Picture from USGS Scientific Investigations Report 2008–5220

Software Training Workshop

Arc-NLET: ArcGIS-Based Nitrate Load Estimation Toolkit

Department of Scientific Computing, Florida State University
Section of Groundwater and Spring Protection, Florida Department of Environmental Protection

July 8th, 2011

Logistics

- Computer accounts of desktops
- Use of laptops
- Software website
- Lunch places

Project Team Members

- Contract Manager:
  - Rick Hicks (FDEP) (Richard.W.Hicks@dep.state.fl.us)
- Principal Investigators:
  - Ming Ye (FSU) (mye@fsu.edu)
  - Paul Lee (FDEP) (paul.lee@dep.state.fl.us)
- Graduate Students:
  - Fernando Rios (FSU, graduated in December 2010)
  - Raoul Fernendes (FSU, graduated in June 2011)
- Post-doc:
  - Liying Wang (FSU)
- No-Cost Collaborators:
  - Hal David (USGS)
  - Tingting Zhao, Amy Chan-Hilton, Joel Kostka (FSU)

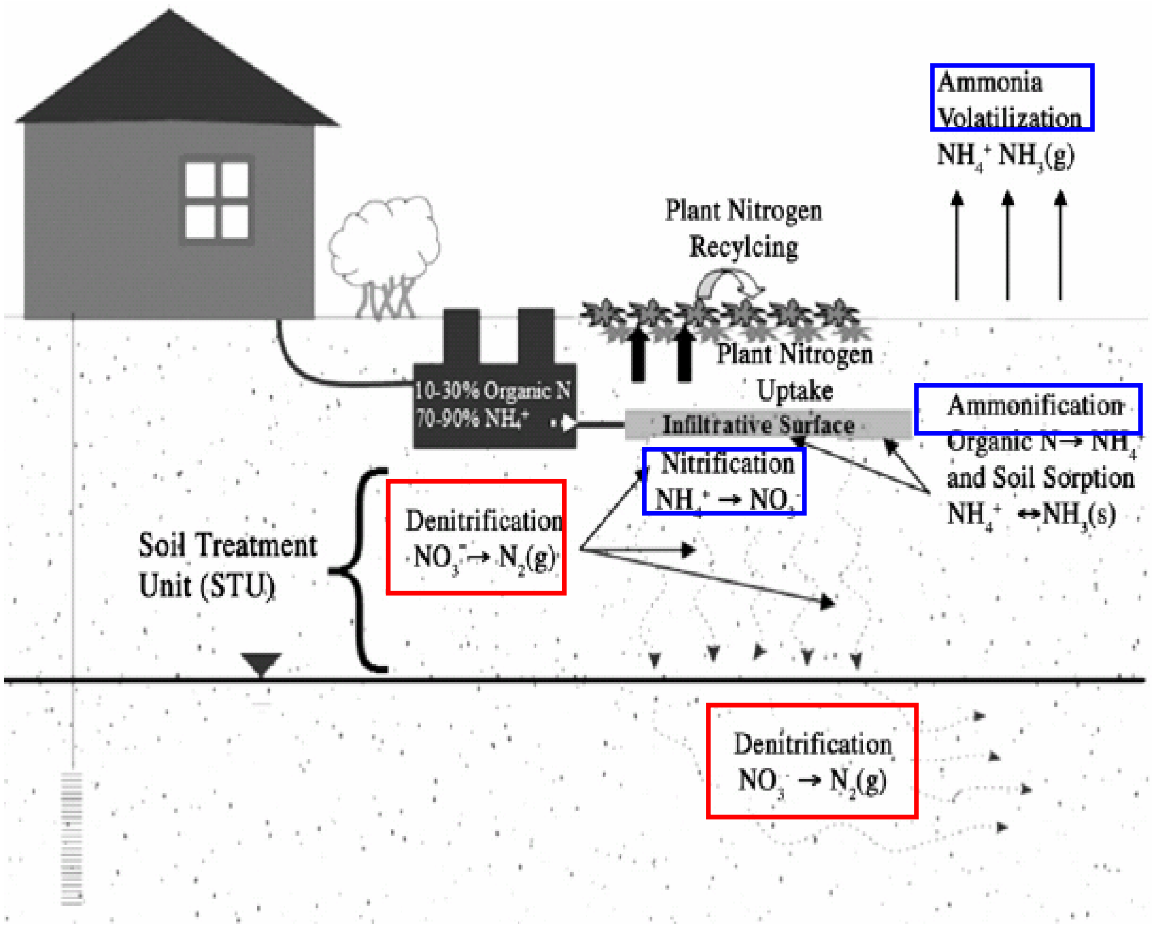
Workshop Agenda

Time	**Agenda**	**Instructor**
8:30 AM	Welcome and Computer Access[†]	Ming Ye
8:45AM	Introduction of Nitrate Fate and Transport Model	Ming Ye
9:30 AM	Model Development and Software Demonstration	Fernando Rios
10:20 AM	Break	
10:30 AM	Software Overview, Execution, and Visualization	Fernando Rios
Noon	Lunch	
1:30 PM	Preparation of Input Files and Result Analysis	Fernando Rios
3:30 PM	Break	
3:40 PM	Guidelines and Examples of Sensitivity Analysis and Model Calibration	Liying Wang
4:20 PM	Discussions	
4:30PM	Adjourn	

Project Overview

Ming Ye

Schematic of an Onsite Wastewater Treatment System (OWTS) and Subsurface Nitrogen Transformation and Removal Processes



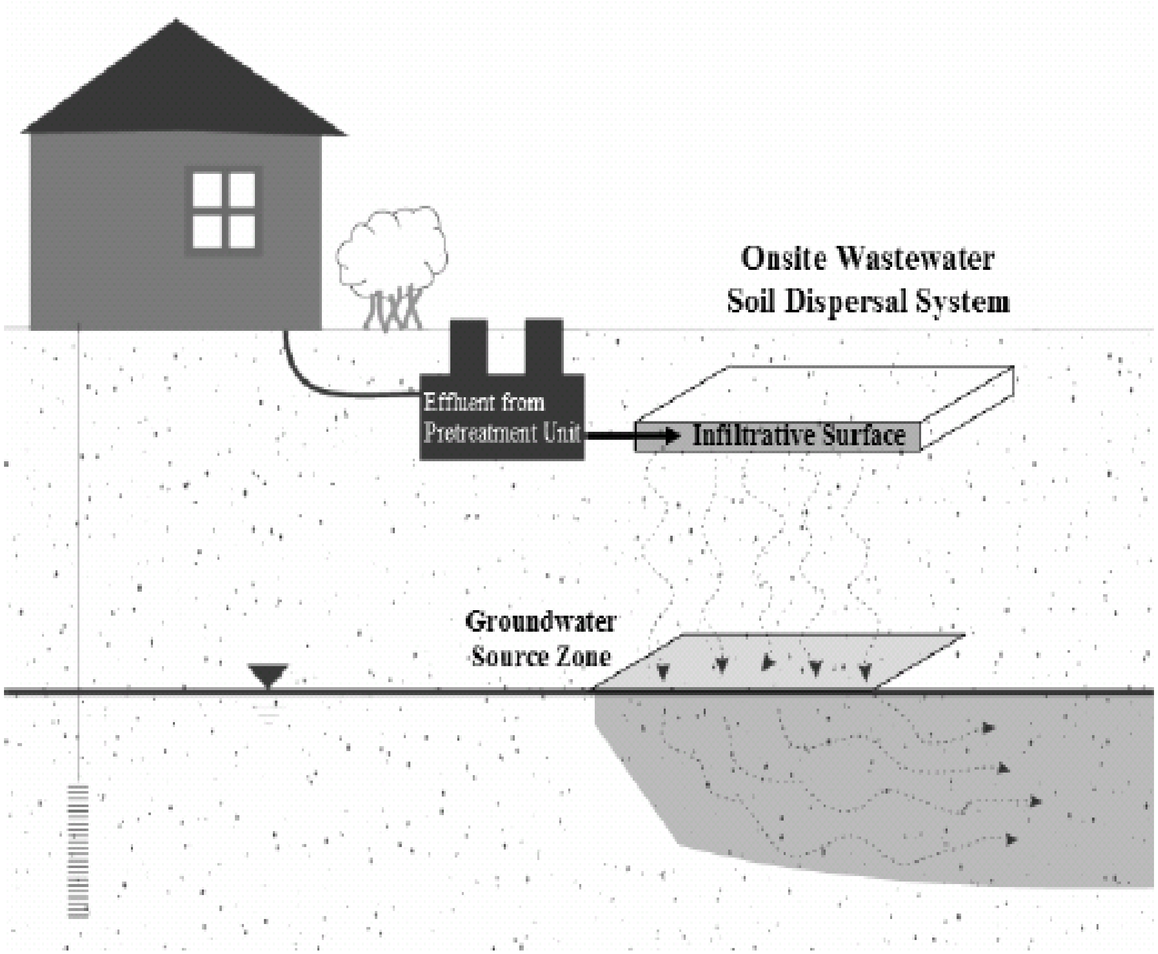
From Heatwole and McCray (2007)

Approximately one-third of the population of Florida utilizes OWTS for wastewater treatment. (Ursin and Roeder, 2008, FDOH)

Denitrification rates are much smaller than nitrification rates in natural soils.

Ninety percent of the water used for drinking comes from the ground water. (FDEP, 2006)

Nitrate Fate and Transport in Groundwater



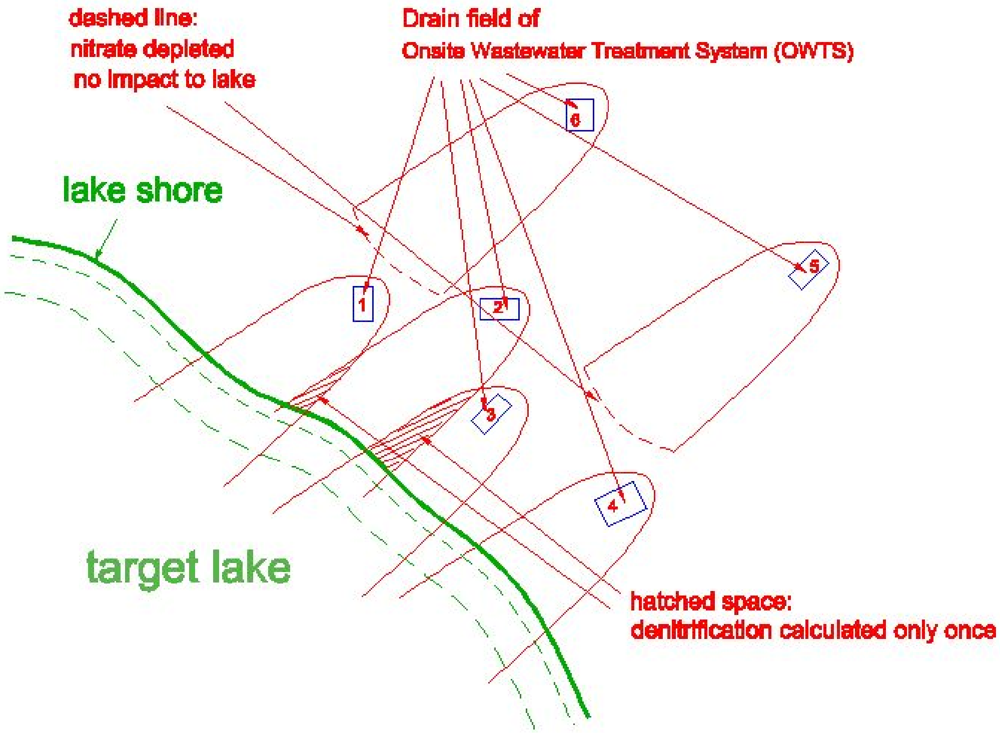
Due to nitrification in the vadose zone, OSW can generate NO_3-N concentration at the water table from 25 to 80 mg N/L in most situations (McCray et al., 2005).

From Heatwole and McCray (2007)

Motivations

Traditional estimate of nitrate loading (e.g., in TMDL) may ignore

- Nitrate from normally working septic systems
- Denitrification process in groundwater occurring between drainfield and surface water body
- Effect of spatial locations of septic systems on nitrate load



Motivations

- Consequence

  Over- or under-estimation of the nitrate load

- Sophisticated numerical models have been developed to study fate and transport of nitrate from septic system, but they may not be the most suitable tool for certain types of estimation (e.g., in TMDL) for the following reasons:
  - Burden for general users to set up model runs
  - Trained professional to operate the models and interpret modeling results
  - Large input and calibration data and long time of model execution and calibration

Project Goal

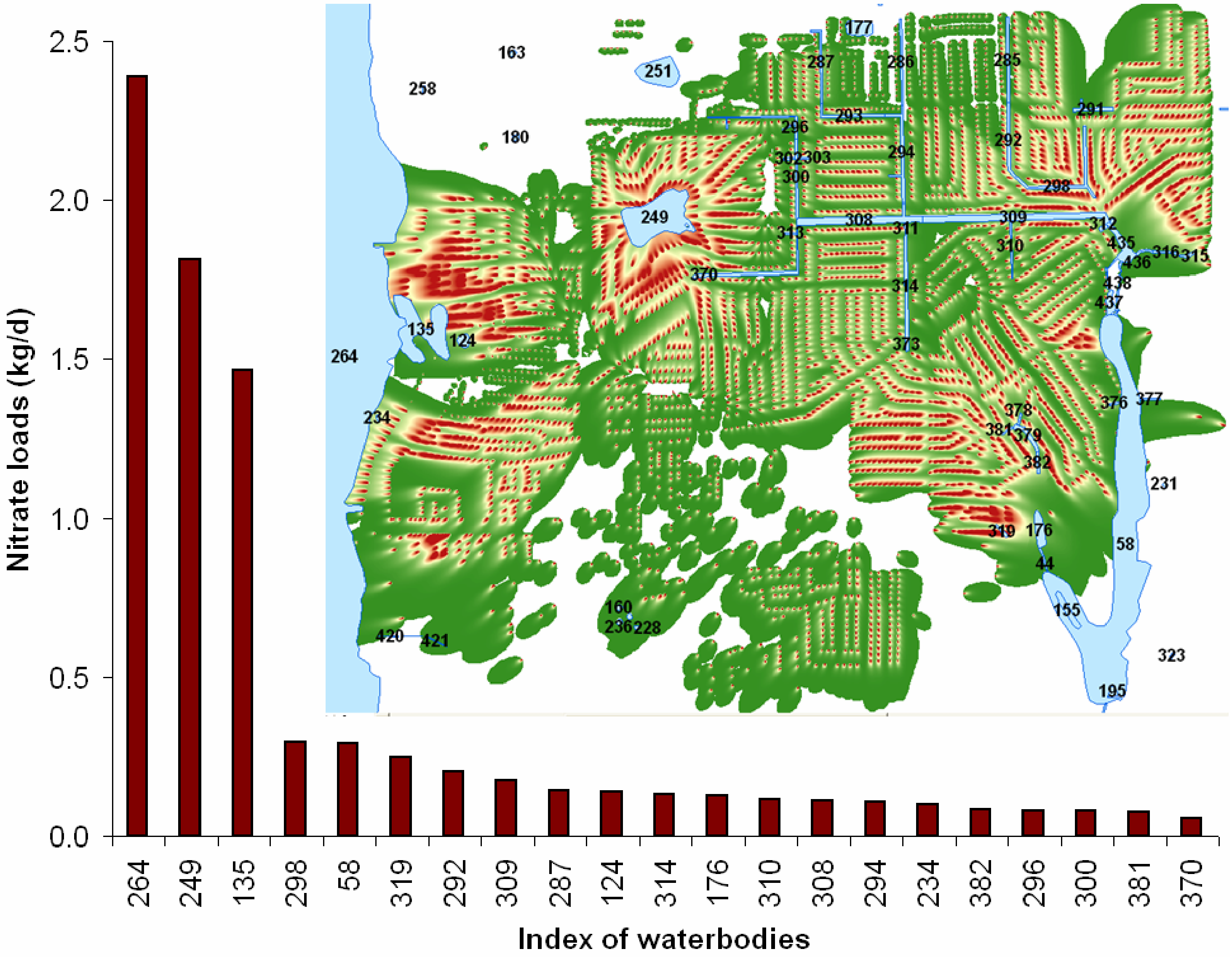
Goal: To develop a simplified model and a user-friendly software to support the TMDL and other environmental projects.

- It should be scientifically defensible under scrutiny.
- It should be user-friendly and GIS-based to incorporate location information for both septic tank cluster and surface water receiving nitrate load.
- It should be available in public domain, to be used by all parties, including the challengers and for comparison reasons

Project Objectives

- Develop a simplified model of groundwater flow and nitrate fate and transport.
- Implement the model by developing a user-friendly ArcGIS extension to
  - Simulate nitrate fate and transport including the denitrification process
  - Consider either individual or clustered septic tanks
  - Provide a management and planning tool for environmental management and regulation
- Apply this software to nitrate transport modeling at the Lower St. Johns River basin to facilitate DEP environmental management and regulation.
- Disseminate the software and conduct technical transfer to DEP staff and other interested parties.

What Can the Software Do?



Food for Thought

Victor Baker, the former President of the Geological Society of America, Member of Academy of Sciences, once said:

“Allowing the public to believe that a problem can be resolved … through elegantly formulated … models is the moral equivalent of a lie.”

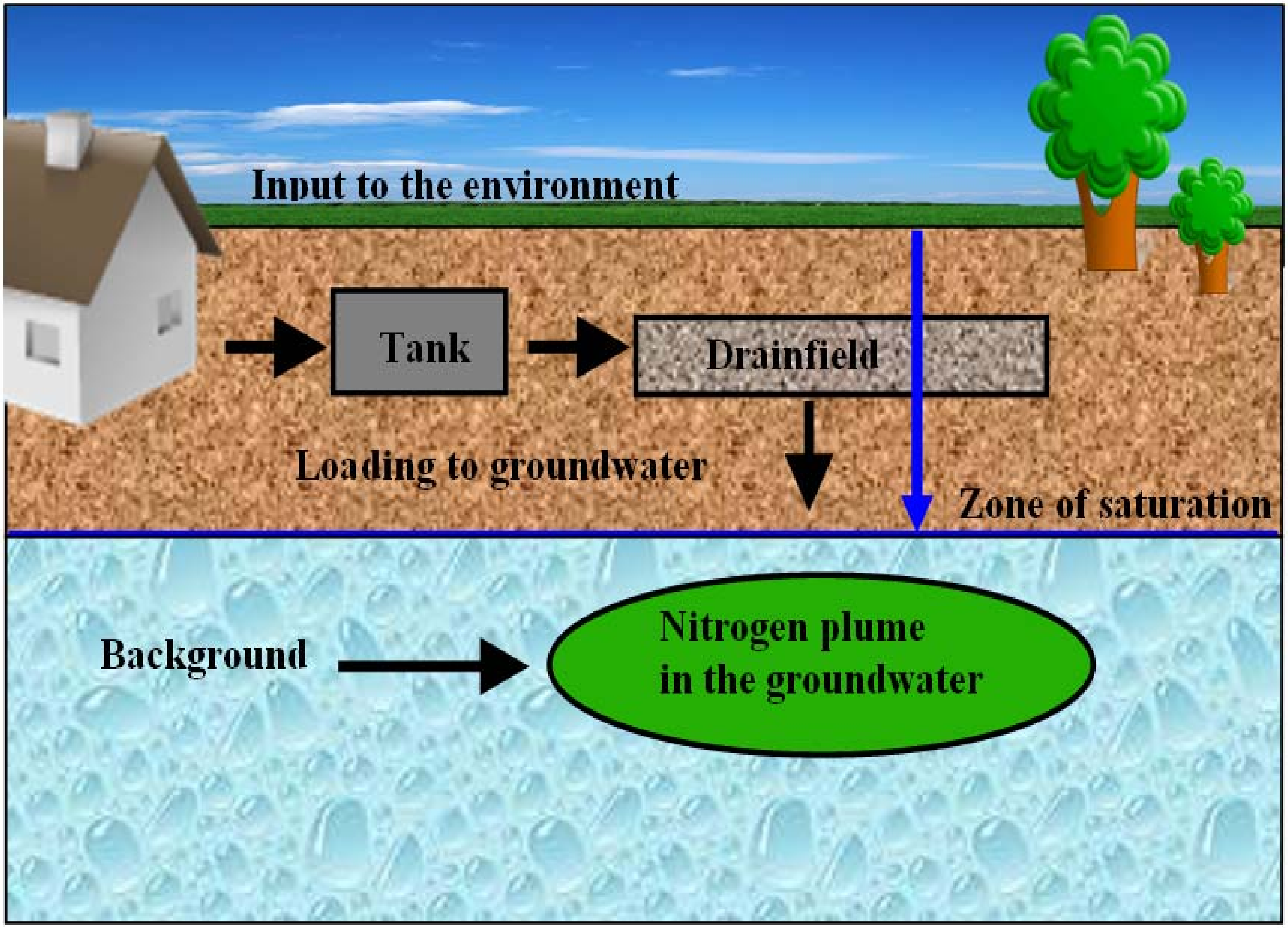
Pilkey, O.H. and L.P. Javis, 2007. Useless Arithmetic – Why Environmental Scientists Can’t Predict the Future, 230. New York, Columbia University Press.

Introduction to Nitrate Fate and Transport Model and Hydrogeology 1000

http://en.wikipedia.org/wiki/Hydrogeology

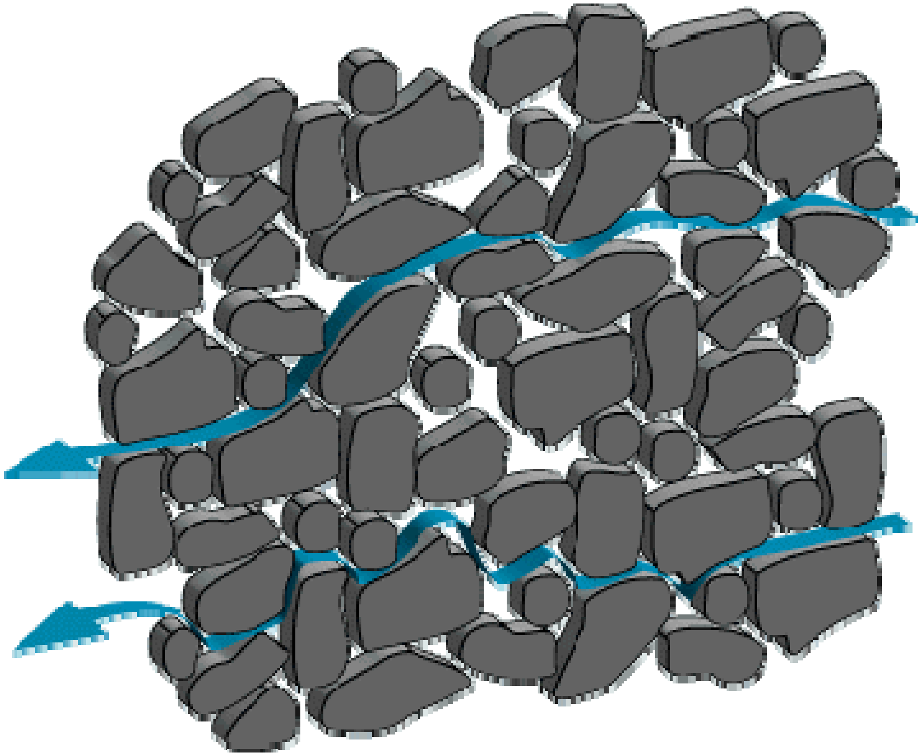
Ming Ye

Groundwater Flow and Transport



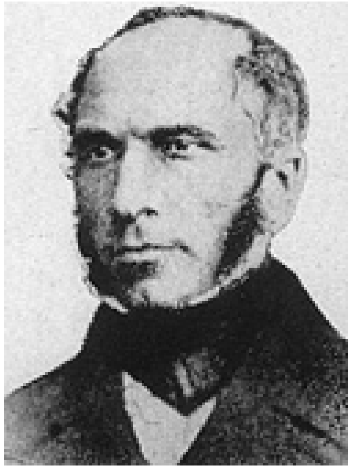
From Ebehard Roeder at FDOH

Groundwater Flow in Porous Media



- Flow in pores or void spaces
- Flow path extremely tortuous
- Geometry of flow channel exceedingly complex
- Friction is warranted

Groundwater Flow: Darcy's Law



Birth of quantitative hydrogeology:

Henry Darcy (1856), The Foundation of the City of Dijon

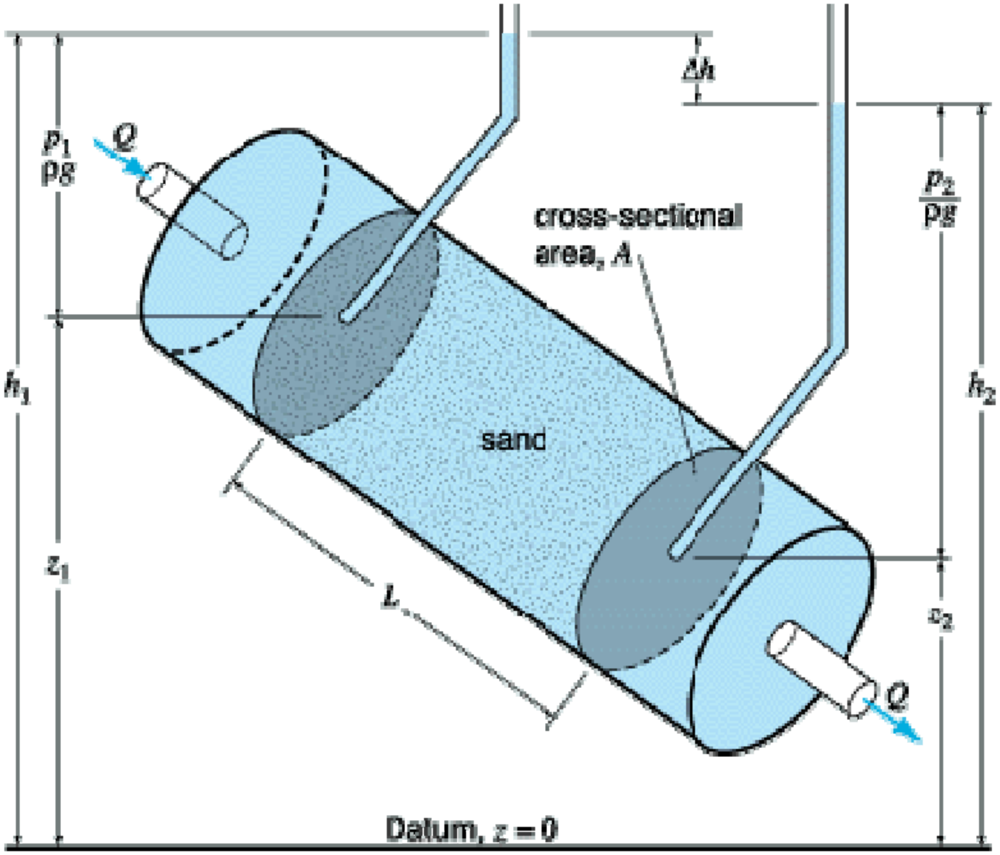
Hydraulic head, h:

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

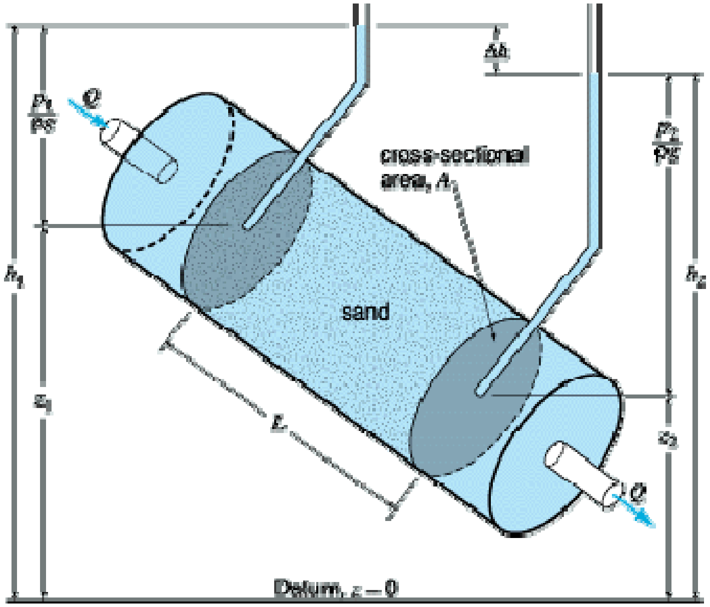
Elevation head

Pressure head

Unit of hydraulic head: [L], meter or foot



$$\frac{Q}{A} = -K\frac{h_2 - h_1}{L} = -K\frac{h_2 - h_1}{l_2 - l_1}$$

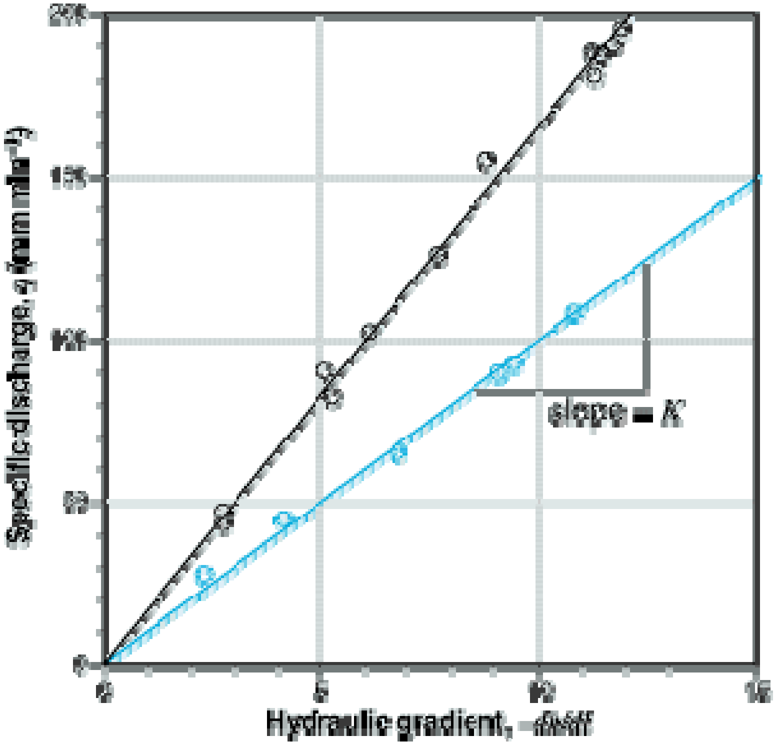


K [L/T] : hydraulic conductivity

q: specific discharge (Darcy velocity) [L/T]

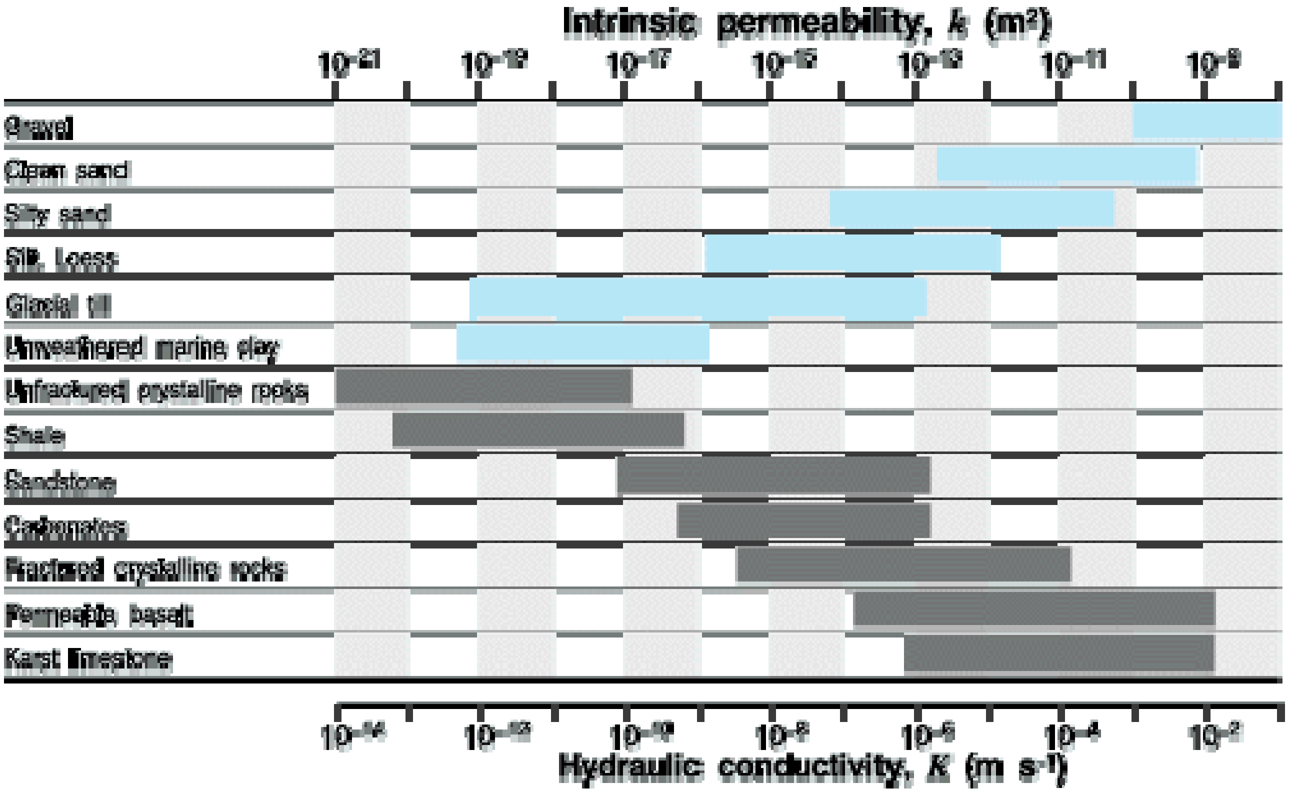
$$q = -K\boxed{\frac{dh}{dl}}$$

Hydraulic gradient <u>along flow path</u>



Hydraulic Conductivity

Different geologic media have different values of hydraulic conductivity.



Field measurement of hydraulic head

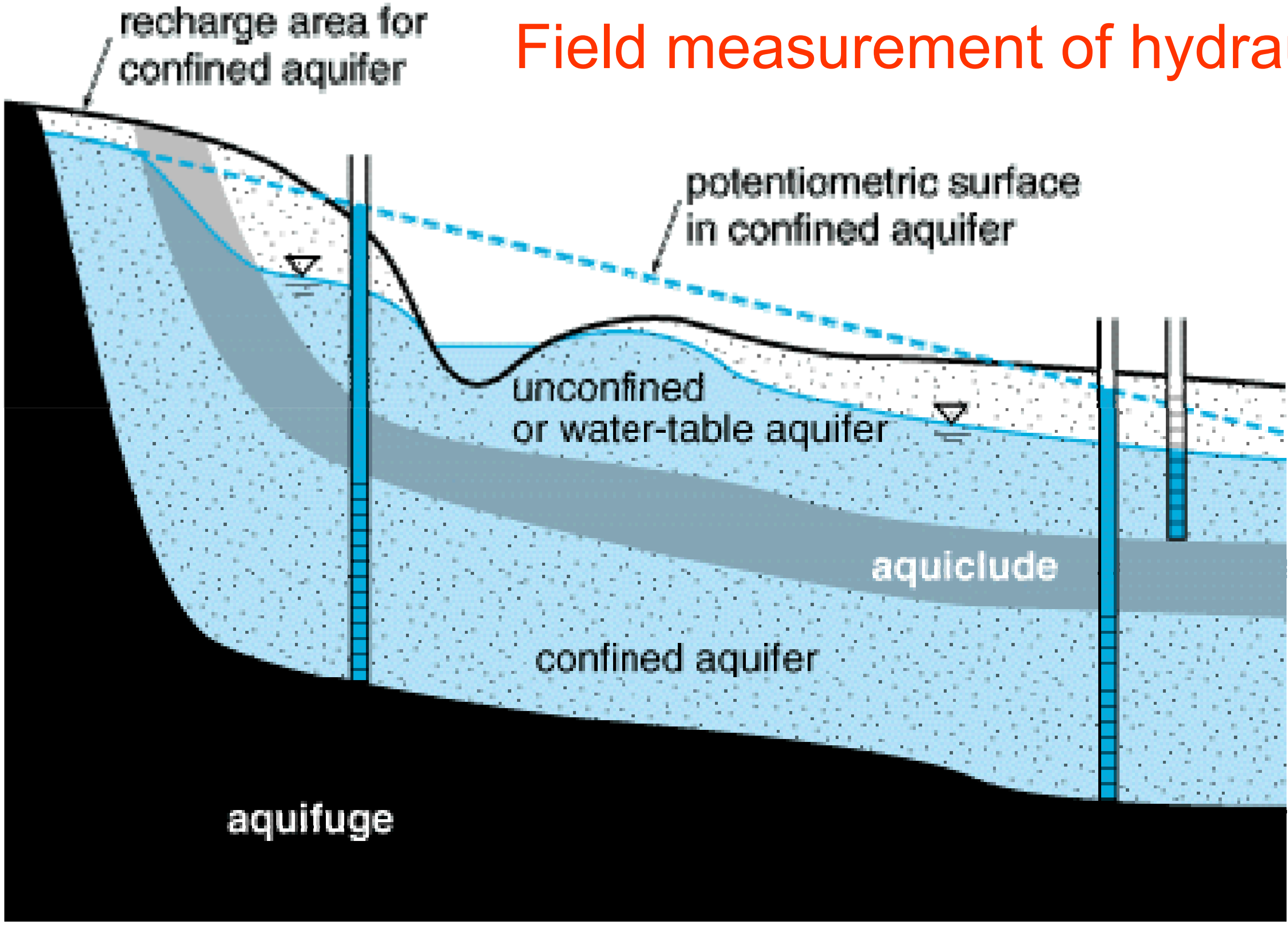


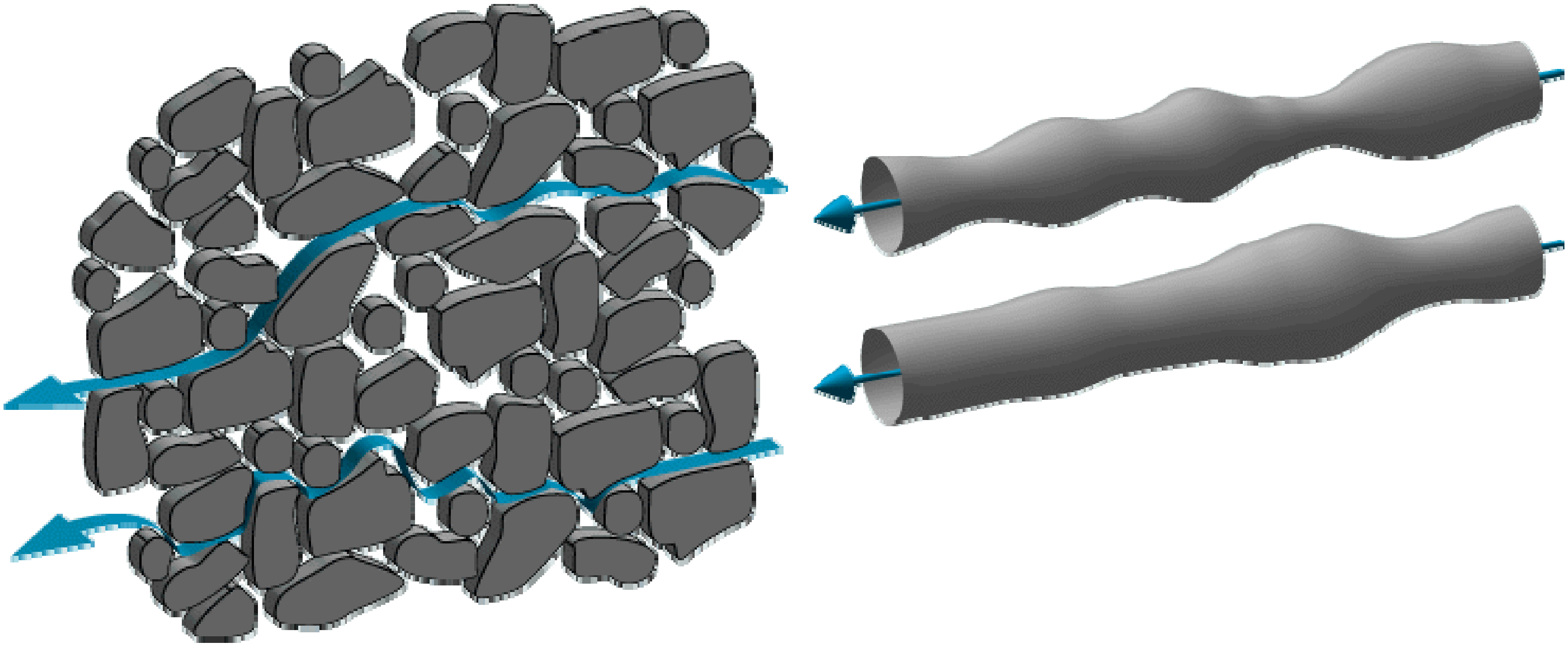
Figure 6.6 Hydrogeological units. Three piezometers are depicted, which are open in either the confined or unconfined aquifer, as indicated by the short horizontal lines. Note that in unconfined aquifers, the water level in the piezometer (far right) indicates the height of the water table; in confined aquifers, the water level in the piezometers (left and center) rises above the top of the aquifer and indicates the position of the potentiometric surface.

Summary of Darcy’s Law

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

- It is used to evaluate the Darcy velocity (or flux = flow rate/area) consists of magnitude and direction.
- Using the Darcy’s law requires knowing
  - Hydraulic conductivity [L/T]
  - Hydraulic head [L]

Groundwater Contaminant Transport



- Darcy velocity is a fictitious velocity since it assumes that flow occurs across the entire cross-section of the soil sample. It is the average over the whole cross section.
- It is NOT the velocity at which a particle travels. Flow actually takes place only through pore space between soil sample.

Seepage Velocity and Porosity

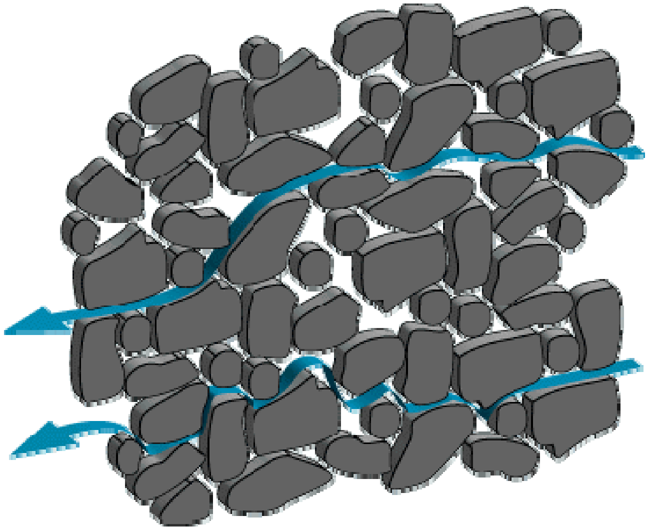
Seepage velocity [L/T]:

$$\bar{v} = \frac{q}{\phi}$$

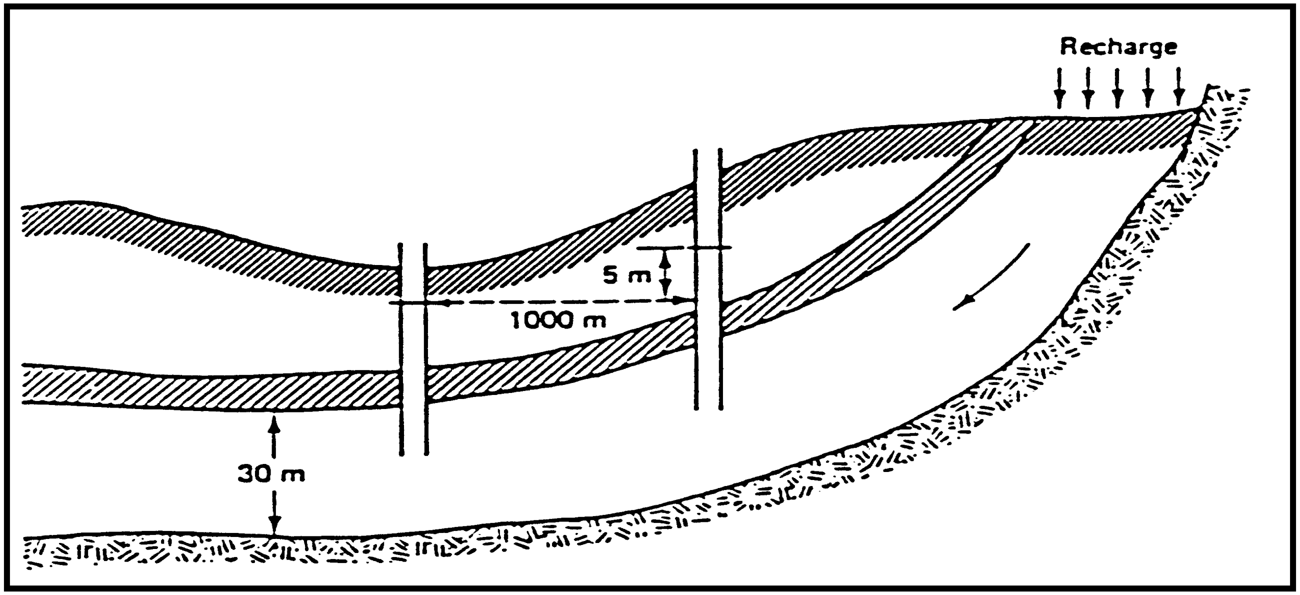
Porosity:

$$\phi = \frac{V_v}{V_t}$$

where V_v is the volume of void space [L^3] and V_t is the total volume [L^3].



Example



- **A confined aquifer has a source of recharge.**
- **K for the aquifer is <u>50 m/day</u>, and *Φ* is <u>0.2</u>.**
- **The piezometric head in two wells <u>1000 m</u> apart is <u>55 m and 50 m</u> respectively, from a common datum.**

A: Darcy velocity?

B: The time of travel from the head of the aquifer to a point 4 km downstream?

$$q = -K\frac{dh}{dl} = -K\frac{h_2 - h_1}{L} = -K\frac{h_2 - h_1}{l_2 - l_1}$$

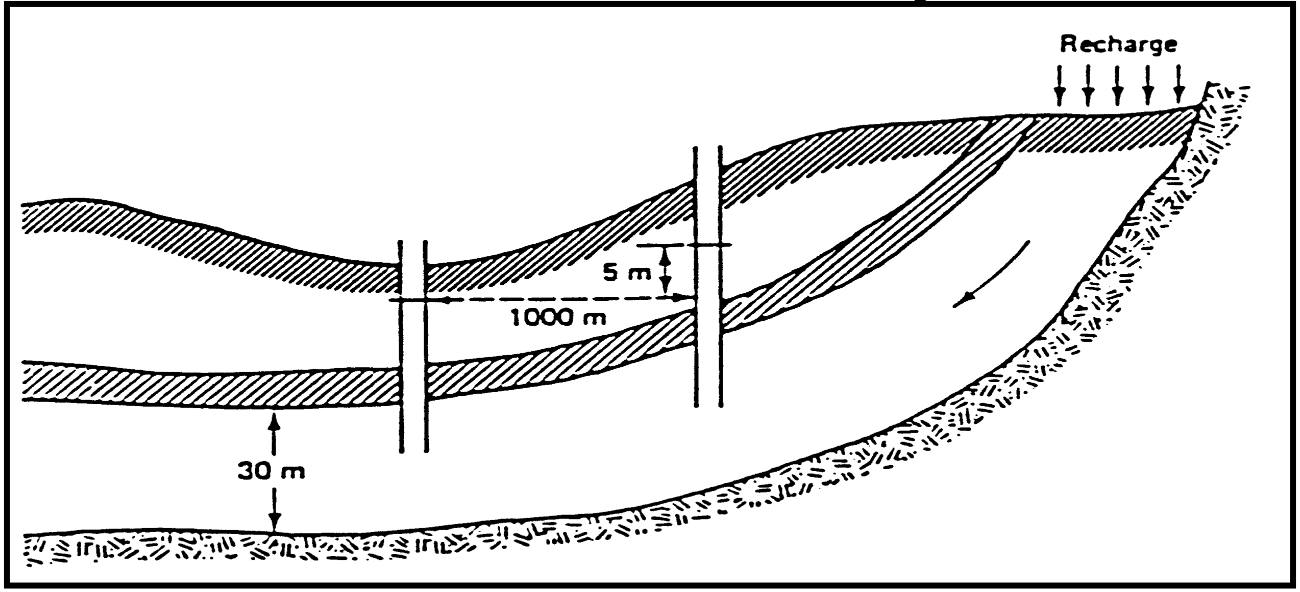
Hydraulic gradient =

(55m-50m)/1000m = 5 x 10^{-3}

Hydraulic conductivity K = 50 m/day

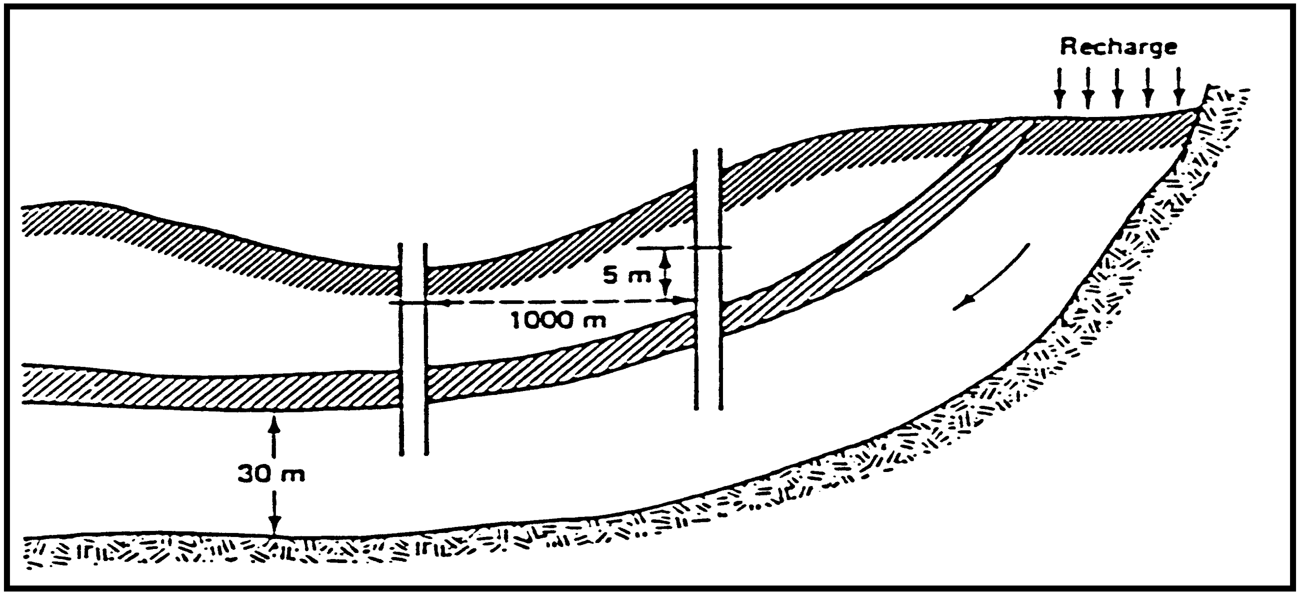
Darcy velocity q = - 50 m/day x 0.005

= - 0.25 m/day

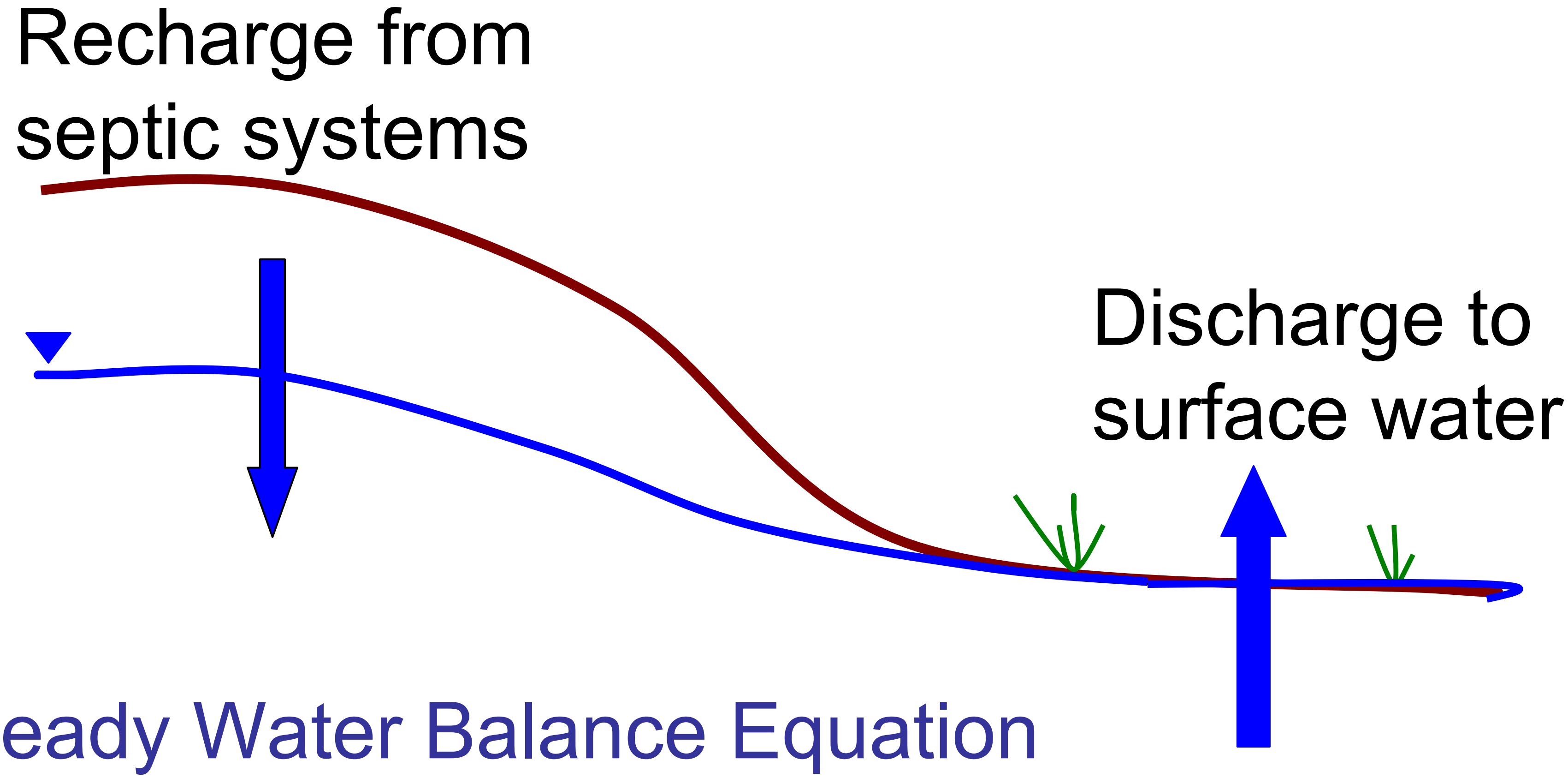


$$\overline{v} = \frac{q}{\phi}$$

- Seepage velocity = 0.25 m/day / 0.2
  = 1.25 m/day
- Travel time = 4000 m / 1.25 m/day
  = 3200 days (8.77 years)



Groundwater Flow: Water Balance Equation



Recharge from septic systems

Discharge to surface water

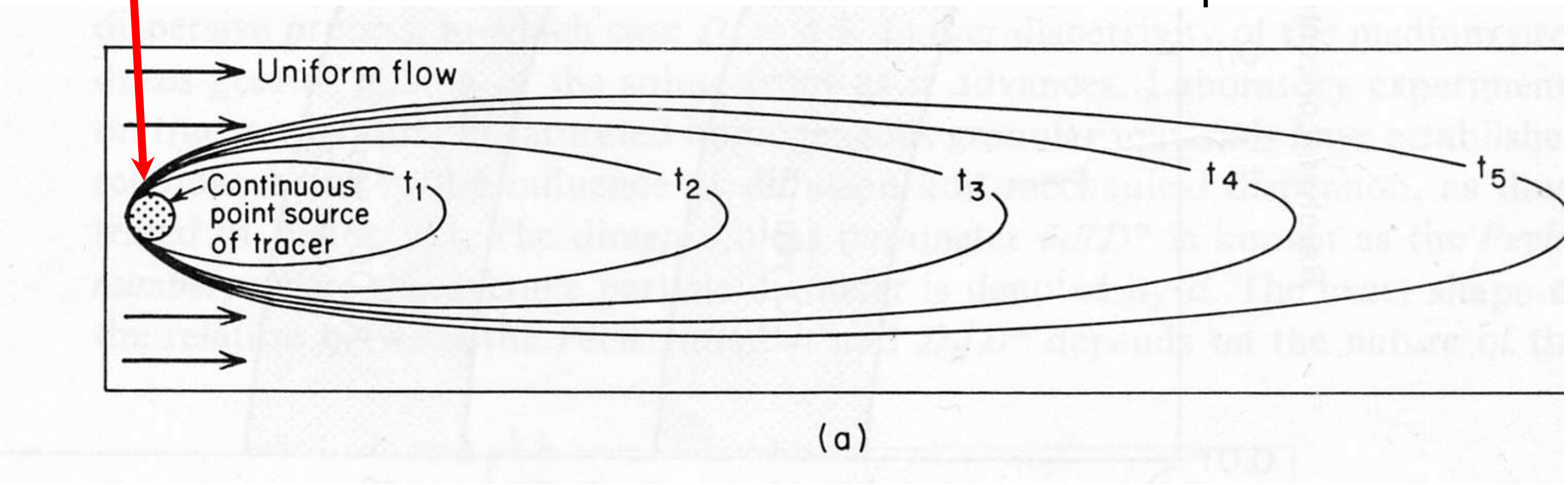
Steady Water Balance Equation

Inflow = Outflow

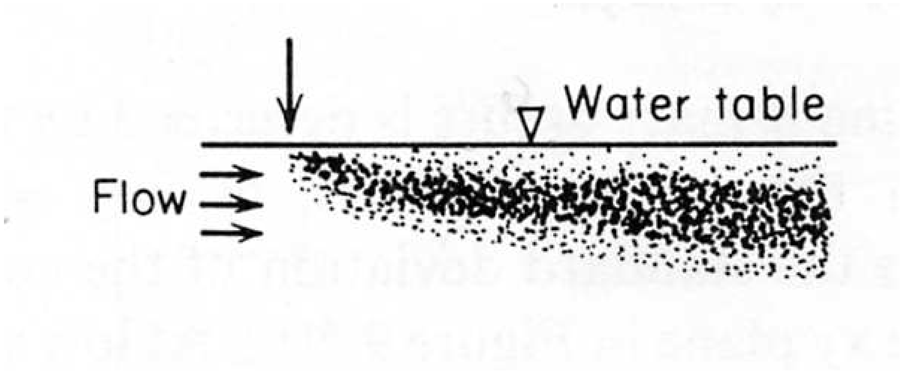
Groundwater Contaminant Transport

Continuous source:

Horizontal cross-section of concentration plume



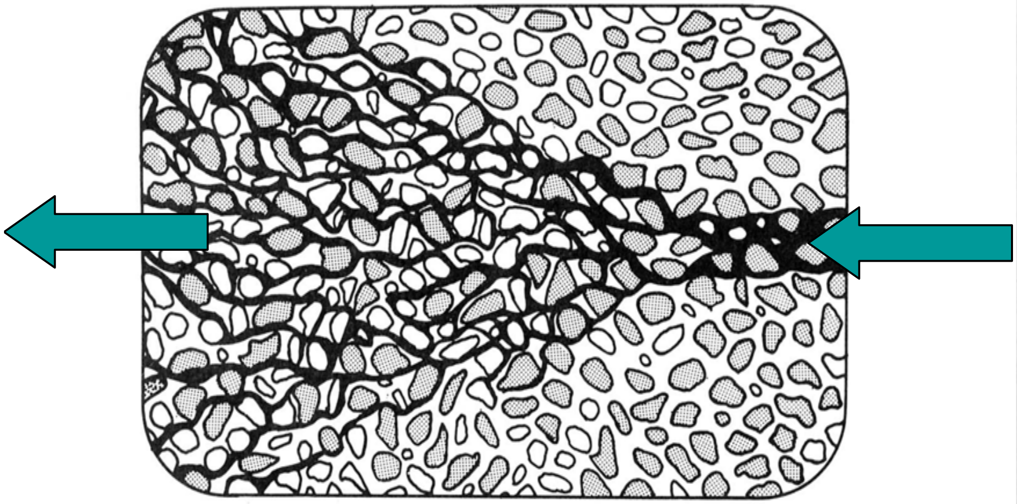
Vertical cross-section of concentration plume

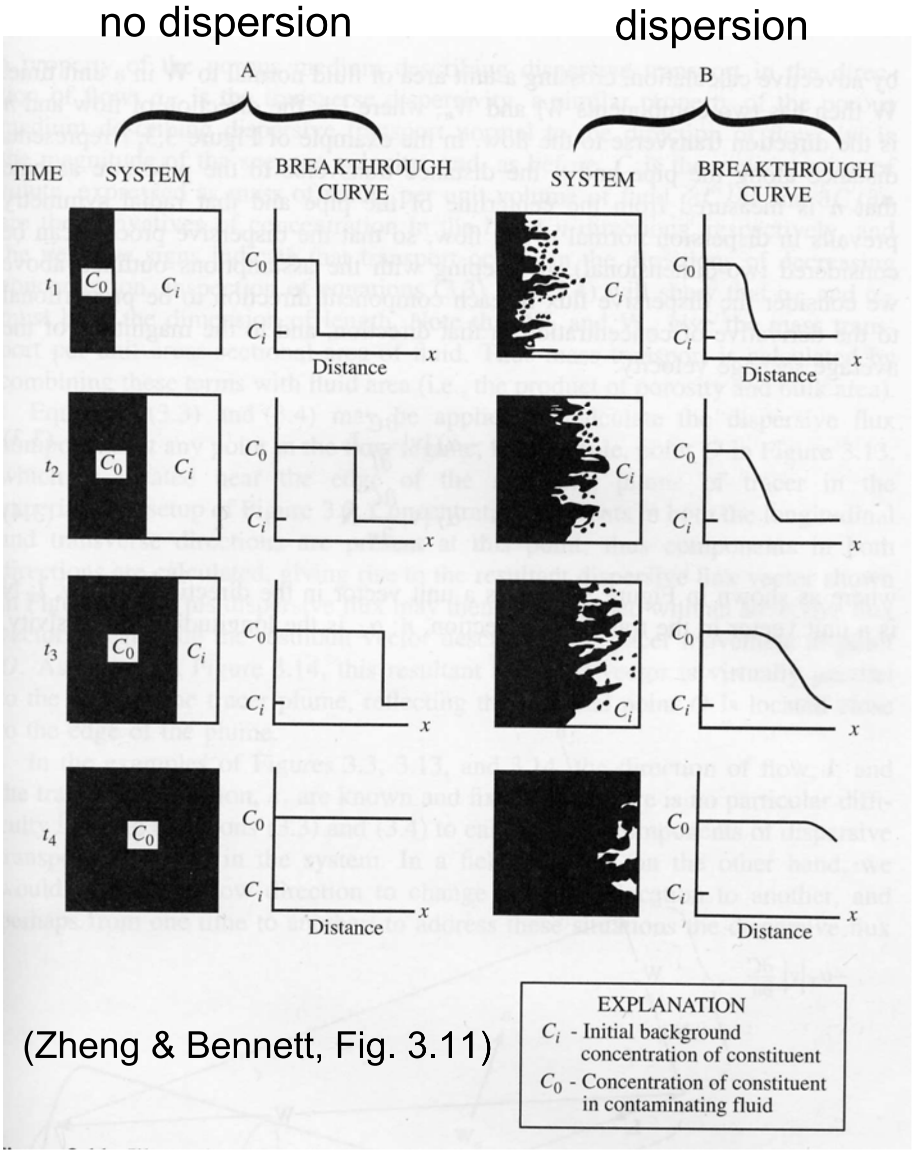


Effects of dispersion on the concentration profile

Advection

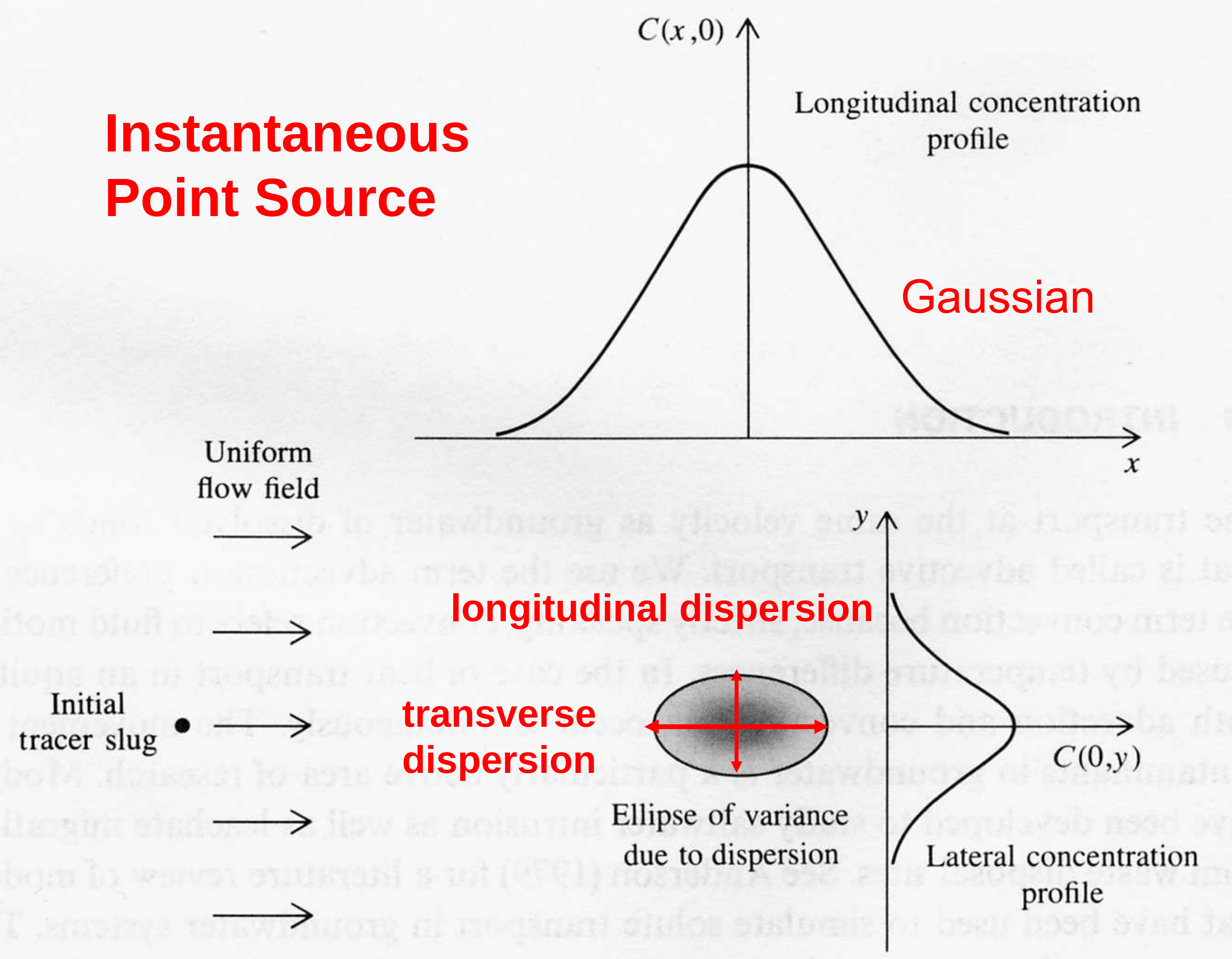
Dispersion





(Zheng & Bennett, Fig. 3.11)

Instantaneous Point Source



Gaussian

longitudinal dispersion

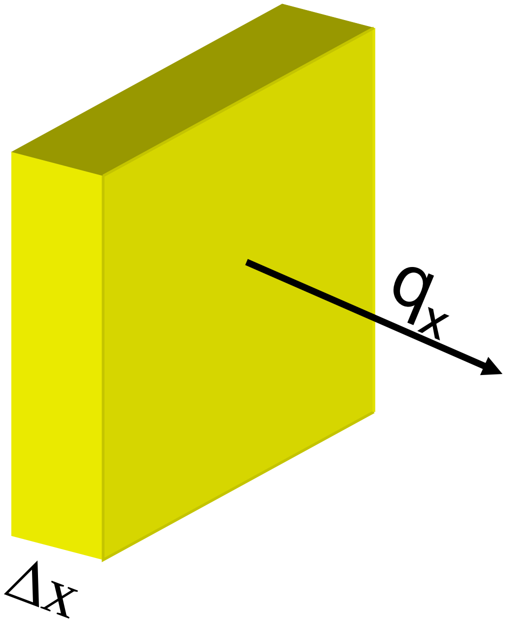
transverse dispersion

Figure from Wang and Anderson (1982)

- Hydrodynamic dispersivity (α_L, α_T) is an empirical factor which quantifies how much contaminants stray away from the path of the groundwater which is carrying it.
- Some of the contaminants will be "behind" or "ahead" the mean groundwater, giving rise to a longitudinal dispersivity (α_L).
- Some will be "to the sides of" the pure advective groundwater flow, leading to a transverse dispersivity (α_T).

Contaminant Mass Flux

Assume 1D flow



Advective flux

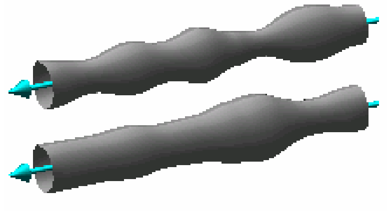
Seepage velocity

Porosity

$$f_A = q_x c = [-K \frac{h_2 - h_1}{\Delta x}]c = v_x \phi c$$

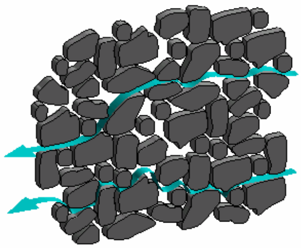
concentration

Darcy velocity



Dispersive flux

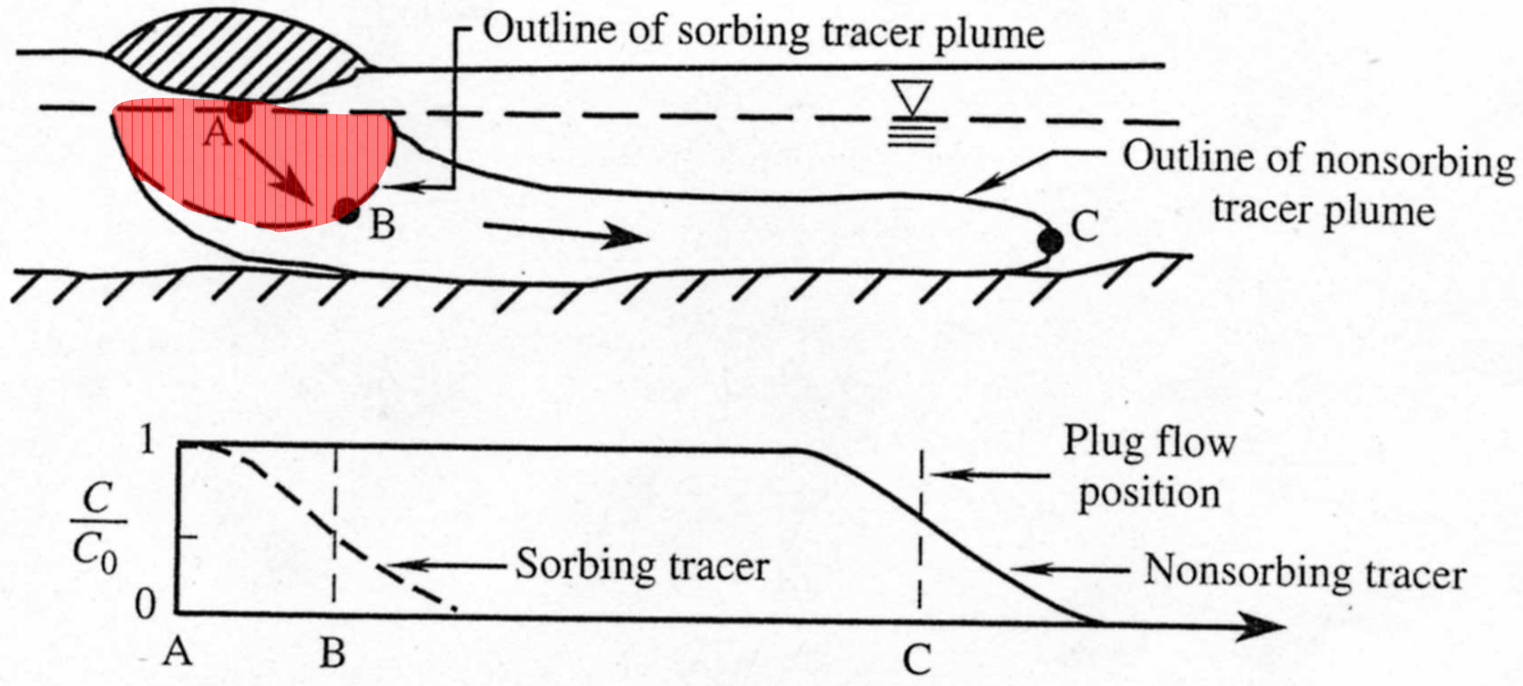
$$f_D = -D_x \phi \frac{c_2 - c_1}{\Delta x}$$



D=vα is the dispersion coefficient. It includes the effects of dispersion and diffusion. D_x is sometimes written as D_L and called the longitudinal dispersion coefficient.

Chemical Reactions

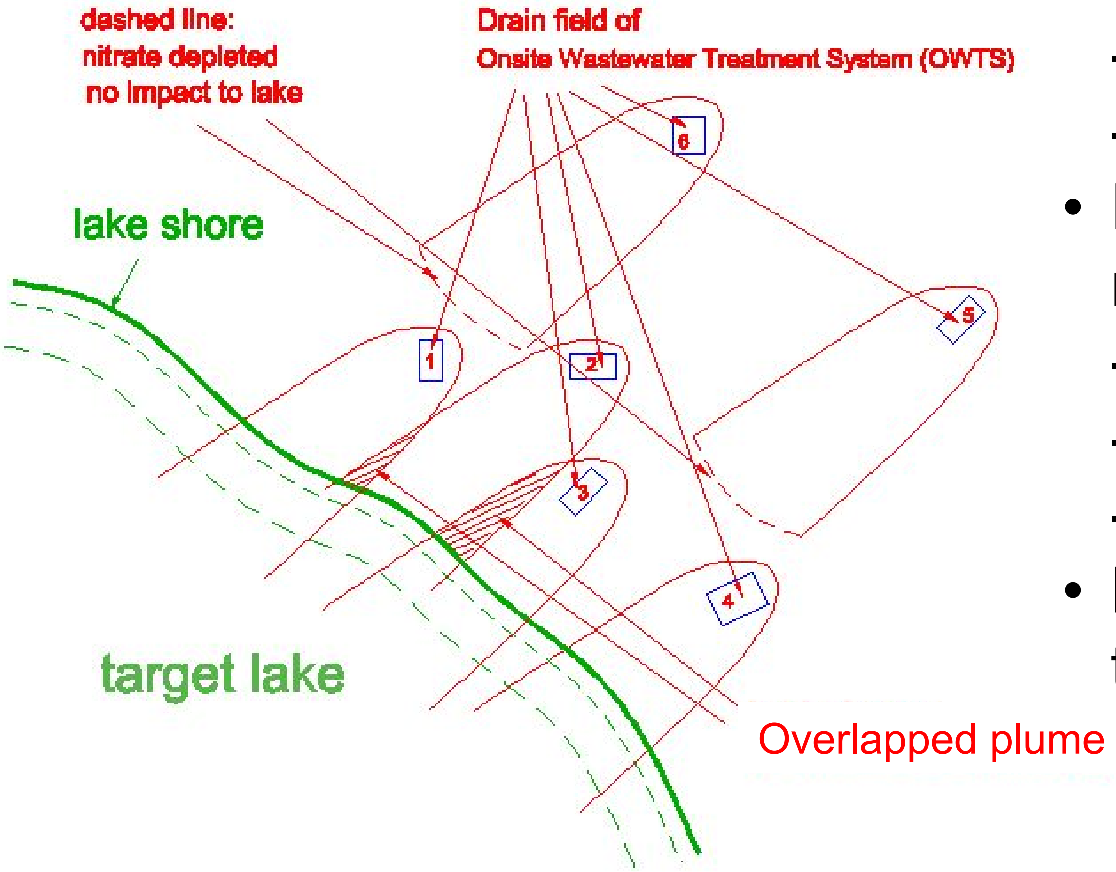
Sorption as an example



$$\text{Retardation factor } (R) = \frac{\text{Distance AC}}{\text{Distance AB}} = v/v_c$$

Conceptual Model of Nitrate Transport

Take into account of nitrate contribution from working septic tanks.



- Groundwater flow model to estimate
  - flow path
  - flow velocity
  - travel time
- Fate and transport model to consider
  - Advection
  - Dispersion
  - Denitrification
- Load calculation model to estimate nitrate load

Denitrification

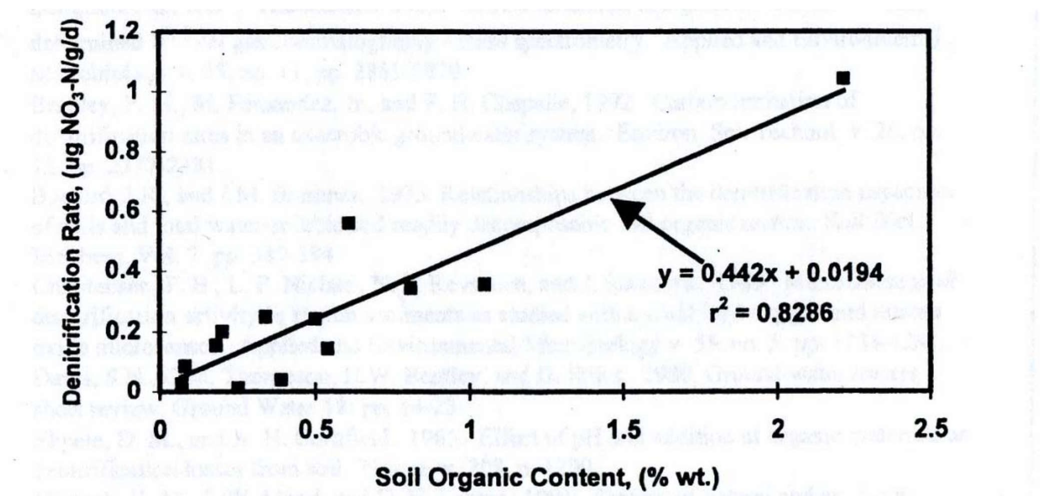
Denitrification refers to the biological reduction of nitrate to nitrogen gas.

$$NO_3^- + \text{Organic carbon} \rightarrow NO_2^- + \text{Organic carbon} \rightarrow N_2 + CO_2 + H_2O$$

$$NO_3^- \rightarrow NO_2^- \rightarrow NO \rightarrow N_2O \rightarrow N_2$$

Denitrification … has been identified as basic factor contributing to the generally low levels of nitrate found in the groundwater of the southeastern United States (Fedkiw, 1991).

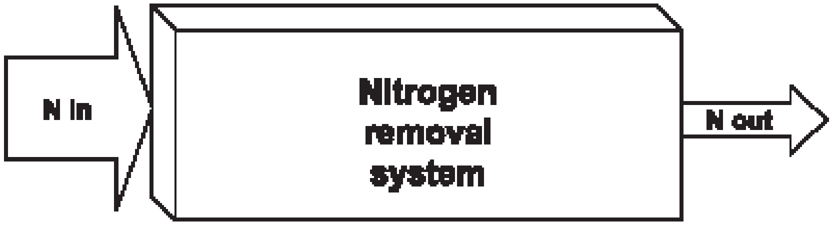
A fairly broad range of heterotrophic anaerobic bacteria are involved in the process, requiring an organic carbon source for energy as follows



Anderson (1989)

Estimation of Nitrate Load

$$M_{in} = M_{out} + M_{dn}$$
$$M_{out} = M_{in} - M_{dn}$$



- M_{out} (M/T): nitrate load to rivers
- M_{in} (M/T): nitrate from septic tanks to surficial aquifer
- M_{dn} (M/T): nitrate loss due to denitrification

$M_{dn} = R_{dn}V_g$

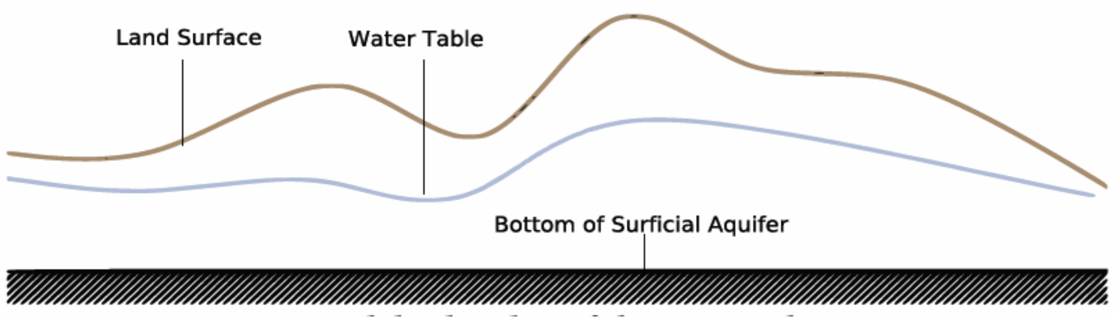
R_{dn} ($M/T/L^3$): denitrification rate

V_g (L^3): volume of groundwater solution, estimated from groundwater flow and reactive transport modeling

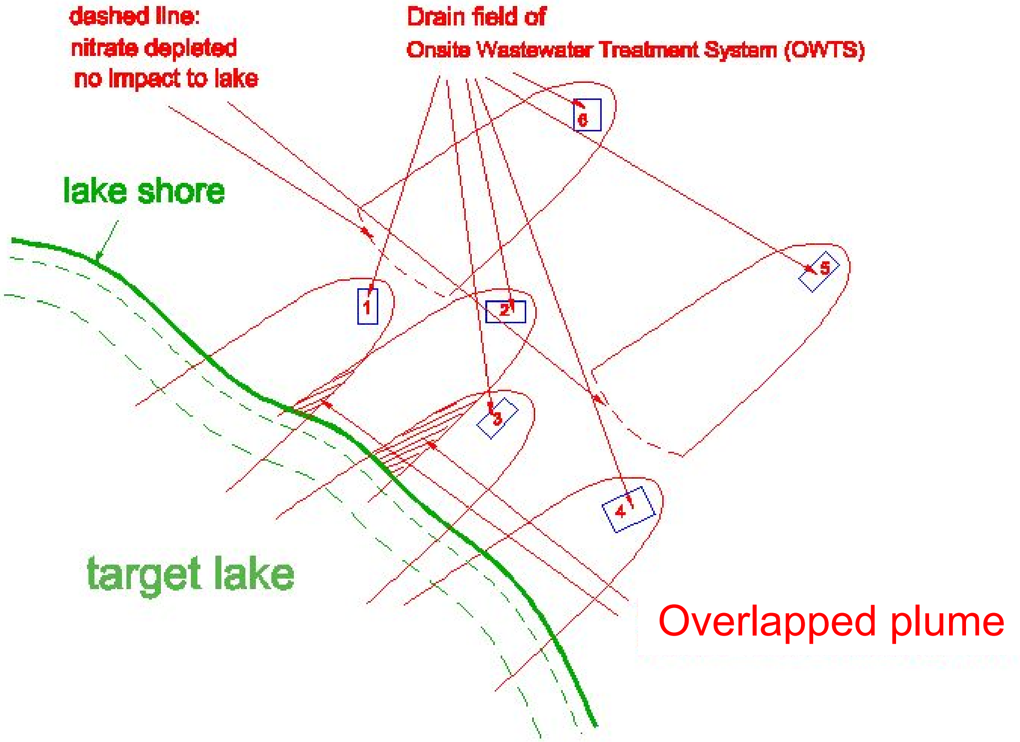
Groundwater Flow Modeling

- Steady-state flow
- Hydraulic conductivity

  Given parameters to ArcNLET
- Hydraulic head
  - Treat water table as subdued replica of the topography
  - Process topographic data and approximate hydraulic gradient using the topographic gradient



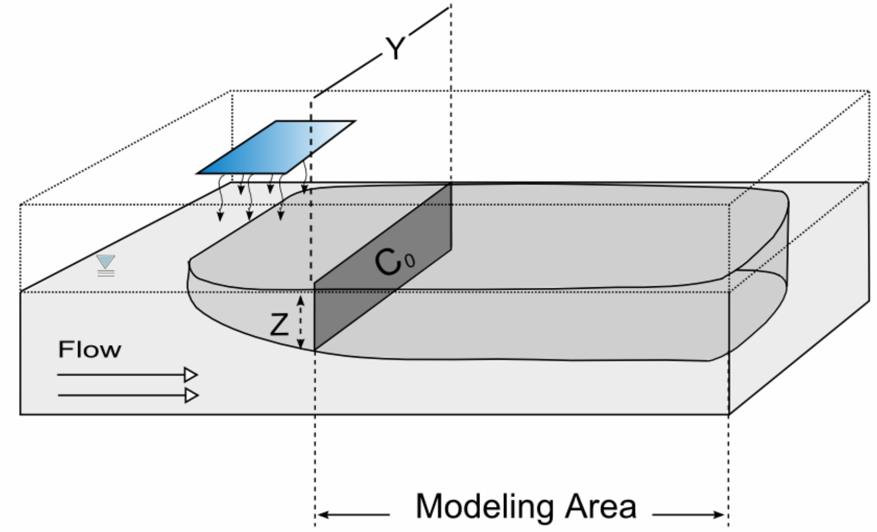
Outputs of Groundwater Flow Modeling



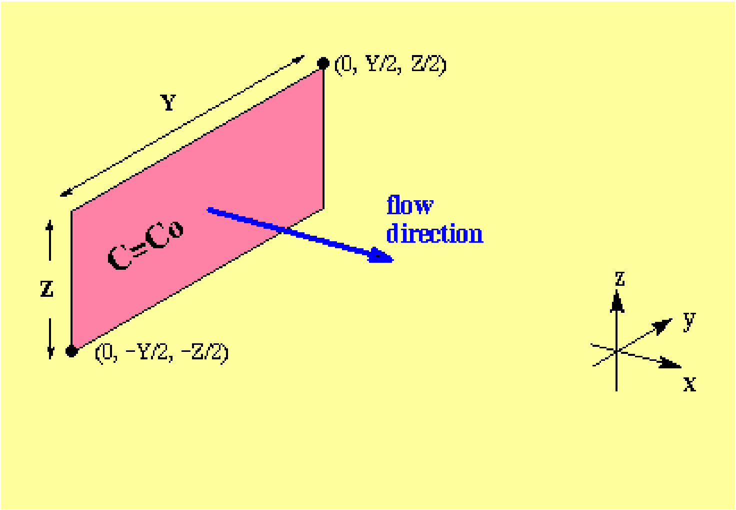
- Flow paths from each septic tank to surface water bodies
- Flow velocity along the flow paths. Heterogeneity of hydraulic conductivity and porosity is considered.
- Travel time from septic tanks to surface water bodies

Nitrate Transport Modeling

EPA BIOCHLOR model



Domenico analytical solution



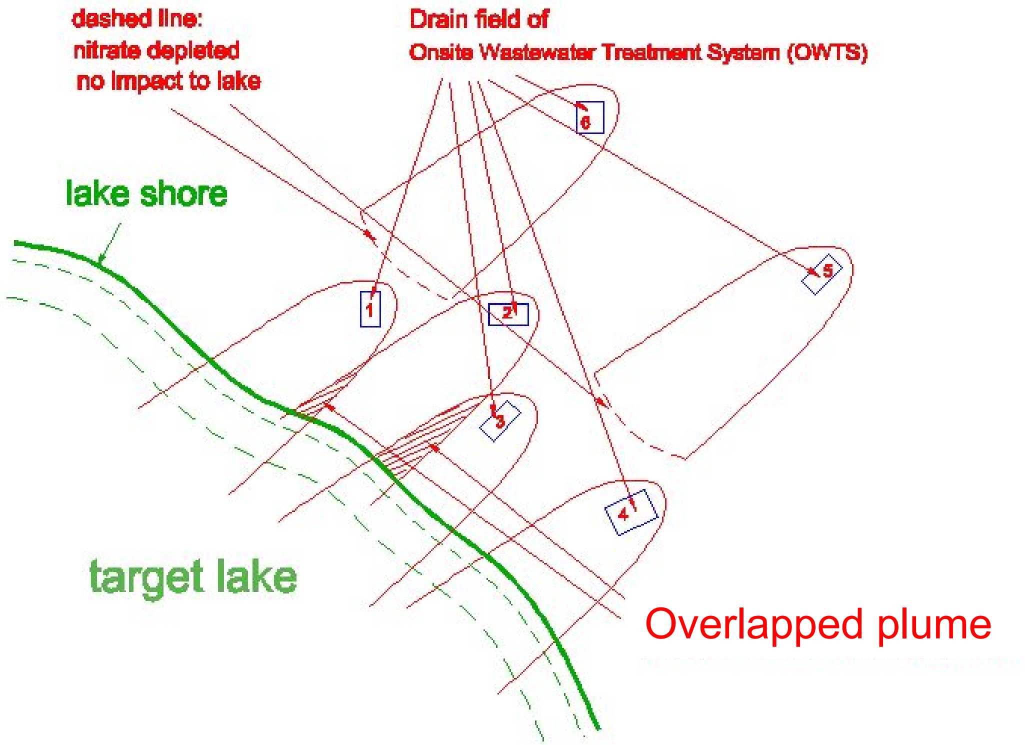
$$\frac{\partial C}{\partial t} = \underbrace{\alpha_\ell v \frac{\partial^2 C}{\partial x^2} + \alpha_{T_h} v \frac{\partial^2 C}{\partial y^2} + \alpha_{T_v} v \frac{\partial^2 C}{\partial z^2}}_{\text{Dispersion}} - \underbrace{v \frac{\partial C}{\partial x}}_{\text{Advection}} - \underbrace{kC}_{\text{Decay}}$$

$\boxed{\text{Denitrification}}$

$$C(x, y, z, t) = \frac{C_0}{8} F_1(x, t) F_2(y, x) F_3(z, x)$$

Outputs of Nitrate Transport Modeling and Calculation of Nitrate Load

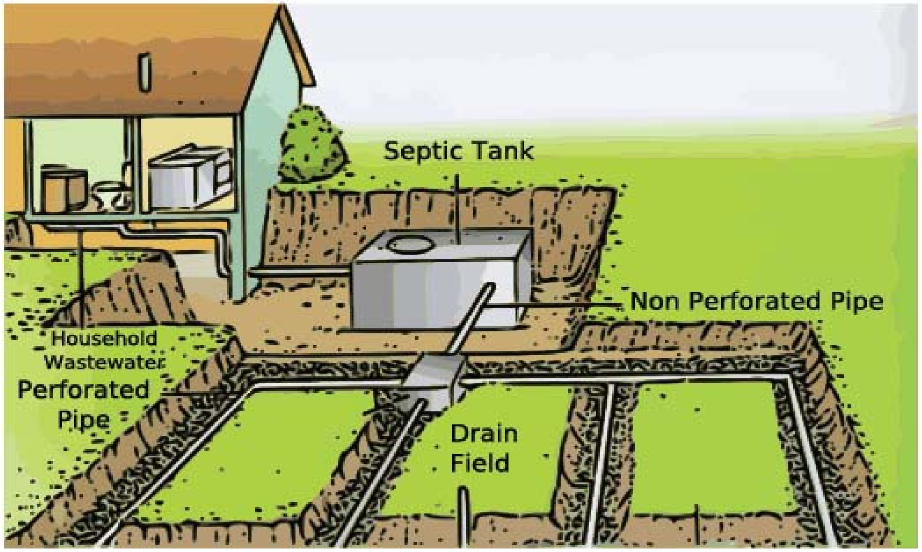
- Apply the analytical solution to each septic tank.
- Obtain the nitrate plume of the entire area.
- Calculate mass of inflow and denitrification.
- Calculate load to rivers



$$M_{out} = M_{in} - M_{dn}$$

$$M_{dn} = R_{dn} V_g = kCVg$$

Questions?


Septic Tank
Non Perforated Pipe
Household
Wastewater
Perforated
Pipe
Drain
Field