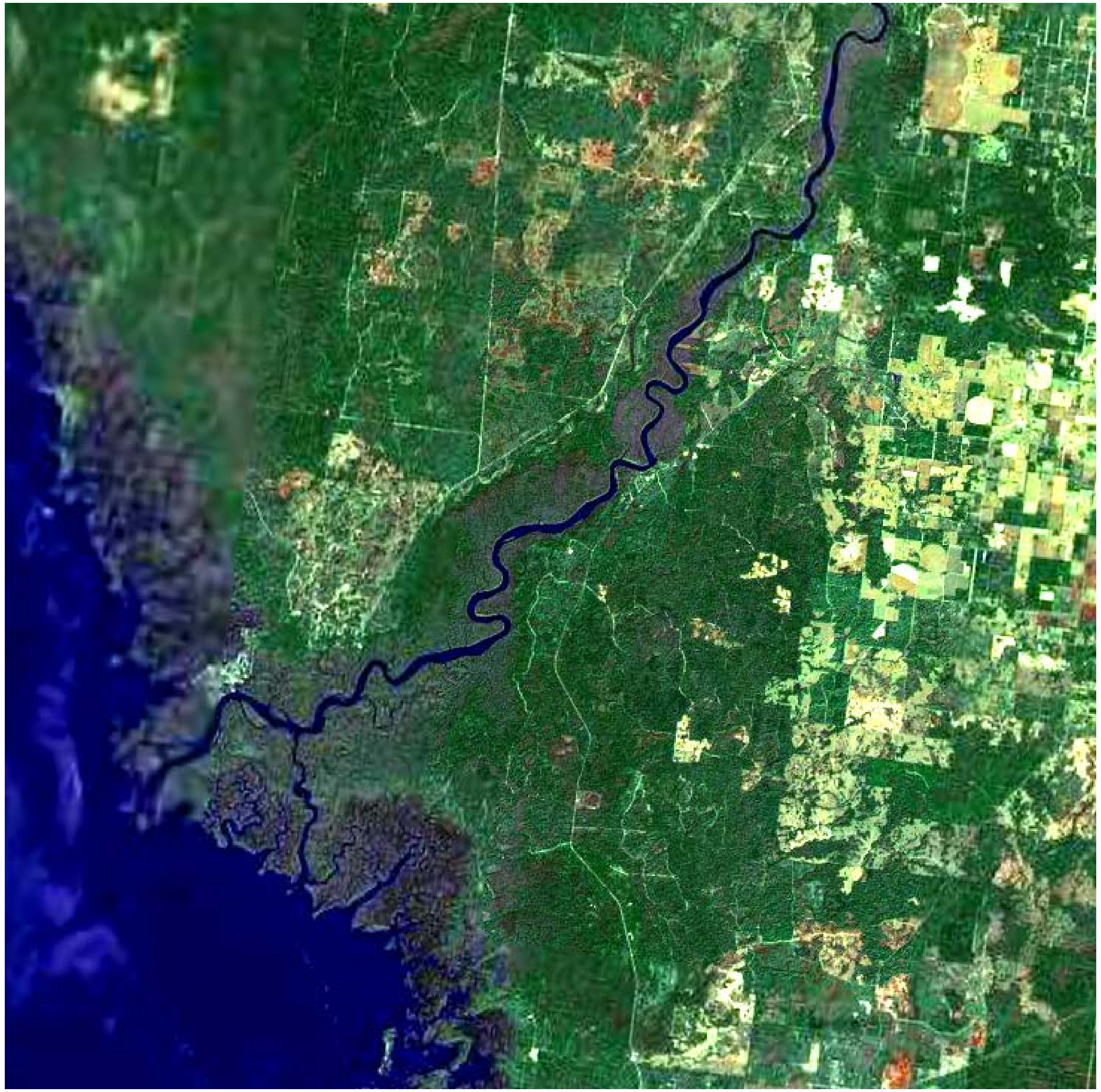
Today’s agenda

- Regional groundwater flow
- Groundwater chemistry

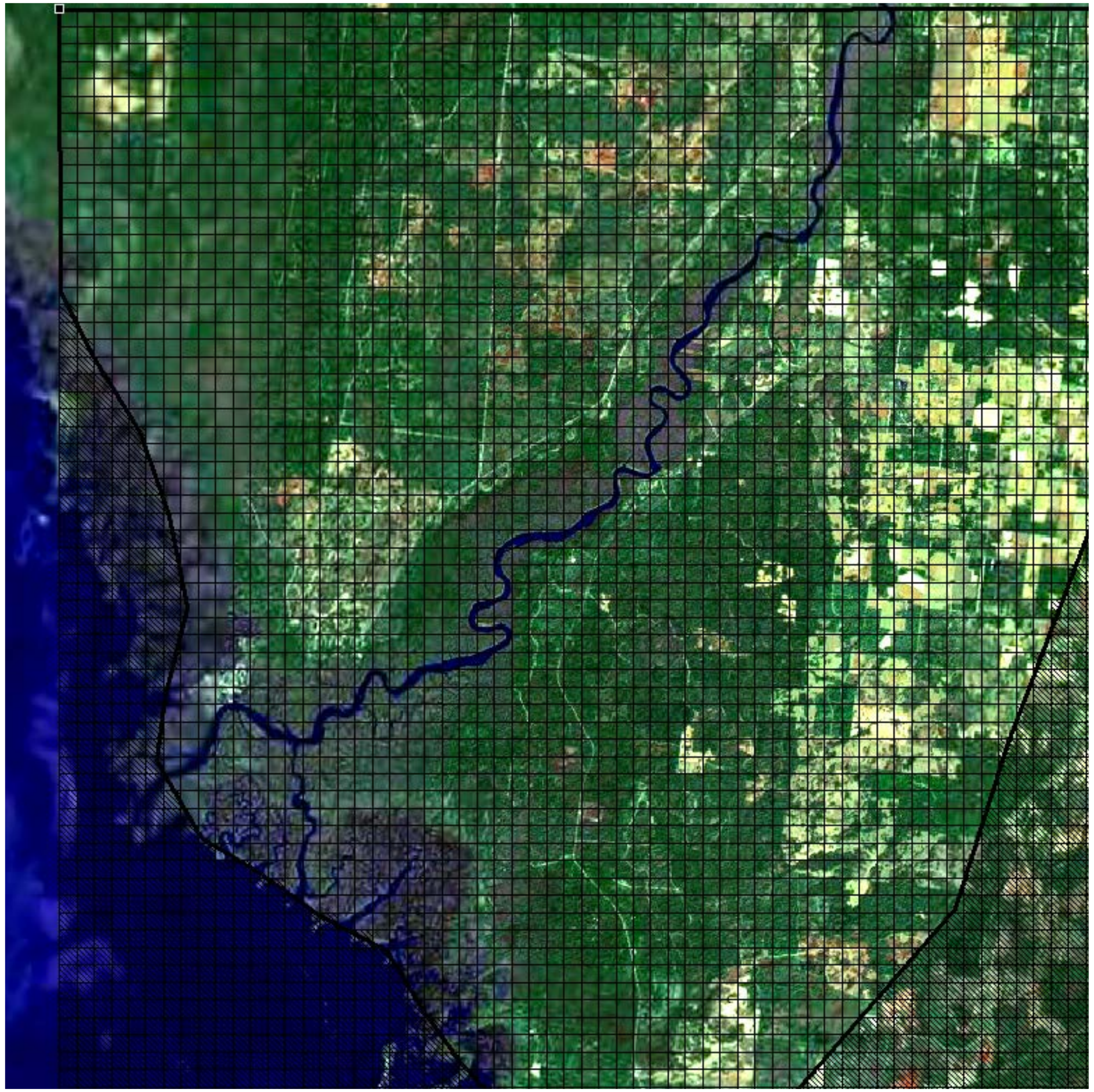
A Numerical Groundwater Model:

Start with a real system

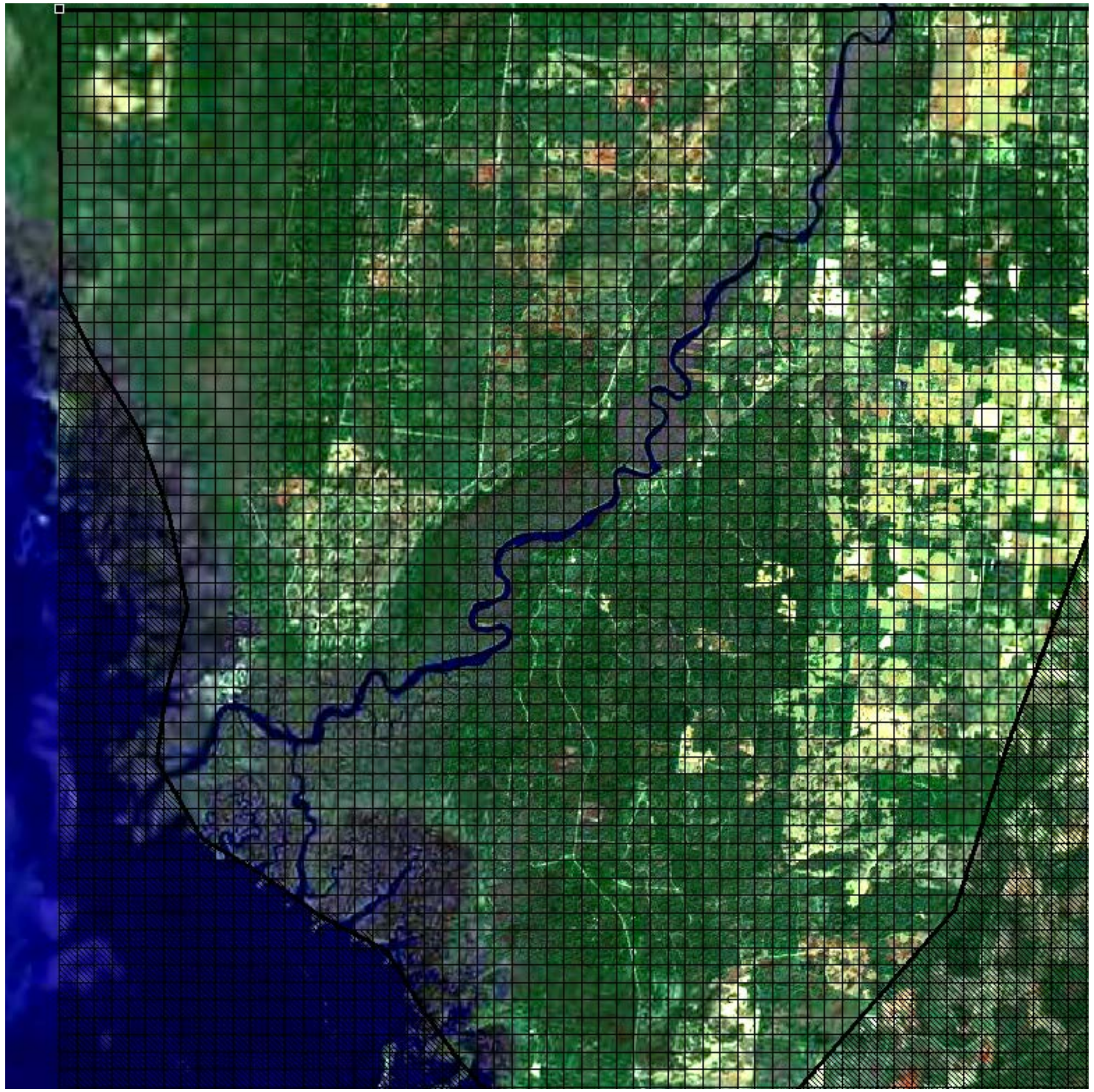


A Numerical Groundwater Model:

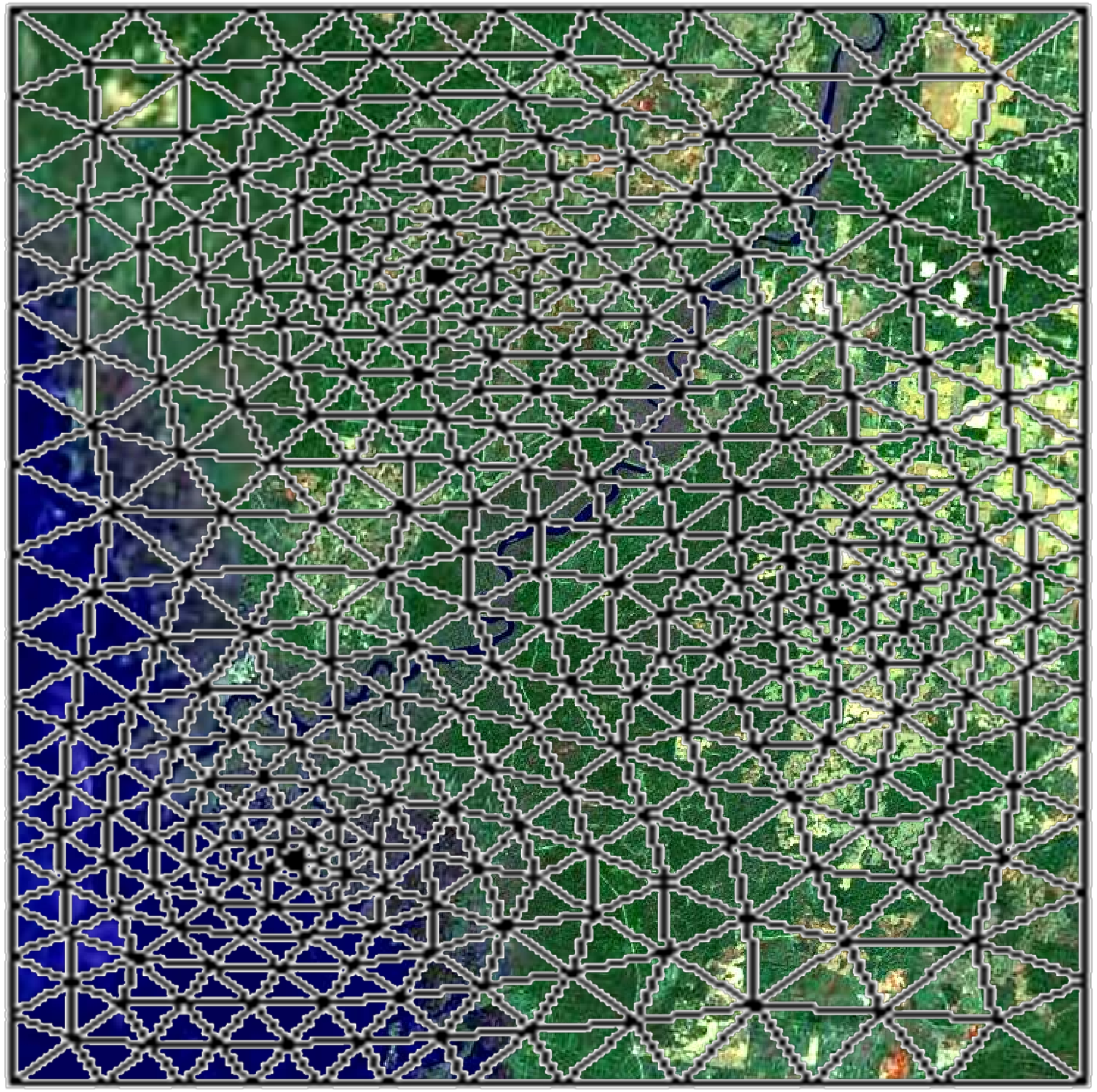
Break it up in space
(and time)



A Numerical Groundwater Model:

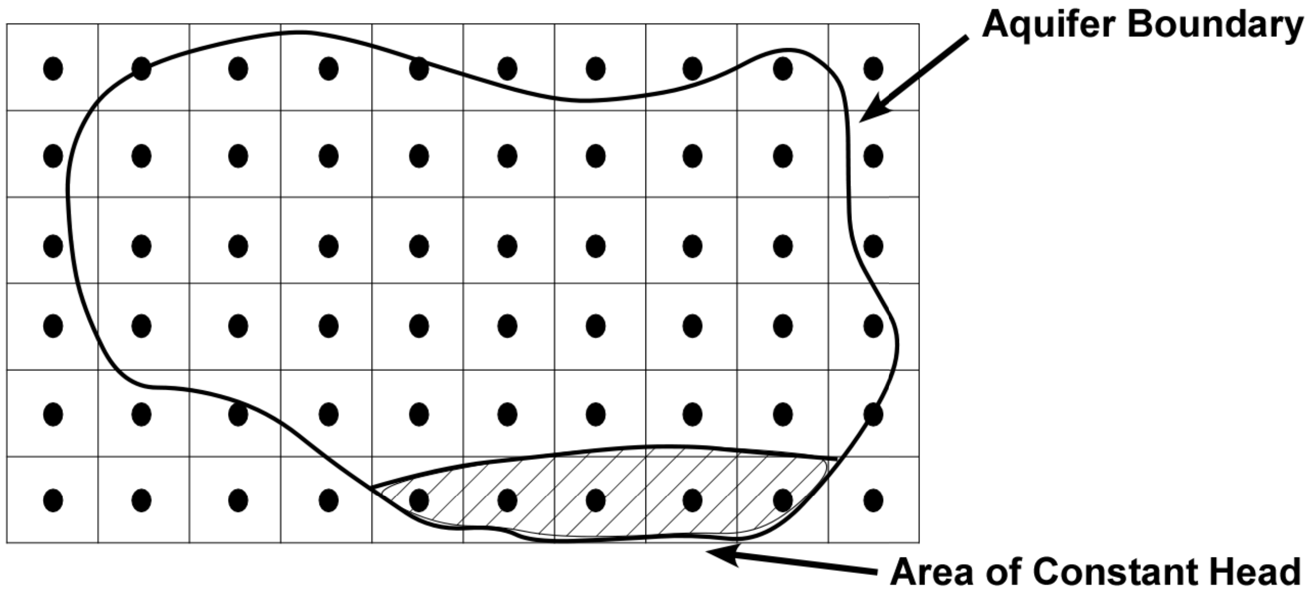


Finite Difference



Finite Element

Discretization

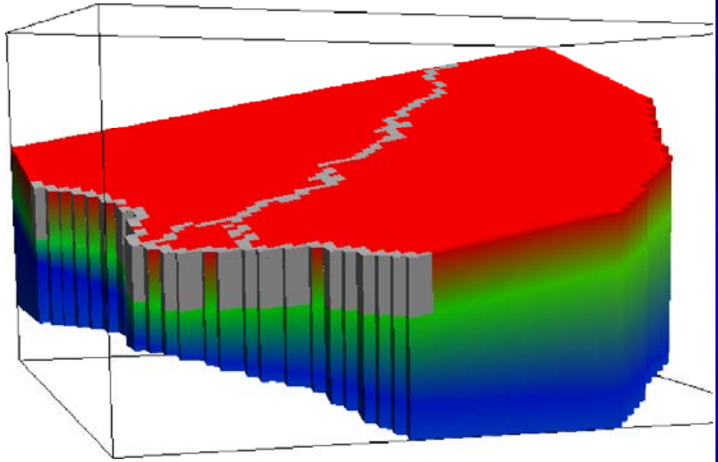


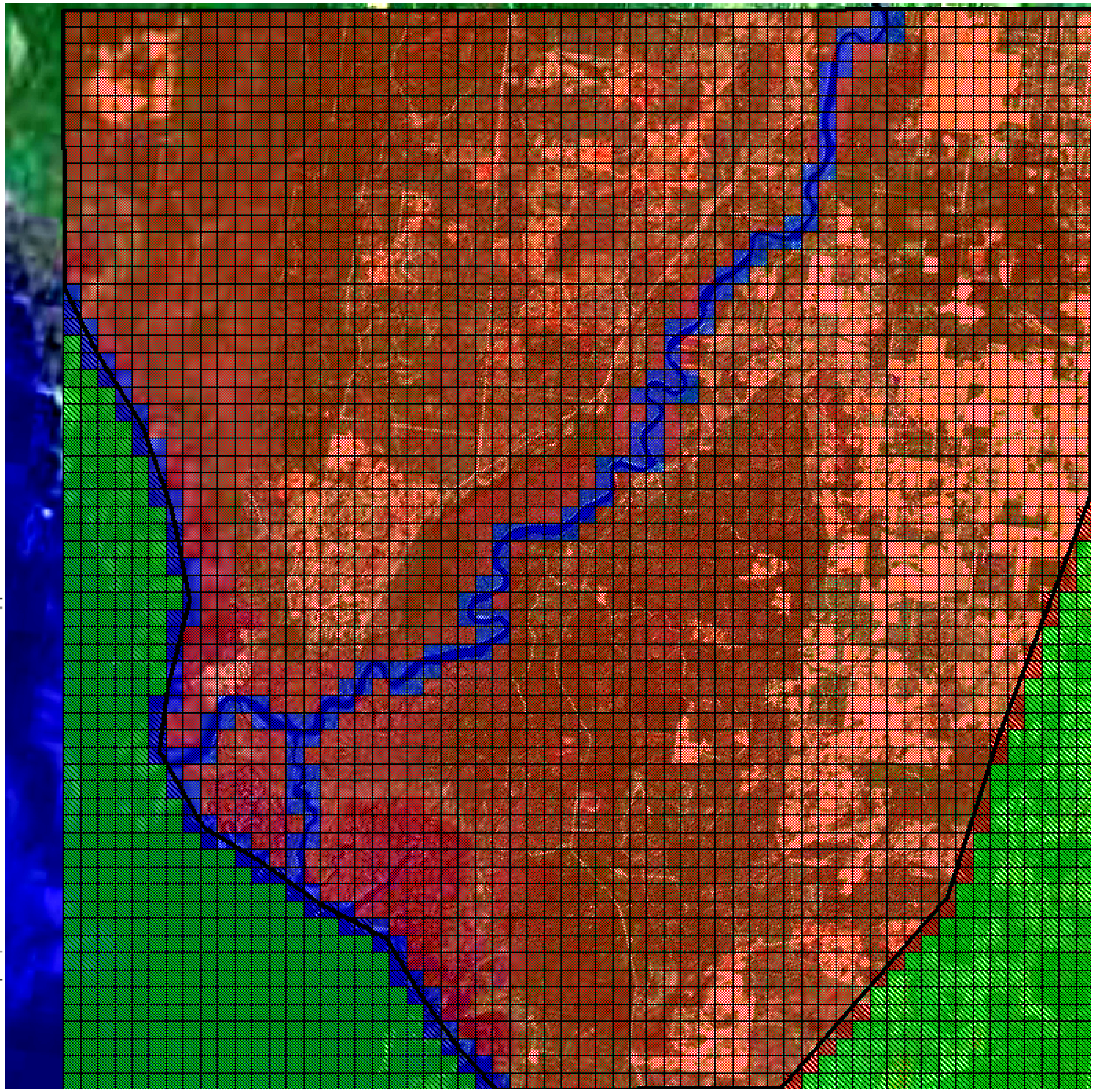
0	1	1	1	1	0	0	0	1	0
0	1	1	1	1	1	1	1	1	0
0	1	1	1	1	1	1	1	1	0
0	1	1	1	1	1	1	1	1	1
0	0	0	1	1	1	1	1	1	1
0	0	0	0	-1	-1	-1	-1	-1	0

A Numerical Groundwater Model:

Assign Parameter Values and Boundary Conditions

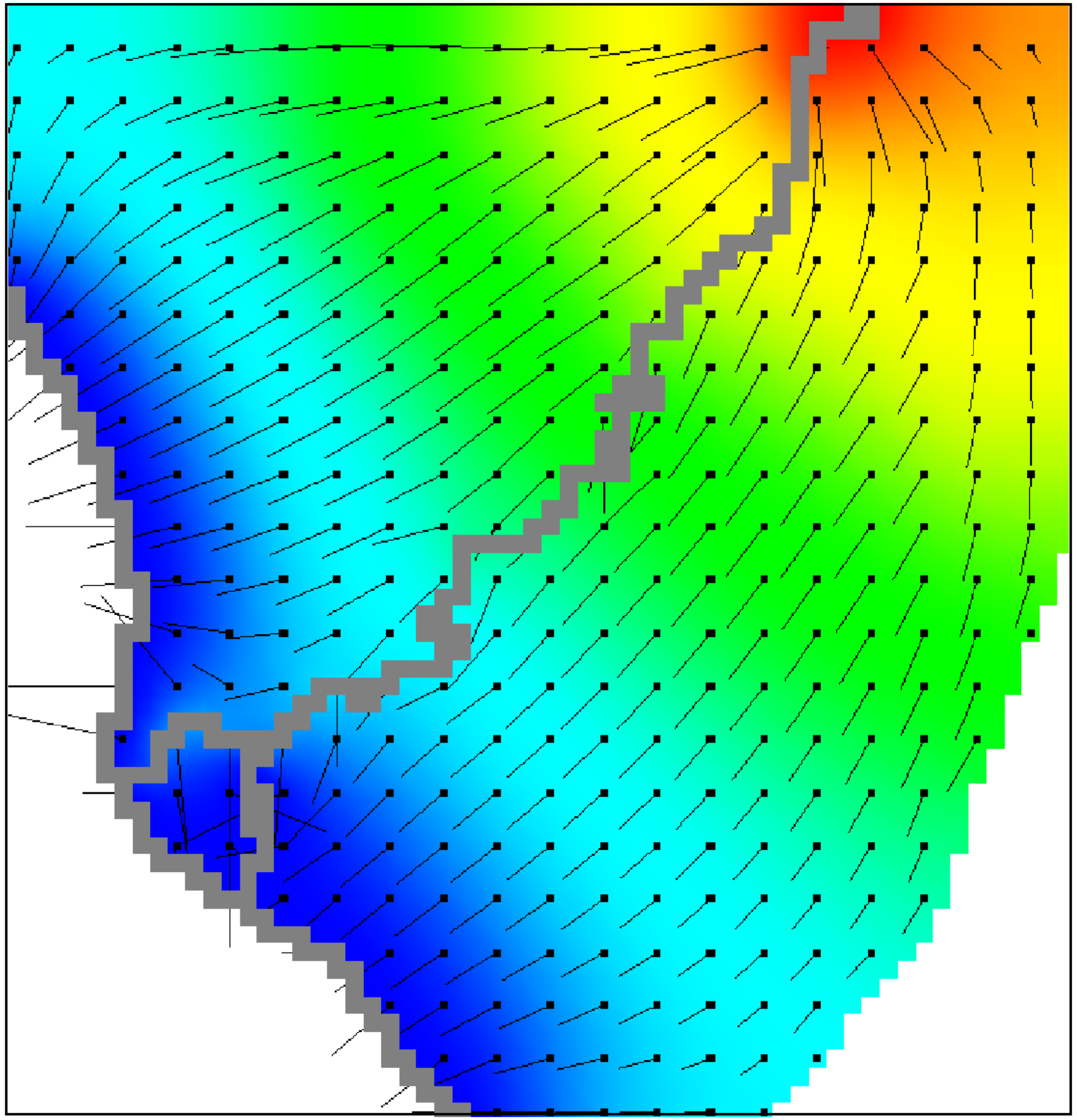
(based on knowledge of the system)



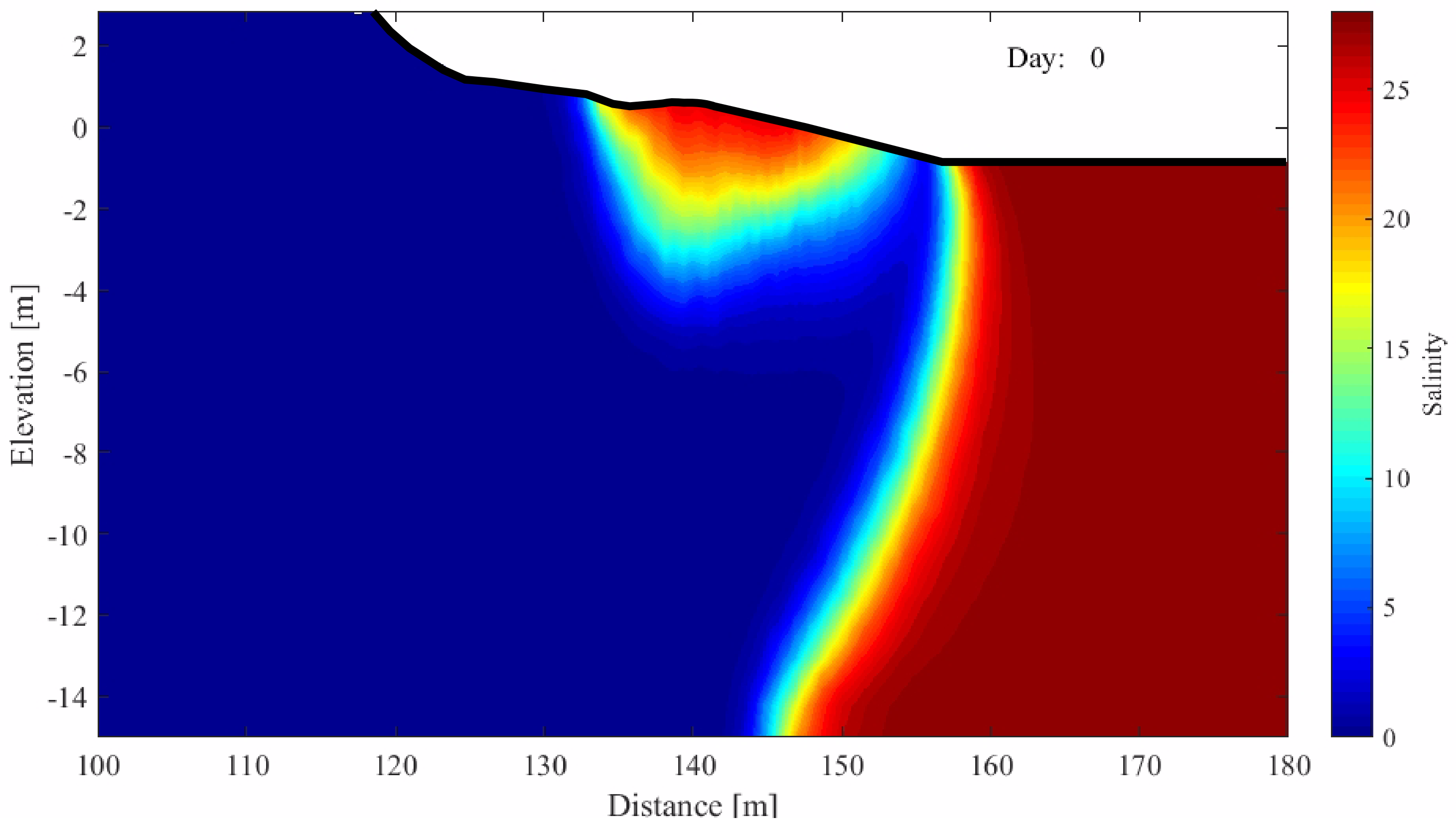


A Numerical Groundwater Model:

Analyze Results



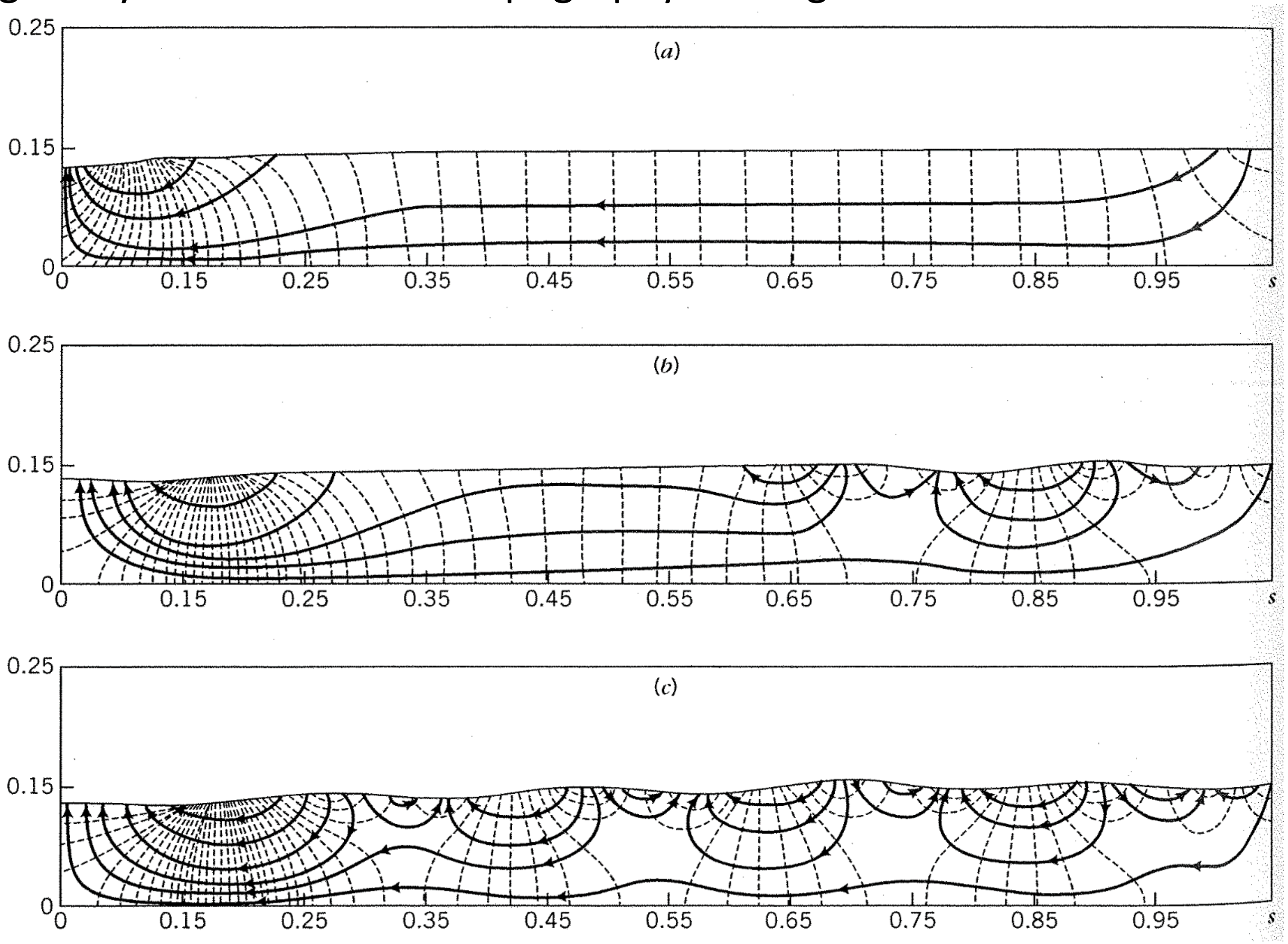
Tidal, spring-neap, and seasonal salinity dynamics



Freeze and Witherspoon (1967)

How does heterogeneity AND water table topography affect groundwater flow?

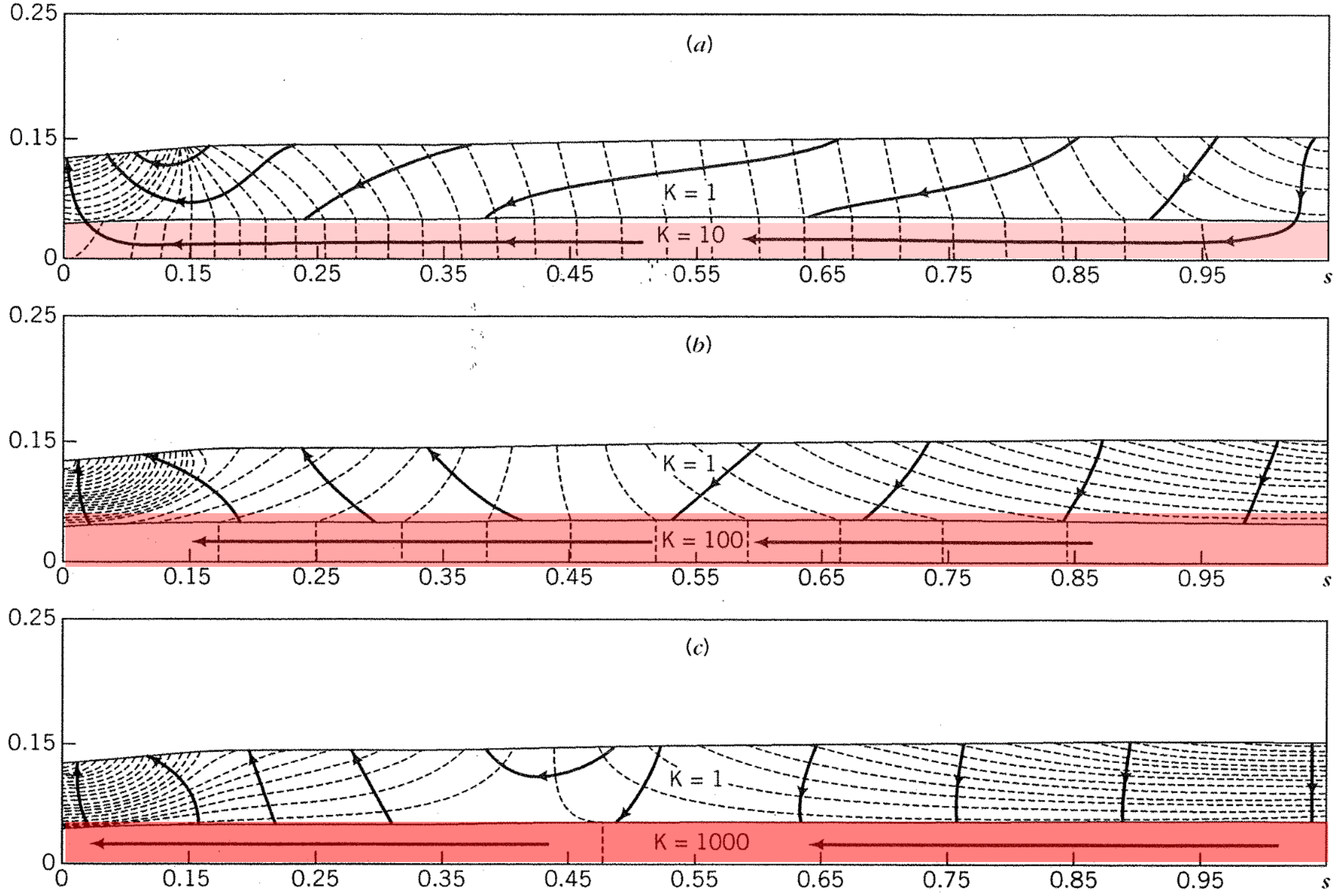
Increasing topographic complexity



Freeze and Witherspoon (1967)

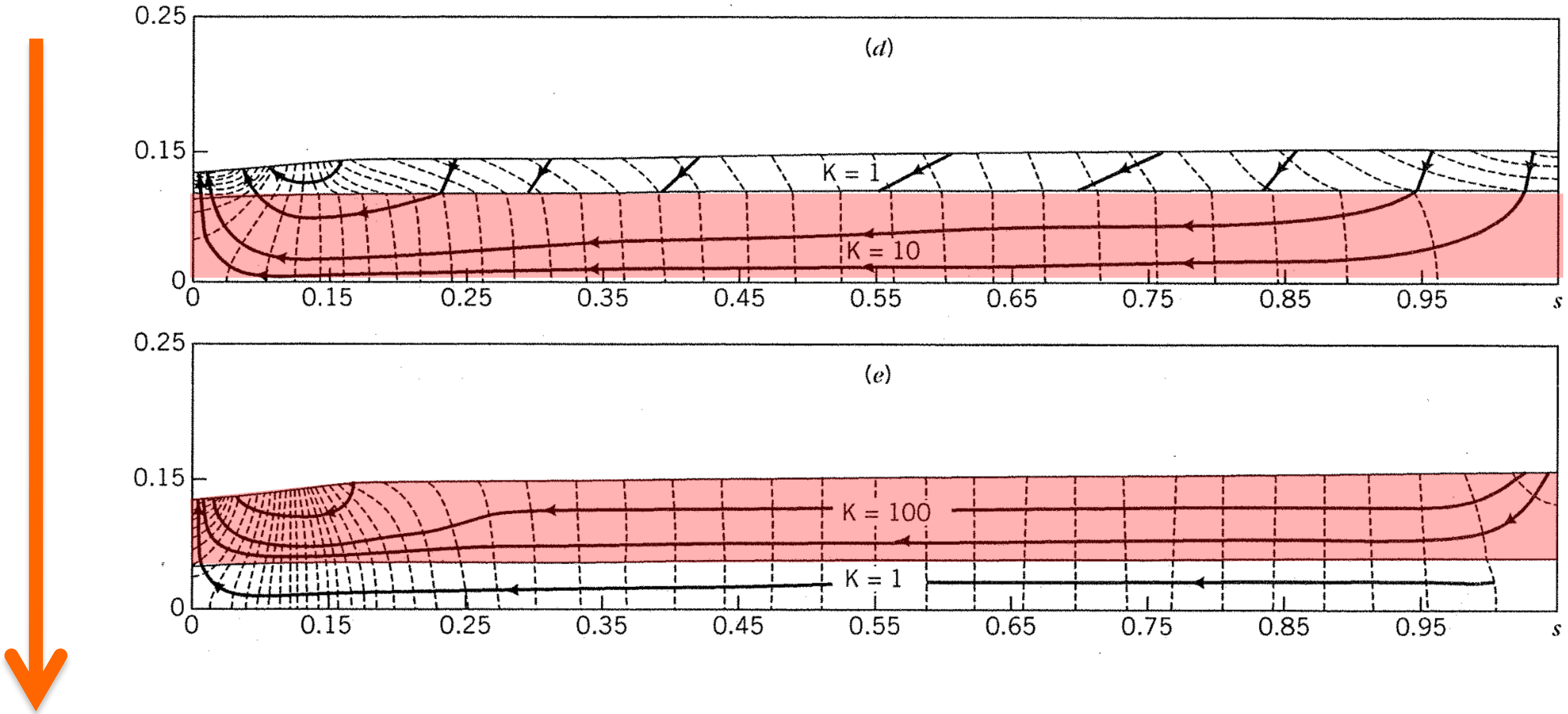
Confined HIGH K unit;

Increasing differences in K between units

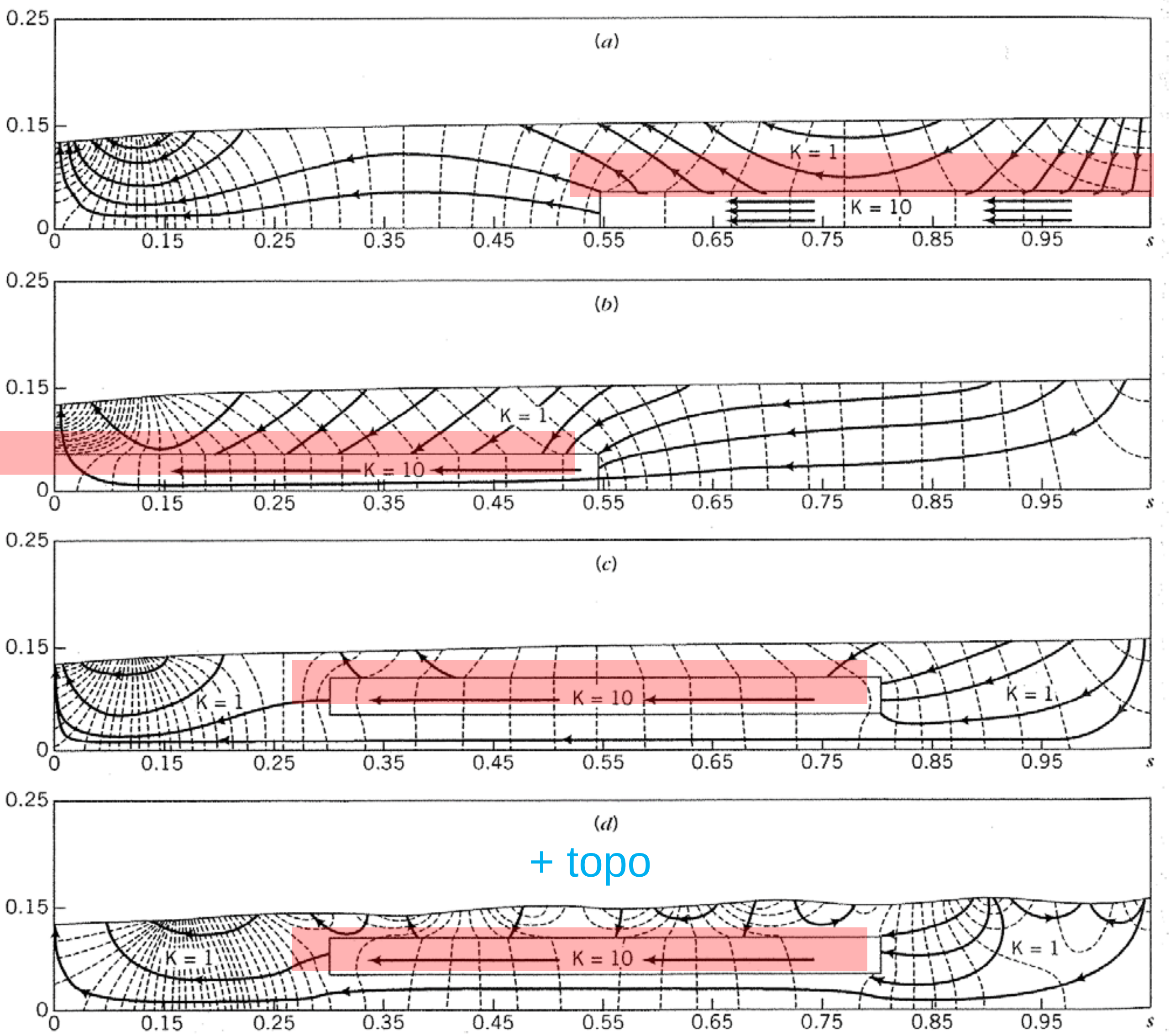


Freeze and Witherspoon (1967)

More permeability contrasts between units:



Freeze and Witherspoon (1967)



TopoDrive and ParticleFlow

http://water.usgs.gov/nrp/gwsoftware/tdpf/tdpf.html

http://pre03.deviantart.net/d066/th/pre/i/2004/175/3/0/wet_newspaper.jpg

Groundwater in the News

The New York Times

Is Poland Spring Water Really From a Spring? 'Not One Drop,' Says a Lawsuit

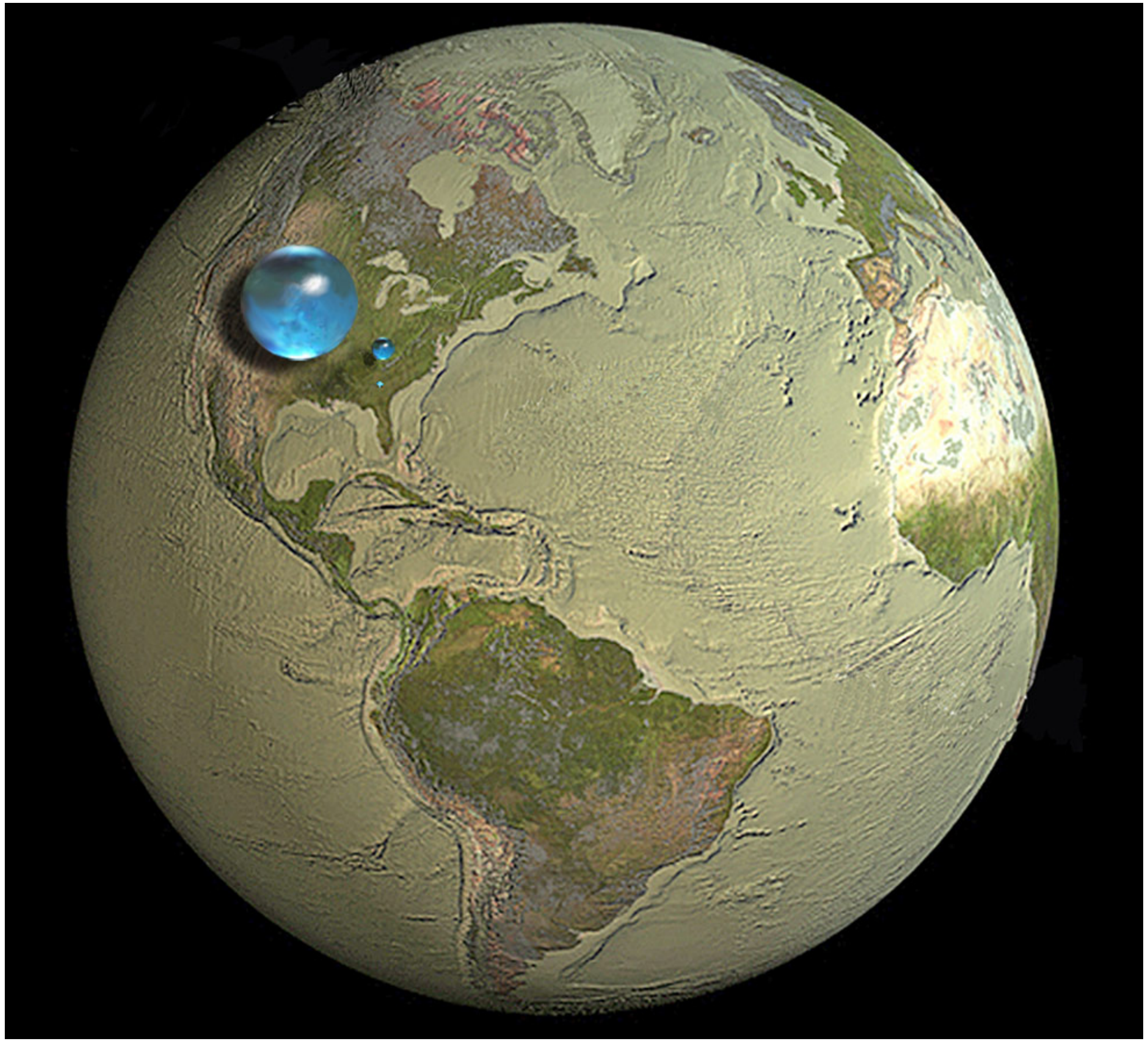
Poland Spring water on display at a grocery store in Tarrytown, N.Y. A lawsuit accuses Nestlé Waters of having fraudulently marketed it as "spring water" when it is not.
Jennifer S. Altman for The New York Times

By Matt Stevens

74 W ater
6 C hemistry 1

(Nothing illicit here)

Why study water chemistry?



Credit: Howard Perlman, USGS; globe illustration by Jack Cook, Woods Hole Oceanographic Institution (©); Adam Nieman. Data source: Igor Shiklomanov's chapter "World fresh water resources" in Peter H. Gleick (editor), 1993, Water in Crisis: A Guide to the World's Fresh Water Resources (Oxford University Press, New York).

Why study water chemistry?

Water chemistry can tell us:

- If water is safe to drink
- Where the water came from
- How ‘old’ the water is

Water is a strange substance

Water is a ‘polar’ molecule

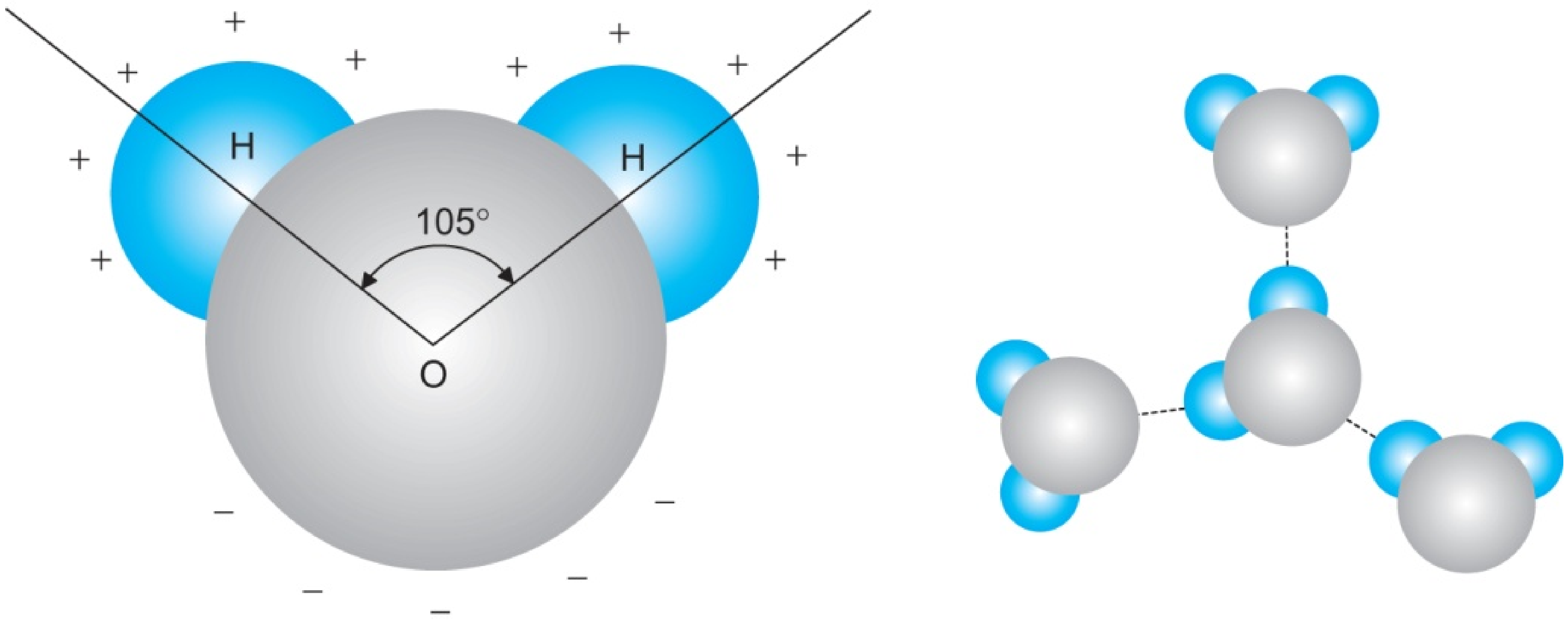
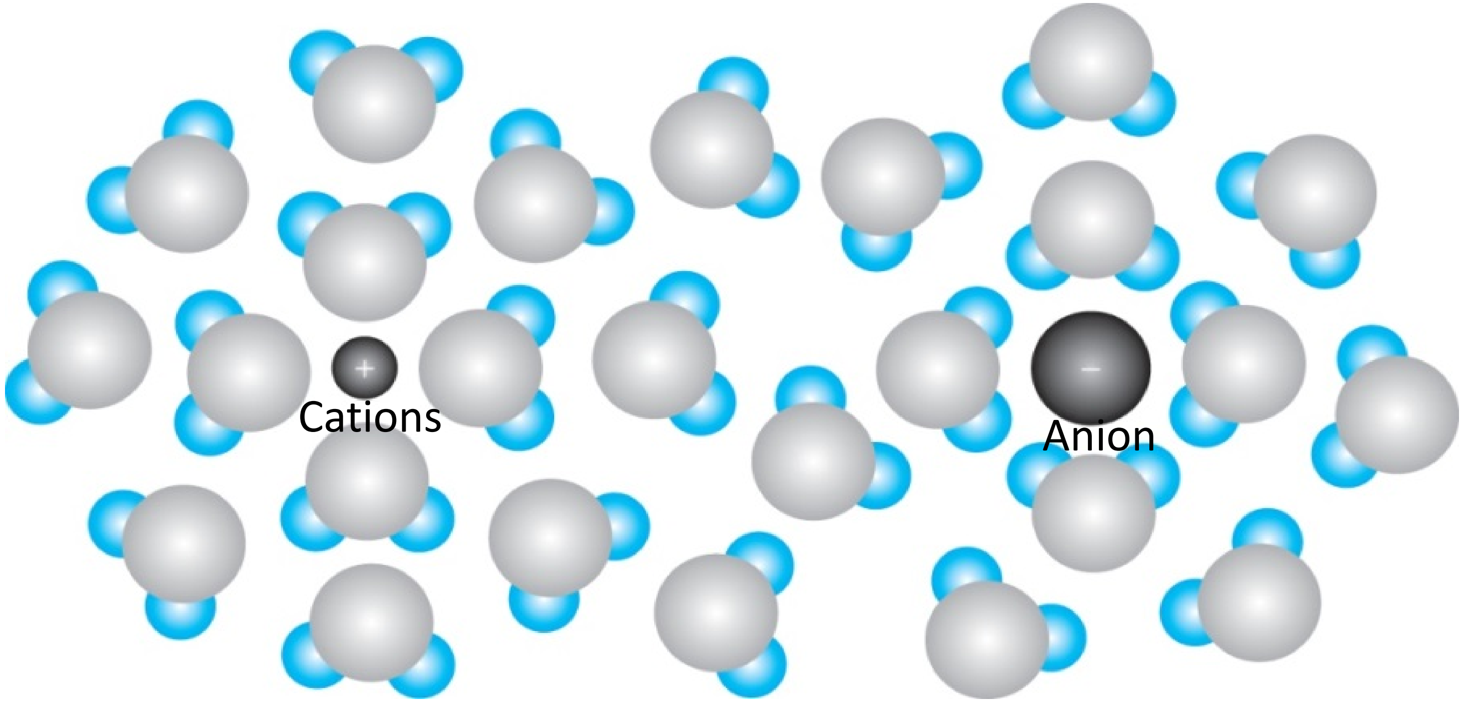


Figure 10.1 Geometry of a water molecule (left) and hydrogen bonding of water molecules (right).

Cations and ions

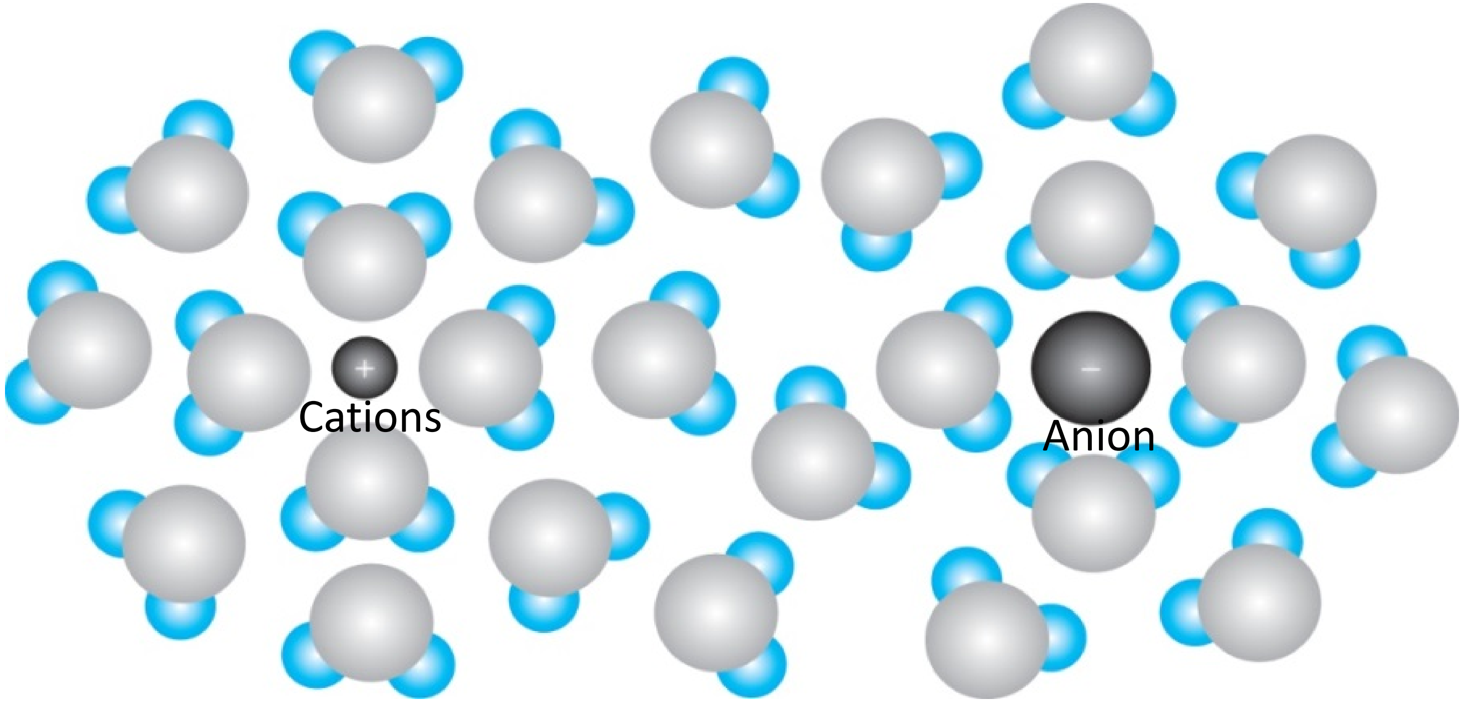
Natural waters are really water based (aqueous) solutions with other elements and compounds (solutes) within the water (solvent)



Polarity and water as a solvent

The polar nature of water makes it an excellent 'solvent'

(a liquid that can dissolve a solute, resulting in a solution)



Stoichiometry and concentration

Stoichiometry deals with reactants and products in (balanced) chemical equations.

e.g.

$$NaCl_{(s)} \rightarrow Na^{+}_{(aq)} + Cl^{-}_{(aq)}$$

Sodium chloride
(as a solid)

Sodium ion
(positive, in aqueous solution)

Chloride ion
(negative, in aqueous solution)

Major Ions (typically > 5 mg/l)

- Calcium (Ca^{2+})
- Magnesium (Mg^{2+})
- Sodium (Na^{+})
- Potassium (K^{+})

Cations (+)

- Sulfate (SO_4^{2-})
- Chloride (Cl^{-})
- Bicarbonate (HCO_3^{-})
- Carbonate (CO_3^{2-})

Anions (-)

Lots of variability between areas, but STILL only ~7-8 ions are found in high concentrations in natural waters

These ions account for 90% of dissolved solids

Units can be expressed in a number of ways

Mass per volume

- g/L or mg/L
- mol/L or mmol/L

Mass per mass

- g/kg or mg/kg
- ppm or ppb

Mass per volume

- g/L or mg/L
- mol/L or mmol/L

Moles

A mole is the amount of a substance (element or compound) containing 6.022×10^{23} atoms.

For example:

2.5 M Ca^{2+} is shorthand for 2.5 mol/L

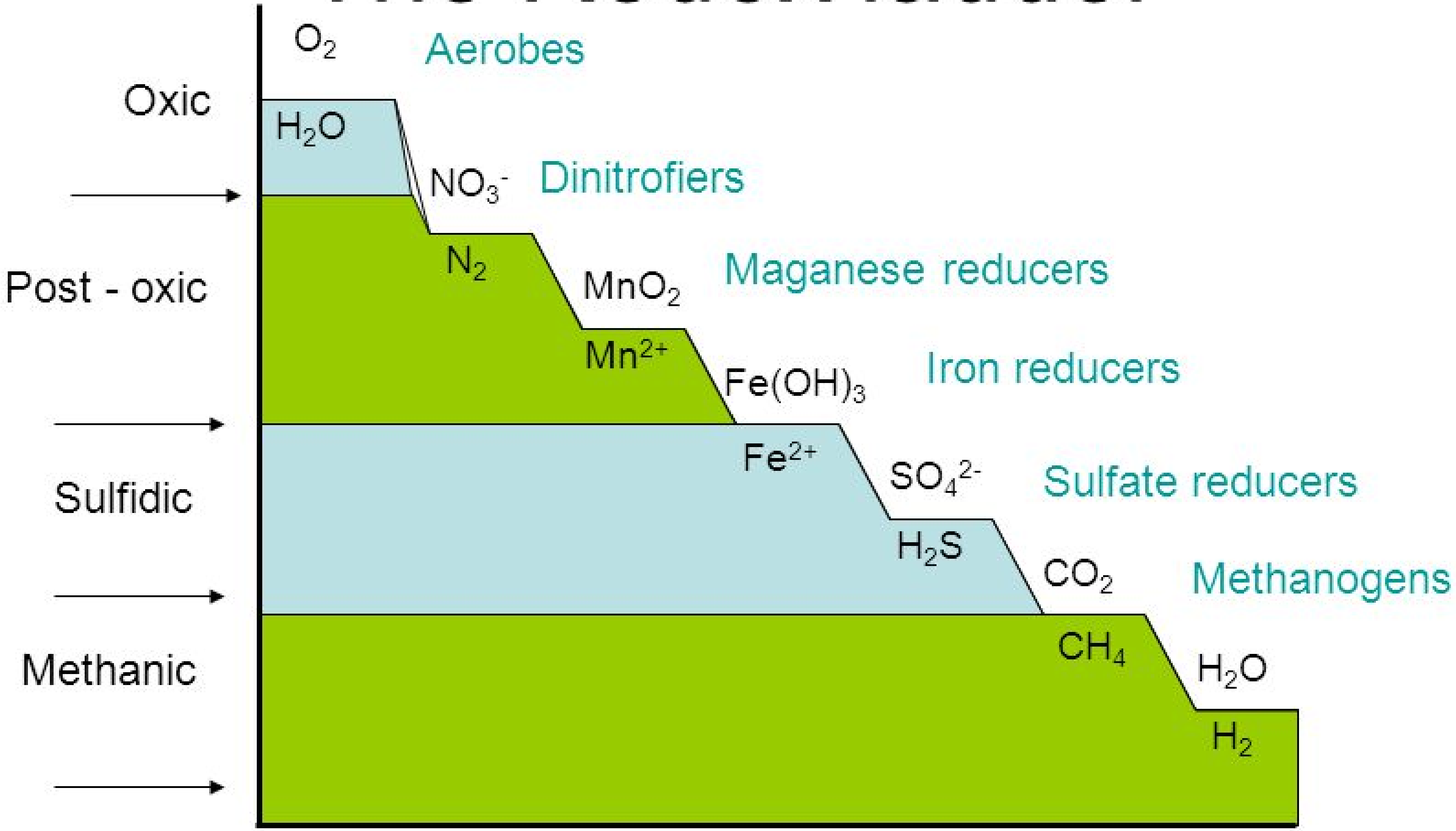
M = Molar = mol/L

Biogeochemistry

Biogeochemistry

- The metabolism of all organisms involves the electron transport chain
- The electron transport chain occurs inside the mitochondria and is responsible for maintaining a proton gradient that allows ATP to be generated inside the cell.
- Must have an electron acceptor and a electron donor as part of the electron transport chain

The Redox ladder



The redox-couples are shown on each stair-step, where the most energy is gained at the top step and the least at the bottom step. (Gibb's free energy becomes more positive going down the steps)

Nitrogen Cycle

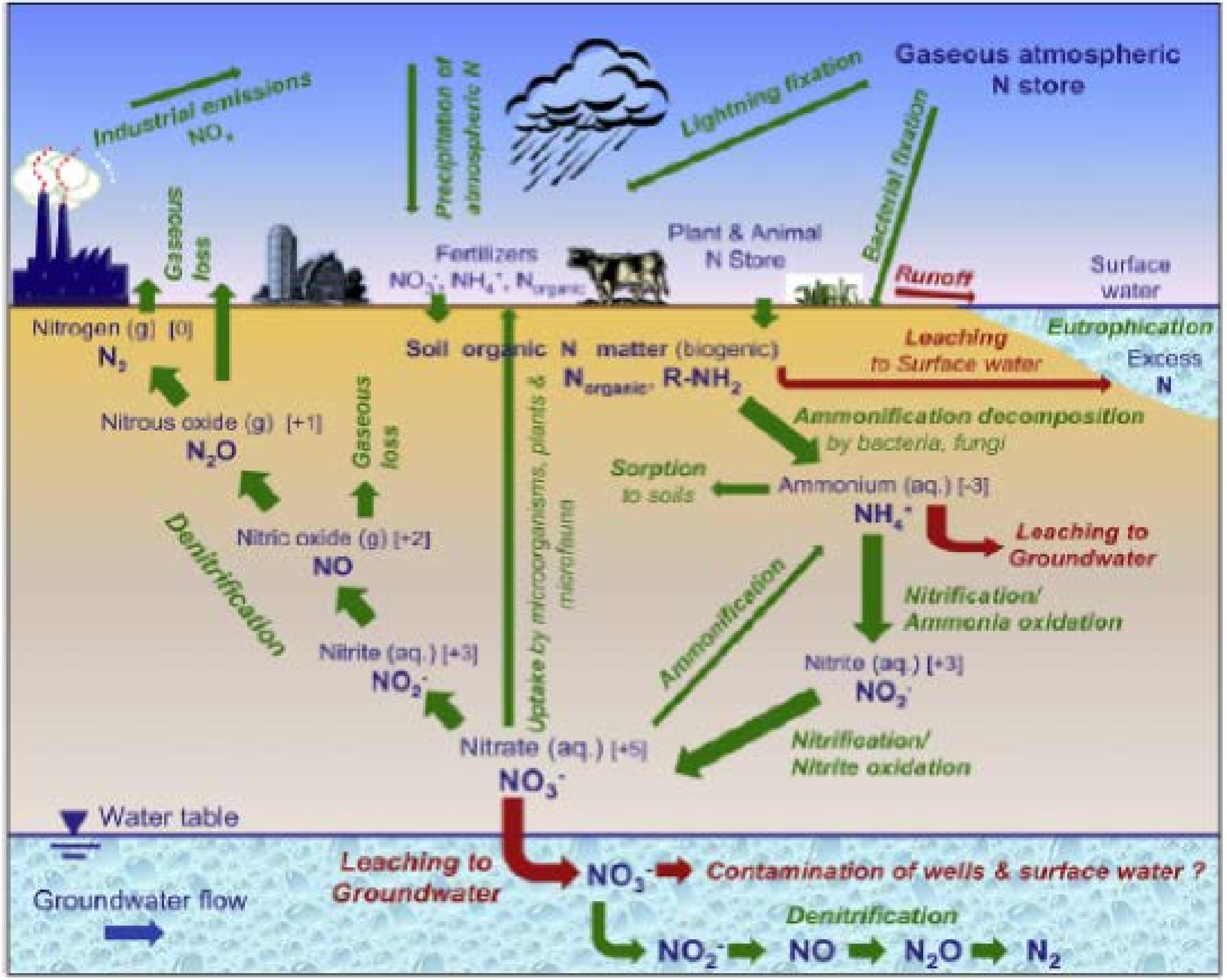


Figure 1. Microbial nitrogen cycle and its influence upon the water environment.
Source: Rivett *et al.* (2008).