Numerical Methods in Mechanics and <u>Environmental Flows</u>

OCT 27, 2017

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Outline for Environmental Flows

Oct 13
- Introduction
- Delft3D Introduction and Assignment 1: Spin-up?

Oct 20
- Box models and solution methods
- Delft3D Assignment 2 - Boundary conditions; initial conditions

Oct 27
- Solution methods: vertical layers / transport processes
- Delft3D Assignment 3 – stratification (wind-driven flows)

Nov 3
- Transport processes in flows (2)
- Delft3d Project

Nov 10
- Transport processes in flows (3)
- Delft3d assignment 4 – model extend (estuarine stratification as an example)

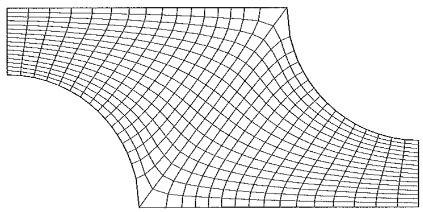
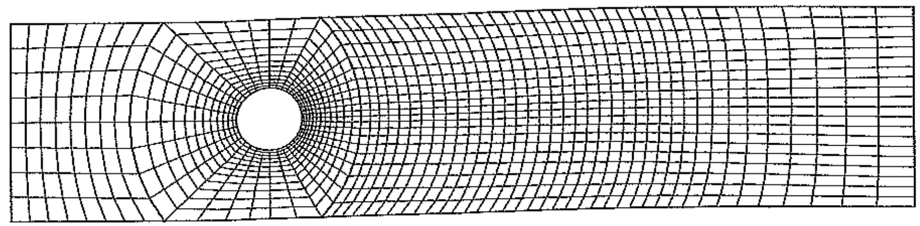
Nov 17
- Presentation of term assignment (5 groups)

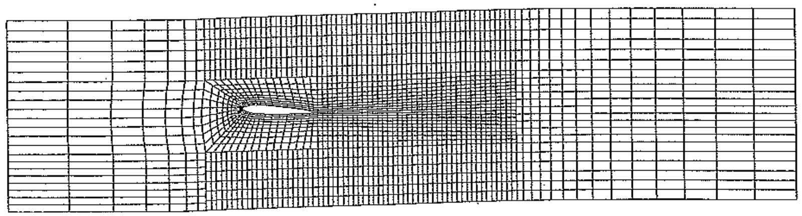
Last week

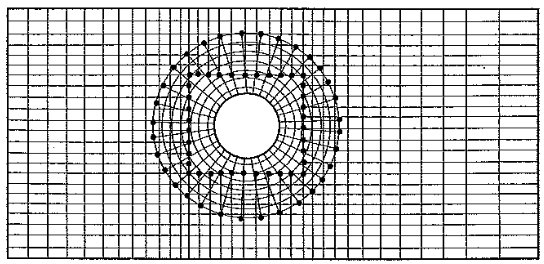
Looked at numerical solutions:

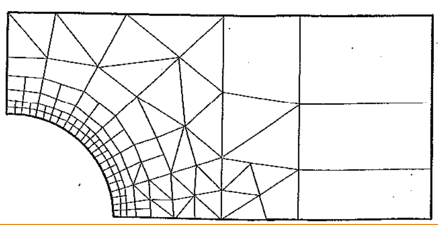
- What are needed for numerical solutions?
  - The Mathematical model
  - Discretization method
  - Solver
- Expected errors
  - Modeling
  - Discretization
  - Iteration
- Why? Due to the components which affect the solutions:
  - Grids
  - Approximations
  - Solution methods

Types of grid

- 1  

- 2 

- 3 

- 4 

Important concepts that arise due to the use of Numerical Methods

Convergence

Consistency

Stability

Conservation

Boundedness

Realizability

Similar concept

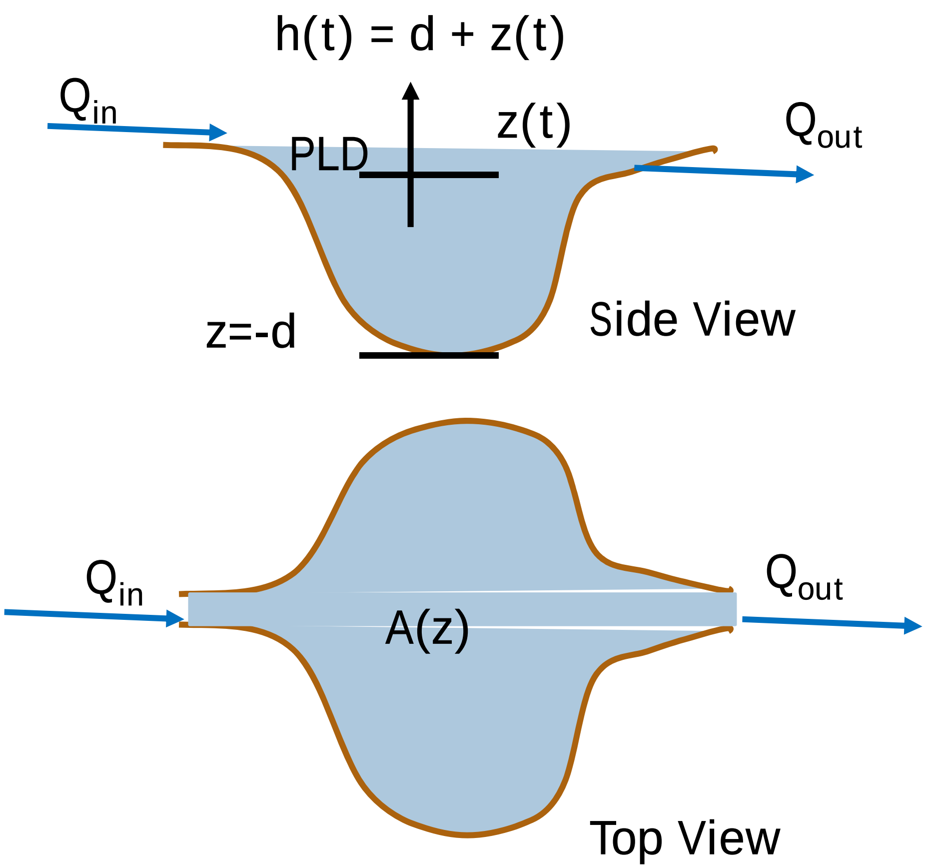
A quick look at the various discretization methods

Mainly FV; FD; FE

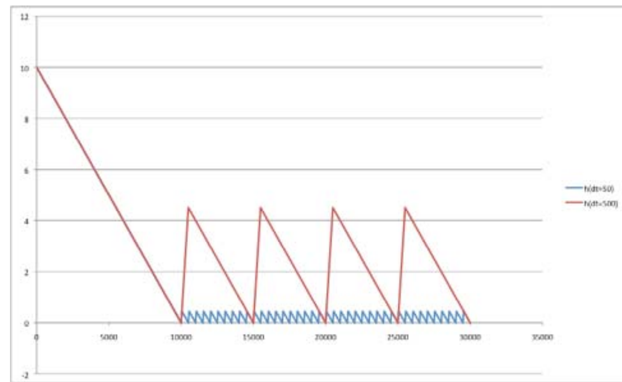
- Their advantages and disadvantages

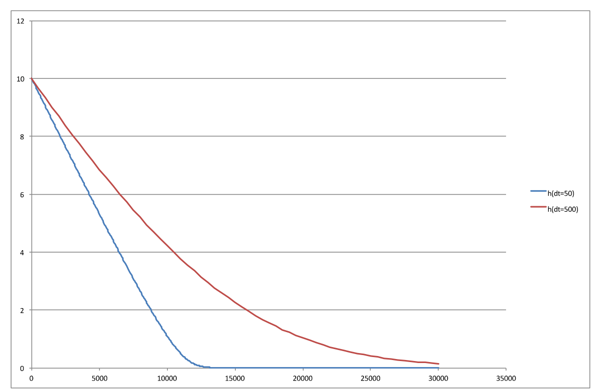
How to discretize in space and time

A look at the lake problem to explore solution issues (1) – Ill-posed



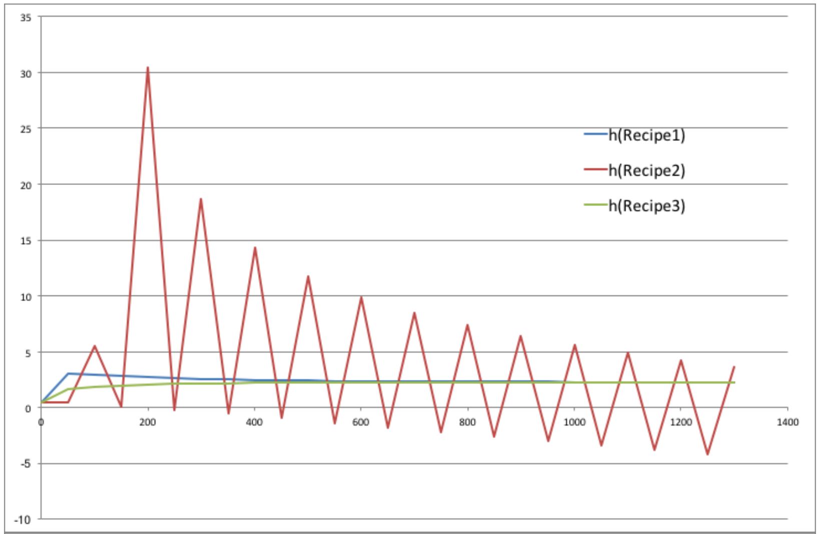
Why ill-posed?

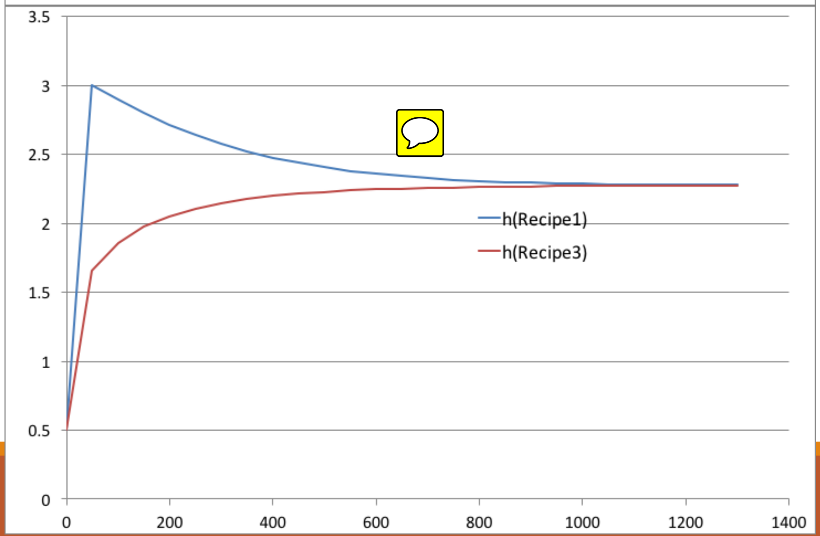




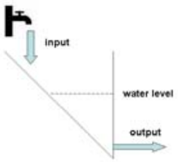
A look at the lake problem to explore solution issues (2) – Schematic problems

Is there a right scheme?





Example



$$\frac{dV(h(t))}{dt} = Q_{input} - Q_{output}(h(t))$$

$h(0) = 0.5\ m$

$$V(h) = 2 \times \frac{1}{2} h^2,\ Q_{input} = 0.05,\ Q_{output}(h) = 0.01\sqrt{2g\max(0, h - 1.0)},\ g = 9.81\ m^2/s$$

Recipe 1: $h_{n+1} = h_n + \Delta t\left(\frac{0.05 - 0.01\sqrt{2g\max(0, h_n - 1.0)}}{2h_n}\right)$

Recipe 2: $h_{n+1} = h_{n-1} + 2\Delta t\left(\frac{0.05 - 0.01\sqrt{2g\max(0, h_n - 1.0)}}{2h_n}\right)$

Recipe 3: $h_{n+1} = \sqrt{(h_n)^2 + \Delta t\left(0.05 - 0.01\sqrt{2g\max(0, h_n - 1.0)}\right)}$

Take home from this part

Two different examples with different reasons for the results you have seen

- Example 1: Actual reason for the fluctuations was due to the problem being ill-posed. But that can be solved through a numerical trick (known as the Patankar trick)

- Example 2: The fluctuations are due to the choice of the numerical schemes

Reservoir with pollutant

Reservoir with following conditions:

- $V = 2x10^5 m^3$; $Q_{u/s} = 9x10^4 m^3/yr$; $Q_{evap} = 1x10^4 m^3/yr$; Assume steady state; upstream c = 6 mg/l; c decays at K = 0.12/year

Find c

- What is budget?
- What is then c?

What if now upstream c = 0 due to changes in management?

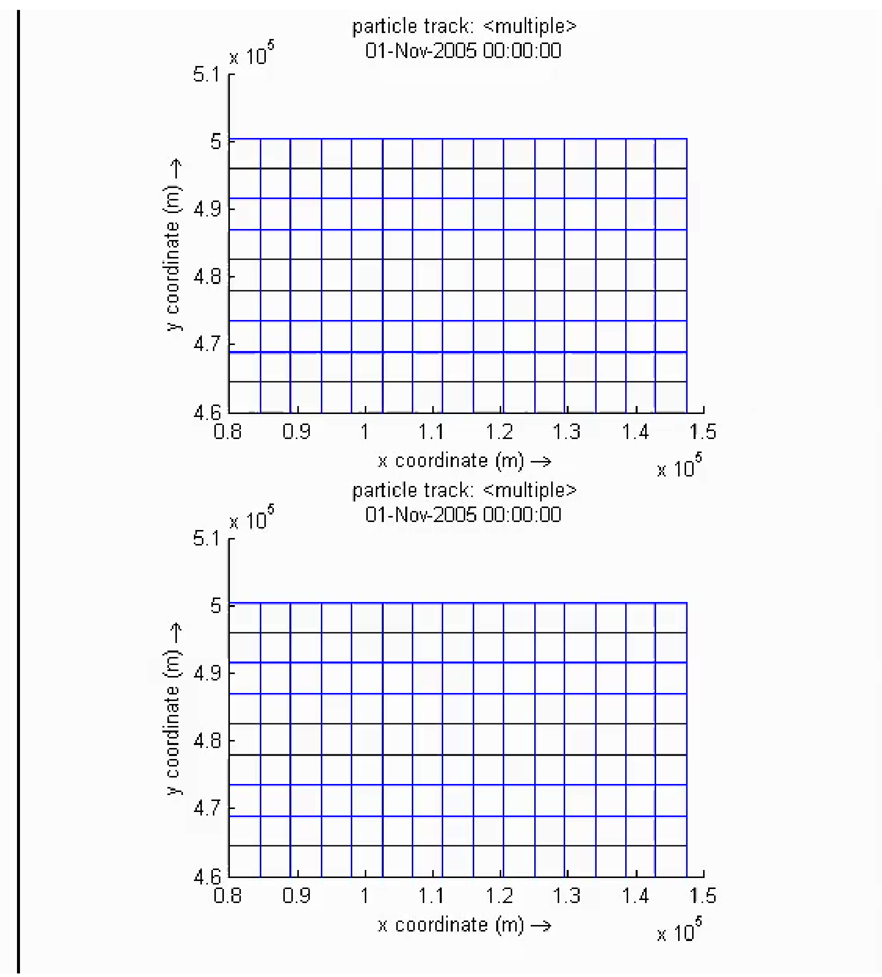
- What is budget?
- How long does it take to drop to 50%
- How long does it take to reach 0.1 mg/l?
- What is the main cause of the improvement in c?

Basic Flow Transport Processes

Flow transport processes that affect fate of substances

Flow transport processes can be generally separated into

- Advection
- Diffusion
- Settling (Not shown here)



The box model for transport

The incompressible flow version of the transport equation can be written as:

$$\frac{\partial c}{\partial t} + \boxed{u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z}} = \boxed{D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right)}$$

Does this equation look similar?

$$\frac{\partial u_i}{\partial t} + u_j\frac{\partial u_i}{\partial x_j} = \frac{\mu}{\rho}\frac{\partial^2 u_i}{\partial {x_j}^2} + g_i$$

What is the primary difference between advection and diffusion?

- Let's use a simple 1-D example: $\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D_x\left(\frac{\partial^2 c}{\partial x^2}\right)$

What is diffusion?

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} = \boxed{D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right)}$$

A fundamental transport process.

Diffusion occurs because of:

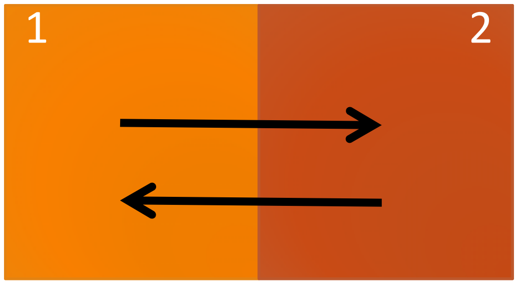
- Gradients → seeking to achieve an equilibrium
- Random motion due to:
  - A.
  - B.

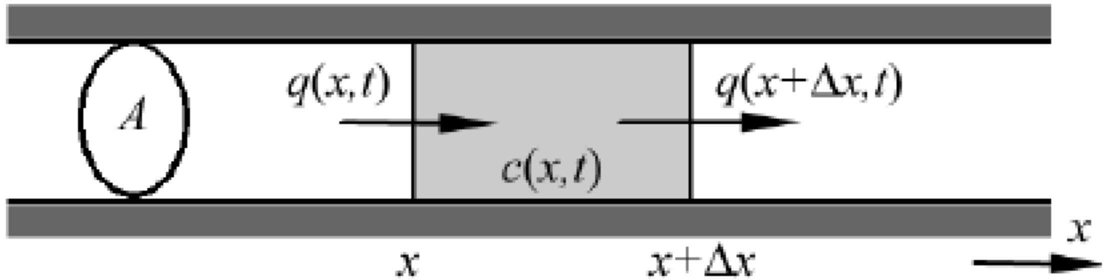
Unfortunately when we introduce numerical schemes we can and often do create artificial diffusion

1-D Diffusion

WHY IT IS RELEVANT

1-D Diffusion Equation





Fick's law $q = -D\frac{\partial c}{\partial x}$

Conservation of mass $\frac{\partial c}{\partial t} = -\frac{\partial q}{\partial x}$

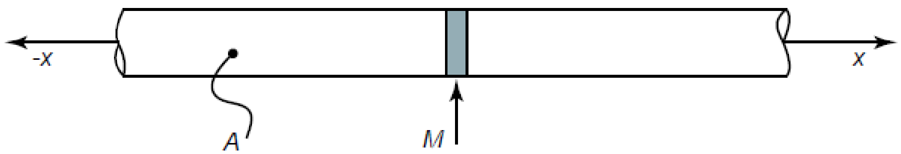
Putting both together you obtain $\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right)$

- Detailed derivation will be provided later

Why is this equation important?

Applications of the 1D Diffusion Equation (1)

Basic solution for 1D narrow infinite pipe



- Concentration at any location and time: $$c(x,t)=\frac{M}{A\sqrt{4\pi Dt}}\exp\left(\frac{-x^2}{4Dt}\right)$$

- Spread $$\frac{c}{c_{\max}}=\exp\left[-\frac{1}{2}\left(\frac{x}{\sigma}\right)^2\right]$$

So what?

- Well because it is a linear equation we can superimpose solutions and obtain solutions for finite domains!

Applications of the 1D Diffusion Equation (2)

Solution for finite domain

- Concentration at any location and time:

$$c(x,t)=\frac{M}{\sqrt{4\pi Dt}}\left[\exp\left(-\frac{\left(x-2mL-a\right)^2}{4Dt}\right)+\exp\left(-\frac{\left(x-2mL+a\right)^2}{4Dt}\right)\right]$$

- Estimate mixing time for an average final concentration depending on where the initial concentration of pollutant was released:
  - For release in the middle of the domain; L/2 → $T = 0.134\frac{L^2}{D}$
  - For release at x= 0 or x = L → $T = 0.536\frac{L^2}{D}$

Applications of the 1D Diffusion Equation (3)

With Decay or Source

- Decay; simple to derive

$$c(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt} - Kt\right)$$

- Source; requires simplification to steady state

$$c(x) = \frac{\dot{M}}{2\sqrt{DK}} \exp\left(+\sqrt{\frac{K}{D}}x\right) \quad for \quad 0 > x$$

$$c(x) = \frac{\dot{M}}{2\sqrt{DK}} \exp\left(-\sqrt{\frac{K}{D}}x\right) \quad for \quad 0 < x$$

Scales & the issue of physical diffusion (1)

Different D (or K, k) values depending on scale.

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right)$$

- All scales solved: true $D \sim O(10^{-9})\frac{m^2}{s} < \upsilon$
- Averaged 3D: $K_z \sim O(\quad)\frac{m^2}{s}$
- 2D Depth-average: $k_{x,y} \sim O(\quad)\frac{m^2}{s}$
- 1D :$K \sim O(\quad)\frac{m^2}{s}$

Scales & the issue of physical diffusion (2)

How does averaging create this difference?

- What is averaging? $u = \bar{u} + u' \; (etc.)$

All scales solved:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right)$$

- Averaged 3D:

$$\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} + \frac{\partial (vc)}{\partial y} + \frac{\partial (wc)}{\partial z} =$$

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right)$$

- 2D Depth-average: $\dfrac{\partial (ch)}{\partial t} + \dfrac{\partial (uhc)}{\partial x} + \dfrac{\partial (vhc)}{\partial y} = \dfrac{\partial}{\partial x}\left(hk_x\dfrac{\partial c}{\partial x}\right) + \dfrac{\partial}{\partial y}\left(hk_y\dfrac{\partial c}{\partial y}\right)$

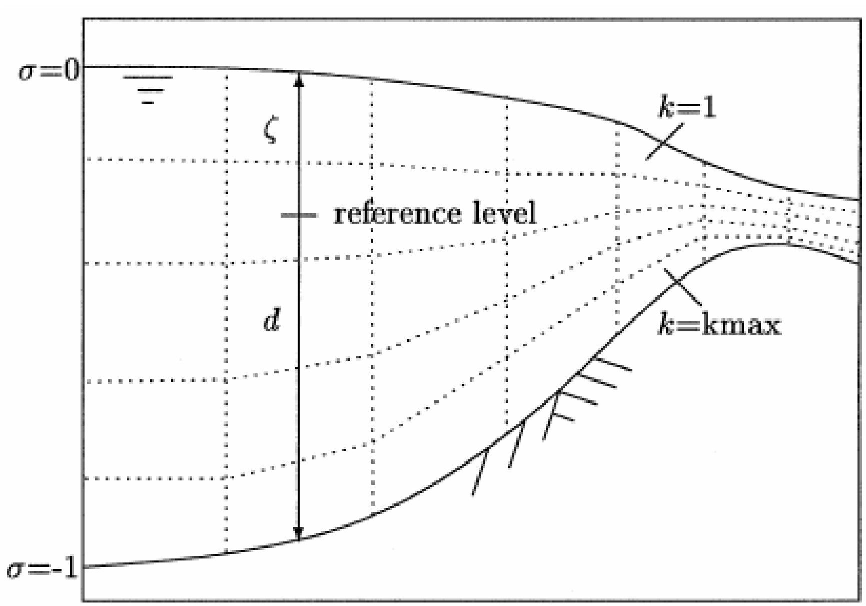
- 1D : $\dfrac{\partial (cA)}{\partial t} + \dfrac{\partial (uAc)}{\partial x} = \dfrac{\partial}{\partial x}\left(AK\dfrac{\partial c}{\partial x}\right)$

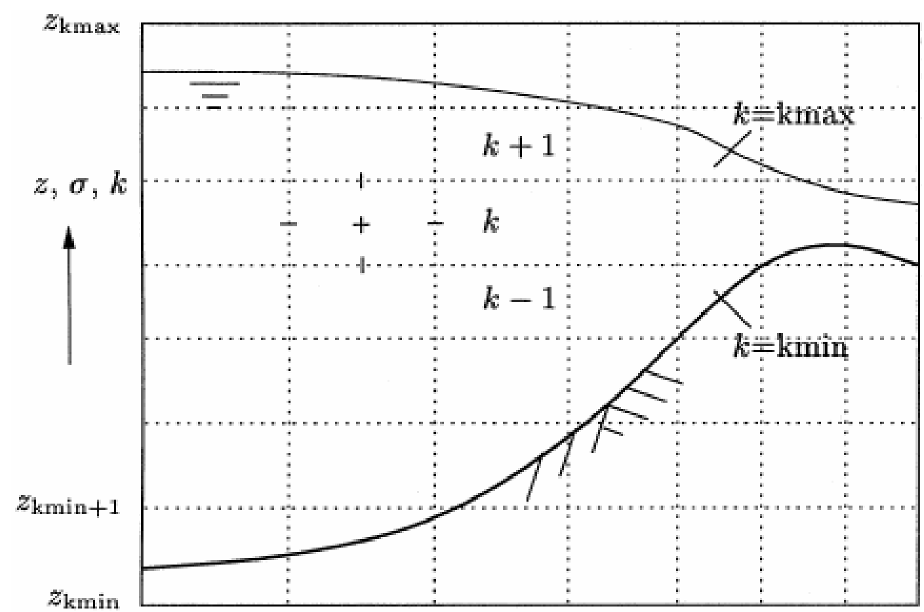
Vertical Planes

THE ISSUE OF ARTIFICIAL DIFFUSION

What is the difference?

Two primary vertical layer systems





a) Sigma-layer

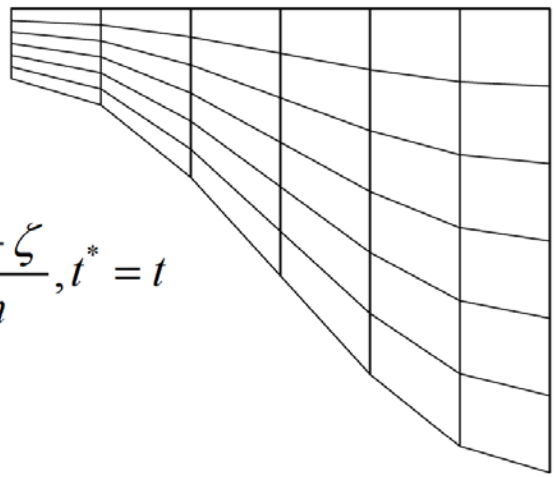
b) z-layer

What is the issue?

Sigma layers essentially require transformation of the equations:

Transformation in

σ coordinates



$$x^* = x, y^* = y, \sigma = \frac{z-\zeta}{h}, t^* = t$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t^*} + \frac{\partial \sigma}{\partial t}\frac{\partial}{\partial \sigma}$$

$$\frac{\partial}{\partial x_i} = \frac{\partial}{\partial x_i^*} + \frac{\partial \sigma}{\partial x_i}\frac{\partial}{\partial \sigma}, i = 1,2$$

$$\frac{\partial}{\partial x_3} = \frac{1}{h}\frac{\partial}{\partial \sigma}$$

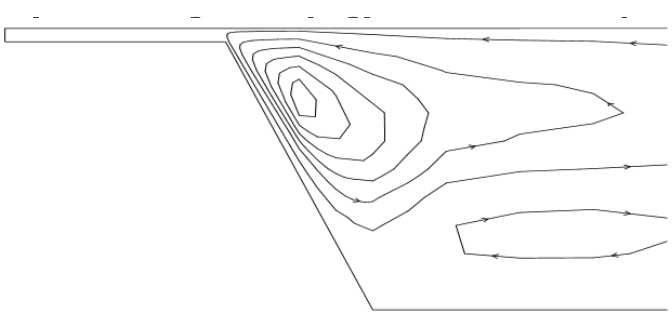
$$u_i^* = u_i, i = 1,2 \quad u_3^* = \omega = h\frac{D\sigma}{Dt}$$

What is the issue (2)?

Transformation however results in incomplete transformation of the gradient transport. For example the pressure gradient can create artificial flow in regions of steep slopes. Why?

$$\frac{\partial p}{\partial x} = \frac{\partial p^*}{\partial x^*} + \frac{\partial \sigma}{\partial x}\frac{\partial p^*}{\partial \sigma} = \frac{\partial p^*}{\partial x^*} - \frac{1}{H}\left(\frac{\partial \zeta}{\partial x} + \sigma\frac{\partial H}{\partial x}\right)\frac{\partial p^*}{\partial \sigma}$$

C
b



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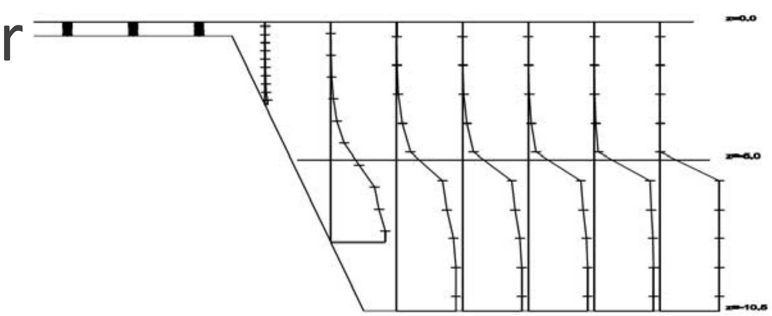
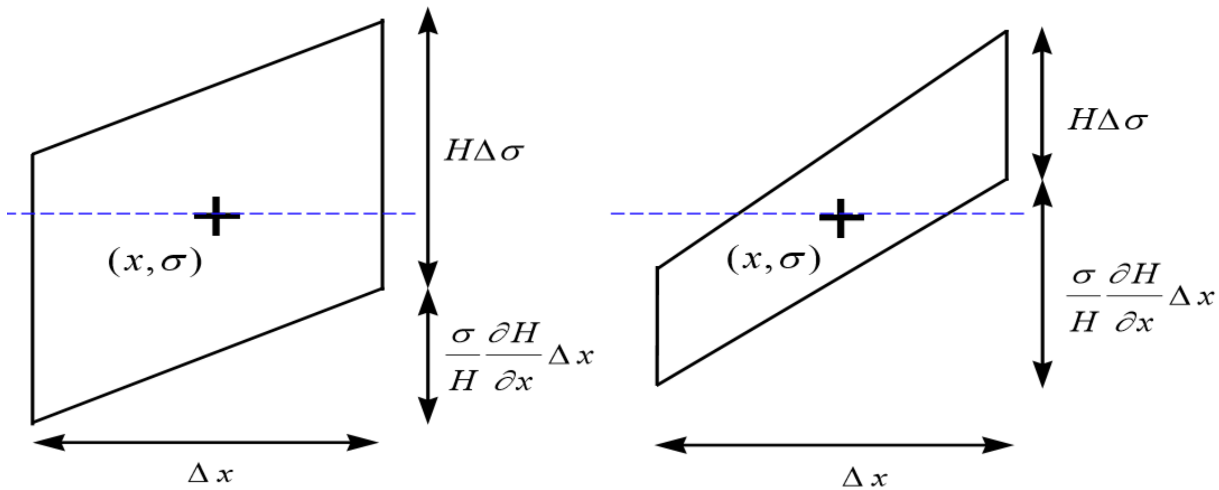


- The issue: Hydrostatic inconsistency

Hydrostatic consistency?

The grid cell size changes too fast in the vertical

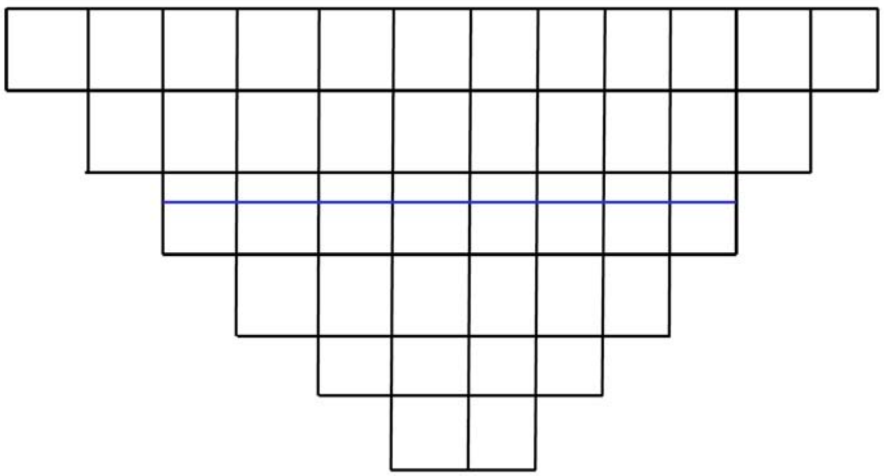


a. Hydrostatic consistent grid cell b. Hydrostatic inconsistent grid

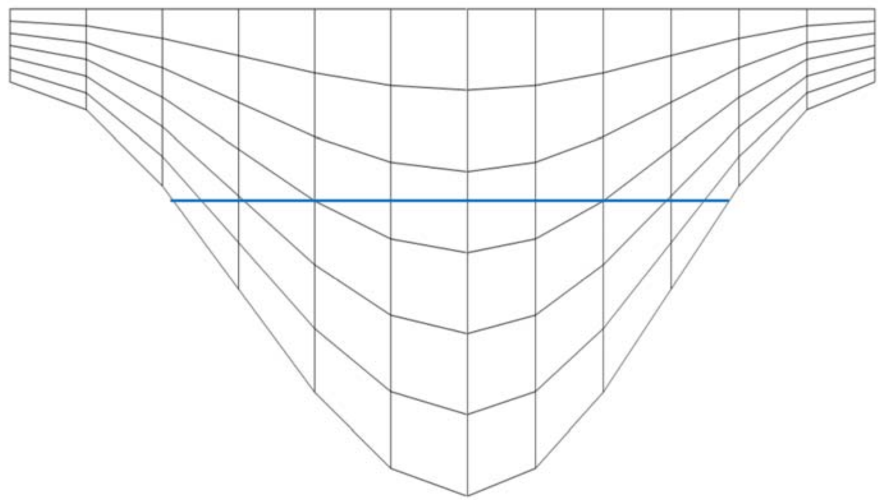
Essentially → $\frac{\sigma}{H}\frac{\partial H}{\partial x}\Delta x < \Delta\sigma$

What is the issue (3)

This will result in artificial diffusion and mixing for weakly stratified systems e.g. lakes



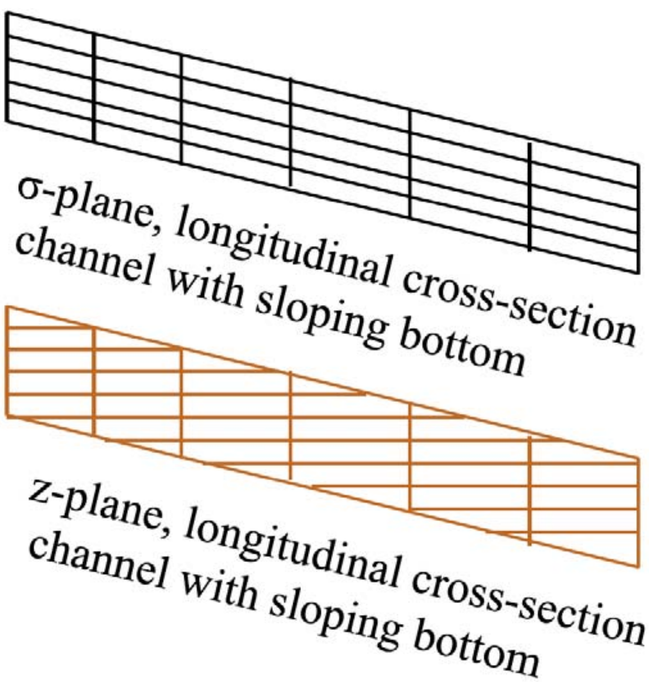
z-plane, cross-section estuary channel

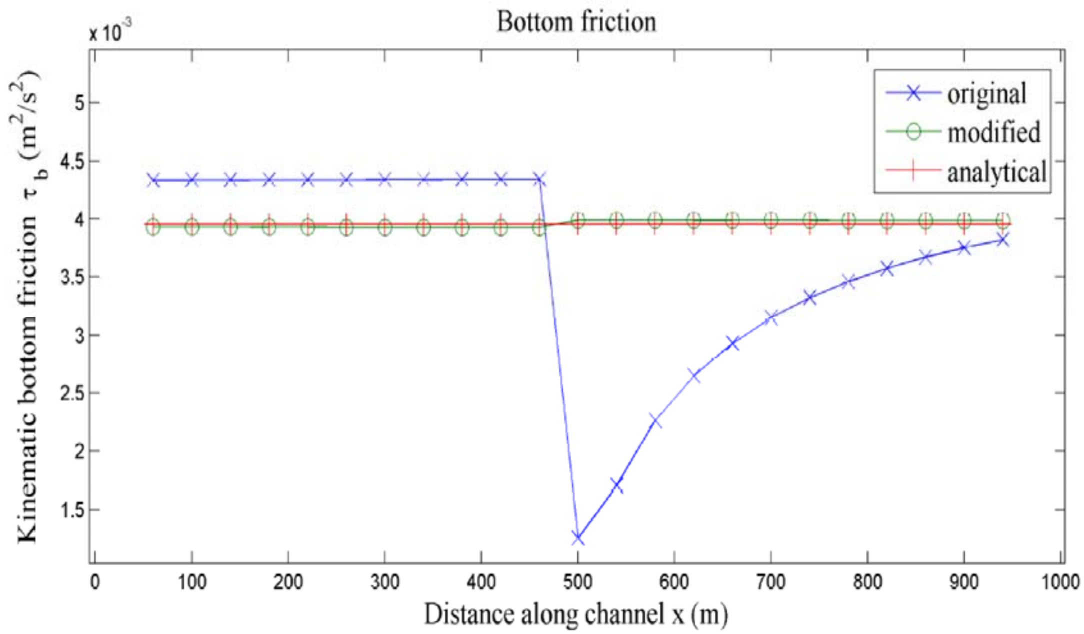


σ-plane, cross-section estuary channel

What is the issue (3)

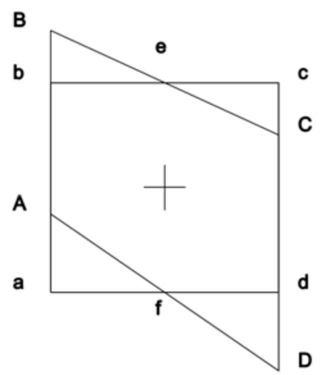
The reverse can occur when constant slopes are in the domain e.g. a river

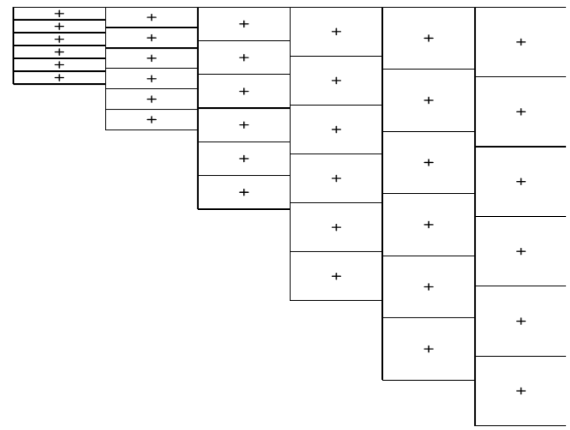




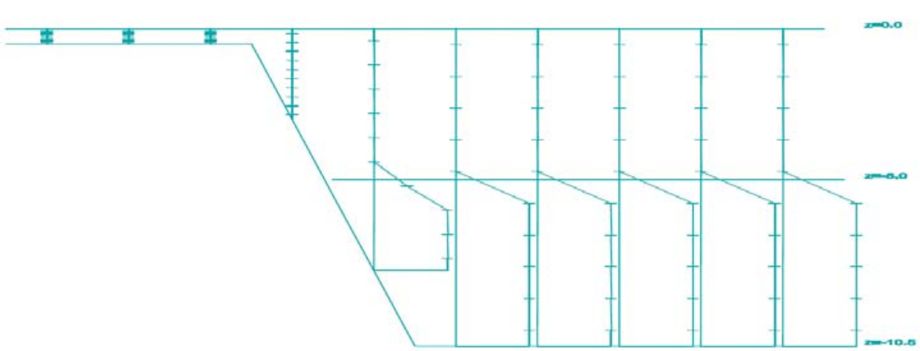
How to solve the problem?

Stelling & Kester (1994); IJNMF 18(10)

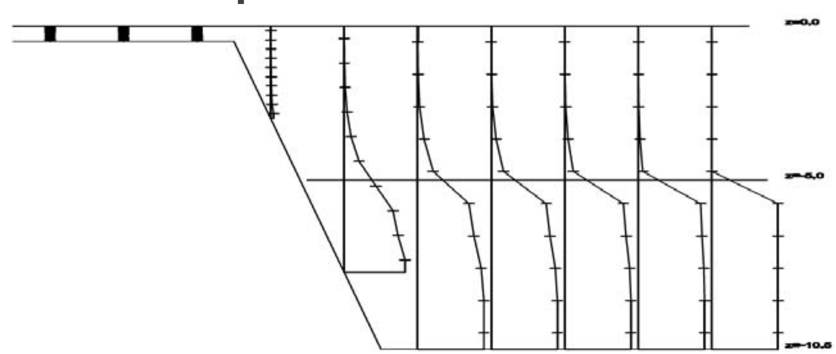




The results



Compared to



Assignment 3

LAKES?

What are lakes/reservoirs?

Body of water surrounded by land

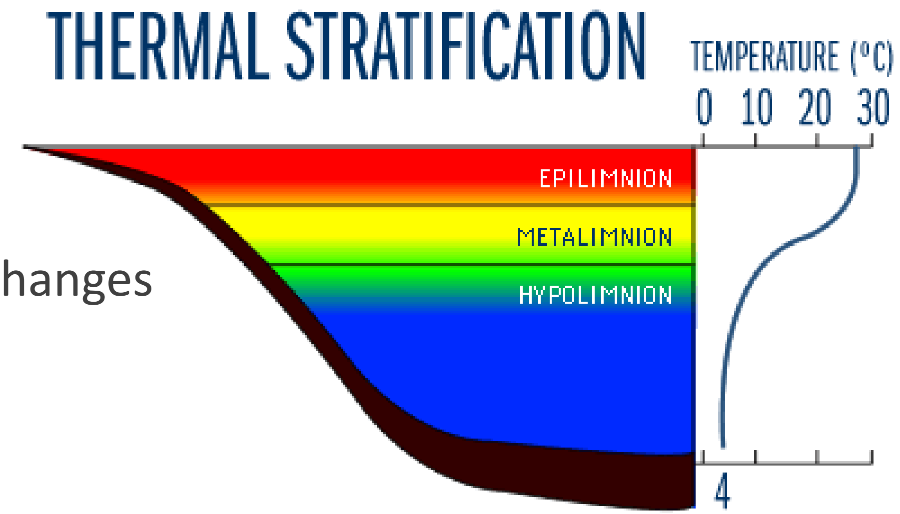
What affects them?

The issue of stratification

Lakes are normally thermally stratified (even in the tropics – where they have to be deep – but where temporal scales are the main difference)

What does stratification do?

- 3 layers
- Epilimnion (upper; well-mixed)
- Metalimnion (mid; temp [density] changes rapidly with depth)
- Hypolimnion



What does wind do?

- Influences the epilimnion depth

The issue of wind

Besides influencing the epilimnion depth. What else can wind do?

- Seiches

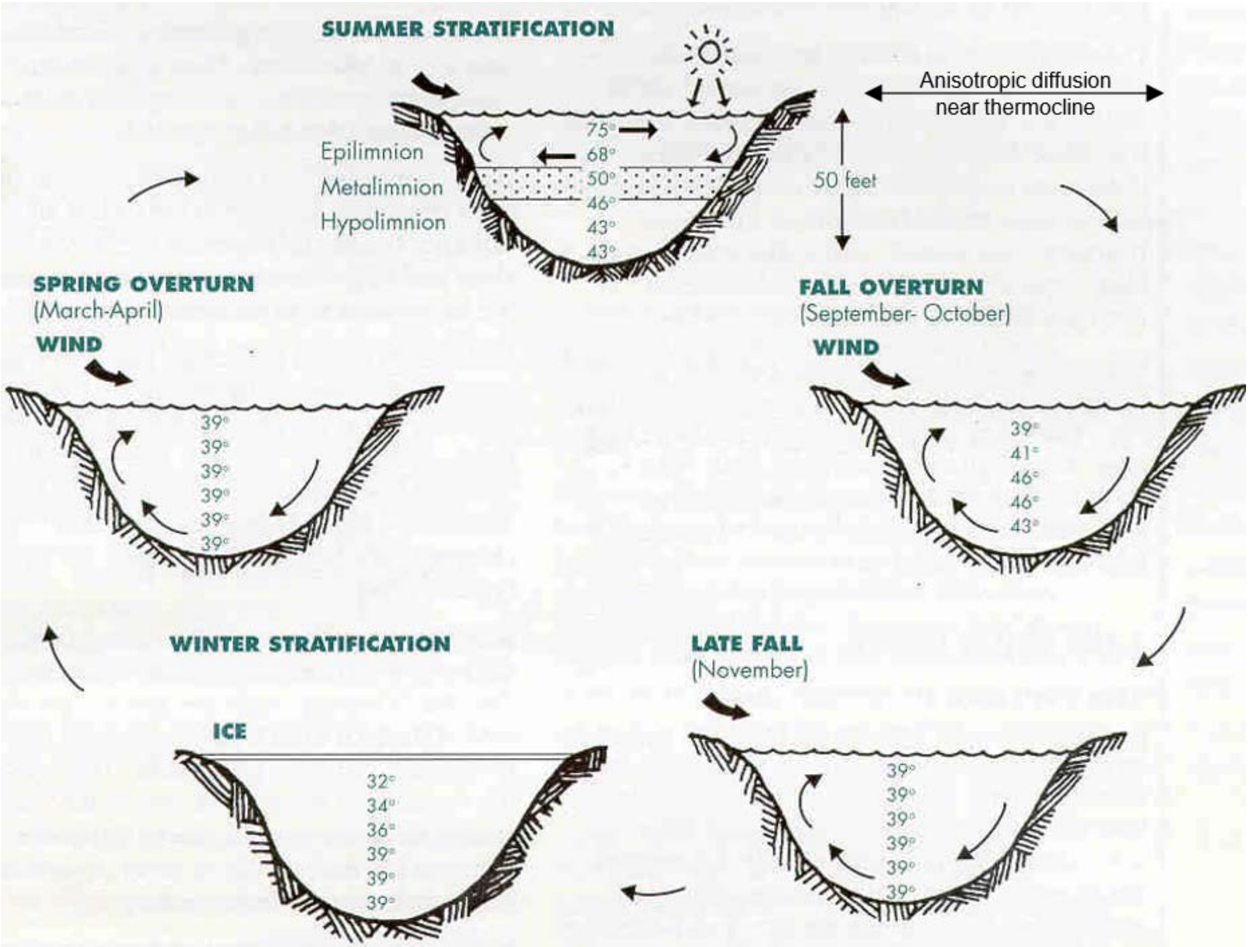
- Enhanced mixing (how?)

And how does it do this?

- Exerts drag force on water: $\tau = \rho_a C_d U_{10}^2$
  - Explanation of all the terms

The issue of wind and mixing

Depends on heat from the sun as well



Mixing is influenced by diffusion

Remember that diffusion has 2 properties?

Well we have to deal with the 2nd property in Part 2

And because of averaging we have to deal with this with respect to both mixing and momentum.

There are 4 ways in Delft3D, 3 of which are based on this assumption: $\nu_t = C_\mu \sqrt{k} L$

- Constant viscosity
- Zero equation
- 1-equation
- 2-equation

So how does it impact us if we get the solution of turbulent viscosity?

Momentum

$$\frac{\partial u}{\partial t}+\frac{u}{\sqrt{G_{\xi\xi}}}\frac{\partial u}{\partial \xi}+\frac{v}{\sqrt{G_{\eta\eta}}}\frac{\partial u}{\partial \eta}+\frac{\omega}{d+\zeta}\frac{\partial u}{\partial \sigma}-\frac{v^2}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\frac{\partial\sqrt{G_{\eta\eta}}}{\partial \xi}+$$
$$+\frac{uv}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\frac{\partial\sqrt{G_{\xi\xi}}}{\partial \eta}-fv=-\frac{1}{\rho_0\sqrt{G_{\xi\xi}}}P_\xi+F_\xi+$$
$$+\frac{1}{(d+\zeta)^2}\frac{\partial}{\partial \sigma}\left(\nu_V\frac{\partial u}{\partial \sigma}\right)+M_\xi, \quad (9.6)$$

$$\frac{\partial v}{\partial t}+\frac{u}{\sqrt{G_{\xi\xi}}}\frac{\partial v}{\partial \xi}+\frac{v}{\sqrt{G_{\eta\eta}}}\frac{\partial v}{\partial \eta}+\frac{\omega}{d+\zeta}\frac{\partial v}{\partial \sigma}+\frac{uv}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\frac{\partial\sqrt{G_{\eta\eta}}}{\partial \xi}+$$
$$-\frac{u^2}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\frac{\partial\sqrt{G_{\xi\xi}}}{\partial \eta}+fu=-\frac{1}{\rho_0\sqrt{G_{\eta\eta}}}P_\eta+F_\eta+$$
$$+\frac{1}{(d+\zeta)^2}\frac{\partial}{\partial \sigma}\left(\nu_V\frac{\partial v}{\partial \sigma}\right)+M_\eta. \quad (9.7)$$

Basic Transport

$$\frac{\partial (d+\zeta)c}{\partial t}+\frac{1}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\left\{\frac{\partial\left[\sqrt{G_{\eta\eta}}(d+\zeta)uc\right]}{\partial \xi}+\frac{\partial\left[\sqrt{G_{\xi\xi}}(d+\zeta)vc\right]}{\partial \eta}\right\}+\frac{\partial \omega c}{\partial \sigma}=$$
$$\frac{d+\zeta}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\left\{\frac{\partial}{\partial \xi}\left[\frac{D_H}{\sigma_{c0}}\frac{\sqrt{G_{\eta\eta}}}{\sqrt{G_{\xi\xi}}}\frac{\partial c}{\partial \xi}\right]+\frac{\partial}{\partial \eta}\left[\frac{D_H}{\sigma_{c0}}\frac{\sqrt{G_{\xi\xi}}}{\sqrt{G_{\eta\eta}}}\frac{\partial c}{\partial \eta}\right]\right\}+$$
$$+\frac{1}{d+\zeta}\frac{\partial}{\partial \sigma}\left[\frac{\nu_{mol}}{\sigma_{mol}}+\max\left(\frac{\nu_{3D}}{\sigma_c},D_V^{back}\right)\frac{\partial c}{\partial \sigma}\right]-\lambda_d(d+\zeta)c+S, \quad (9.29)$$