Numerical Methods in Mechanics and Environmental Flows

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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 extents (estuarine stratification as an example)

Nov 17
- Presentation of term assignment (4 groups)
- Revision / past exam questions

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

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

Basic transport processes:

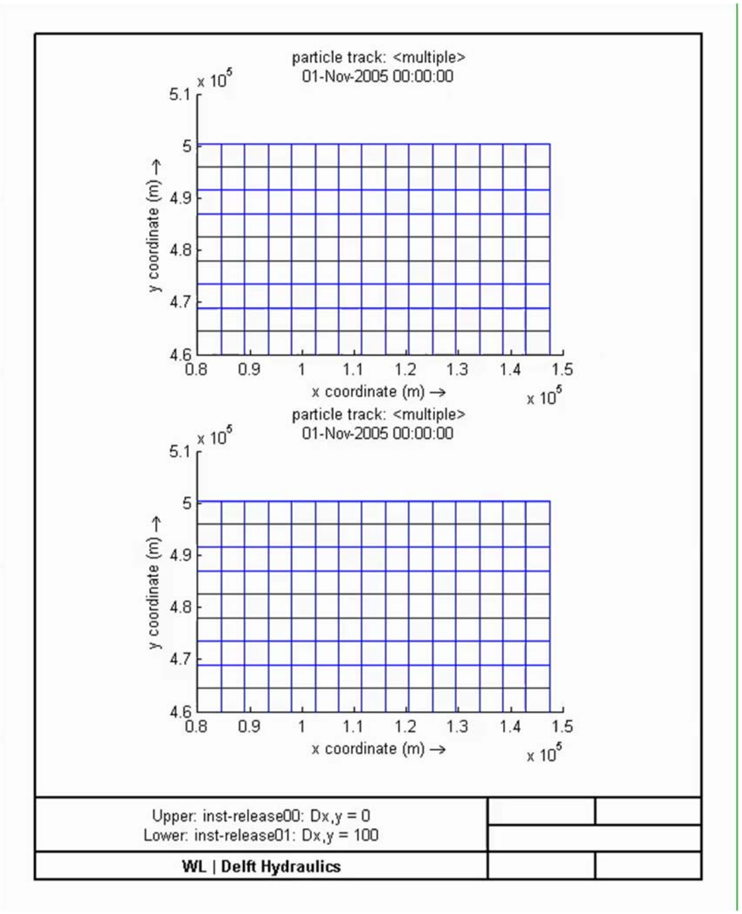
- A, D, S

Main difference between advection and diffusion:

- 1-D Example $$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D_x\left(\frac{\partial^2 c}{\partial x^2}\right)$$

Diffusion occurs because of:

- 1.
- 2.



The use of the 1-D Diffusion Equation

Derivation from Fick's Law and conservation of mass: $\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial c}{\partial x} \right)$

- Important because it is a linear equation!

Started with solution for infinite domain.

Obtained solutions for finite domains

- Concentration $c(x,t) = \frac{M}{\sqrt{4\pi D t}} \left[\exp\left(-\frac{(x - 2mL - a)^2}{4Dt} \right) + \exp\left(-\frac{(x - 2mL + a)^2}{4Dt} \right) \right]$
- Mixing time: $T = 0.134 \frac{L^2}{D}$ or $T = 0.536 \frac{L^2}{D}$
- Extended to include Decay and Source

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

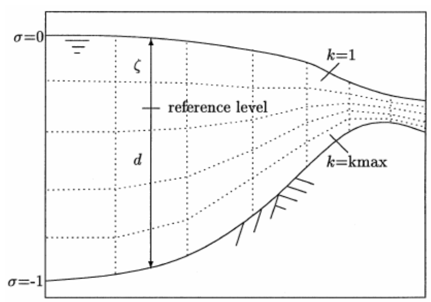
- Averaged 3D: $$\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} + \frac{\partial (vc)}{\partial y} + \frac{\partial (wc)}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right)$$

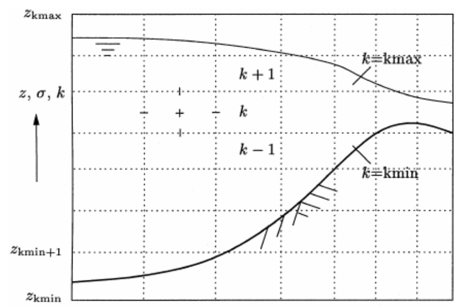
- 2D Depth-average: $$\frac{\partial (ch)}{\partial t} + \frac{\partial (uhc)}{\partial x} + \frac{\partial (vhc)}{\partial y} = \frac{\partial}{\partial x}\left(hk_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(hk_y\frac{\partial c}{\partial y}\right)$$

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

Artificial diffusion due to vertical grid coordinate system

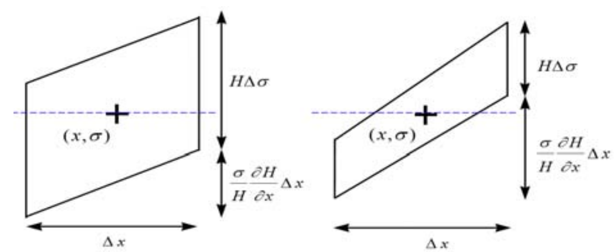
Two main types:





Issue arises due to transformation of equations

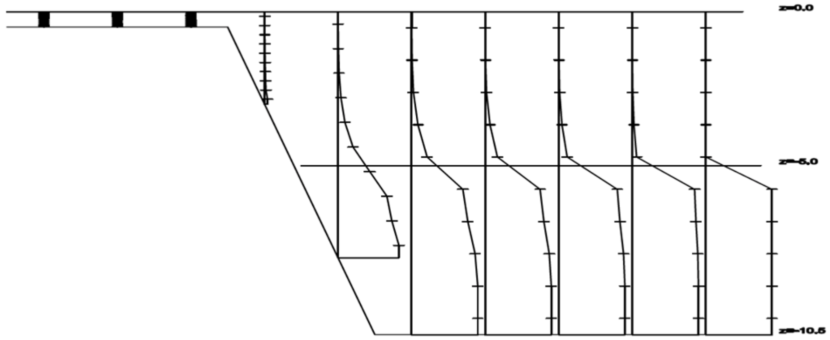
- Results in hydrostatic inconsistency
- Essentially → $\frac{\sigma}{H}\frac{\partial H}{\partial x}\Delta x < \Delta\sigma$



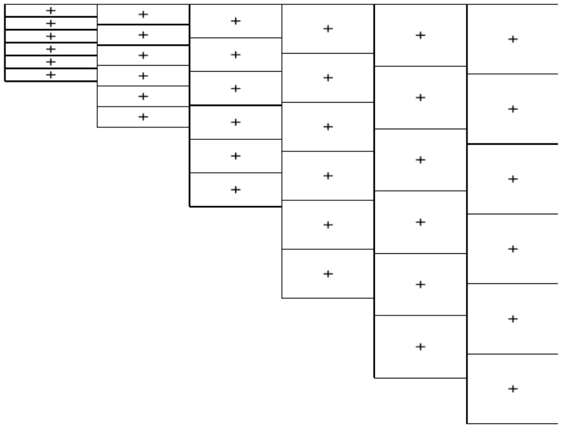
a. Hydrostatic consistent grid cell   b. Hydrostatic inconsistent g

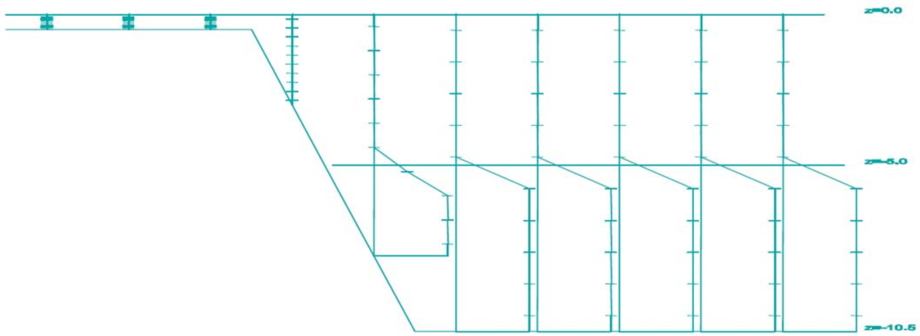
Discussed the Effect and solution

Artificial diffusion and mixing



Possible solution:





Turbulent mixing and models

Introduced the issue of turbulent mixing and its importance on mixing

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

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

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

Mixing and Turbulence

WHAT, WHY, HOW

What, where is turbulence?

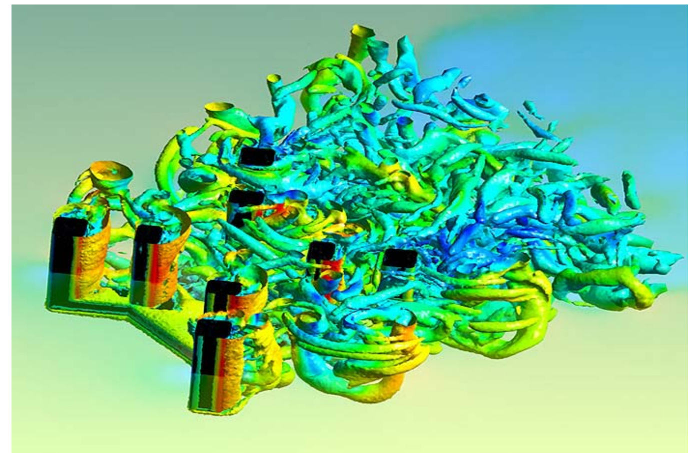
Everywhere

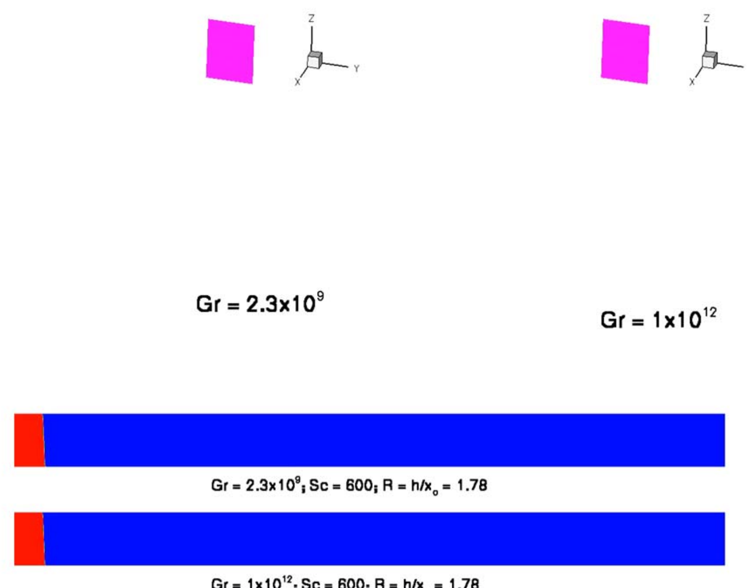
- Essentially all environmental flows are turbulent

Characteristics of turbulent flows:

- Highly unsteady
- 3-Dimensional
- High vorticity
- Fluctuates over a large range of length and time scales.
- Unpredictable (inherent instability)

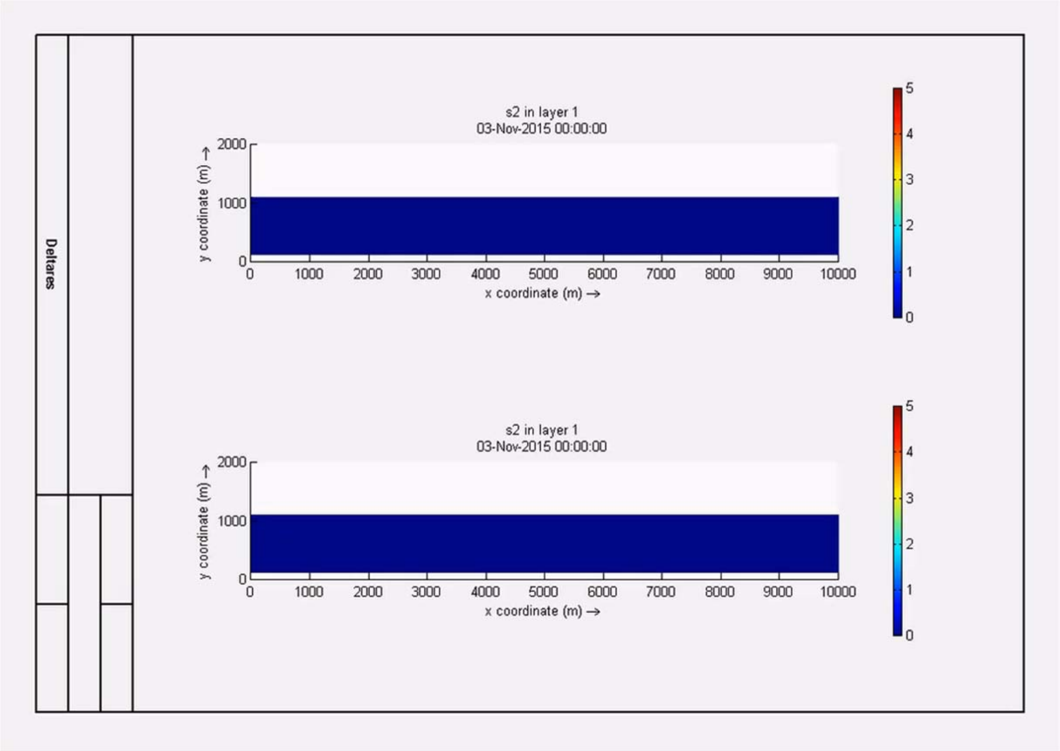
Great → More effective mixing as there is more agitation→ Larger D!





Are there simple ways to analyze turbulent mixing?

Shear flows are a starting point:

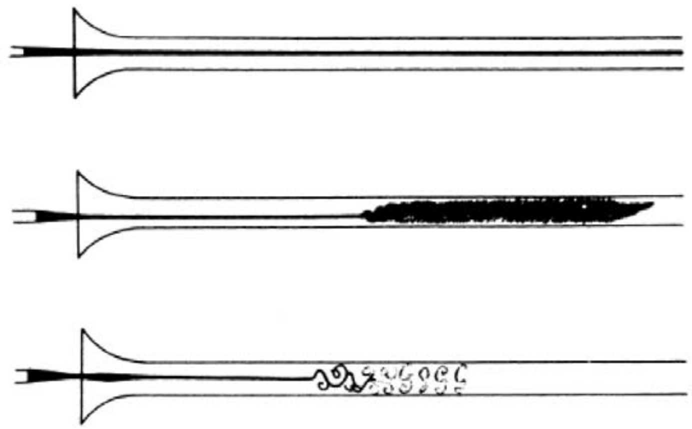


But fully turbulent flows have an unsteady velocity profile which restricts this method of analysis

- So how do we proceed?

Let’s classify turbulence

3 observations by Reynolds about dye streaks



Types of flows and its implications:

- Laminar → dependent on molecular diffusion
- Turbulent → creation of eddies which are unstable and grow

What does turbulence do then?

Describing turbulence

Simplest turbulent flow concept: Homogeneous turbulence..?

- Statistically steady (no spatial gradients)

Energy cascade

- Eddies going from large → small
- HOWEVER very little loss of energy until viscosity takes over → very small scales!
- Conversion of KE to heat at small scales → DISSIPATION: $\epsilon = \dfrac{\text{dissipated kinetic energy}}{\text{time}}$
- → P must equal E in a homogeneous turbulent flow

Which leads to the 2nd concept - length scale, L_K

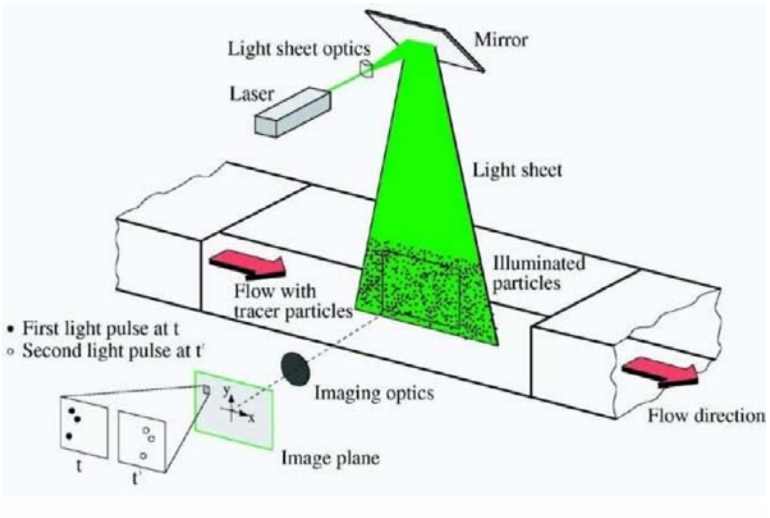
- How Large?
- Dimensional Analysis and physical understanding
- L_K must depend on rate of dissipation and viscosity

Can we prove it?

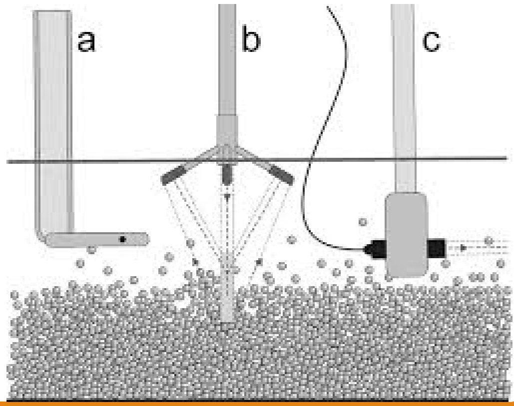
Can we measure eddies?

A few different methods exist to measure

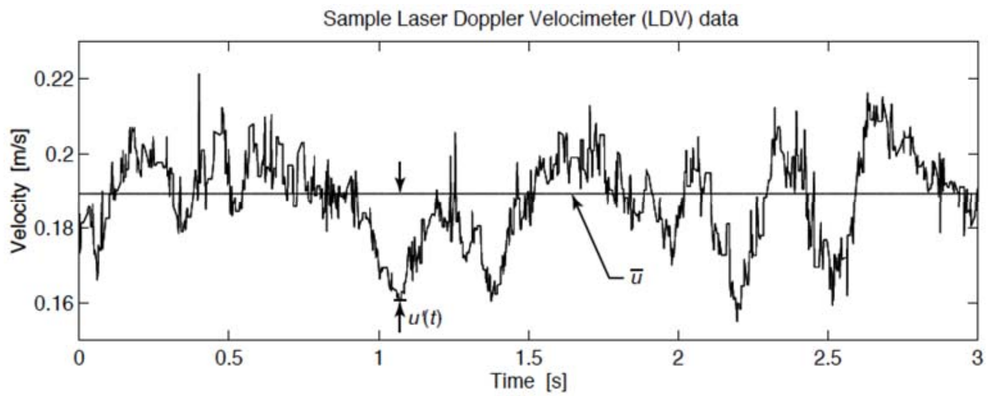
- Lagrangian view (PTV / PIV)



- Eulerian view (velocity probes)



A sample result and its implication



What do we see?

- A large spectrum of velocity fluctuations
- Different periods which we can correlate to eddy sizes
  - Large Eddy → Long Period; Small Eddy → Short Period
- Short time → High correlation;
- Longer time → lower correlation → eventually seemingly random
  - Integral Time Scale → Characteristic Length, Velocity

This allows us to use Reynolds Decomposition!

Remember Reynolds Decomposition?

Decompose velocity into mean and fluctuating components → $u_i(x_i,t) = \overline{u_i}(x_i) + u_i'(x_i,t)$.

- Essentially Integral Time Scale becomes the time for $\overline{u}_i$ to become steady/constant

Which allows us to have a 3rd important quantity

$$u_{rms} = \sqrt{\overline{u'u'}}$$

- Why is this important?

Turbulence and mixing (1)

Let's investigate using the 1D transport equation and introduce 2 concepts

- Reynolds Decomposition

$$C(x,t) = \bar{C}(x) + C'(x,t)$$

- And Time Averaging

$$q_x = \overline{uC}$$

$$\overline{uC} = \frac{1}{t_I}\int_{t_I}^{t+t_I} uC\, d\tau = \overline{\left(\bar{u}_i + u'_i\right)\left(\bar{C} + C'\ \right)} = \overline{u'C'} + \overline{uC}$$

Turbulence and mixing (2)

The advective-diffusive equation $\frac{\partial c}{\partial t}+\frac{\partial uc}{\partial x}=\frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right)$

Transforms into $\frac{\partial \overline{c}}{\partial t}+\overline{u}\frac{\partial \overline{c}}{\partial x}=-\frac{\partial \overline{u'c'}}{\partial x}+\frac{\partial}{\partial x}\left(D\frac{\partial \overline{c}}{\partial x}\right)$

A Fickian Relationship can be derived →

$$\overline{u'c'}=D_t\frac{\partial \overline{c}}{\partial x};\quad where \quad D_t=u_I L_I$$

Allowing us to re-write the equation as

$$\frac{\partial \overline{c}}{\partial t}+\overline{u}\frac{\partial \overline{c}}{\partial x}=\frac{\partial}{\partial x}\left(D_t\frac{\partial \overline{c}}{\partial x}\right)+\frac{\partial}{\partial x}\left(D\frac{\partial \overline{c}}{\partial x}\right)$$

Can we estimate D_t for Open Channel Flows?

Take a river as an example

Assume

- Wide (W >> H); how does this help?
- Turbulence is generated in high shear zones →
  - Where would you expect this to occur?
  - How does this help us → Shear velocity : $u_* = \sqrt{\frac{\tau_0}{\rho}}$
- Uniform flow → so?
- This allows us to obtain a turbulent diffusion relationship

$$D_t \propto u_* d$$

A logical deduction is that D_t will not be isotropic. Why?

Then how do we estimate D_t?

In the vertical (z)

- From log-law $\overline{u_t}(z) = \overline{u} + \frac{u_*}{\kappa}(1 + \ln(z/h))$ → $D_t = 0.067 u_* d$

In the transverse (y)

- From measurements
  - Lab $D_t = 0.15 u_* d$
  - Field $D_t = 0.60 u_* d$

And in the longitudinal (x)

- One can expect this to be the same as transverse dispersion. If we assume…
- However, since the vertical profile is not uniform → there is another process that dominates mixing in the longitudinal direction, which allows us to ignore this

So let's compare

B = 10m, d = 0.3m, Q = 1 m^3/s, S = 0.0005

From these formulas

$$D_t = 0.067 u_* d$$

$$D_t = 0.60 u_* d$$

TURBULENCE CLOSURE MODELS

MODELING TURBULENT MIXING

The need for turbulence closure models

If we could solve all flow scales practically, then there is no need for turbulence closure models.

The issue arises from the need to achieve a solution practically

- Without averaging, one has to carry out Direct Numerical Simluation (DNS) which requires MASSIVE computational resources (memory, CPUs and CPU speed) due to this approximate relationship

$$N^3 \geq \mathrm{Re}^{2.25}$$

However averaging over space (LES) or time (RANS) results in the problem of an additional tensor term.

The additional tensor term:

LES:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\overline{u_i u_j}) = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial}{\partial x_j}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + 2\nu \frac{\partial}{\partial x_j} S_{ij},$$

RANS:

- Momentum $$\frac{\partial \overline{u}_i}{\partial t} + \overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 \overline{u_i}}{\partial x_i x_j} - \frac{\partial \overline{u_i' u_j'}}{\partial x_j}$$
- Scalar $$\frac{\partial \overline{c}}{\partial t} + \overline{u}_j \frac{\partial \overline{c}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D \frac{\partial \overline{c}}{\partial x_j}\right) - \frac{\partial \overline{u_j' c'}}{\partial x_j}$$

Focusing on RANS, how do we solve this?

What is the issue of the additional term?

$$\frac{\partial \overline{u}_i}{\partial t} + \overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_i x_j} - \frac{\partial \overline{u_i' u_j'}}{\partial x_j}$$

We now have more unknowns than equations!

- These terms didn't exist originally and arise due to the averaging process.
- Called the Reynolds Stress Tensor!

To solve this problem one needs either extra parameters or equations (called closure models) to have a unique solution

- Simplest models use the Boussinesq hypothesis

$$\overline{u_i' u_j'} = \frac{2}{3} k \delta_{ij} - \nu_t \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right)$$

EDDY VISCOSITY

where $k = \frac{1}{2} \overline{u_i' u_i'}$

Where is this term?

In Delft3D for example:

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

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

Closing the Eddy Viscosity Relation

4 ways that have been proposed to calculate the eddy viscosity include

- Constant coefficient [Not strictly a Boussinesq assumption]
- Zero Equation
- One Equation
- Two Equation

Boussinesq assumption of eddy viscosity assumes that there is a relationship between characteristic length and velocity scales

$$\nu_t = C_\mu \sqrt{k} L$$

Zero Equation Models

The zero-equation is the simplest turbulence closure model, we only need to use analytical formulas to obtain *k* and *L* to solve the relationship:

$$\nu_t = C_\mu \sqrt{k} L$$

- Typically k is calculated directly from the flow; in Delft3D

$$k = \frac{1}{\sqrt{c_\mu}} L^2 \left[\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 \right] \quad \text{or} \quad k = \frac{1}{\sqrt{c_\mu}} \left[\left(u_*^b \right)^2 \left(1 - \frac{z+d}{H} \right) + u_{*8}^2 \frac{z+d}{H} \right]$$

- And a relationship to obtain *L* is derived from either

$$L = \kappa (z+d) \sqrt{1 - \frac{z+d}{H}} f(Ri) \quad \text{or} \quad \sqrt{k} = L \frac{\partial u}{\partial y}$$

Where $$Ri = \frac{-g \frac{\partial \rho}{\partial z}}{\rho \left[\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 \right]}$$

One Equation Model

One equation models

- solve for *k* through a transport equation e.g.

$$\frac{\partial k}{\partial t} + \overline{u}_j \frac{\partial k}{\partial x_j} = +D_t \frac{\partial^2 k}{\partial x_i x_j} + P_k + P_{kw} + B_k - \varepsilon$$

- And prescribe *L* (typically using the previous relationships shown for the zero-equation model) and then using the same viscosity relationship to calculate viscosity → $\nu_t = C_\mu \sqrt{k} L$

In Delft3D the transport equation for k is:

$$\frac{\partial k}{\partial t} + \frac{u}{\sqrt{G_{\xi\xi}}} \frac{\partial k}{\partial \xi} + \frac{v}{\sqrt{G_{\eta\eta}}} \frac{\partial k}{\partial \eta} + \frac{\omega}{d+\zeta} \frac{\partial k}{\partial \sigma} = + \frac{1}{(d+\zeta)^2} \frac{\partial}{\partial \sigma} \left[\left(\nu_{mol} + \frac{\nu_{3D}}{\sigma_k} \right) \frac{\partial k}{\partial \sigma} \right] + P_k + P_{kw} + B_k - \varepsilon$$

$$P_k = \nu_V \frac{1}{(d+\zeta)^2} \left[\left(\frac{\partial u}{\partial \sigma} \right)^2 + \left(\frac{\partial v}{\partial \sigma} \right)^2 \right]$$

$$B_k = \frac{\nu_{3D}}{\rho \sigma_\rho} \frac{g}{H} \frac{\partial \rho}{\partial \sigma}$$

$$\varepsilon = c_D \frac{k\sqrt{k}}{L}$$

$$c_D = c_\mu^{3/4} \approx 0.1925.$$

Two Equation Models

Two-equation models solve for

- Transport of *k* and the dissipation rate of *k*, ε.
- From *k* and ε the mixing length and viscosity are calculated.

For hydrostatic models, the equations can be written as:

$$\frac{\partial k}{\partial t} + \frac{u}{\sqrt{G_{\xi\xi}}}\frac{\partial k}{\partial \xi} + \frac{v}{\sqrt{G_{\eta\eta}}}\frac{\partial k}{\partial \eta} + \frac{\omega}{d+\zeta}\frac{\partial k}{\partial \sigma} = + \\ + \frac{1}{(d+\zeta)^2}\frac{\partial}{\partial \sigma}\left[\left(\nu_{mol} + \frac{\nu_{3D}}{\sigma_k}\right)\frac{\partial k}{\partial \sigma}\right] + P_k + P_{kw} + B_k - \varepsilon,$$

$$\frac{\partial \varepsilon}{\partial t} + \frac{u}{\sqrt{G_{\xi\xi}}}\frac{\partial \varepsilon}{\partial \xi} + \frac{v}{\sqrt{G_{\eta\eta}}}\frac{\partial \varepsilon}{\partial \eta} + \frac{\omega}{d+\zeta}\frac{\partial \varepsilon}{\partial \sigma} = \\ \frac{1}{(d+\zeta)^2}\frac{\partial}{\partial \sigma}\left[\left(\nu_{mol} + \frac{\nu_{3D}}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial \sigma}\right] + P_\varepsilon + P_{\varepsilon w} + B_\varepsilon - c_{2\varepsilon}\frac{\varepsilon^2}{k}.$$

$$\nu_{3D} = c'_\mu L\sqrt{k} = c_\mu \frac{k^2}{\varepsilon}$$

After all that…

This is how it is taken care of in your model

Note that there are

- 3 horizontal components $$\nu_H = \nu_{SGS} + \nu_V + \nu_H^{back}$$
- And 2 vertical components: $$\nu_V = \nu_{mol} + \max(\nu_{3D}, \nu_V^{back})$$

model description	ν_{SGS}	ν_H^{back} (represents)	ν_{3D}	ν_V^{back}
2D, no HLES	-	2D-turbulence + dispersion coefficient	-	-
2D, with HLES	computed by HLES	3D-turbulence + dispersion coefficient	-	-
3D, no HLES	-	2D-turbulence	computed by vertical turbulence model.	background vertical viscosity
3D, with HLES	computed by HLES	-	computed by vertical turbulence model.	background vertical viscosity

What about the turbulent diffusivity?

That solved the turbulent viscosity and taken care of turbulence in our momentum equation.

What about mixing processes for our transport equations?

Simplest model assumes a gradient-diffusion hypothesis that is

$$\overline{u_j'c'} = -D_t \frac{\partial \overline{c'}}{\partial x_j}$$

where

$$D_t = \frac{\nu_t}{Sc_t}$$

What about Diffusion?

Where is Diffusion and what is it affected by?

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

Diffusion in Delft3D

Similar to the momentum equation:

- Horizontal $D_H = D_{SGS} + D_{3D} + D_H^{back}$
- Vertical $$D_V = \frac{\nu_{mol}}{\sigma_{mol}} + \max(D_V^{back}, D_{3D})$$

But what is D_{3D}? $$D_{3D} = \frac{\nu_{3D}}{\sigma_c}$$

- What is σ_c? $\sigma_c = \sigma_{c_0} F_\sigma(Ri).$
- What is actually put in the code? $$D_{3D} = \max\left(D_{3D}, 0.2L_{oz}^2\sqrt{-\frac{g}{\rho}\frac{\partial\rho}{\partial z}}\right)$$

The issue of stratification, the Prandtl-Schmidt Number, σ_c

This is a dimensionless number that relates viscous diffusion to

- Molecular diffusion ν/D (Schmidt); or
- Turbulent diffusion ν_t/D_t; or
- Thermal diffusion: ν/α (Prandtl)

In the Delft3D formulation:

$$\sigma_c = \sigma_{c_0} F_\sigma(Ri).$$

- σ_{c0} is a constant (0.7; 1.0[k]; 1.3[ε])
- F_σ is a damping function for the ALM when the flow is strongly stratified

In summary:

model description	D_{2D}	D_H^{back}	D_{3D}	D_V^{back}
2D, no HLES	0	2D-turbulence + dispersion coefficient	-	-
2D, with HLES	computed by HLES	3D-turbulence + dispersion coefficient	-	-
3D, no HLES	0	2D-turbulence	maximum of value of turbulence model and the Ozmidov length scale. *2	background eddy diffusivity
3D, with HLES	computed by HLES		maximum of value of turbulence model and the Ozmidov length scale. *2	background eddy diffusivity

Diffusion is accounted for as:

$$D_{3D} = \max\left(D_{3D}, 0.2L_{oz}^2\sqrt{-\frac{g}{\rho}\frac{\partial\rho}{\partial z}}\right).$$

where $D_{3D} = \frac{\nu_{3D}}{\sigma_c}$

- HOWEVER by default $L_{OZ} = 0$; why?