A Brief Summary of Contaminant Transport in Surface Waters

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How are sunscreens transported?

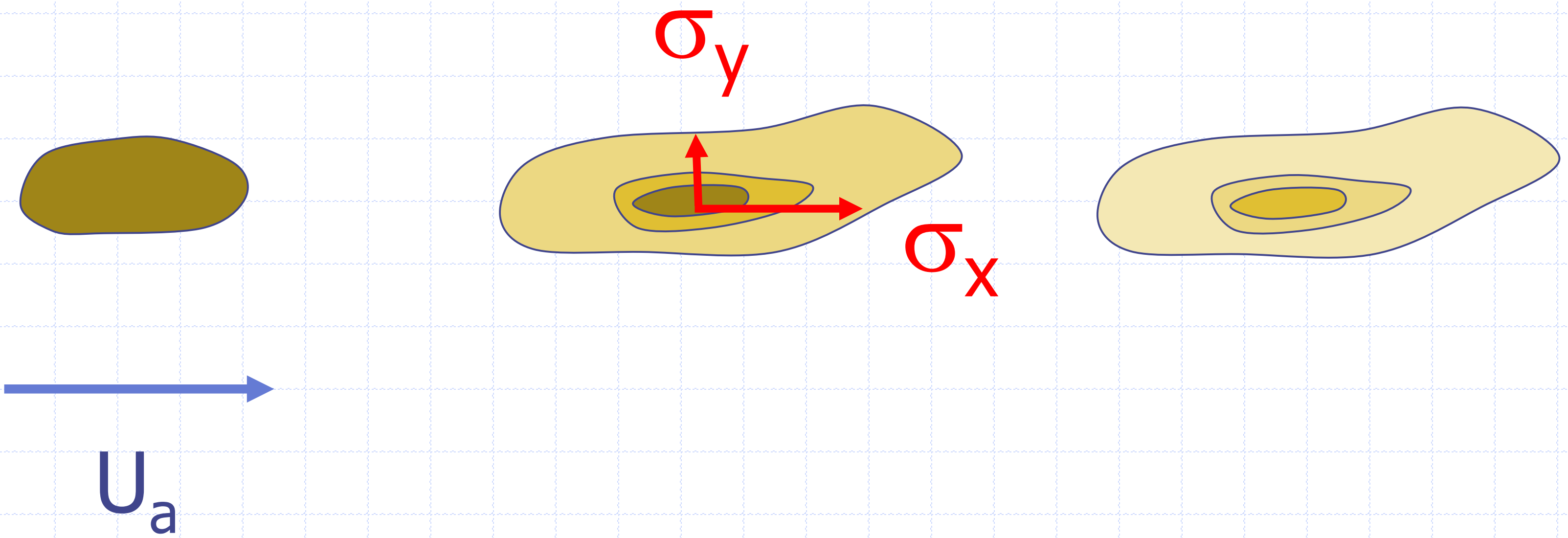
Some sunscreen components are immiscible in water, thus behave as dispersed phase(s).

Their density ~ 1 g/mL, and they form small globules, so they are nearly neutrally buoyant, and are thus transported like water.

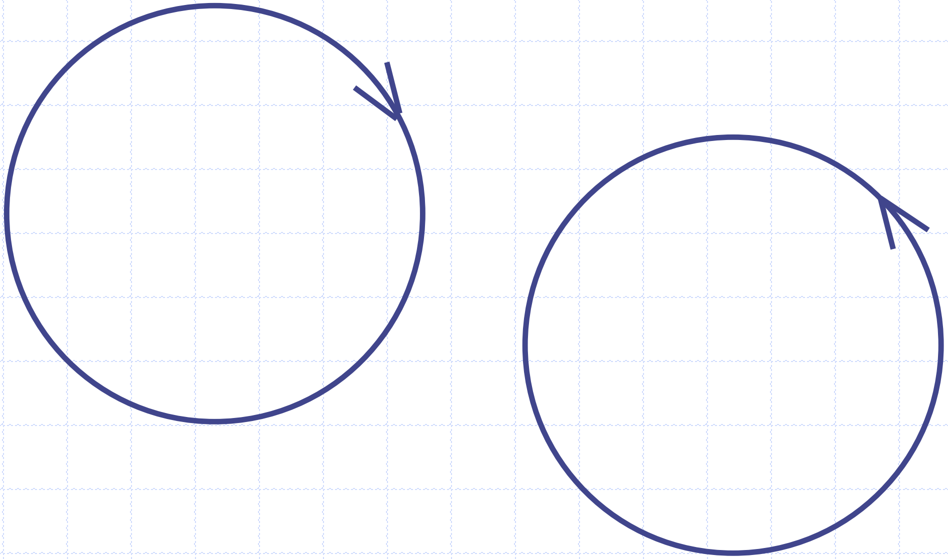
Thus a wide range of water quality models is available to predict transport. Advection Diffusion Reaction equations.

A bit about transport mechanisms, then a bit about models

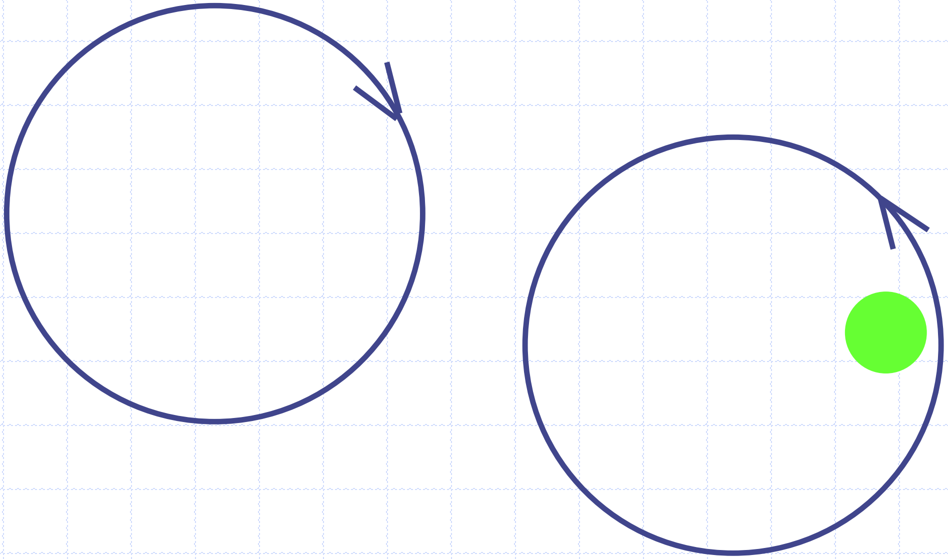
Advection Diffusion/Dispersion Reaction/ Transformation



Relative Diffusion

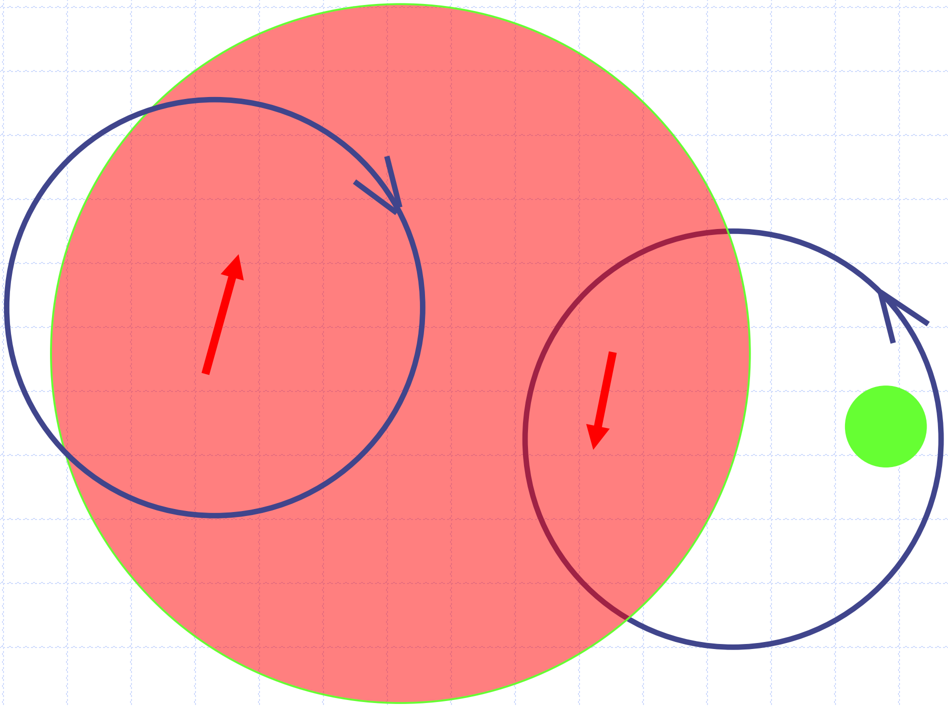


Relative Diffusion



Contaminant patches smaller than eddies are advected.

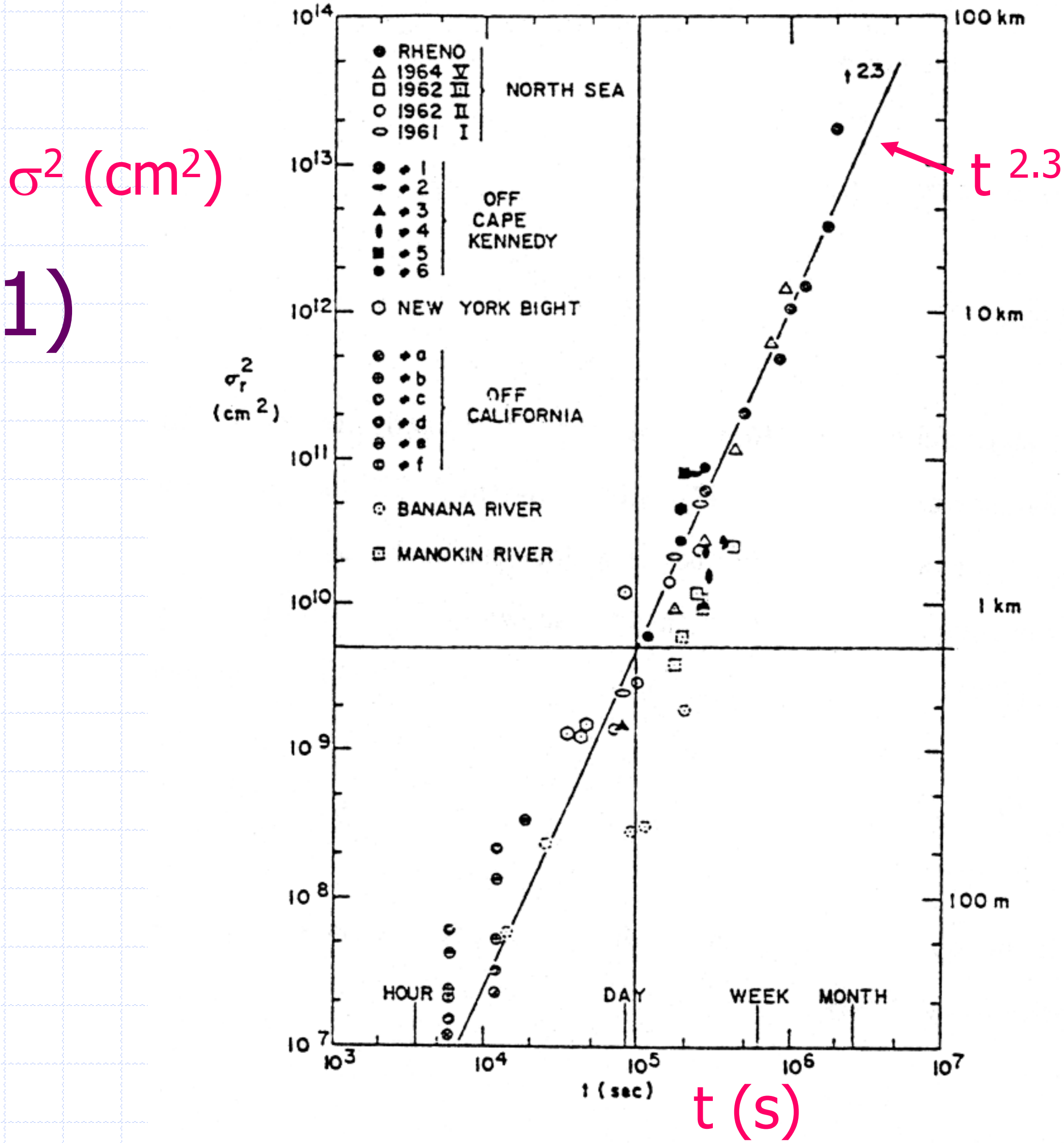
Relative Diffusion



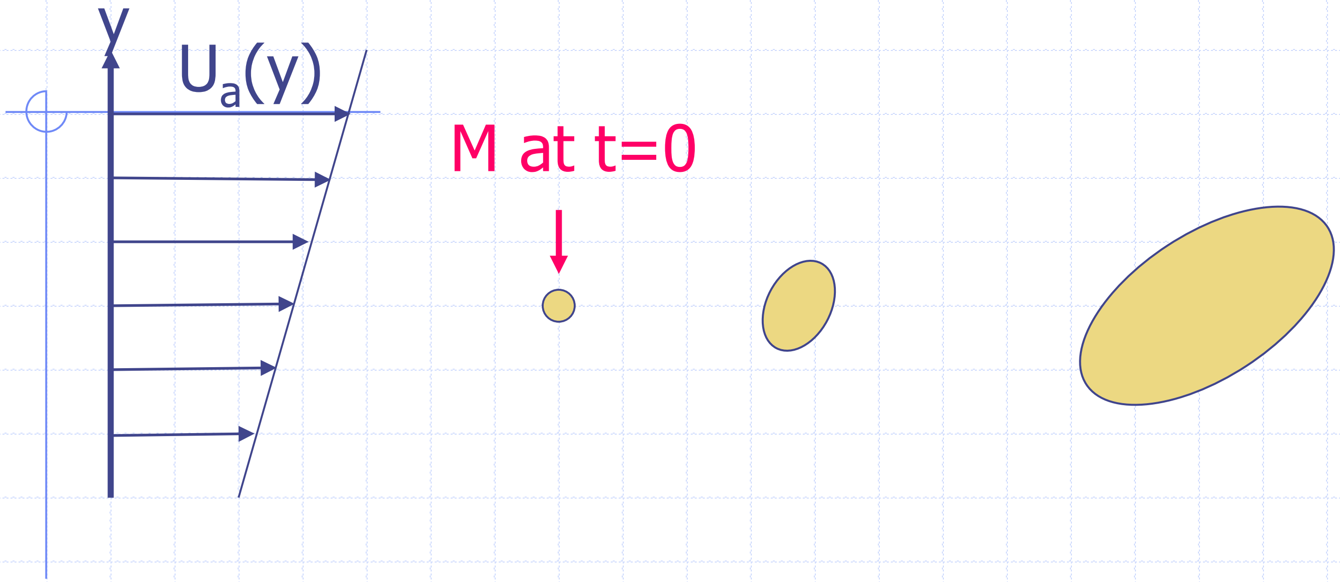
Contaminant patches smaller than eddies are advected.

Contaminant patches larger than eddy are mixed; as patches grow they encounter larger eddies (scale dependent diffusion): $\sigma^2 \sim t^{2.3}$ (Fickian diffusion: $\sigma^2 \sim t^1$)

Horizontal Diffusion Diagram (Okubo 1971)



Shear Dispersion

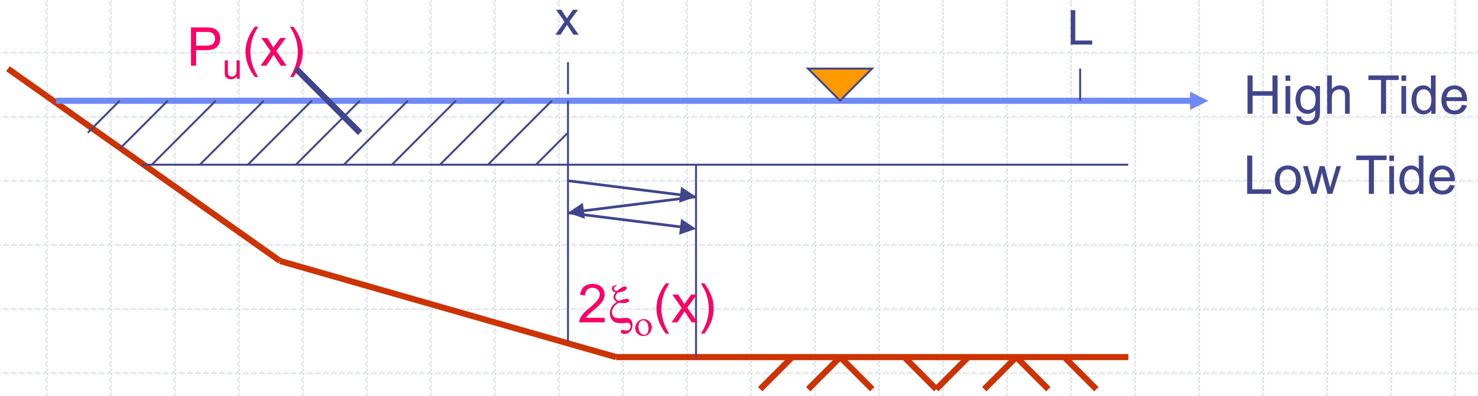


Differential advection combined with transverse diffusion

Process continues until the velocity gradients cease (patch runs into a bank, shoreline; the tide reverses, etc.)

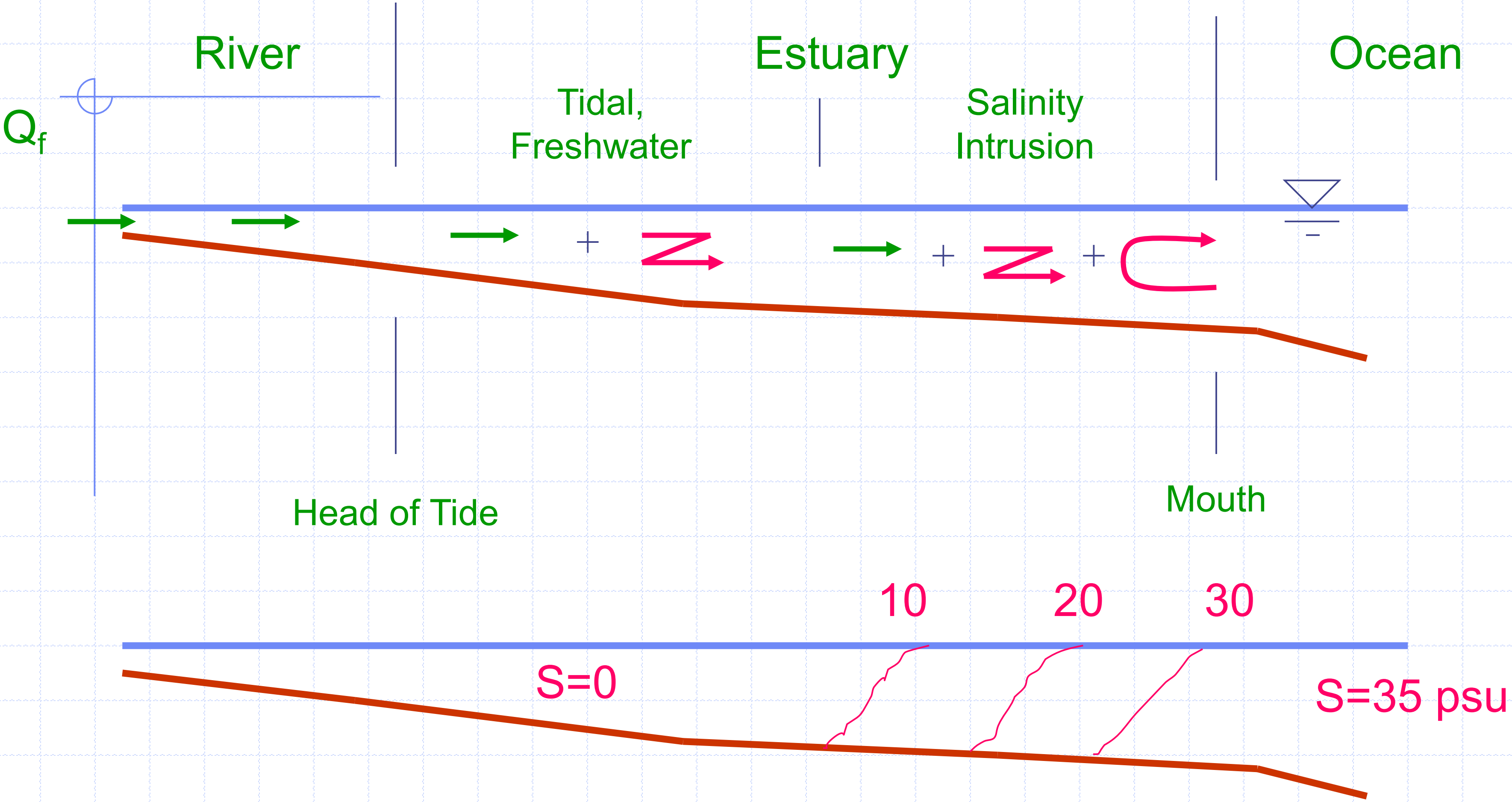
Similar processes in groundwater (macro-dispersion) and atmosphere (shear dispersion)

Simple Tidal Inlet



Upstream Tidal Prism (P_u), and Tidal Excursion increase going downstream

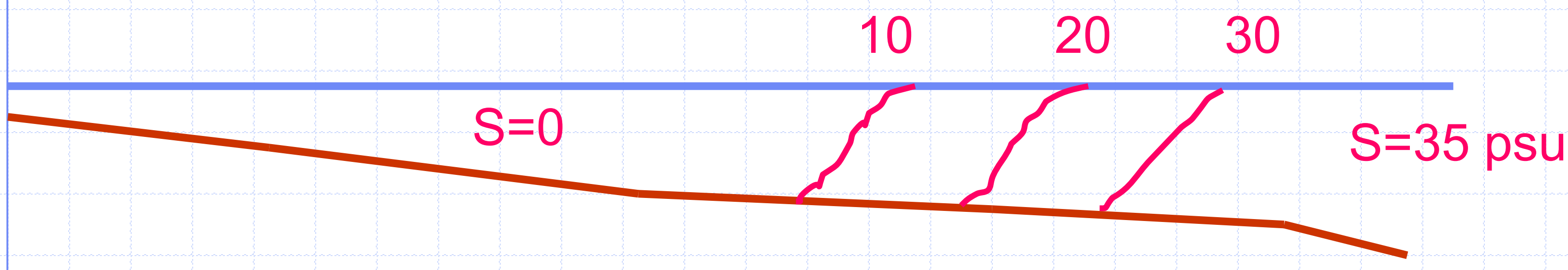
Now introduce freshwater, salinity



PSU = practical salinity unit,

an operational definition of salinity (mass fraction: ppt, $^{o}/_{oo}$ or g/kg)

Estuary classification



Well mixed: isohaline lines approach vertical (Delaware R)

Partially mixed: isohaline lines slant

Vertically stratified (salt wedge): isohaline lines approach horizontal (Mississippi R.)

Desire to classify to know what type of model/analysis to use; several options available; none is perfect

Estuary classification, cont'd

Estuary Richardson number (Fischer, 1972; 1979)

$$R = \frac{\Delta\rho_o g Q_f / W}{\rho u_t^3}$$

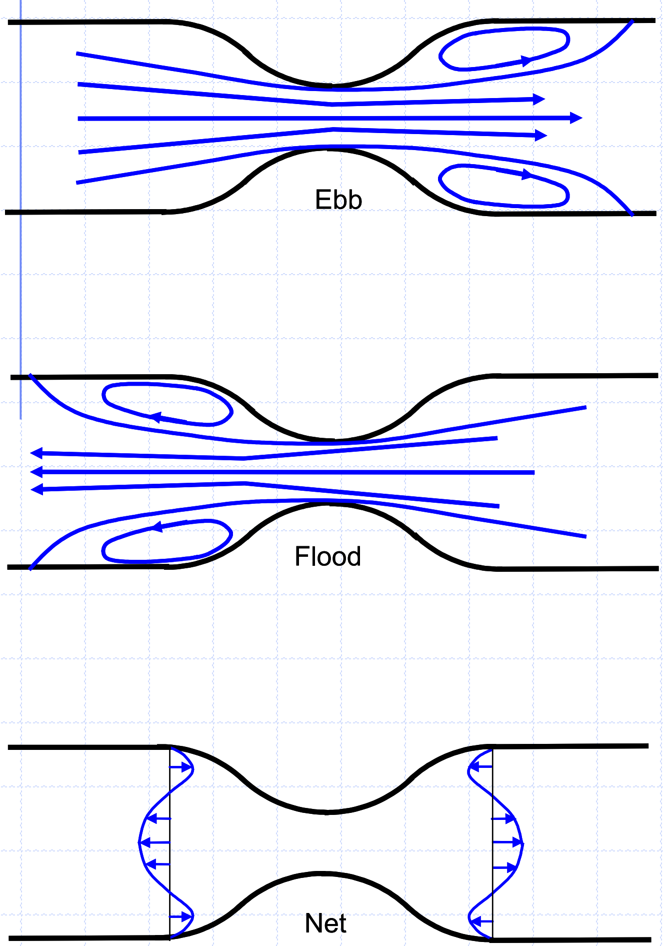
W = estuary width;

u_t = RMS tidal velocity ≅ $0.71 u_o$

R ~ potential energy rate/kinetic energy rate

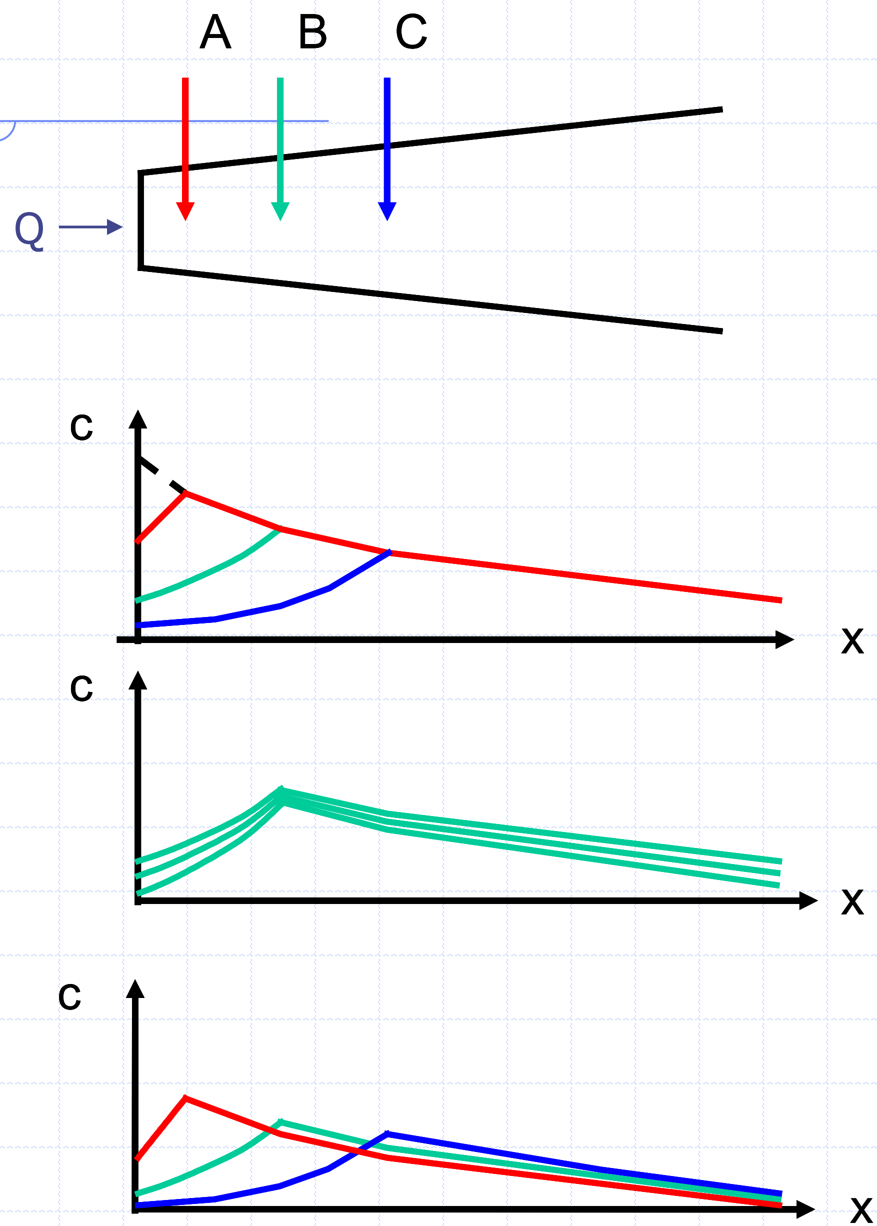
R < 0.08	well-mixed
0.08 < R < 0.8	partially stratified
0.8 < R	vertically stratified (salt wedge)

Tidal dispersion



- Tidal pumping (shown)
  - Asymmetric ebb (a) & flood (b)
  - Tidal averaging => mean velocity (c)
  - Trans mixing + trans velocity gradients => dispersion!
- Similar drivers
  - Tidal trapping
  - Coriolis + density
  - Depth-dependent tidal reversal
- $E_L \sim (2\xi_o)^2/T_t$

General result



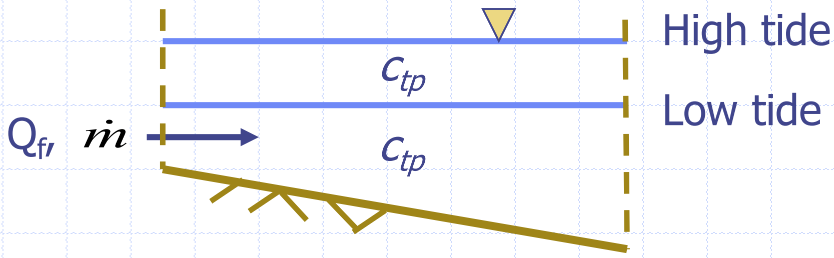
Conservative Tracer;
3 injection locations

Non-conservative
tracer; middle location

Non-conservative
tracer; 3 locations

Tidal Prism Method

- Treats whole channel as single well-mixed box (harbors, marinas)
- Mass that leaves on ebb does not returns
- Except for harbors/short channels, this overestimates flushing; underestimates c.
- Hence common to "discount" P by defining the effective volume P' of "clean" water. E.g., P' = 0.5 P
- Formal ways to compute return factor using phase of circulation outside harbor



$$\frac{P c_{tp}}{T_t} = \dot{m}$$

$$c_{tp} = \frac{\dot{m} T_t}{P}$$

P = total tidal prism

Vertical Diffusion (open waters, near surface)

$$E_z = \frac{0.028 H_w^{\;2}}{T_w} e^{-4\pi z / L_w}$$

Ichiye (1967); z = depth; H_w, T_w, L_w = significant wave height, period and length

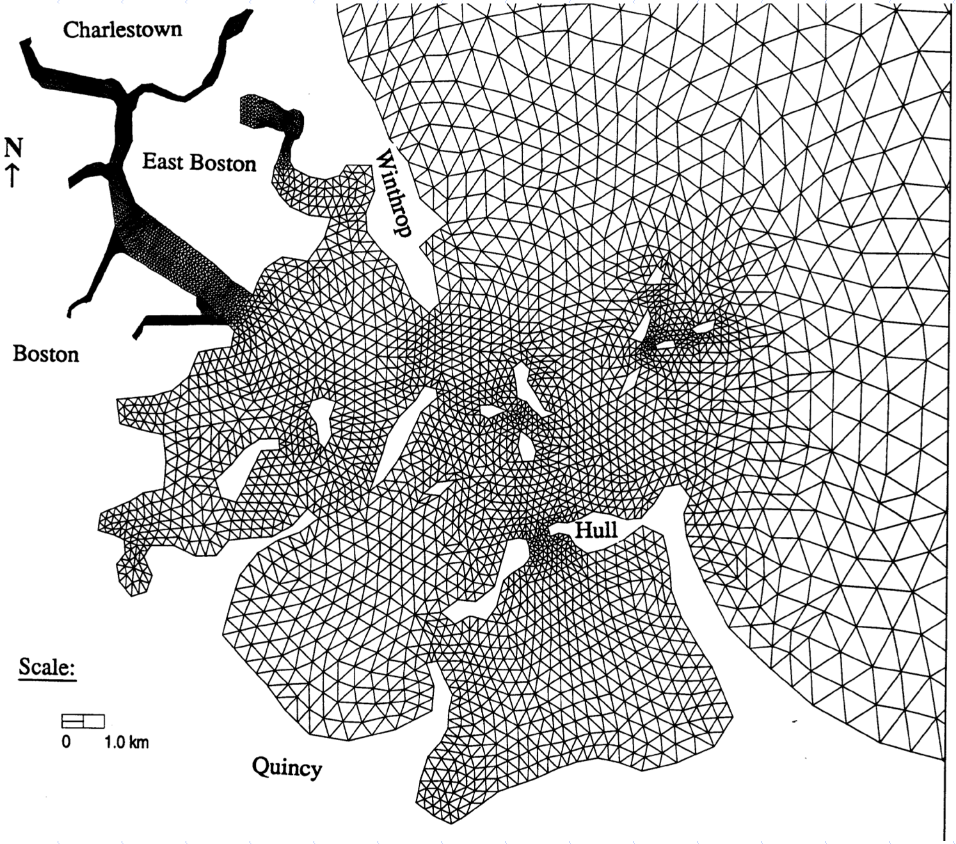
If you must pollute, do it downstream (or into large waterbodies)

- Larger eddies, greater tidal excursion, larger tidal prism, higher waves
- Closer to the “open door”

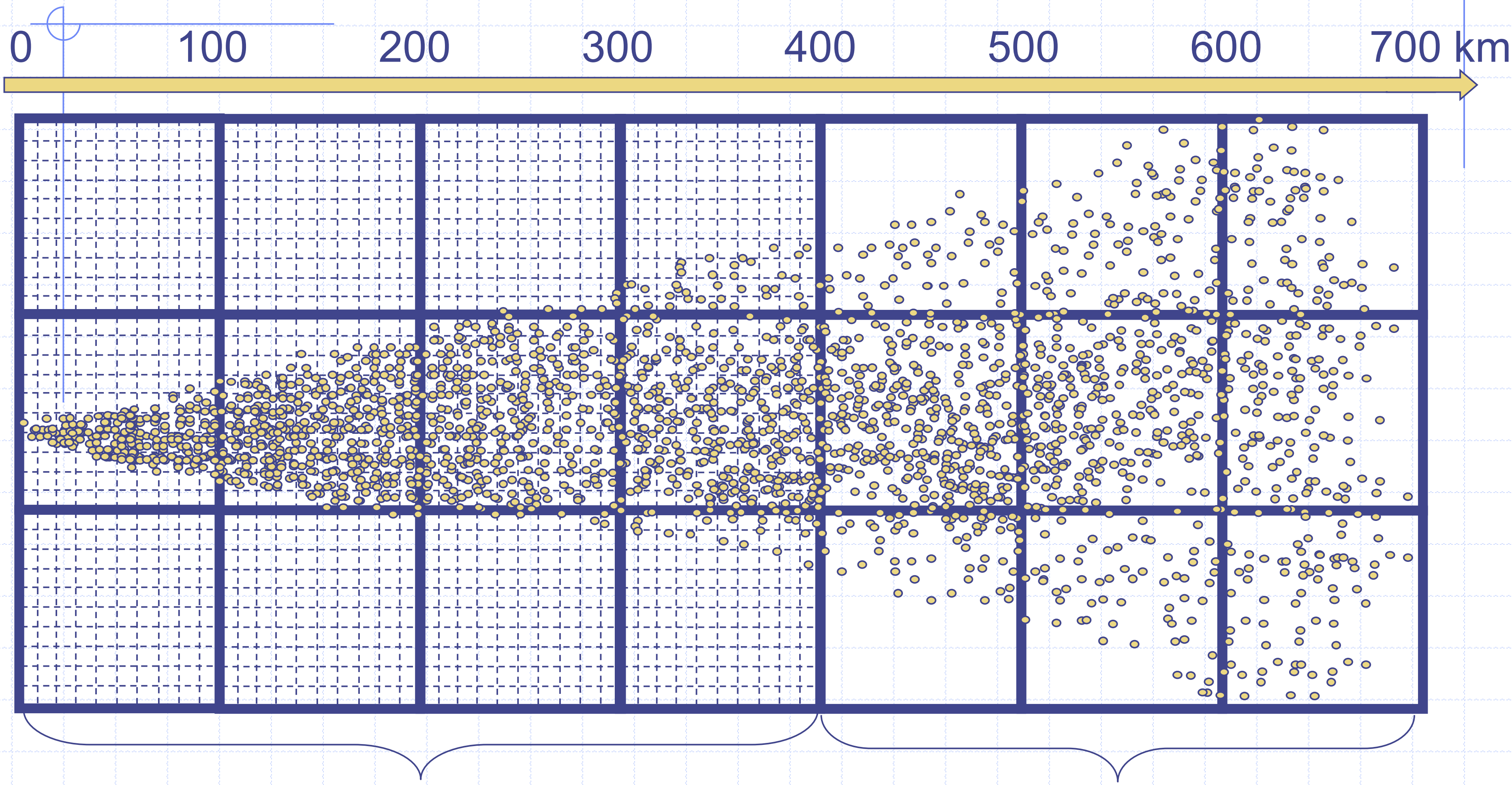
Types of Models

- Dimensionality: 0, 1, 2, 3-D
- Time resolution: steady, unsteady
- Coupling (hydrodynamics and water quality combined or treated separately)
- Solution Scheme
  - Analytical
  - Numerical (Eulerian/fixed grid): Finite Difference, Finite element, Finite Volume
  - Numerical (Lagrangian): Random walk-particle tracking, Hybrid

Unstructured Grid of Boston Harbor



Hybrid Random Walk Particle Tracking/Grid Based Model



Use finer grid to visualize intermediate-field concentrations

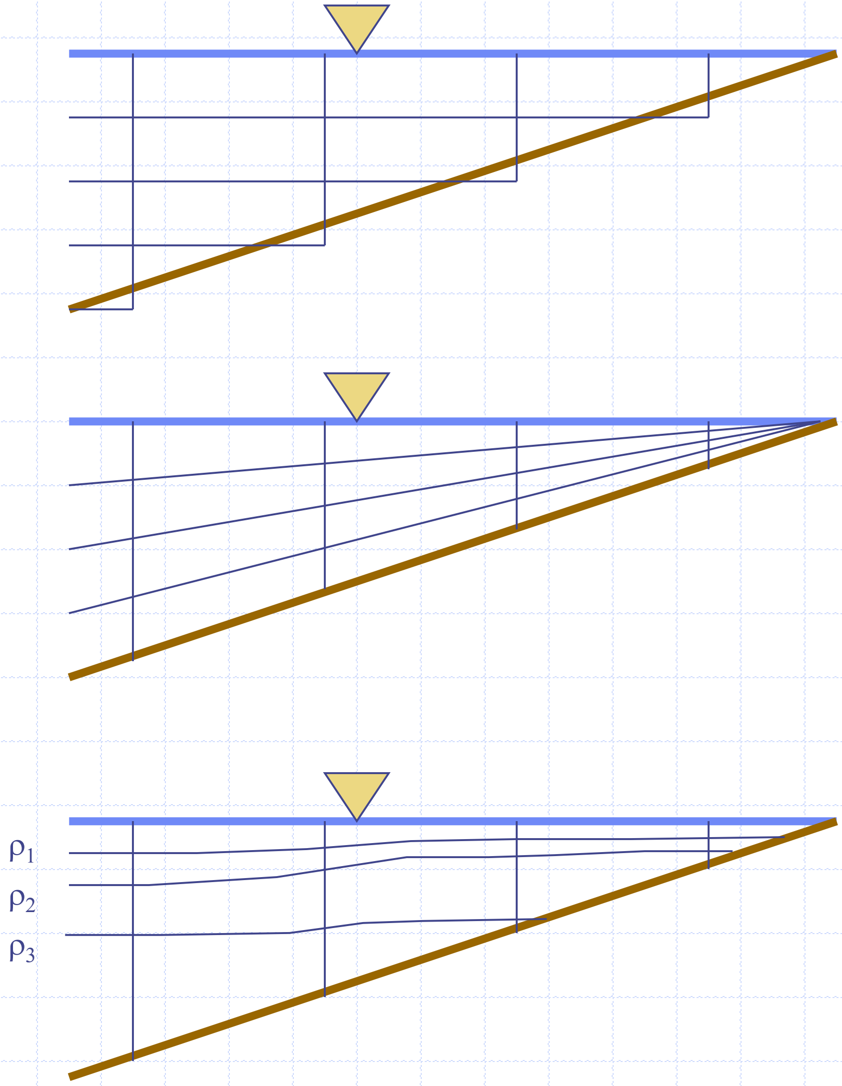
Project particles onto OGCM grid → far-field concentrations

Types of Models (cont'd)

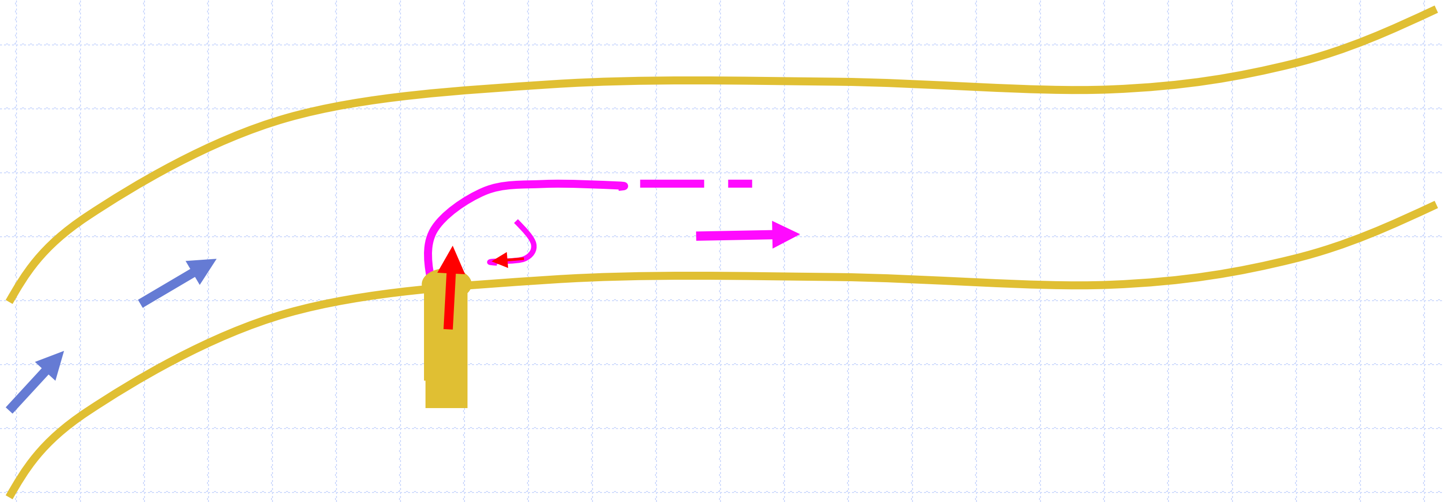
- Source: instantaneous, intermittent, continuous
- Mixing schemes/turbulence closure: RANS, LES, DNS
- Gridding: horizontal, vertical
- Near-far field coupling
- Etc.

Grids

- Horizontal
  - Rectangular
  - Curvilinear
  - Unstructured
- Vertical
  - Stair-stepped (z coordinate)
  - Bottom fitting (σ coordinate)
  - Isopycnal



Near Field Mixing



- Dilution of at least 2 is possible (indeed, inevitable) even with passive discharge
- Many Near Field (Initial Mixing Models): CORMIX, VISJET, Visual Plumes, etc.
- Many ways to couple to far field.

Questions ?