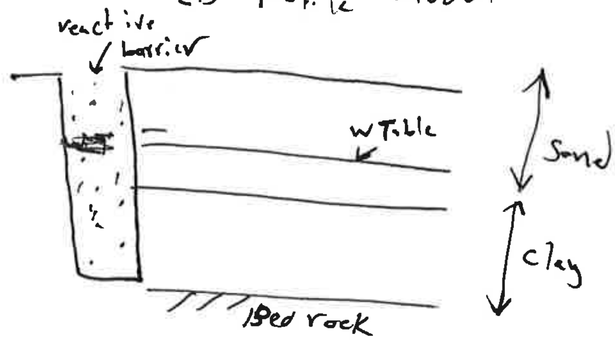




multiple 1D model

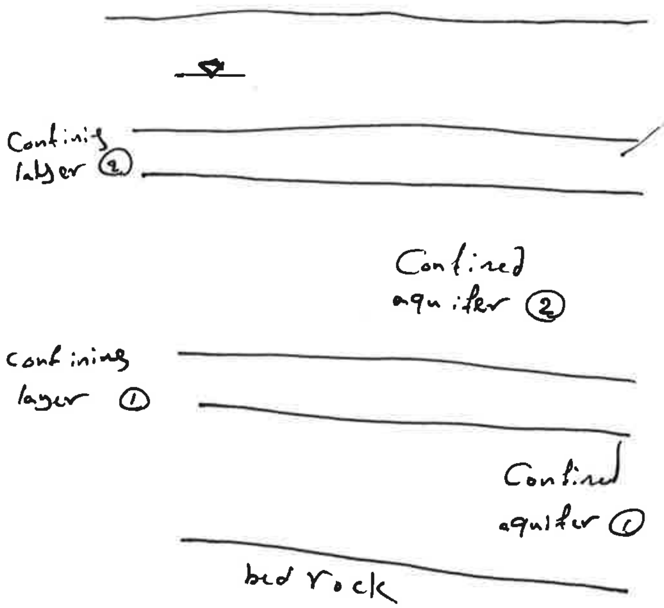
2 D areal

2D Profile model



Saturated soil

Saturated/unsaturated soil ← if you do a profile you need to do it for sat/unsat soil because you need boundry also 3D



← better to take it as leaking if hydrolic conductivity of aquifer ≤ 3 clay

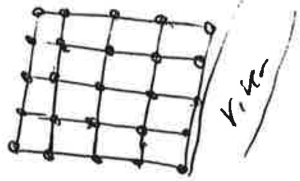
quasi 3D if partial from full 3D

$$\text{leakance term} = \frac{\text{vertical Conductivity}}{\text{Radius}}$$

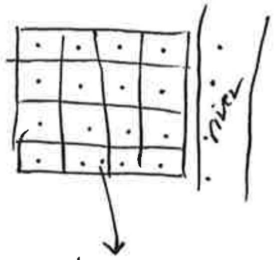
Grid design

Mesh Centered

block centered



better to use mesh in this case because you have the data on the edge of the mesh



You can use false node here to solve for the block Centered

* false node = Inactive node

this point has no value only center point has values (~~difference element~~ finite difference method)

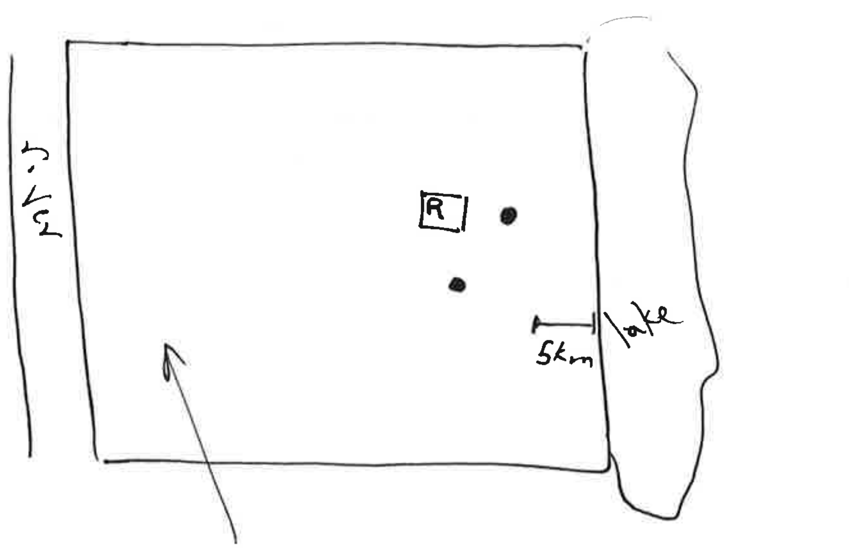
problem

* in finite element you have values everywhere

with finite element you can have different shapes of elements in the Grid
in finite difference you can't.

in finite difference if you have a small source it will not be captured accurately in the Grid

Telescopic mesh refining

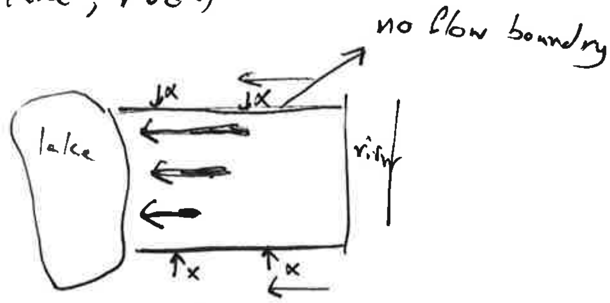


model spacing increases by 1.5 times (max)

use big grid here and slowly smaller your grid as you approach the target area

Boundries

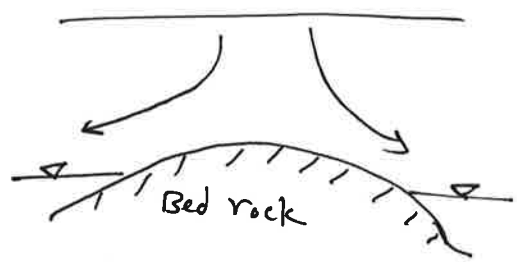
- physical boundries (ex. river, lake, rock)
- hydrolic boundries



You dont want stress to affect your boundries (ex. Pumping well)

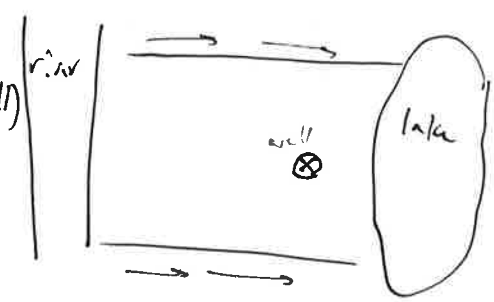
if the hydrulic gradient is too low you can have a no flow boundry

Impemeable rock is a boundry if the difference in K (hydrulic conductivity) > 2 orders of magnitude



Ground water divide
(very good boundry)

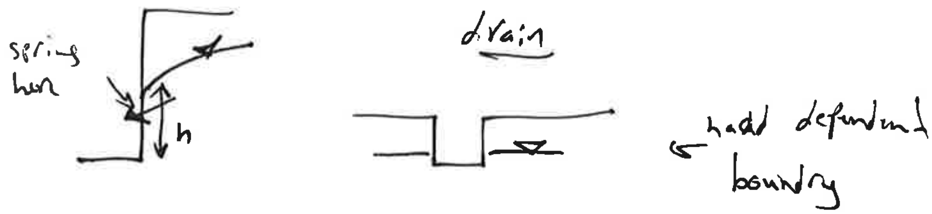
You can establish the initial condition starting with a steady state condition (no well) and then move to transiate state



* Using hydrolic boundry is not allowed when you have a stress. unless its very far and not affecting the boundry

specified head is better than specified flux.

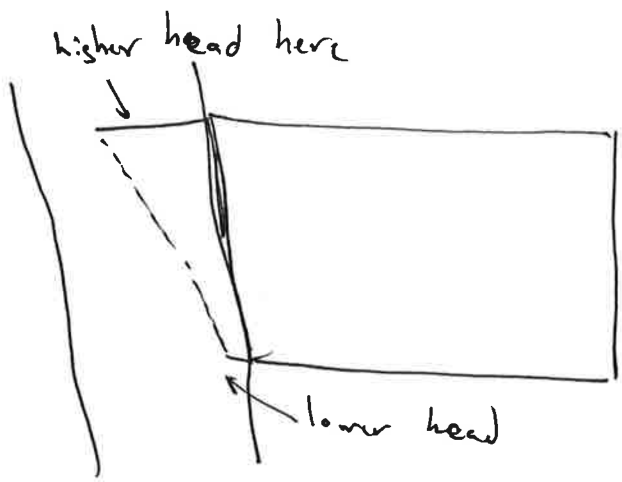
Head dependent boundry



Sources / sink

injecting well

pumping well



write it down

what does the field look like
what is the geology, topography look like
take a walk at the site

choose 1D, 2D, 3D models & depends on data available

do I want a finite element model
How would my mathematical model work

there are well established codes
and non tested codes

Bore hole

Sensitivity analysis within the calibration stage → what happens if a number changes (e.g. v + 50%) How would it effect C

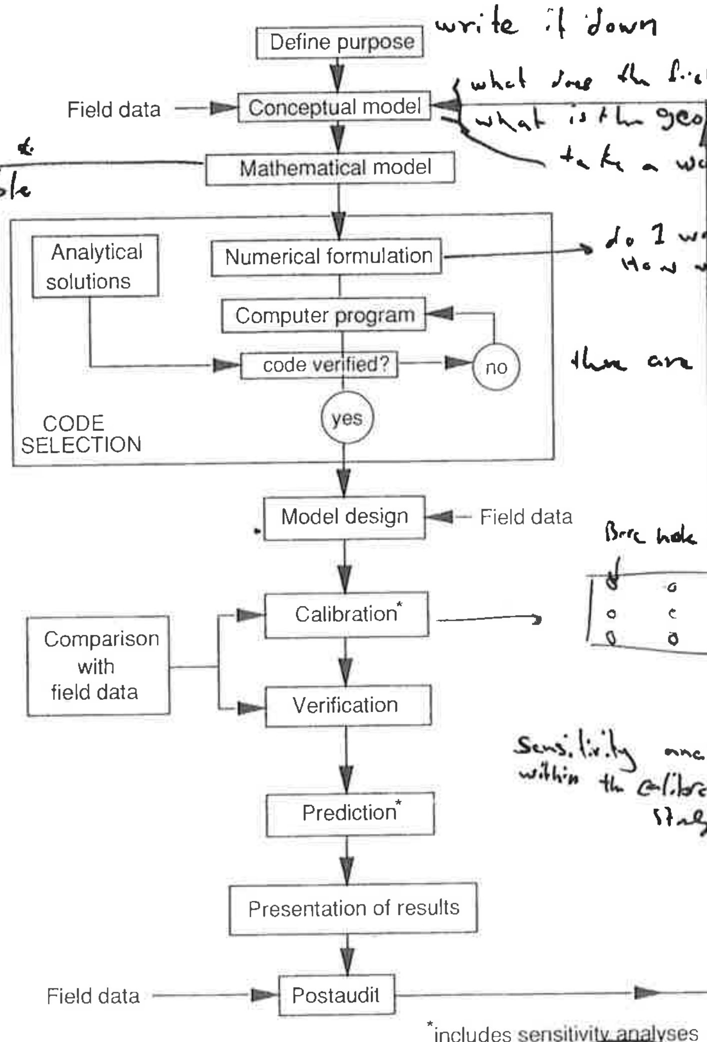


Fig. 1.1 Steps in a protocol for model application.

will help keep the modeler tied into reality and will exert a positive influence on the subjective decisions that will be made during the modeling study.

3. Select the governing equation and a **computer code** (Chapters 2 and 8). The code is the computer program that contains an algorithm to solve the mathematical model numerically. Both the governing equation and the code should be verified. Verification of the governing equation demonstrates that it accurately describes the physical processes occur-

$$\frac{\partial c}{\partial t} = -v\frac{dc}{dt} + D\frac{d^2C}{dx^2} - kC$$

to solve we need v, D, k and BCs

1. take half the data (2000 - 2005) calibrate it (calibration)
2. use your calibrated model and use it to predict the other half of data (2005 - 2013)
3. go back an calibrate

Notes

- $acc = \frac{dV}{dt}$ for water $= \frac{dVC}{dt}$ for a solute (V is constant) $= \frac{dc}{dt} \cdot V$

- $Q = v \cdot A = \frac{V}{t}$

- Avogadro's law : $\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$ $T_{\text{in kelvin}} = T_C + 273$ $0^\circ C = 273$ kelvin

- one mole of ideal gas occupies 22.4 Litres at $0^\circ C$ and 1 Atm

- weight of 1 mole CO_2 is $12 + 32 = 44$ g

- $\frac{\partial c}{\partial t} = - v_x \frac{\partial c}{\partial x}$ - $J = QC$ (mass flux) for advective tranport

- $J = -DA \frac{dc}{dx}$ (Fick's 1st (Dispresive transport)) steady state

- $\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$ (Fick's 2nd) transient state

- Darcy's law $Q = -kiA$, $i = \frac{\Delta h}{L}$, $\frac{Q}{A}$ = ~~seepage~~ Darcy velocity $(q) = -ki =$

seapage velocity $= \frac{q}{\theta}$

- $k = R \frac{\rho g}{\mu}$

- Quotient rule (derivative) $\rightarrow f/g = \frac{(f'g - g'f)}{g^2}$

- hydrolic gradiant $= \frac{\Delta h}{L} = i$

- $D_L = \alpha_L v_i + D^*$

α_L → longitudinal dispersivity

D_L → hydrodynamic dispersion

$\alpha_L v_i$ → longitudinal mechanical dispersion

D^* → diffusion Coefficent

- $P_e = \frac{v_i L}{D_L}$ (Peclet Number)

$m = \frac{b \pm \sqrt{b^2 + 4ac}}{2a}$