

Tobias Bleninger

MECÂNICA DOS FLUIDOS AMBIENTAL I

Balanço de massa

$$0 = \frac{\partial}{\partial t} \int_{V_c} \rho dV + \int_{S_c} \rho (\mathbf{v} \cdot \mathbf{n}) dS.$$

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0,$$

Balanço de massa de um soluto

$$\frac{\partial}{\partial t} \int_{V_c} C_A \rho dV + \int_{S_c} C_A \rho (\mathbf{v} \cdot \mathbf{n}) dS = - \int_{S_c} (\mathbf{j} \cdot \mathbf{n}) dS.$$

$$\frac{\partial C_A}{\partial t} + (\mathbf{v} \cdot \nabla) C_A = D_{AB} \nabla^2 C_A.$$

Balanço de quantidade de movimento

$$\frac{\partial}{\partial t} \int_{V_c} \mathbf{v} \rho dV + \int_{S_c} \mathbf{v} \rho (\mathbf{v} \cdot \mathbf{n}) dS = \int_{V_c} \rho \mathbf{g} dV + \int_{S_c} (\mathbf{T} \cdot \mathbf{n}) dS.$$

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla (p + \rho g h) + \mu \nabla^2 \mathbf{v}$$

Balanço de energia

$$\frac{\partial}{\partial t} \int_{V_c} e \rho dV + \int_{S_c} e \rho (\mathbf{v} \cdot \mathbf{n}) dS = - \int_{S_c} (\mathbf{q} \cdot \mathbf{n}) dS + \int_{S_c} [(\mathbf{T} \cdot \mathbf{v}) \cdot \mathbf{n}] dS$$

Forma geral

$$\frac{\partial \eta}{\partial t} + (\mathbf{v} \cdot \nabla) \eta - K \nabla^2 \eta = f(x, y, z, t)$$

$$\rho \frac{\partial e}{\partial t} + \rho (\mathbf{v} \cdot \nabla) e = \nabla \cdot (\mathbf{T} \cdot \mathbf{v}) + \nabla \cdot (\rho c_p \alpha \nabla T)$$

$$\frac{DT}{Dt} = \frac{\partial T}{\partial t} + (\mathbf{v} \cdot \nabla) T = \alpha \nabla^2 T,$$

Equação de difusão

Concentração:

$$C = \frac{M_{substancia}}{V_{total}}$$

Fluxo de massa:

$$j_x = -D \frac{\partial C}{\partial x}$$

(compare: $q_x = -\lambda \frac{\partial T}{\partial x}$)

Impulso

$$\tau = \mu \frac{dV}{dy} = \rho v \frac{dV}{dy} = v \frac{d\rho V}{dy}$$

Conservação:

$$\frac{\partial C}{\partial t} + \text{div } \vec{j} = 0 \text{ ou } R$$

Equação de difusão (1D):

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} + R(x, t)$$

(compare: $\frac{\partial T}{\partial t} = \alpha^2 \frac{\partial^2 T}{\partial x^2} + F(x, t)$)

$R(x, t)$: fonte ou sumidor (reações, transformações)

Soluções da equação de difusão

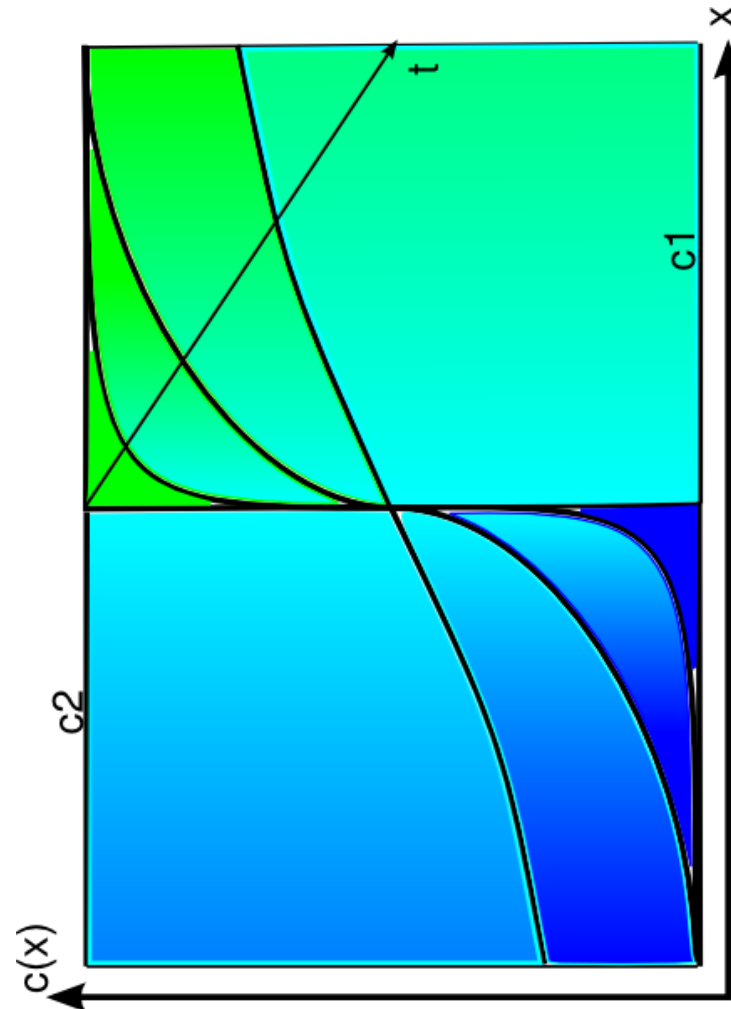
Mistura de fluidos com concentrações diferentes (experimento)

- $F(x,t) = 0$
- Condições iniciais $C(x,0) = C_0 \varphi(\mathbf{x})$
 - transparente: água com $C_{\text{sal}} = 0$
 - colorido: água com $C_{\text{sal}} = C_0$
- Condições de contorno:
 - superfície: $C(\infty,t) = 0$
 - fundo: $C(-\infty,t) = C_0$
- Solução (análogo eq. do calor)

$$c(x, t) = \frac{c_0}{2\sqrt{\pi Dt}} \int_0^\infty dx' \exp\left(-\frac{(x-x')^2}{4Dt}\right) = \frac{c_0}{2} \left(1 + \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right)$$

Soluções da equação de difusão

Mistura de fluidos com concentrações diferentes (experimento)



Exemplo 2

Definição:

- Equações diferenciais parciais (edp) são equações contendo
 - duas (ou mais) variáveis independentes x e y
 - a função procurada $f(x,y)$
 - derivadas de f da ordem n

Motivação:

- Problemas mais importantes na engenharia ambiental: edp2
- Problemas de condução/difusão, equação do calor, de onda

Equação do calor (ec1):

$$q_x = -\lambda \frac{\partial T}{\partial x} \quad \frac{\partial T}{\partial t} = \alpha^2 \frac{\partial^2 T}{\partial x^2} + F(x,t) \quad \alpha^2 = \frac{\lambda}{c_p \rho}$$

- $0 < x < l$, $t > 0$
- **λ : condutividade térmica, c : calor específico a p const., ρ : densidade, α : difusividade térmica**

Definição do problema de valor de contorno 1

Equação do calor

■ $0 < x < l$, $t > 0$

homogêneo

cc1:

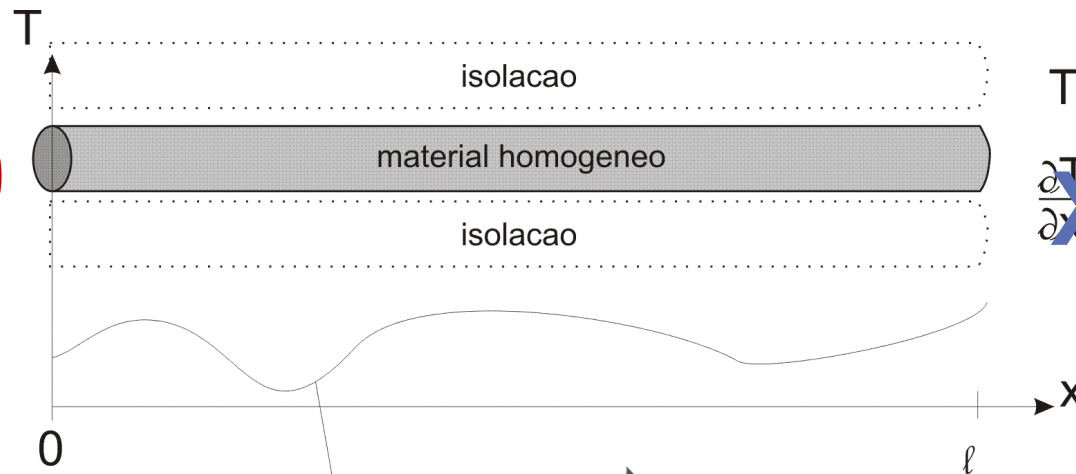
$$\frac{\partial T}{\partial t} = \alpha^2 \frac{\partial^2 T}{\partial x^2} + 0$$

cc2:

Dirichlet
(T fixo)

$$\left. \begin{array}{l} T(0,t) \\ \text{ou} \\ \frac{\partial T}{\partial x}(0,t) \end{array} \right\} = 0$$

von Neumann
(fluxo fixo)



$$\left. \begin{array}{l} T(l,t) \\ \text{ou} \\ \frac{\partial T}{\partial x}(l,t) \end{array} \right\} = 0$$

condição inicial (ci):

$T(x,0)=\varphi(x)$
distr. inicial

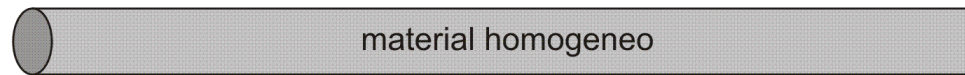
~~ $F(x,t)$ produção de calor~~

$$\varphi(0) = \psi_1(0)$$

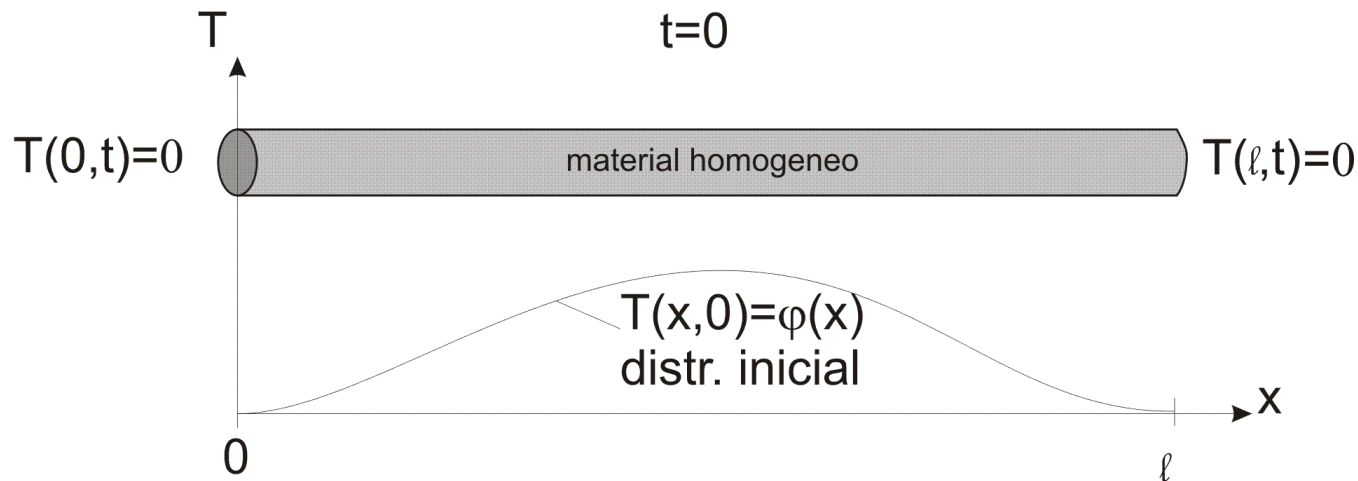
$$\varphi(l) = \psi_2(0)$$

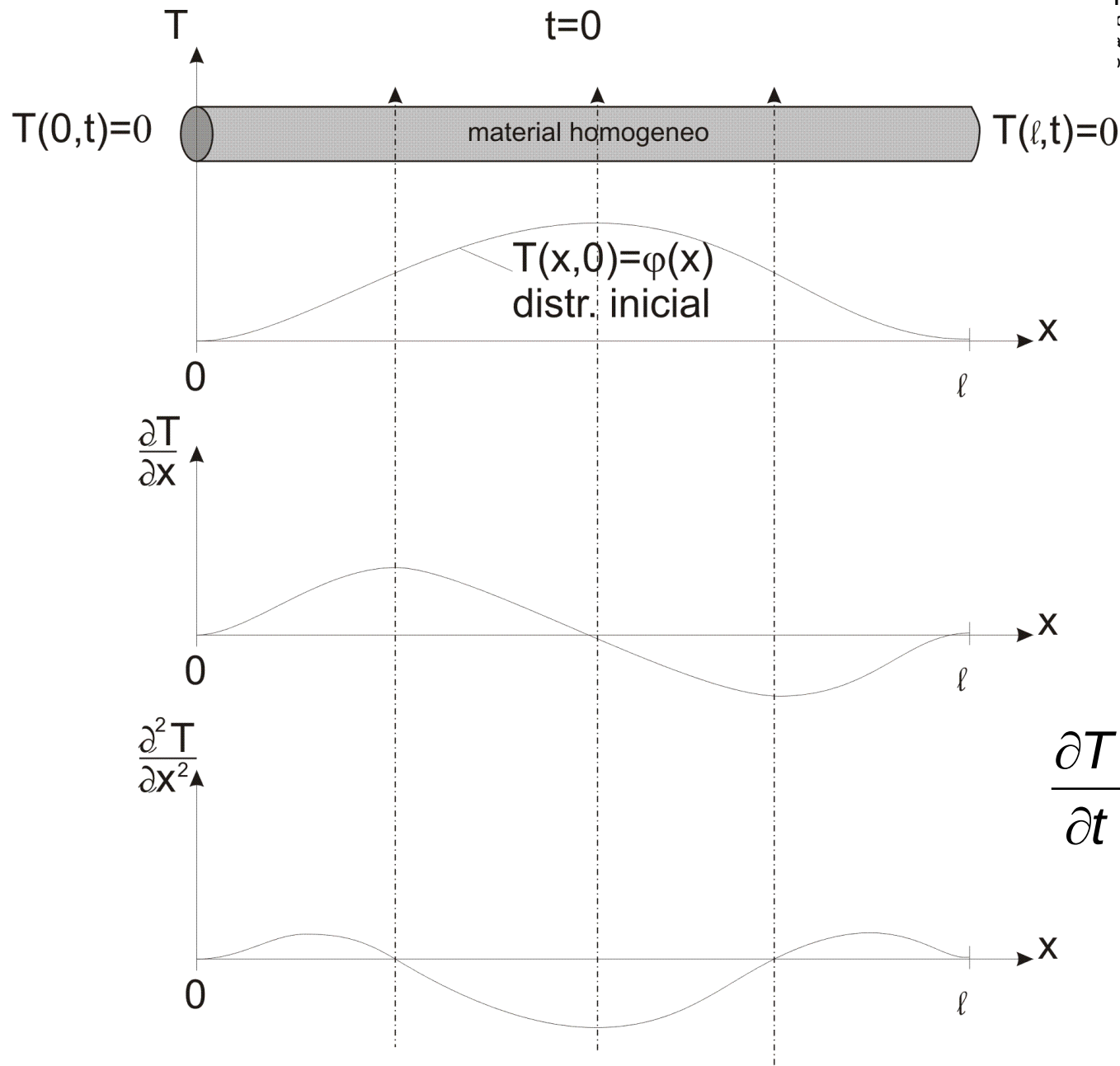
Equação do calor homogênea: Ilustração do problema de valor de contorno 1

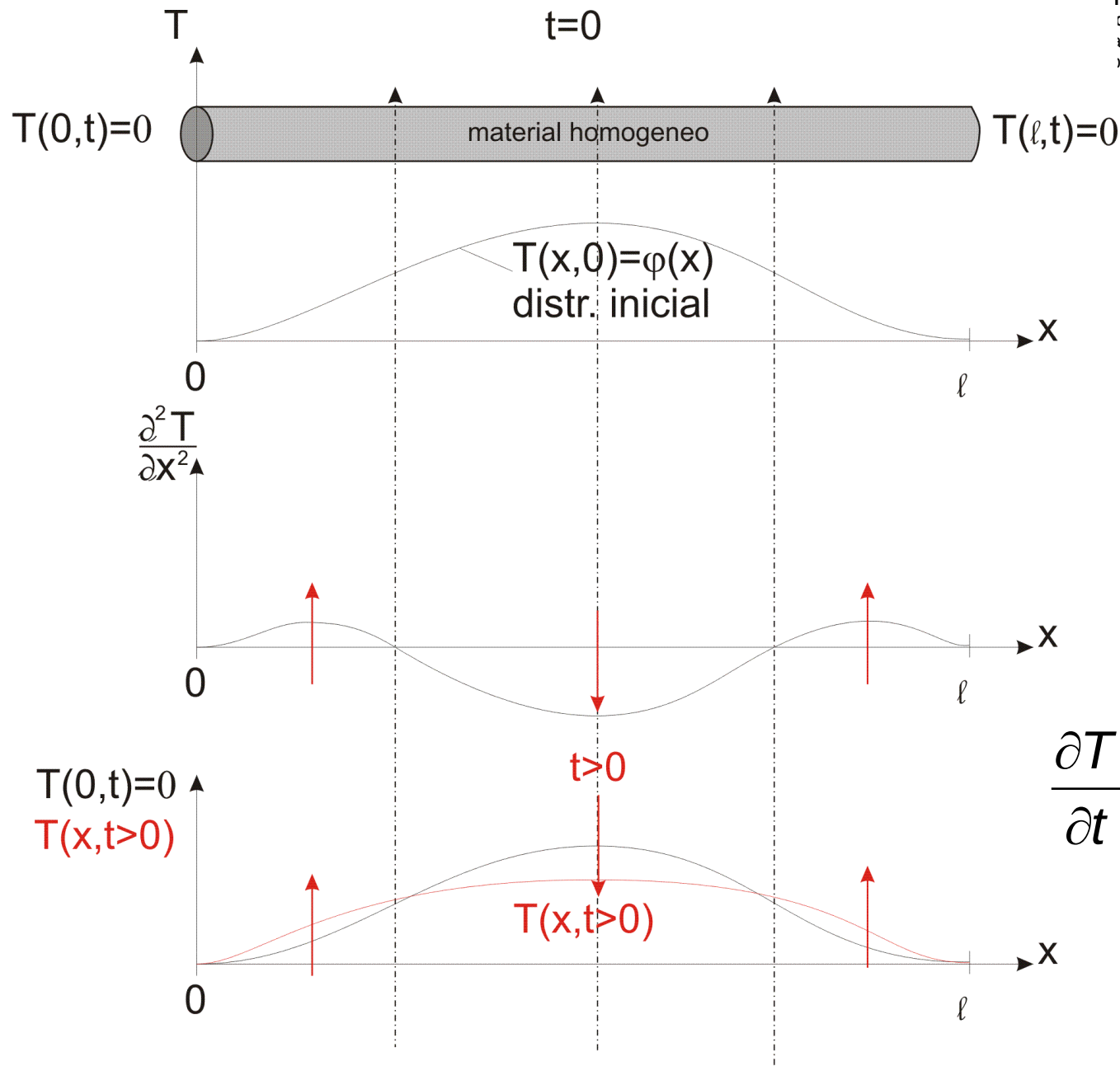
$t < 0$



$t = 0$







Equação do calor homogênea: Solução do problema de contorno 1

Matemática!

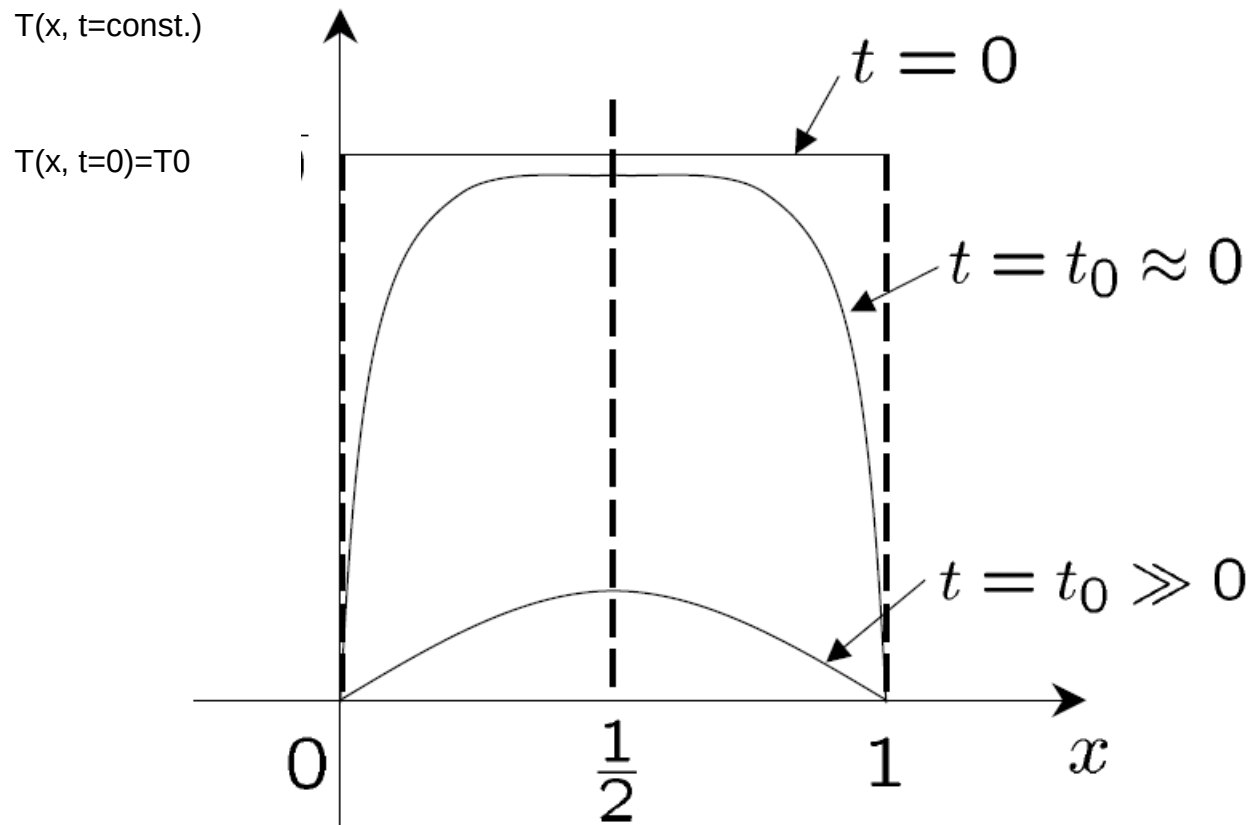
$$T(x,t) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{\ell}\right) \exp\left(\frac{-n^2\pi^2\alpha^2 t}{\ell^2}\right)$$

Observações:

- falta mostrar convergência e continuidade, mas se pode mostrar
- $t \rightarrow \infty \rightarrow T(x,t) \rightarrow 0$ com limites maiores
- assim $\lambda_n = -n^2\pi^2/\ell^2$, $n=1,2,\dots$ são auto valores com a
- auto função

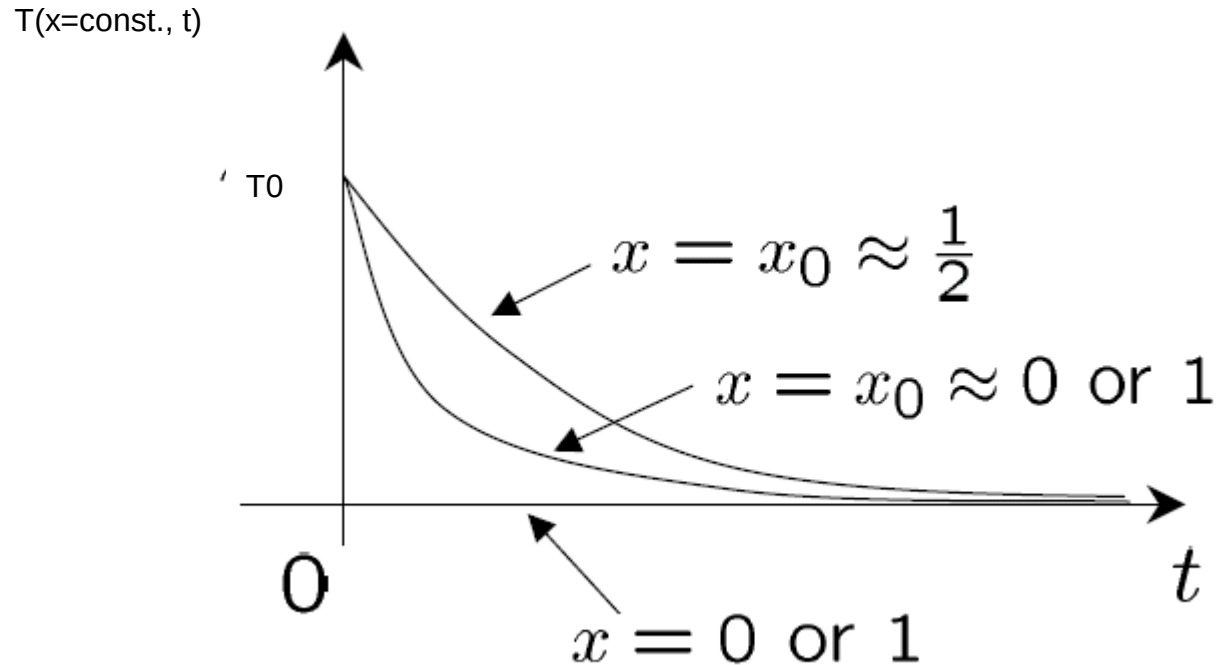
$$u_n(x) = c_n \sin\left(\frac{n\pi x}{\ell}\right)$$

Equação do calor homogênea: Solução do problema de contorno 1 $T(x, t = \text{const.})$



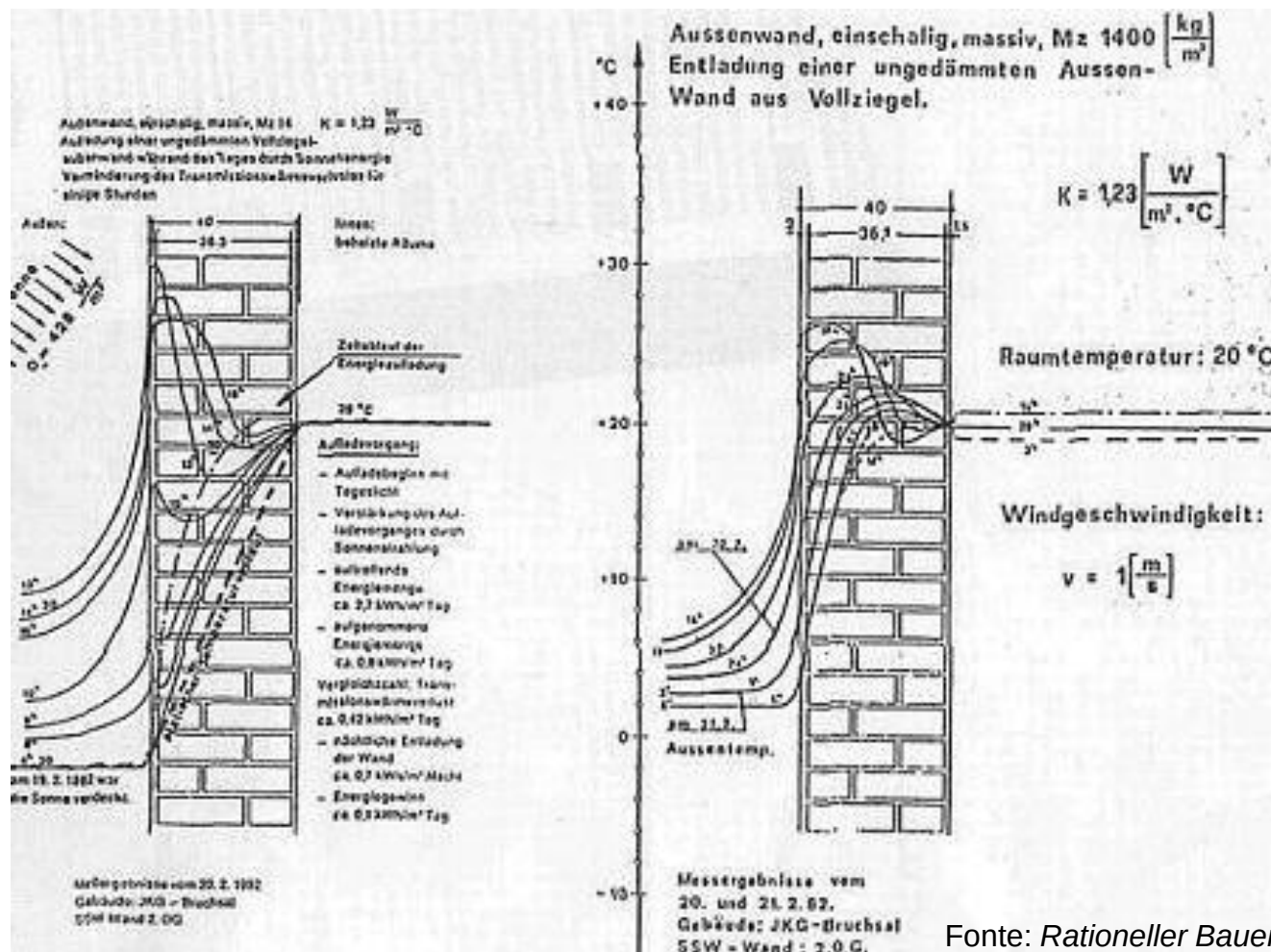
Fonte: Hancock, 2006

Equação do calor homogênea: Solução do problema de contorno 1 $T(x=\text{const.}, t)$



Fonte: Hancock, 2006

Equação do calor : Aplicações

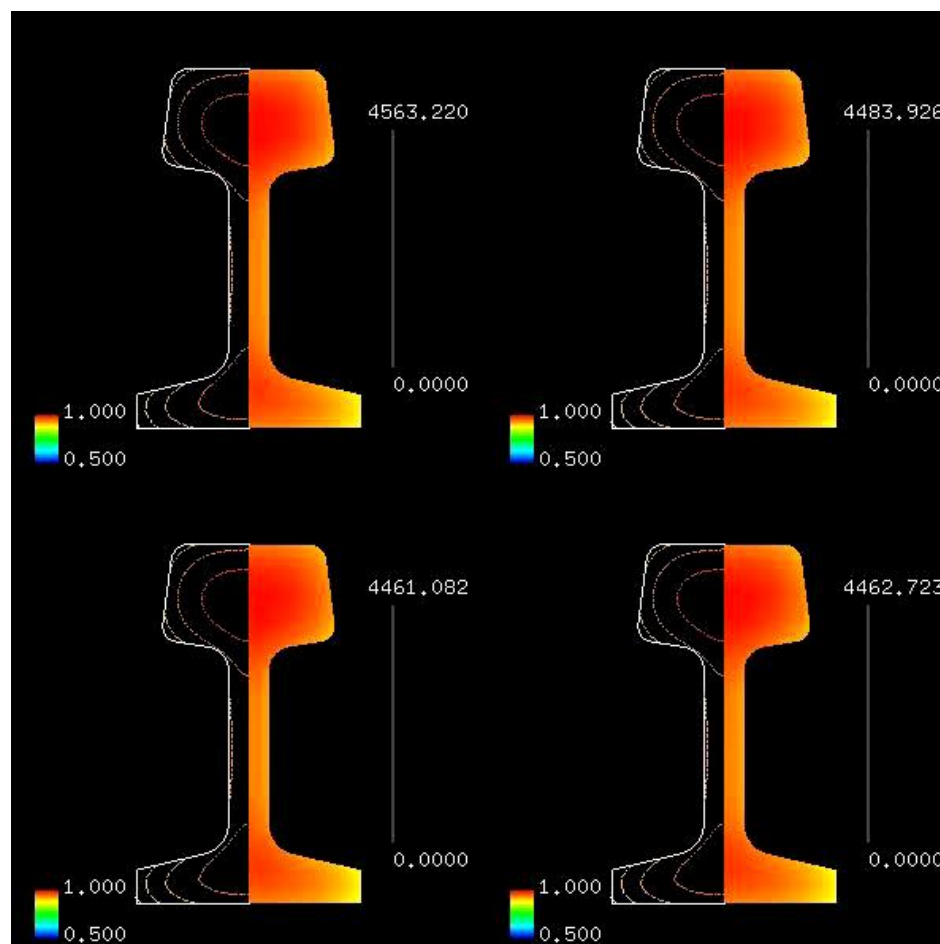


Fonte: Rationeller Bauen, 1983

Medições de temperatura numa parede em inverno (nublado).

$T_{ar,amb} = 6-10^\circ\text{C}$, $T_{par,amb} = 14-30^\circ\text{C}$, $T_{par,int.} = T_{ar,int.} = 20^\circ\text{C}$ $T_{ar,amb} < T_{par} \rightarrow$ não ocorre condensação. Obs.: distribuição permanente não corresponde com medições!

Equação do calor : Aplicações



Modelagem da refrigeração controlada de barras de aço (trilha) no processo de produção. Objetivo: definir condições de contorno (refrigeração controlada) e/ou condições iniciais (produção controlada) para obter uma distribuição de temperatura equilibrada para cada momento. Fonte: Dipl. Math. Jens Saak

Equação de difusão

Concentração:

$$C = \frac{M_{substancia}}{V_{total}}$$

Fluxo de massa:

$$j_x = -D \frac{\partial C}{\partial x}$$

- **D: difusividade molecular de A em B**

Equação de difusão:

$$\frac{\partial C}{\partial t} = -D \frac{\partial^2 C}{\partial x^2} + F(x,t) \quad \left(\text{compare: } \frac{\partial T}{\partial t} = \alpha^2 \frac{\partial^2 T}{\partial x^2} + F(x,t) \right)$$

- $F(x,t)$: fonte ou sumidor (reações, transformações)

Soluções da equação de difusão

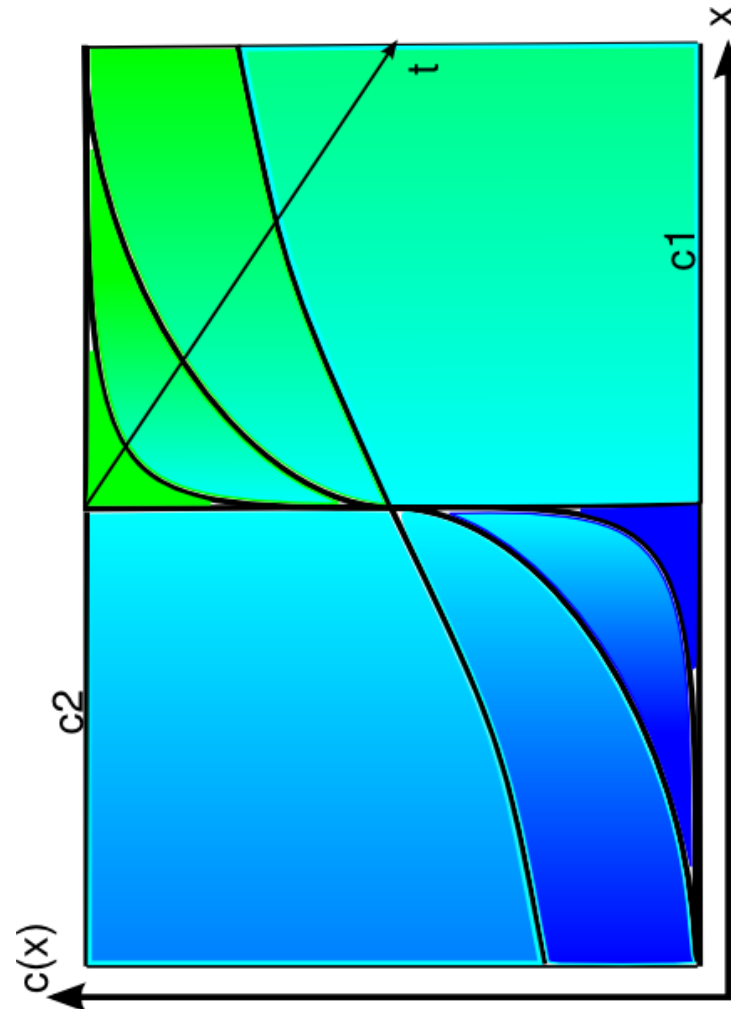
Mistura de fluidos com concentrações diferentes (experimento)

- $F(x,t) = 0$
- Condições iniciais $C(x,0) = C_0 \varphi(\mathbf{x})$
 - transparente: água com $C_{\text{sal}} = 0$
 - colorido: água com $C_{\text{sal}} = C_0$
- Condições de contorno:
 - superfície: $C(\infty,t) = 0$
 - fundo: $C(-\infty,t) = C_0$
- Solução (análogo eq. do calor)

$$c(x, t) = \frac{c_0}{2\sqrt{\pi Dt}} \int_0^\infty dx' \exp\left(-\frac{(x-x')^2}{4Dt}\right) = \frac{c_0}{2} \left(1 + \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right)$$

Soluções da equação de difusão

Mistura de fluidos com concentrações diferentes (experimento)



Referências

- Boyce, W. E., DiPrima, R. C., 1998, “Equações Diferenciais Elementares e Problemas de Valores de Contorno”, traduzido do inglês por Horacio Macedo, LTC - Livros Técnicos e Científicos Editora S.A., Rio de Janeiro, ISBN 85-216-1131-5
- Kreyszig, E., 1999, “Advanced Engineering Mathematics”, John Wiley & Sons, Inc., New York, ISBN 0-471-15496-2
- Hancock, M. 2006, “Linear Partial Differential Equations”, MIT Open Course Ware, Massachusetts Institute of Technology, <http://ocw.mit.edu/courses/mathematics/18-303-linear-partial-differential-equations-fall-2006/>
- Robert E. Terrell, 2011, “PDE applets heat equation in 1d and 2d“, Cornell University, Department of Mathematics, <http://www.math.cornell.edu/~bterrell/>

Coupling case study Cartagena outfall (Colombia)

Outfall:

2.8 km long

20 m deep

3.8 m³/s

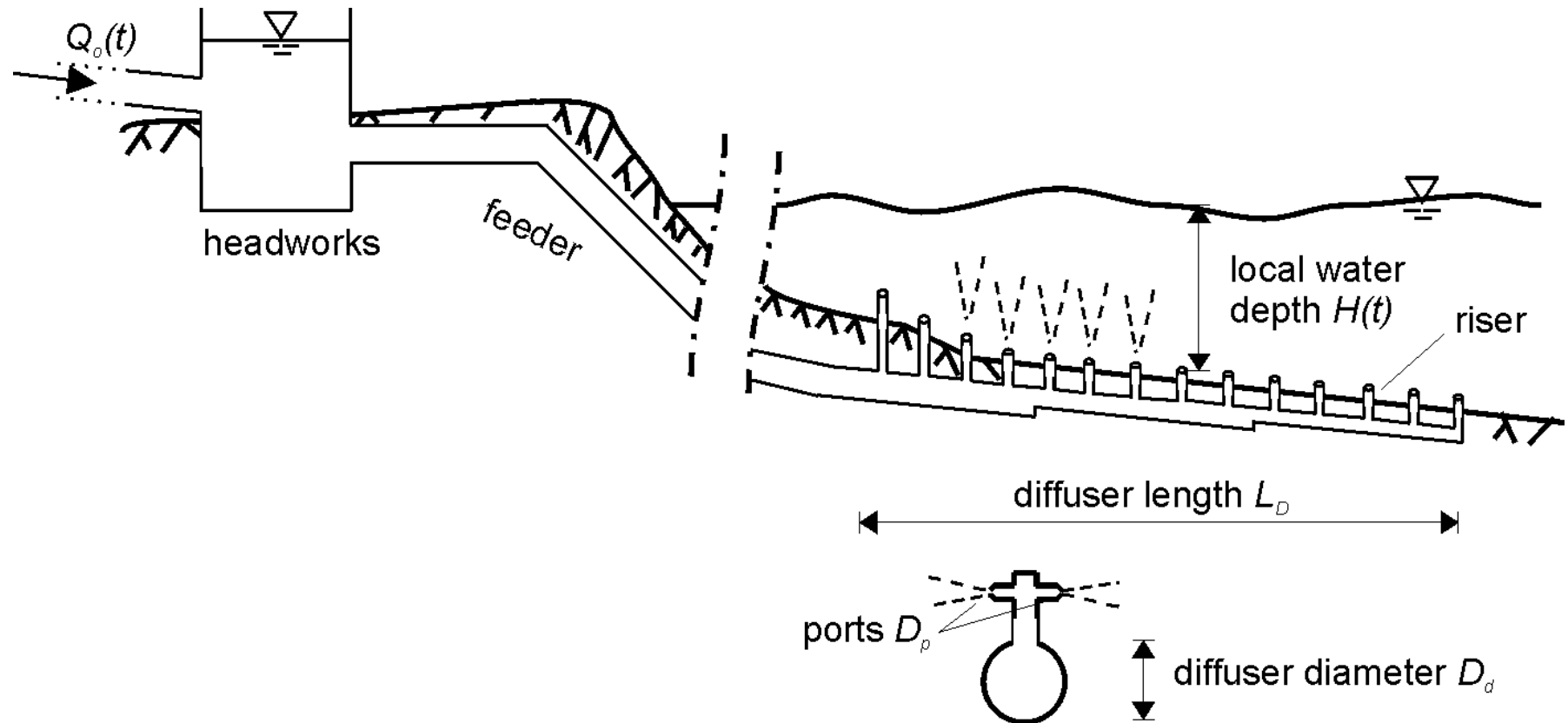


Cartagena

Source: World Bank

A) Multiport diffuser design program - CorHyd

Definition diagram



Governing equations for CorHyd

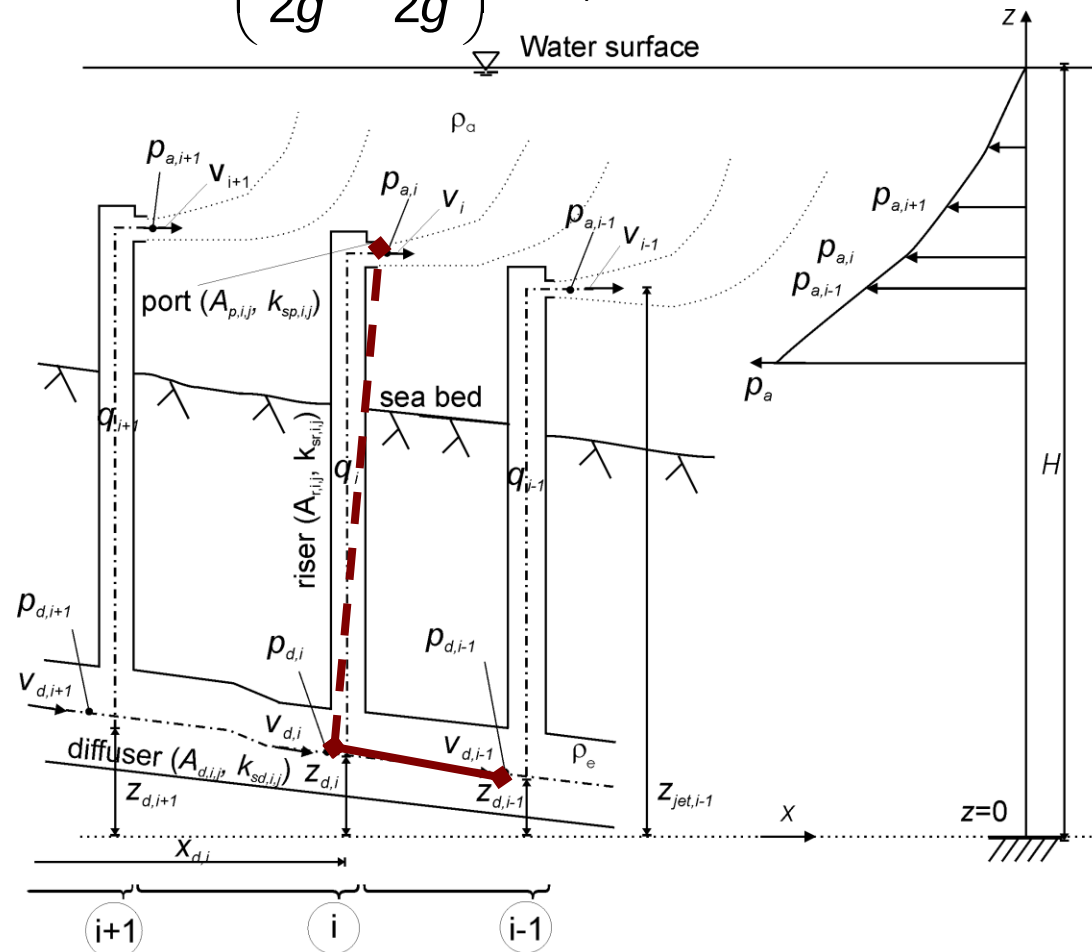
- 1-D continuity and steady-state work-energy equations

$$p_{d,i} = p_{d,i-1} + \gamma_e (z_{d,i-1} - z_{d,i}) + \gamma_e \left(\frac{v_{d,i-1}^2}{2g} - \frac{v_{d,i}^2}{2g} \right) + p_{\ell,d,i}$$

$$p_{d,i} = p_{a,i} + \gamma_e (z_{jet,i} - z_{d,i}) + \gamma_e \left(\frac{v_{p,i}^2}{2g} - \frac{v_{d,i}^2}{2g} \right) + p_{\ell,p,i}$$

Automatic consideration of:

- friction losses along every single pipe section
- local losses at every geometrical change (e.g. contractions, bends)



Solving scheme

$$q_i = \sqrt{\frac{\frac{2}{\rho_e} \underbrace{(p_{d,i-1} - p_{a,i})}_{\text{pressure diff.}} + 2g \underbrace{(z_{d,i-1} - z_{jet,i})}_{\text{geod. diff.}} + \left(\sum_{k=1}^{i-1} q_k \right)^2 \left[\frac{1}{A_{d,i-1}^2} + \underbrace{\sum_{j=1}^{n_{d,i-1}} \frac{1}{A_{d,i-1,j}^2} \left(\zeta_{d,i-1,j} + \lambda_{d,i-1,j} \frac{L_{d,i-1,j}}{D_{d,i-1,j}} \right)}_{\text{diffuser losses}} \right]}{\frac{\alpha_i^2}{(C_{c,i} A_{p,i})^2} + \underbrace{\sum_{j=1}^{n_{p,i}} \left(\frac{\alpha_i}{A_{p,i,j}} \right)^2 \left(\zeta_{p,i,j} + \frac{\lambda_{p,i,j} L_{p,i,j}}{D_{p,i,j}} \right)}_{\text{port losses}} + \underbrace{\sum_{j=1}^{n_{r,i}} \left(\frac{1}{A_{r,i,j}} \right)^2 \left(\zeta_{r,i,j} + \frac{\lambda_{r,i,j} L_{r,i,j}}{D_{r,i,j}} \right)}_{\text{riser losses}}}}$$

Solving for flow distribution and total head with given total flow

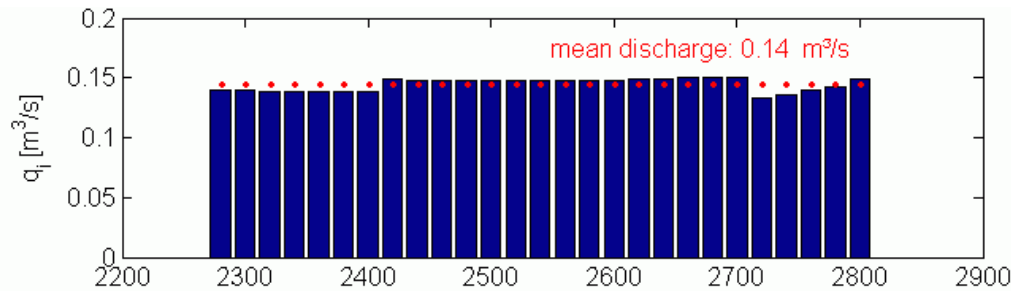
- q_1 is estimated, q_i calculated, iteration until $\sum q_i = Q$

optional: Solving for total flow with given total head

- $p_{d,1}$ is estimated, q_i calculated, iteration until $\sum h_\ell = H_t$

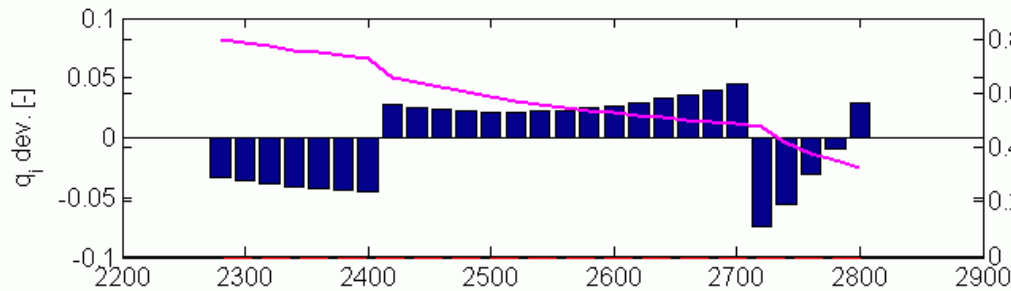
Algorithm coded in Matlab®, including GUI and graphical output

CorHyd - results for Cartagena outfall ($L_D = 540$ m)



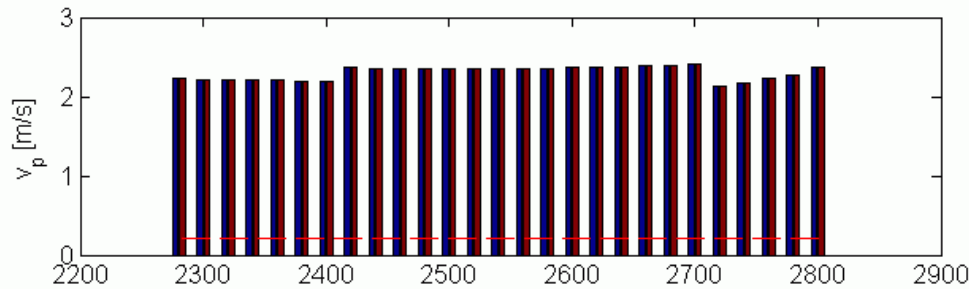
$$Q = 3.9 \text{ m}^3/\text{s}, H_t = 2.8 \text{ m}$$

- Discharge per riser (27 risers)



- Relative discharge deviation

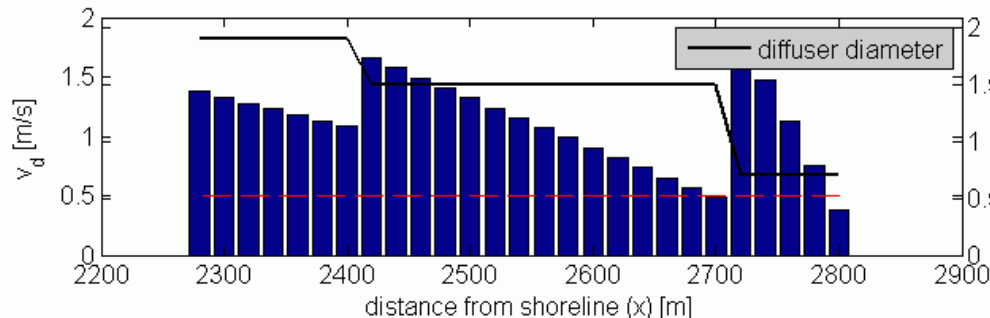
- Port/riser losses (54 ports, $D_p = 0.2$ m; $D_r = 0.3$ m)



- Discharge velocity at ports

- critical velocity for intrusion

$$F_p = v_p / (\Delta\rho / \rho g D_p)^{0.5} > 1$$



- Velocity in diffuser ($D_d = 1.9$ m)

- Critical velocity (deposition)

Shallow water equation

$$\frac{\partial h}{\partial t} + \frac{\partial(uh)}{\partial x} + \frac{\partial(vh)}{\partial y} = 0$$

mass conservation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - f v = -g \frac{\partial h}{\partial x} - b u,$$

momentum conservation

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + f u = -g \frac{\partial h}{\partial y} - b v,$$

h : total fluid column height

(u,v) : fluid's horizontal velocity

g : acceleration due to gravity

b : viscous drag coefficient

f : coriolis coefficients

Waves in the atmosphere, rivers, lakes and oceans as well as gravity waves in a smaller domain (e.g. surface waves in a bath)

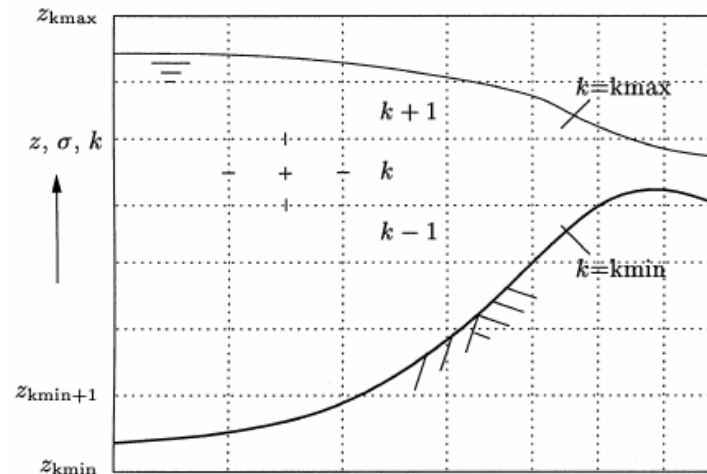
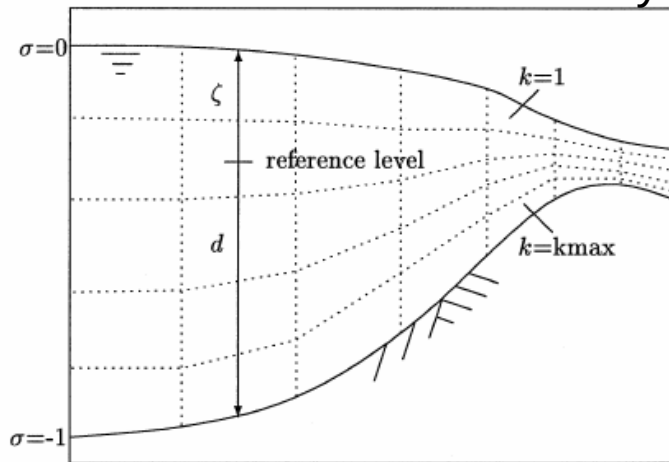
Limitations: wave length of phenomenon much larger than depth of domain (e.g. tides)

two horizontal co-ordinate systems

- Cartesian co-ordinates (ξ, η)
- Spherical co-ordinates (λ, ϕ)

two vertical systems

- surface and bottom following σ -layers
- fixed horizontal z-layers



$$\sigma = \frac{z - \zeta}{d + \zeta} = \frac{z - \zeta}{H},$$

the total water depth, given by

$$H = d + \zeta.$$

with:

z

the vertical co-ordinate in physical space

ζ

the free surface elevation above the reference plane (at $z = 0$)

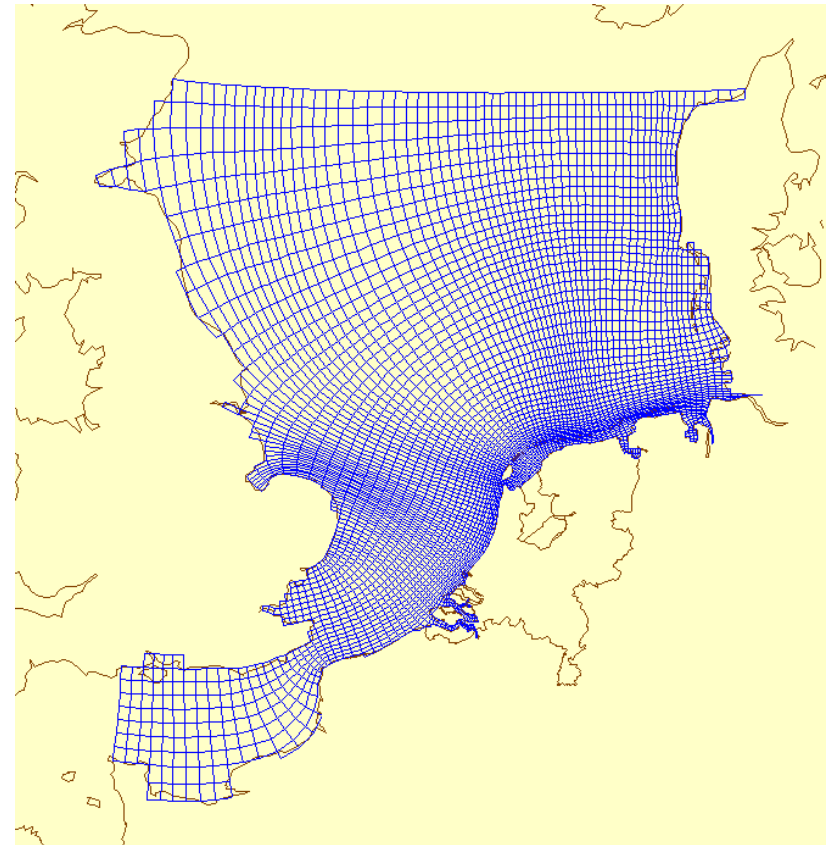
d

the depth below the reference plane

Fonte: Deltares, Delft3d, 2013

Numerical domain: Curvi-linear grid

- local refinements where required
- boundary fitted (no 'stair-case')
- follows channels and shallow areas
- follows river bends



Fonte: Deltares, Delft3d, 2013

Continuity equation

$$\frac{\partial h}{\partial t} + \frac{\partial(uh)}{\partial x} + \frac{\partial(vh)}{\partial y} = 0$$

The depth-averaged continuity equation is given by:

$$\frac{\partial \zeta}{\partial t} + \frac{1}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}} \frac{\partial [(d + \zeta) U \sqrt{G_{\eta\eta}}]}{\partial \xi} + \frac{1}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}} \frac{\partial [(d + \zeta) V \sqrt{G_{\xi\xi}}]}{\partial \eta} = Q, \quad (9.4)$$

with Q representing the contributions per unit area due to the discharge or withdrawal of water, precipitation and evaporation:

$$Q = H \int_{-1}^0 (q_{in} - q_{out}) d\sigma + P - E, \quad (9.5)$$

$\sqrt{G_{\xi\xi}}$	m	coefficient used to transform curvilinear to rectangular coordinates
$\sqrt{G_{\eta\eta}}$	m	coefficient used to transform curvilinear to rectangular coordinates

Fonte: Deltares, Delft3d, 2013

Momentum equations

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - f v = -g \frac{\partial h}{\partial x} - b u,$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + f u = -g \frac{\partial h}{\partial y} - b v,$$

Momentum equations in horizontal direction

The momentum equations in ξ - and η -direction are given by:

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

and

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

Reynolds stresses (horizontal)

$$F_{\xi} = \frac{1}{\sqrt{G_{\xi\xi}}} \frac{\partial \tau_{\xi\xi}}{\partial \xi} + \frac{1}{\sqrt{G_{\eta\eta}}} \frac{\partial \tau_{\xi\eta}}{\partial \eta}, \quad (9.20)$$

$$F_{\eta} = \frac{1}{\sqrt{G_{\xi\xi}}} \frac{\partial \tau_{\eta\xi}}{\partial \xi} + \frac{1}{\sqrt{G_{\eta\eta}}} \frac{\partial \tau_{\eta\eta}}{\partial \eta}. \quad (9.21)$$

For small-scale flow, i.e. when the shear stresses at the closed boundaries must be taken into account, the shear stresses $\tau_{\xi\xi}$, $\tau_{\xi\eta}$, $\tau_{\eta\xi}$ and $\tau_{\eta\eta}$ are determined according to:

$$\tau_{\xi\xi} = \frac{2\nu_H}{\sqrt{G_{\xi\xi}}} \left(\frac{\partial u}{\partial \xi} + \frac{\partial u}{\partial \sigma} \frac{\partial \sigma}{\partial \xi} \right), \quad (9.22)$$

$$\tau_{\xi\eta} = \tau_{\eta\xi} = \nu_H \left\{ \frac{1}{\sqrt{G_{\eta\eta}}} \left(\frac{\partial u}{\partial \eta} + \frac{\partial u}{\partial \sigma} \frac{\partial \sigma}{\partial \eta} \right) + \frac{1}{\sqrt{G_{\xi\xi}}} \left(\frac{\partial v}{\partial \xi} + \frac{\partial v}{\partial \sigma} \frac{\partial \sigma}{\partial \xi} \right) \right\}, \quad (9.23)$$

$$\tau_{\eta\eta} = \frac{2\nu_H}{\sqrt{G_{\eta\eta}}} \left(\frac{\partial v}{\partial \eta} + \frac{\partial v}{\partial \sigma} \frac{\partial \sigma}{\partial \eta} \right). \quad (9.24)$$

Vertical velocities

The vertical velocity ω in the adapting σ -co-ordinate system is computed from the continuity equation:

$$\frac{\partial \zeta}{\partial t} + \frac{1}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}} \frac{\partial [(d + \zeta) u \sqrt{G_{\eta\eta}}]}{\partial \xi} + \frac{1}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}} \frac{\partial [(d + \zeta) v \sqrt{G_{\xi\xi}}]}{\partial \eta} + \frac{\partial \omega}{\partial \sigma} = H (q_{in} - q_{out}) . \quad (9.8)$$

At the surface the effect of precipitation and evaporation is taken into account. The vertical velocity ω is defined at the iso σ -surfaces. ω is the vertical velocity relative to the moving σ -plane. It may be interpreted as the velocity associated with up- or downwelling motions. The “physical” vertical velocities w in the Cartesian co-ordinate system are not involved in the model equations. Computation of the physical vertical velocities is only required for post-processing purposes. These velocities can be expressed in the horizontal velocities, water depths, water levels and vertical ω -velocity according to:

$$w = \omega + \frac{1}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}} \left[u \sqrt{G_{\eta\eta}} \left(\sigma \frac{\partial H}{\partial \xi} + \frac{\partial \zeta}{\partial \xi} \right) + v \sqrt{G_{\xi\xi}} \left(\sigma \frac{\partial H}{\partial \eta} + \frac{\partial \zeta}{\partial \eta} \right) \right] + \left(\sigma \frac{\partial H}{\partial t} + \frac{\partial \zeta}{\partial t} \right) . \quad (9.9)$$

Hydrostatic assumption

$$\frac{\partial P}{\partial \sigma} = -g\rho H. \quad (9.10)$$

After integration, the hydrostatic pressure is given by:

$$P = P_{atm} + gH \int_{\sigma}^0 \rho(\xi, \eta, \sigma', t) d\sigma'. \quad (9.11)$$

For water of constant density and taking into account the atmospheric pressure, the pressure gradients read:

$$\frac{1}{\rho_0 \sqrt{G_{\xi\xi}}} P_{\xi} = \frac{g}{\sqrt{G_{\xi\xi}}} \frac{\partial \zeta}{\partial \xi} + \frac{1}{\rho_0 \sqrt{G_{\xi\xi}}} \frac{\partial P_{atm}}{\partial \xi}, \quad (9.12)$$

$$\frac{1}{\rho_0 \sqrt{G_{\eta\eta}}} P_{\eta} = \frac{g}{\sqrt{G_{\eta\eta}}} \frac{\partial \zeta}{\partial \eta} + \frac{1}{\rho_0 \sqrt{G_{\eta\eta}}} \frac{\partial P_{atm}}{\partial \eta}. \quad (9.13)$$

Hydrostatic assumption

$$\frac{\partial P}{\partial \sigma} = -g\rho H. \quad (9.10)$$

After integration, the hydrostatic pressure is given by:

$$P = P_{atm} + gH \int_{\sigma}^0 \rho(\xi, \eta, \sigma', t) d\sigma'. \quad (9.11)$$

In case of a non-uniform density, the local density is related to the values of temperature and salinity by the equation of state, see Section 9.3.4. Leibnitz' rule is used to obtain the following expressions for the horizontal pressure gradients:

$$\frac{1}{\rho_0 \sqrt{G_{\xi\xi}}} P_{\xi} = \frac{g}{\sqrt{G_{\xi\xi}}} \frac{\partial \zeta}{\partial \xi} + g \frac{d + \zeta}{\rho_0 \sqrt{G_{\xi\xi}}} \int_{\sigma}^0 \left(\frac{\partial \rho}{\partial \xi} + \frac{\partial \rho}{\partial \sigma} \frac{\partial \sigma}{\partial \xi} \right) d\sigma' \quad (9.14)$$

$$\frac{1}{\rho_0 \sqrt{G_{\eta\eta}}} P_{\eta} = \frac{g}{\sqrt{G_{\eta\eta}}} \frac{\partial \zeta}{\partial \eta} + g \frac{d + \zeta}{\rho_0 \sqrt{G_{\eta\eta}}} \int_{\sigma}^0 \left(\frac{\partial \rho}{\partial \eta} + \frac{\partial \rho}{\partial \sigma} \frac{\partial \sigma}{\partial \eta} \right) d\sigma' \quad (9.15)$$

Coupling case study Cartagena outfall (Colombia)

Outfall:

2.8 km long

20 m deep

3.8 m³/s



Cartagena

Source: World Bank

Delft 3D - Hydrodynamic modeling

B.C.:

- unsteady currents (logarithmic) (merged ELCOM and measurements)
- density profile

B.C.:

- unsteady water levels (tidal measurements)
- density profile

B.C. (surface):

- free surface (sigma layer)
- unsteady, uniform wind shear

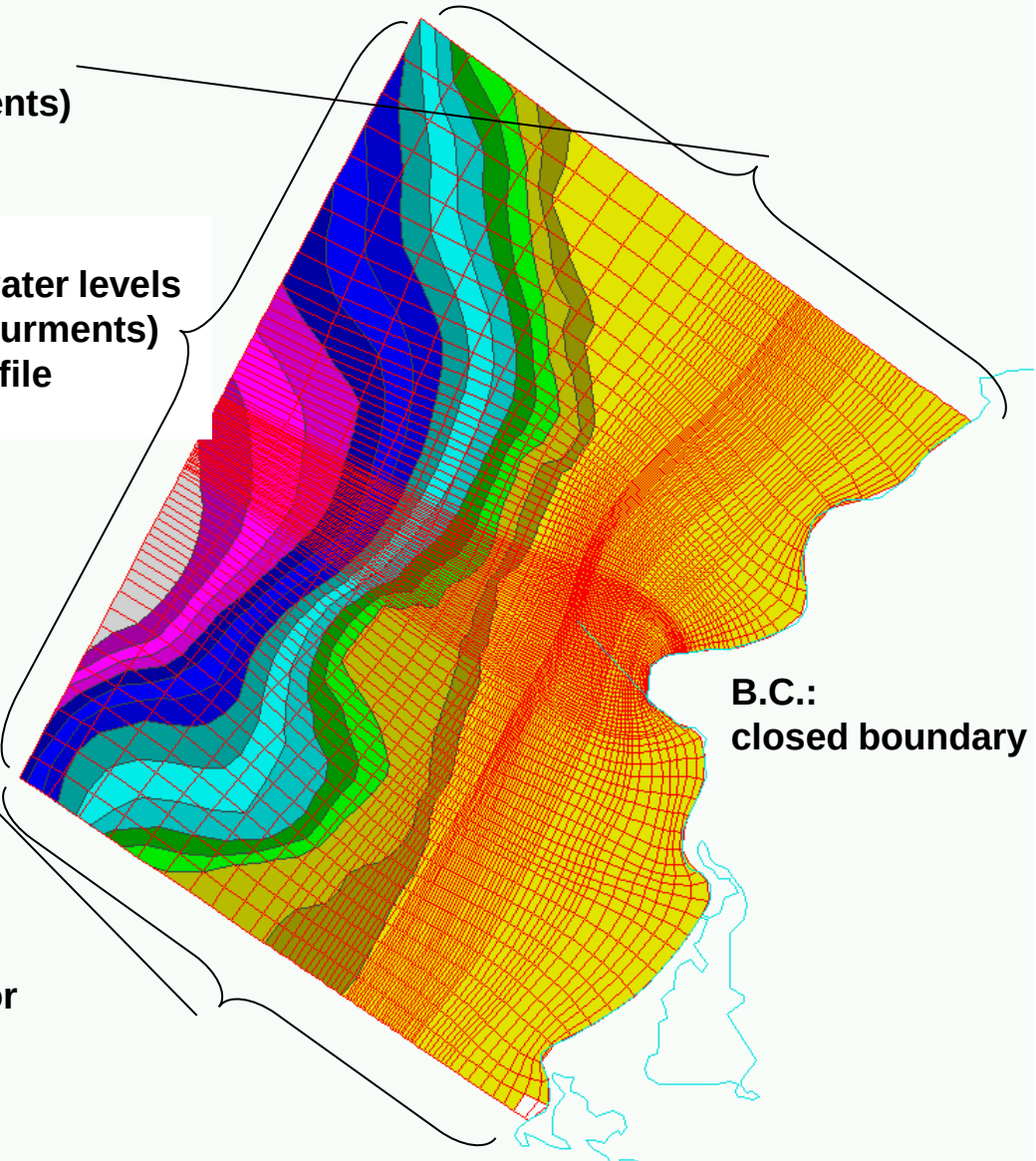
B.C.:

closed boundary

10,000 cells in horizontal
13 layers in vertical
→ 10 h calculation time for
1 month simulation

B.C. (bottom):

- bed stress (quadratic formulation)



25 km

Closed boundary conditions (bed)

9.4.1.1 Vertical boundary conditions

Kinematic boundary conditions

In the σ co-ordinate system, the free surface ($\sigma = 0$, or $z = \zeta$) and the bottom ($\sigma = -1$, or $z = -d$) are σ co-ordinate surfaces. ω is the vertical velocity relative to the σ -plane. The impermeability of the surface and the bottom is taken into account by prescribing the following kinematic conditions:

$$\omega|_{\sigma=-1} = 0 \text{ and } \omega|_{\sigma=0} = 0 \quad (9.48)$$

For the Z -grid the kinematic conditions read:

$$w|_{z=-d} = 0 \text{ and } w|_{z=\zeta} = 0 \quad (9.49)$$

Bed boundary condition

At the seabed, the boundary conditions for the momentum equations are:

$$\left. \frac{\nu_V}{H} \frac{\partial u}{\partial \sigma} \right|_{\sigma=-1} = \frac{1}{\rho_0} \tau_{b\xi}, \quad (9.50)$$

$$\left. \frac{\nu_V}{H} \frac{\partial v}{\partial \sigma} \right|_{\sigma=-1} = \frac{1}{\rho_0} \tau_{b\eta}, \quad (9.51)$$

Closed boundary conditions (bed)

Depth-averaged flow

For 2D depth-averaged flow the shear-stress at the bed induced by a turbulent flow is assumed to be given by a quadratic friction law:

$$\vec{\tau}_b = \frac{\rho_0 g \vec{U} |\vec{U}|}{C_{2D}^2}, \quad (9.52)$$

where $|\vec{U}|$ is the magnitude of the depth-averaged horizontal velocity.

- Chézy formulation:

$$C_{2D} = \text{Chézy coefficient } [\text{m}^{1/2}/\text{s}]. \quad (9.53)$$

- Manning's formulation:

$$C_{2D} = \frac{\sqrt[6]{H}}{n} \quad (9.54)$$

- White Colebrook's formulation:

$$C_{2D} = 18 \cdot {}^{10}\log \left(\frac{12H}{k_s} \right) \quad (9.55)$$

Closed boundary conditions (bed)

Three-dimensional flow

For 3D models, a quadratic bed stress formulation is used that is quite similar to the one for depth-averaged computations. The bed shear stress in 3D is related to the current just above the bed:

$$\vec{\tau}_{b_{3D}} = \frac{g\rho_0\vec{u}_b|\vec{u}_b|}{C_{3D}^2}, \quad (9.56)$$

$$\vec{u}_b = \frac{\vec{u}_*}{\kappa} \ln \left(1 + \frac{\Delta z_b}{2z_0} \right), \quad (9.57)$$

where z_0 is user-defined. In the numerical implementation of the logarithmic law of the wall for a rough bottom, the bottom is positioned at z_0 . The magnitude of the bottom stress is defined as:

$$|\vec{\tau}_b| = \rho_0\vec{u}_*|\vec{u}_*|. \quad (9.58)$$

Using Eqs. 9.56 to 9.58, C_{3D} can be expressed in the roughness height z_0 of the bed:

$$C_{3D} = \frac{\sqrt{g}}{\kappa} \ln \left(1 + \frac{\Delta z_b}{2z_0} \right). \quad (9.59)$$

The parameter z_0 can be linked to the actual geometric roughness as a fraction of the RMS-value of the sub-grid bottom fluctuations. For rough walls Nikuradse (1933) found:

$$z_0 = \frac{k_s}{30}, \quad (9.60)$$

Closed boundary conditions (surface)

$$\left. \frac{\nu_V}{H} \frac{\partial u}{\partial \sigma} \right|_{\sigma=0} = \frac{1}{\rho_0} |\vec{\tau}_s| \cos(\theta), \quad (9.64)$$

$$\left. \frac{\nu_V}{H} \frac{\partial v}{\partial \sigma} \right|_{\sigma=0} = \frac{1}{\rho_0} |\vec{\tau}_s| \sin(\theta), \quad (9.65)$$

where θ is the angle between the wind stress vector and the local direction of the grid-line η

The magnitude is determined by the following widely used quadratic expression:

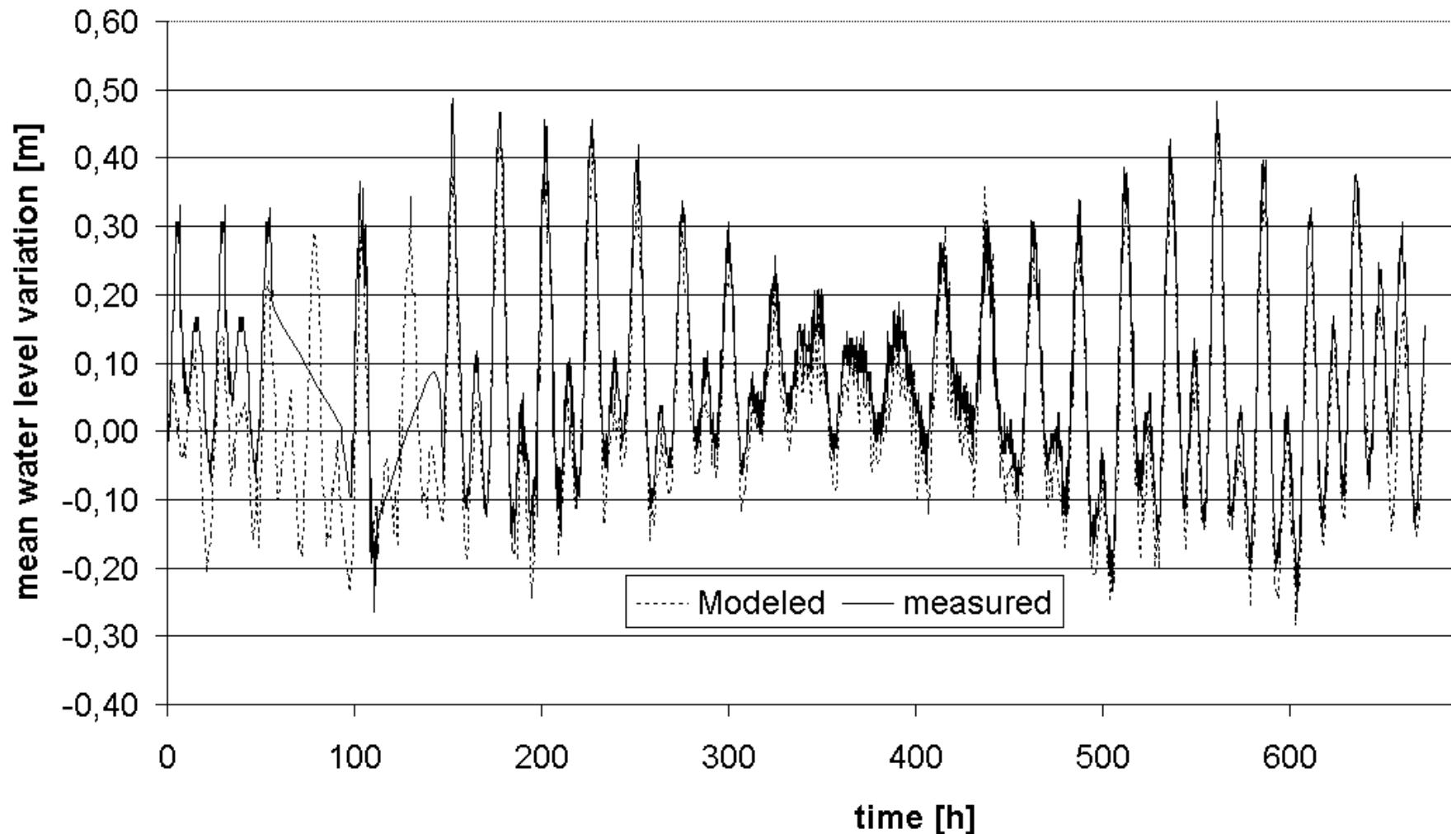
$$|\vec{\tau}_s| = \rho_a C_d U_{10}^2 \quad (9.67)$$

where:

ρ_a	the density of air.
U_{10}	the wind speed 10 meter above the free surface (time and space dependent).
C_d	the wind drag coefficient, dependent on U_{10} .

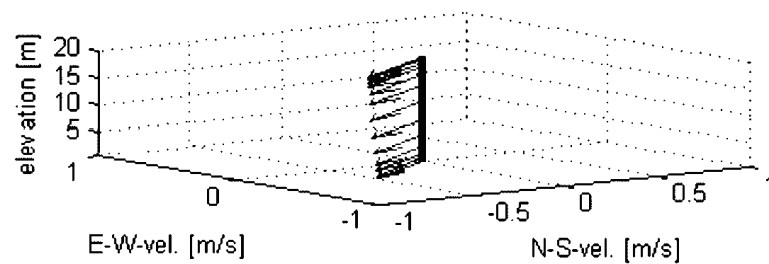
Results 3: Delft3D - hydrodynamics

Comparison of measured and computed water levels at outfall location

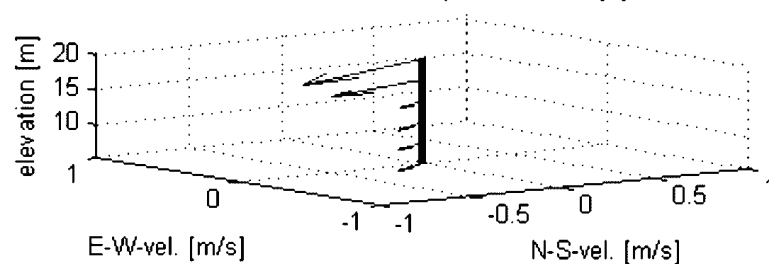


Delft3D - Hydrodynamic model results

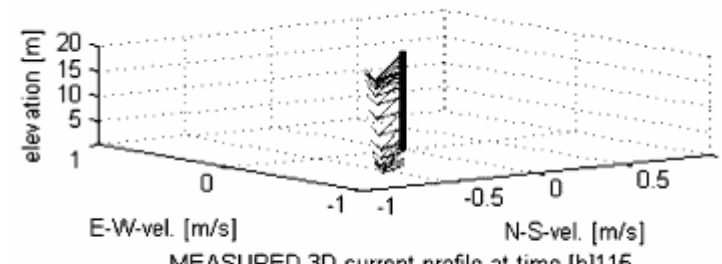
MODELED 3D current profile at time [h]176



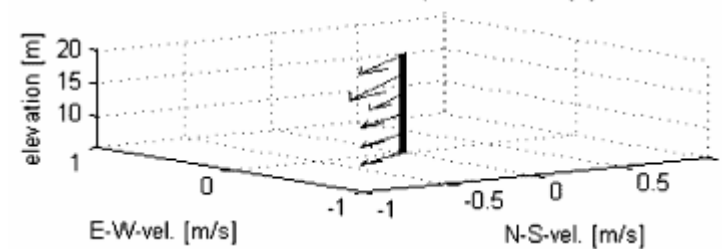
MEASURED 3D current profile at time [h]176



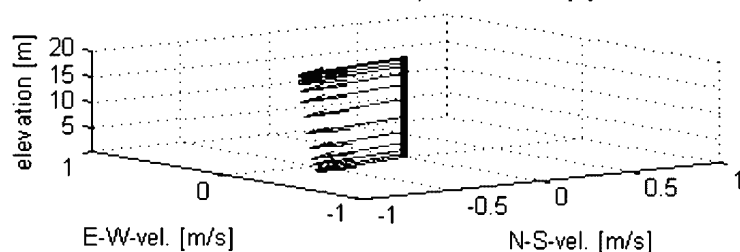
MODELED 3D current profile at time [h]115



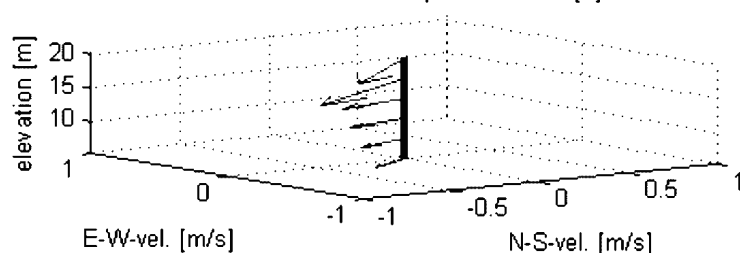
MEASURED 3D current profile at time [h]115



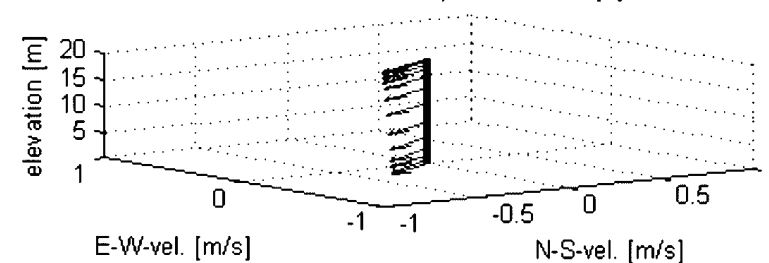
MODELED 3D current profile at time [h]120



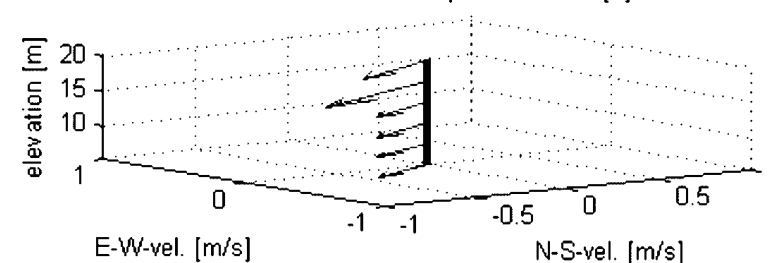
MEASURED 3D current profile at time [h]120



MODELED 3D current profile at time [h]594



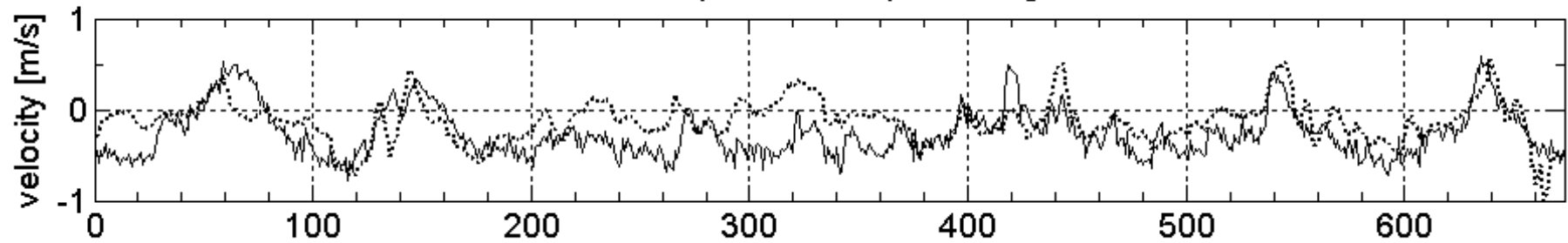
MEASURED 3D current profile at time [h]594



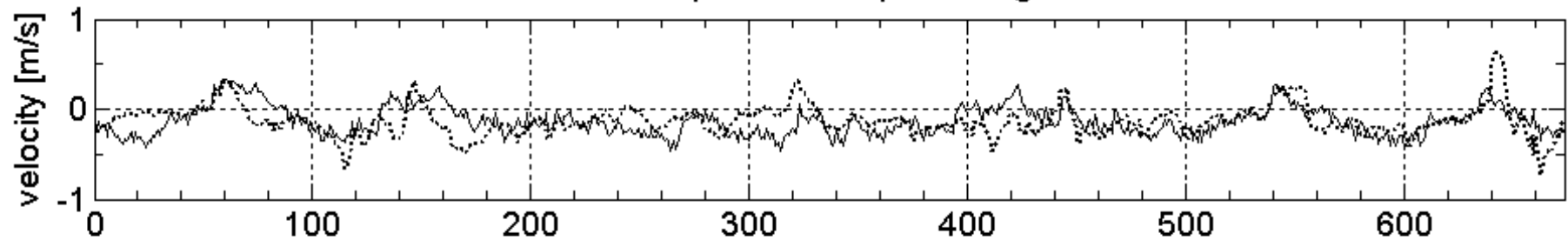
Results 3: Delft3D - hydrodynamics

Comparison of measured and modeled depth averaged currents at outfall location

north-south-component of depth averaged current



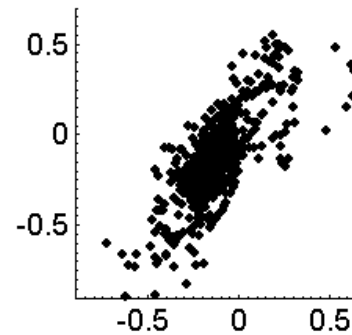
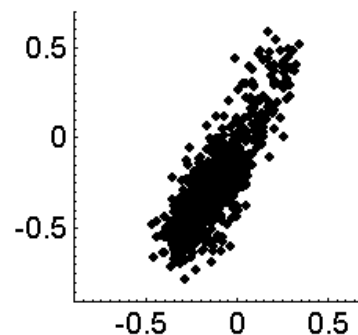
east-west-component of depth averaged current



time [h]

..... modeled
—— measured

scatter of depth averaged velocity [m/s]
measured - modeled



Transport Equation

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\vec{v} c) + R$$

Transport Equation

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\vec{v} c) + R$$

$$\begin{aligned} \frac{\partial (d + \zeta) c}{\partial t} + \frac{1}{\sqrt{G_{\xi\xi}} \sqrt{G_{\eta\eta}}} \left\{ \frac{\partial [\sqrt{G_{\eta\eta}} (d + \zeta) u c]}{\partial \xi} + \frac{\partial [\sqrt{G_{\xi\xi}} (d + \zeta) v c]}{\partial \eta} \right\} + \frac{\partial \omega c}{\partial \sigma} = \\ \frac{d + \zeta}{\sqrt{G_{\xi\xi}} \sqrt{G_{\eta\eta}}} \left\{ \frac{\partial}{\partial \xi} \left(D_H \frac{\sqrt{G_{\eta\eta}}}{\sqrt{G_{\xi\xi}}} \frac{\partial c}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left(D_H \frac{\sqrt{G_{\xi\xi}}}{\sqrt{G_{\eta\eta}}} \frac{\partial c}{\partial \eta} \right) \right\} + \\ + \frac{1}{d + \zeta} \frac{\partial}{\partial \sigma} \left(D_V \frac{\partial c}{\partial \sigma} \right) - \lambda_d (d + \zeta) c + S, \quad (9.29) \end{aligned}$$

with D_H the horizontal diffusion coefficient, D_V the horizontal diffusion coefficient, λ_d representing the first order decay process and S the source and sink terms per unit area due to the discharge q_{in} or withdrawal q_{out} of water and/or the exchange of heat through the free surface Q_{tot} :

$$S = (d + \zeta) (q_{in} c_{in} - q_{out} c) + Q_{tot}. \quad (9.30)$$

The total horizontal diffusion coefficient D_H is defined by

$$D_H = D_{SGS} + D_V + D_H^{back} \quad (9.31)$$

Equation of State

UNESCO formulation

The UNESCO formulation is given by (UNESCO, 1981a):

Range: $0 < t < 40$ °C, $0.5 < s < 43$ ppt

$$\rho = \rho_0 + As + Bs^{3/2} + Cs^2 \quad (9.42)$$

where

$$\begin{aligned} \rho_0 = & 999.842594 + 6.793952 \cdot 10^{-2}t - 9.095290 \cdot 10^{-3}t^2 + \\ & + 1.001685 \cdot 10^{-4}t^3 - 1.120083 \cdot 10^{-6}t^4 + 6.536332 \cdot 10^{-9}t^5 \end{aligned} \quad (9.43)$$

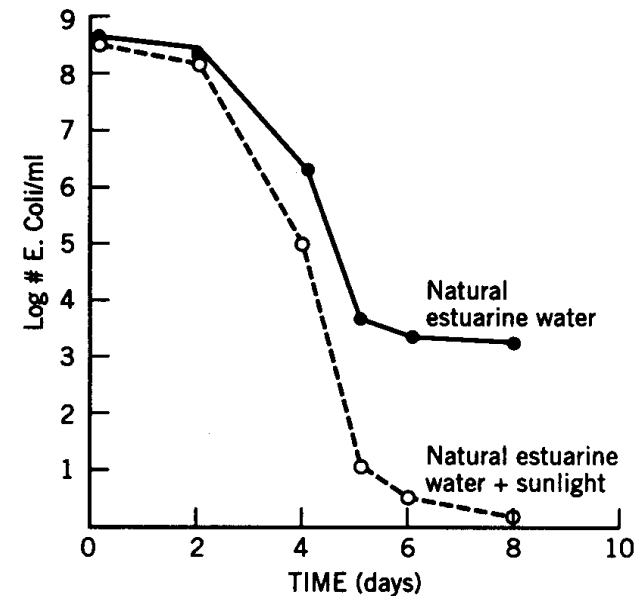
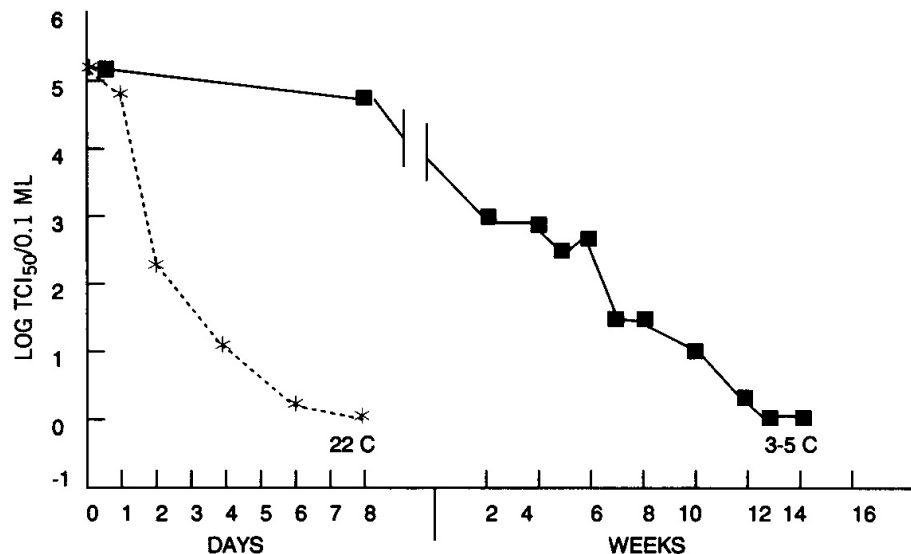
$$\begin{aligned} A = & 8.24493 \cdot 10^{-1} - 4.0899 \cdot 10^{-3}t + 7.6438 \cdot 10^{-5}t^2 + \\ & - 8.2467 \cdot 10^{-7}t^3 + 5.3875 \cdot 10^{-9}t^4 \end{aligned} \quad (9.44)$$

$$B = -5.72466 \cdot 10^{-3} + 1.0227 \cdot 10^{-4}t - 1.6546 \cdot 10^{-6}t^2 \quad (9.45)$$

$$C = 4.8314 \cdot 10^{-4} \quad (9.46)$$

FF water quality model: Delft3D-WAQ

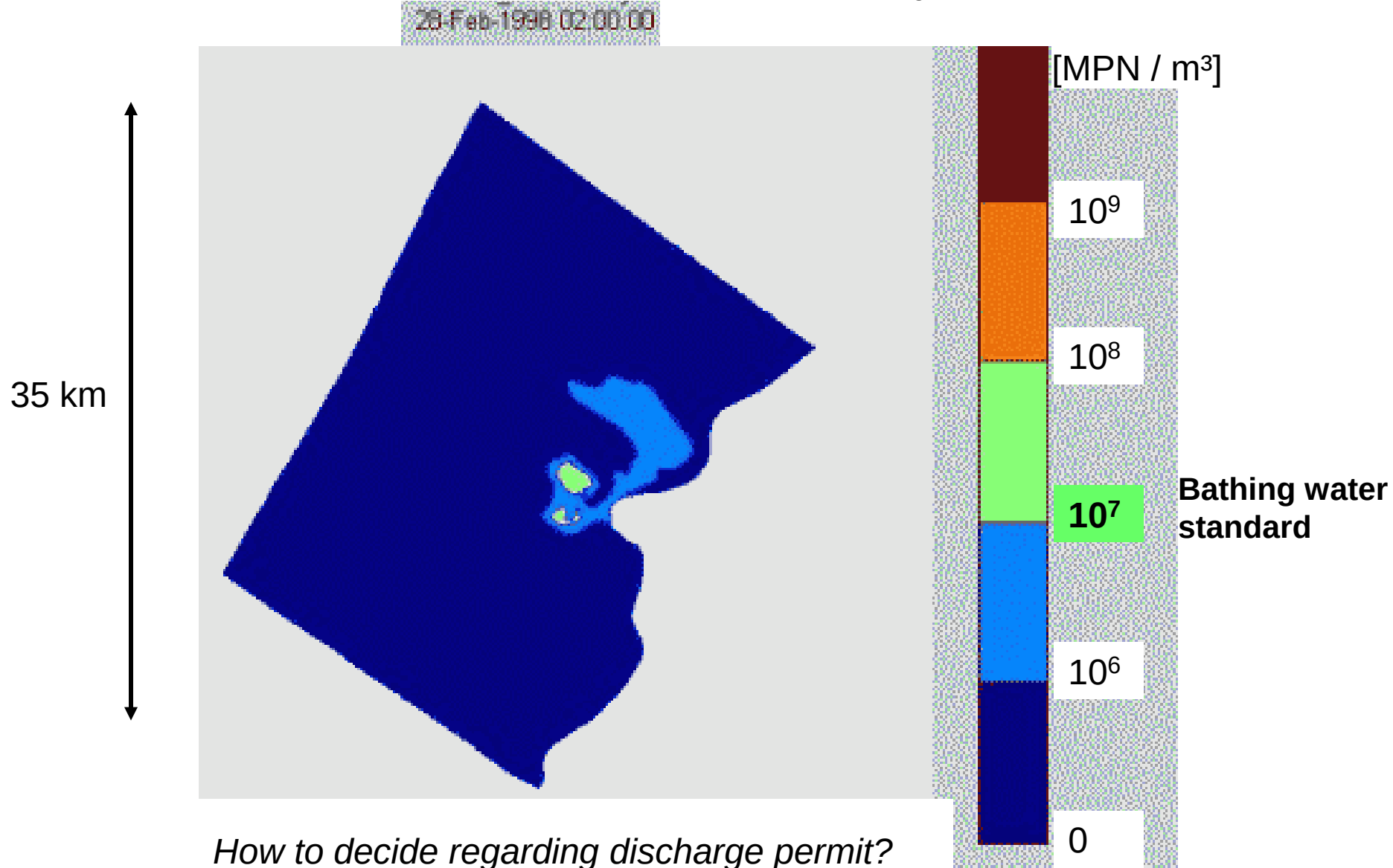
- Water quality indicator (public health): total coliform bacteria
- Indicates probability of pathogens in water
- Bacteria inactivation highly sensitive to environmental parameters
- Significant differences exist between daylight and night and between trapped or surfaced plumes
- Implemented: Mancini model : $k = f(\text{surface radiation, temperature, turbidity, depth, salinity})$



source: Bitton, 1994

Results 4: bacteria concentration distributions

Depth averaged total coliform concentration ($C_o = 10^{11}$ MPN/m³)



C) Regulatory implementation - CorZone

Exceedance frequency of water quality standard

