J. Szantyr – Lecture No. 14 – Modelling of Flows with Free Boundaries

The free boundary of the flow domain is usually a surface separating liquid and gas. On this surface gravity waves occur frequently, caused by the flow of gas (wind) or by motion of solid objects floating in the liquid. Within the linear theory of two-dimensional waves the following equation of the wavy surface may be formulated:

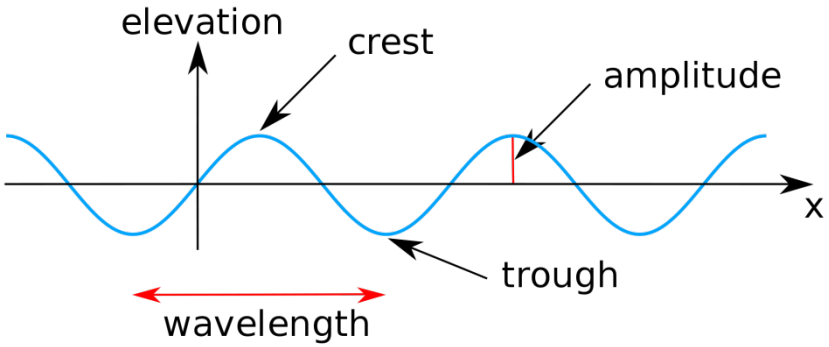
$$\eta(x,t) = a \cdot \cos(k \cdot x - \omega \cdot t)$$

where: $k = \frac{2 \cdot \pi}{\lambda}$ - wave number

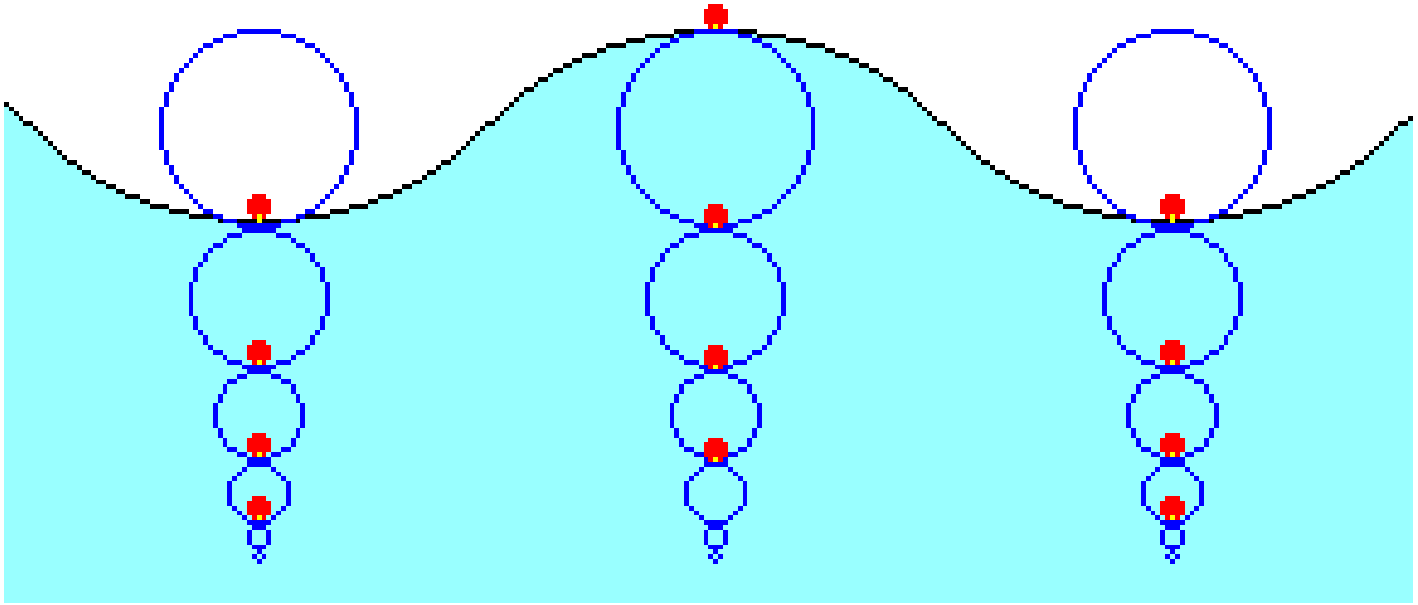
$\omega = \frac{2 \cdot \pi}{T} = 2 \cdot \pi \cdot f$ - circular frequency

λ – wave length T – wave period

a – wave amplitude



The simplest two-dimensional model of surface waves is the Airy's theory



Airy's theory describes the travelling sinusoidal wave.

George Biddle Airy 1801 - 1892

Two-dimensional regular wave may be described by the velocity potential:

$$\Phi(x,z,t) = -\frac{g\cdot a}{\omega}\cdot\frac{\cosh\left[k\cdot(h-z)\right]}{\cosh(k\cdot h)}\cdot\sin(k\cdot x-\omega\cdot t)$$

where: $\cosh(s)=\frac{e^{s}+e^{-s}}{2}$ h – liquid domain depth z – vertical co-ordinate downwards from free surface

Phase wave velocity in deep liquid domain: $c=\frac{\omega}{k}=\frac{\lambda}{T}=\sqrt{\frac{g}{k}}=\sqrt{\frac{g\cdot\lambda}{2\cdot\pi}}=\mathrm{A}$

Phase wave velocity in shallow liquid domain: $c=\sqrt{g\cdot h}=\mathrm{A}$

Group wave velocity in deep liquid domain: $c_g=\frac{1}{2}\cdot\frac{\omega}{k}=\frac{1}{2}\cdot c=\mathrm{B}$

Group wave velocity in shallow liquid domain: $c_g=c=\sqrt{g\cdot h}=\mathrm{B}$

Pressure inside wave in deep water domain: $p=\rho\cdot g\cdot a\cdot\frac{\cosh\left[k\cdot(h-z)\right]}{\cosh(k\cdot h)}\cdot\sin(k\cdot x-\omega\cdot t)$

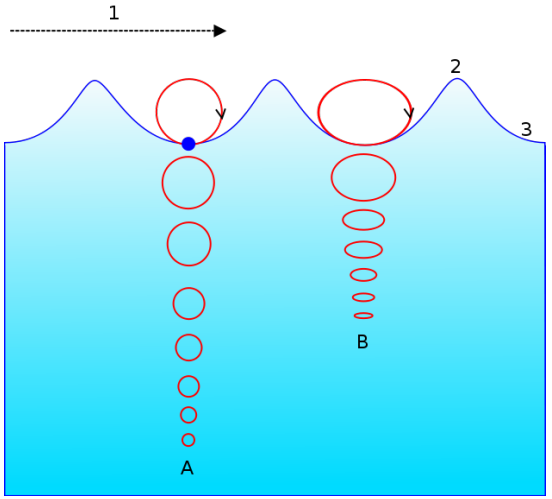
Pressure inside wave in shallow water domain: $p=\rho\cdot g\cdot a\cdot e^{-kz}\cdot\sin(k\cdot x-\omega\cdot t)$

Wave energy (per unit surface):

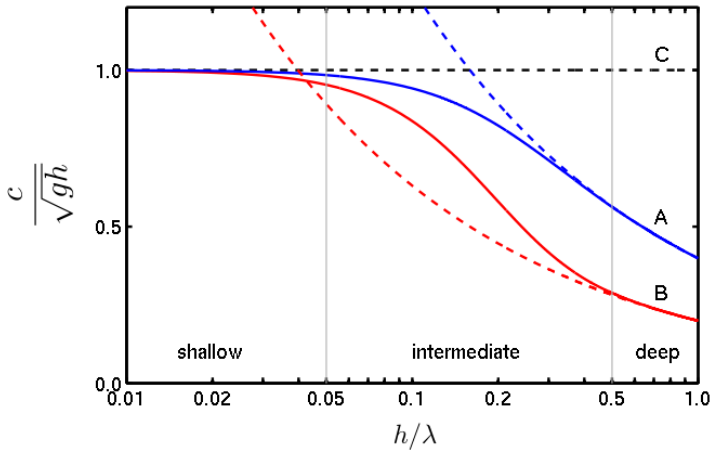
$$E=E_k+E_p=\frac{1}{4}\cdot\rho\cdot g\cdot a^2+\frac{1}{4}\cdot\rho\cdot g\cdot a^2=\frac{1}{2}\cdot\rho\cdot g\cdot a^2$$

The liquid domain may be regarded as „deep” when its depth is larger than half of the wave length:

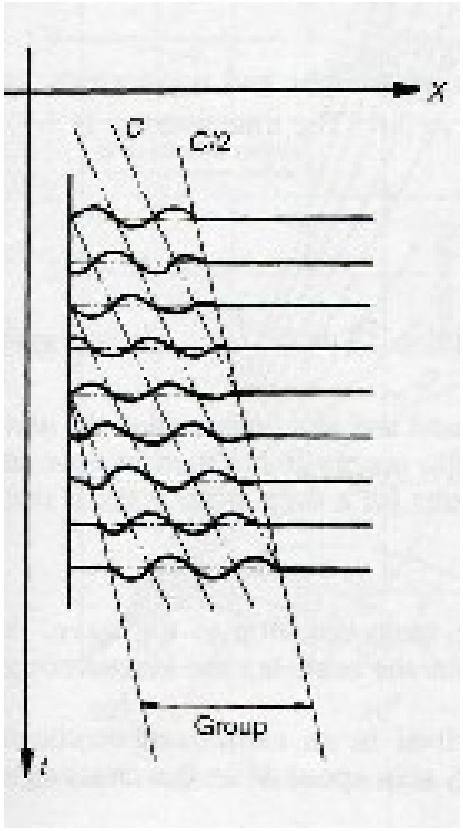
$$h \geq \frac{1}{2} \cdot \lambda$$



Comparison of trajectories of the liquid particles in waves in liquid domain of unlimited depth (A) and in shallow liquid domain (B). →

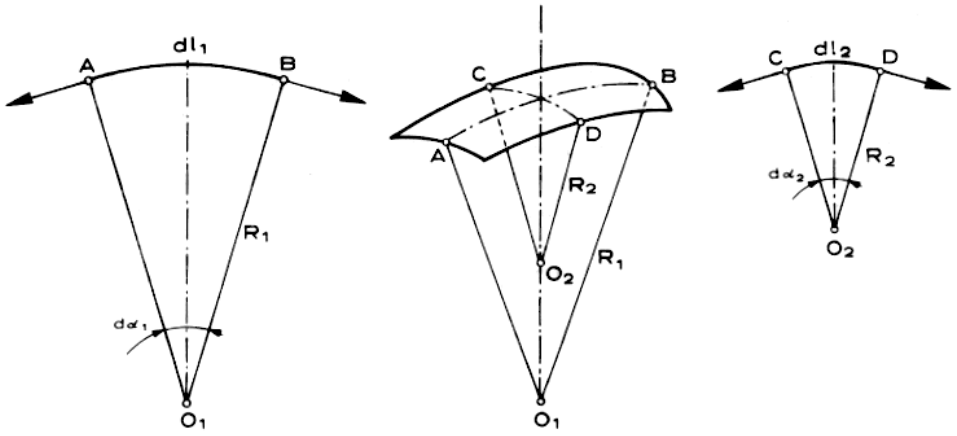


Explanation of the wave phase velocity and wave grupo velocity →



Variation of the phase wave velocity (A) and group wave velocity (B) between deep and shallow liquid domain

Capillary waves or waves under the influence of surface tension



In case when the surface tension acting on the separation surface between liquid and gas is taken into account, the dynamic boundary condition on the free surface takes the form:

$$p - p_a = f_{la} \cdot \left(\frac{1}{R_1} + \frac{1}{R_2} \right)$$

where: f_{la} - surface tension, for water/air there is: $f_{la} = 0.072 \left[N/m \right]$

Then within the linear wave theory we obtain the following relation:

Phase velocity in deep liquid domain:

$$c = \sqrt{\frac{g \cdot \lambda}{2 \cdot \pi} + \frac{2 \cdot \pi \cdot f_{la}}{\rho \cdot \lambda}}$$

Influence of the surface tension on the wave velocity and frequency:

$$\frac{\omega - \omega_0}{\omega_0} = \frac{c - c_0}{c_0} = \sqrt{1 + \frac{f_{la}}{g \cdot \rho} \cdot k^2} - 1$$

The influence of surface tension on the surface waves becomes meaningful for waves shorter than 0.12 [m] and propagation velocity under 0.43 [m/s]. Then we may use the term capillary waves.

Numerical determination of flows with free boundaries

As a rule the shape and location of the free boundary are known in the initial condition only. In the consecutive instants of time they have to be determined as part of the solution. If the phase change processes on the free boundary are neglected, then we have the following boundary conditions:

Kinematic boundary condition: **no flow through the free boundary**, i.e.:

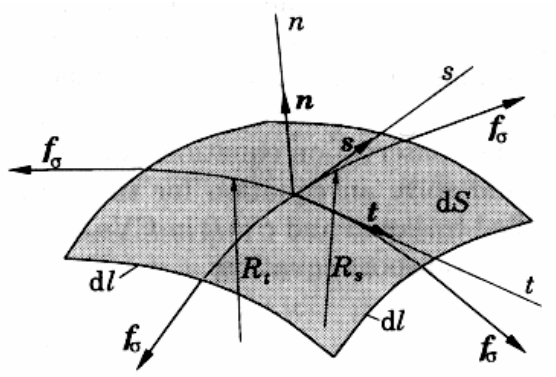
$$\left[\left(\bar{\upsilon}-\bar{\upsilon}_{fs}\right)\cdot\bar{n}\right]_{fs}=0 \qquad \text{or} \qquad \dot{m}_{fs}=0$$

Dynamic boundary condition: **forces on the free boundary are in equilibrium**, i.e.:

$$\bar{F}_c\cdot\bar{n}=\bar{F}_g\cdot\bar{n}+f_{la}\cdot\left(\frac{1}{R_1}+\frac{1}{R_2}\right)$$

$$\bar{F}_c\cdot\bar{t}=\bar{F}_g\cdot\bar{t}+\frac{\partial f_{la}}{\partial t}$$

$$\bar{F}_c\cdot\bar{s}=\bar{F}_g\cdot\bar{s}+\frac{\partial f_{la}}{\partial s}$$



In case when meaningful temperature gradients are present on the free surface, the value of surface tension may vary, this may cause forces tangential to the surface and may generate a flow from „warm” region to the „cold” region.

There are two groups of computational methods enabling determination of the free boundary geometry:

Interface Capturing Methods

In this case the calculations are performed on the fixed discrete grid (e.g. finite volume grid), which extends beyond the initial location of the free boundary. The consecutive locations of the free boundary are determined either through tracing the motion of mass-less particles located in the liquid close to the free boundary (Marker and Cell Method - MAC),or through solving an additional transport equation for „degree of vacuum" in the liquid phase (Volume of Fluid Method - VOF).

The MAC method is quite simple but it requires high computer power for tracing motion of a large number of marker particles. In VOF method the transport equation for the parameter C must be solved in addition to the mass and momentum conservation equations:

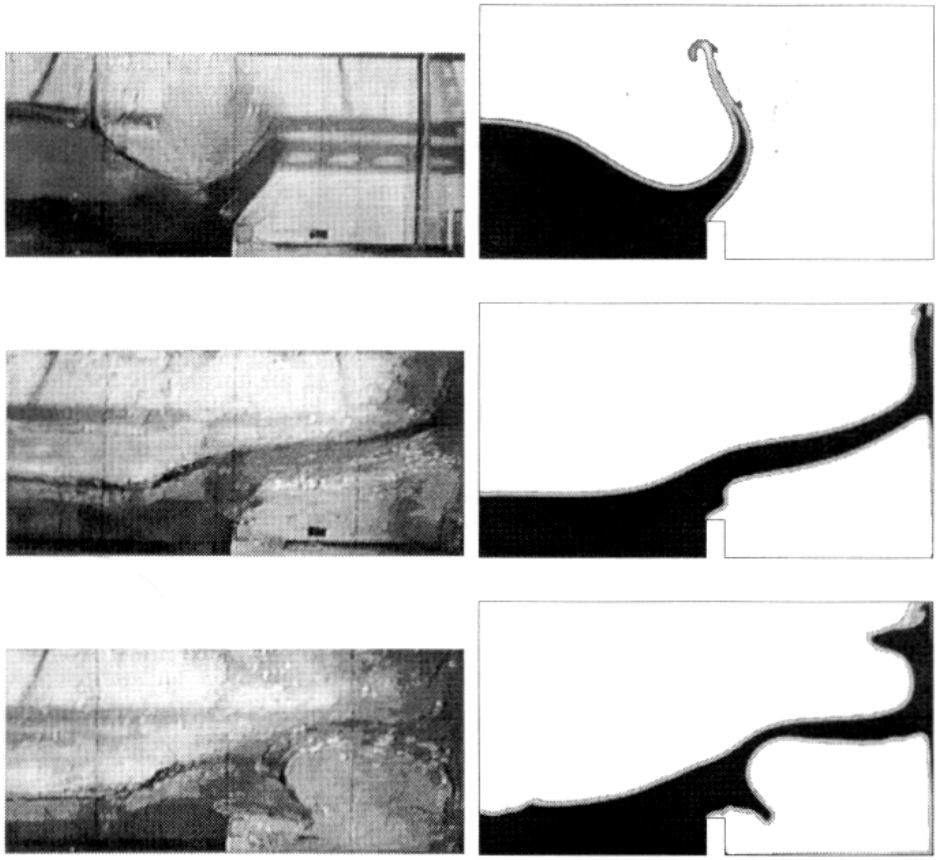
$$\frac{\partial C}{\partial t} + div\left(C\,\bar{v}\right) = 0$$

where C=1 denotes a finite volume completely filled with liquid, and C=0 – finite volume completely filled with gas. The free boundary is determined by finite volumes where C=0.5. The VOF method does not produce a „sharp" definition of the free boundary location – usually it is „smeared" over 2 -3 finite volumes. This problem may be alleviated by an additional increase of grid density in the vicinity of the free boundary.

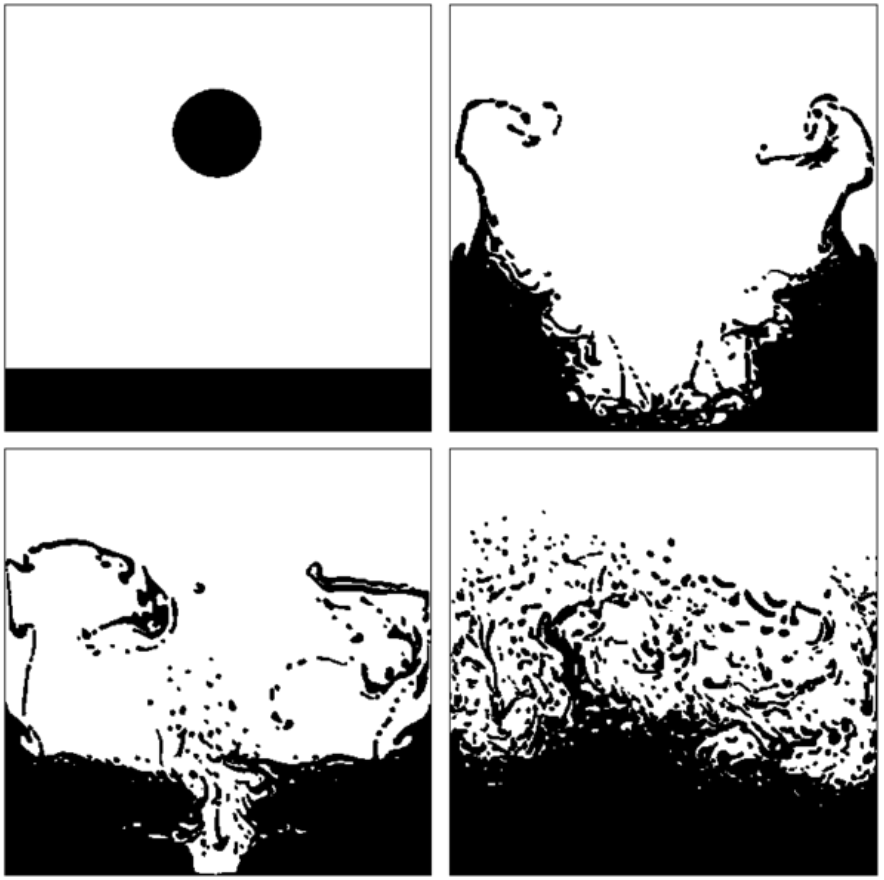
In the VOF method the gas and liquid flows are usually determined separately, with a common boundary condition on the free boundary. Alternatively, both phases may be treated as one fluid with changing properties, i.e.:

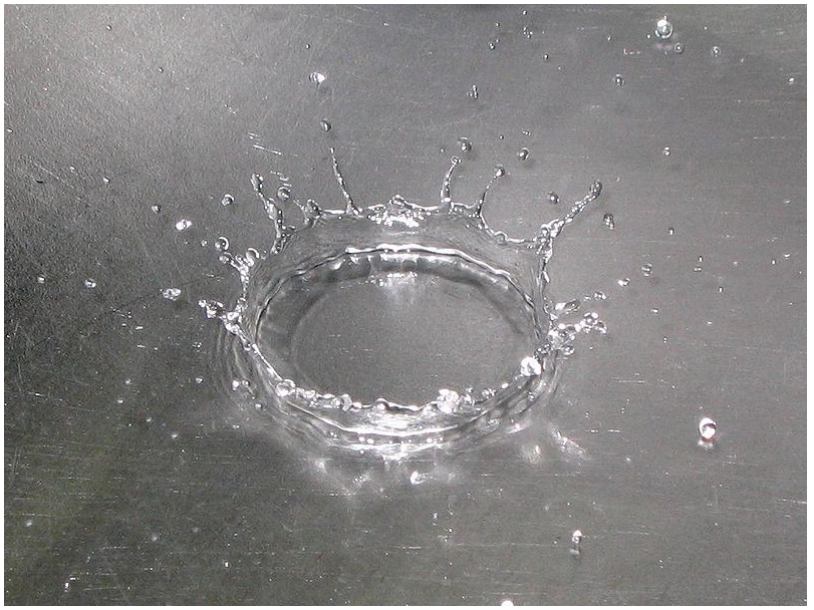
$$\rho = \rho_1 \cdot C + \rho_2 \cdot (1 - C) \qquad \mu = \mu_1 \cdot C + \mu_2 \cdot (1 - C)$$

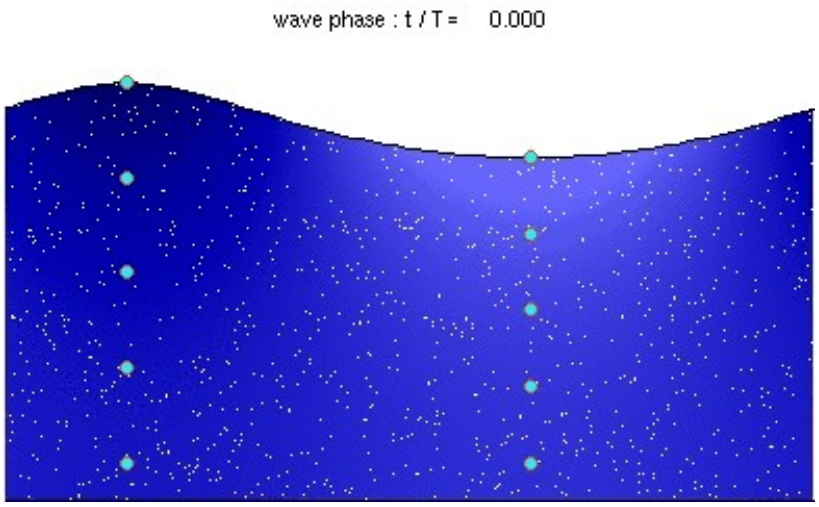
In such a case the formal boundary condition on the free boundary is not taken into account explicitly, because this boundary is treated as a surface of discontinuity of the fluid parameters. However, the boundary conditions are implicitly fulfilled.



The consecutive phases of unsteady flow after sudden breaking of a barrier, calculated by the Volume of Fluid (VOF) method, using „one fluid approach", in comparison with experiment.







Calculated effect of dropping a solid sphere on the free surface of water, calculated by the MAC method. On the right the mass-less particles (markers) distributed in a liquid →

Interface Tracking Methods

These methods require modification of the computational grid in every time step

In most cases the following function describing the elevation of the free boundary above its initial position is introduced: $z = H(x, y, t)$

Then the following relation describing the local variation of H may be developed from the kinematic boundary condition:

$$\frac{\partial H}{\partial t} = v_z - v_x \cdot \frac{\partial H}{\partial x} - v_y \cdot \frac{\partial H}{\partial y}$$

The above relation is integrated numerically in time and in each time step the following internal iterative cycle is performed:

- Solution of the momentum conservation equation with known pressure distribution on the free boundary, leading to the determination of the velocity field

- Solution of the mass conservation equation with known pressure distribution on the free boundary and known geometry of this boundary, leading to the determination of the non-zero mass flow through the free boundary:

$$\dot{m}_{fs} = \int_{S_{fs}} \rho \cdot \bar{v}_{fs} \cdot \bar{n} \cdot dS - \int_{S_{fs}} \rho \cdot \bar{v}_b \cdot \bar{n} \cdot dS \approx \rho \cdot \left(\bar{v} \cdot \bar{n}\right)_{fs}^{T} \cdot S_{fs}^{T} - \rho \cdot \dot{\Omega}_{fs}$$

where: $\bar{v}_{fs}$ - current velocity determined on the free boundary

$\bar{v}_b$ - own velocity of the free boundary from the preceding time step

- Correction of the free boundary location leading to zero mass flow through the corrected boundary:

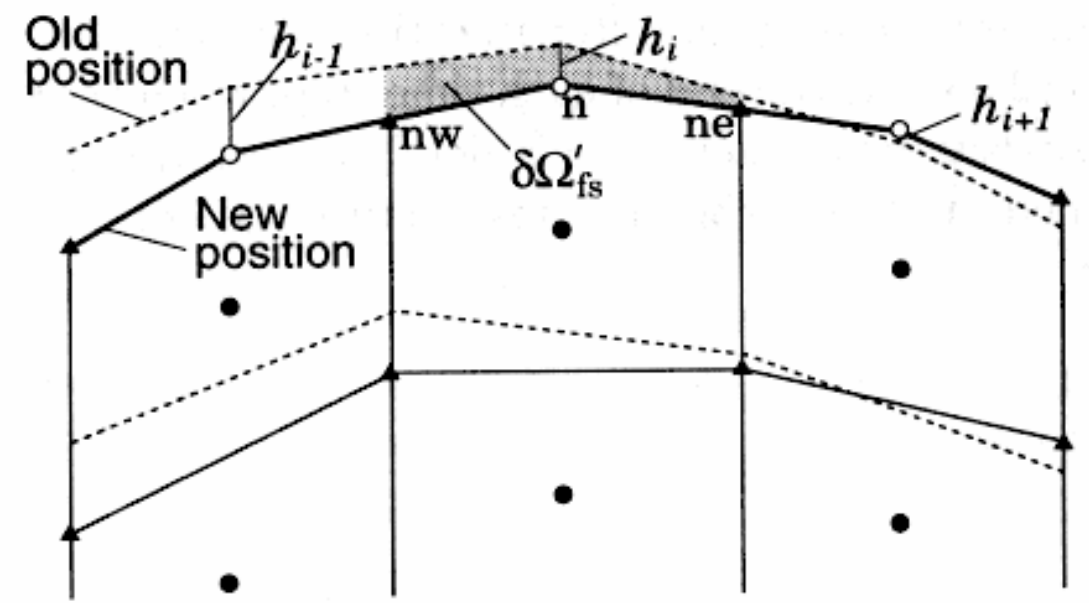
$$\dot{m}_{fs} + \rho \cdot \dot{\Omega}'_{fs} = 0$$

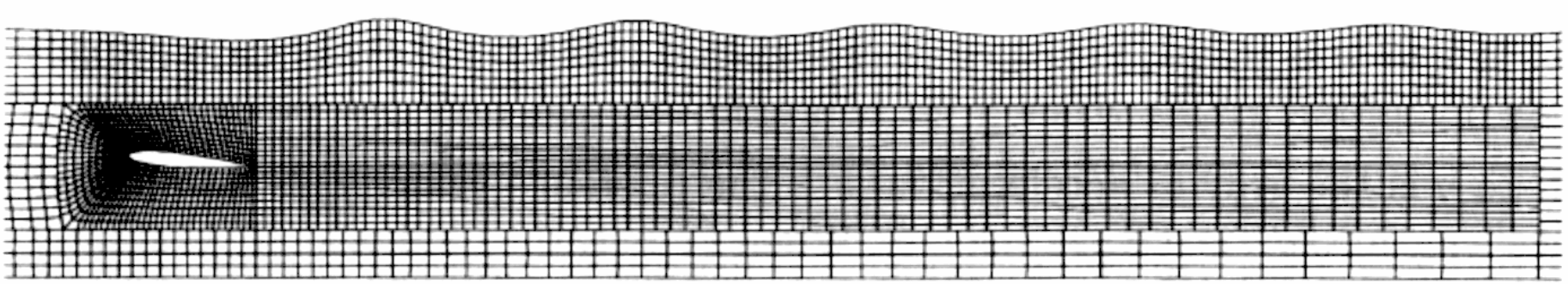
$\dot{\Omega}'_{fs}$ is the volume of liquid which should flow out from (or flow into) the finite volume in order to fulfil the mass conservation equation. On the basis of this volume the appropriate displacement of the grid nodes is determined (cf. the sketch below), e.g. for a two-dimensional grid we have:

$$\partial \dot{\Omega}'_{fs} = \frac{1}{2} \cdot \Delta x \cdot \left(h_{nw} + 2 \cdot h_n + h_{ne} \right)$$

- Repetition of the above actions until the satisfactory convergence is achieved

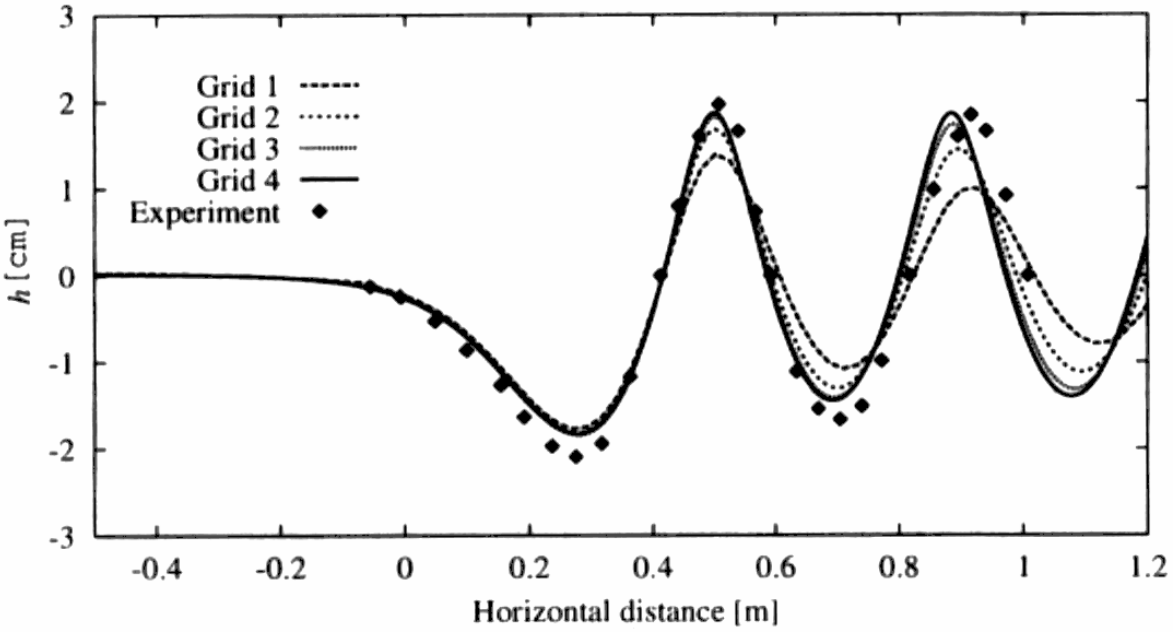
- Moving to the next time step





An example of application of the ITM method for the case of determination of the wave system on the free boundary generated by a hydrofoil moving under the surface (two-dimensional flow).

Comparison of the calculated and experimental results



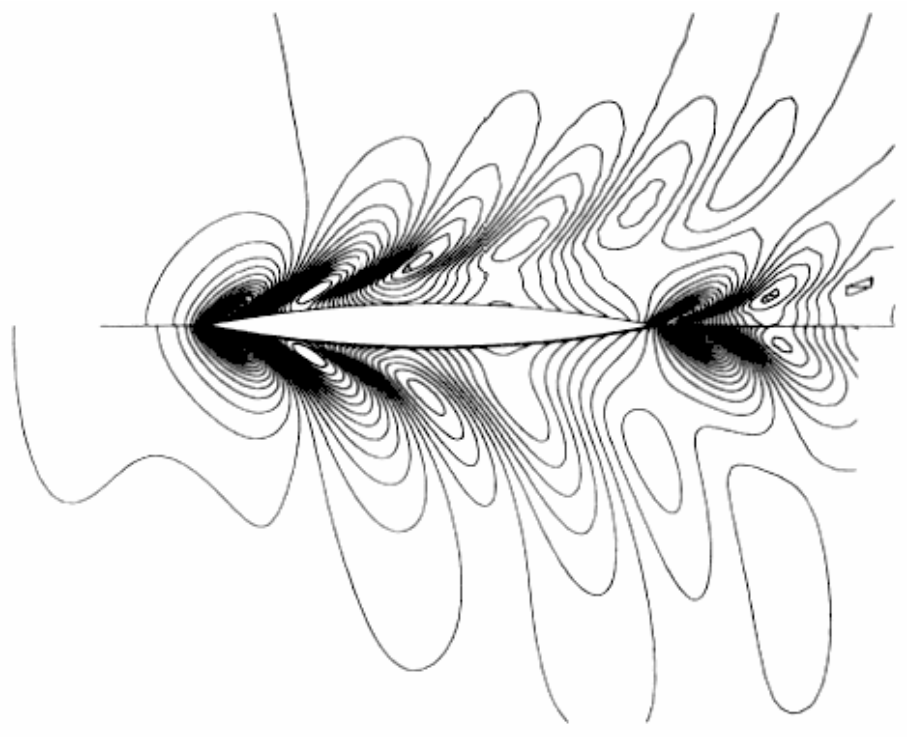
Grid 1 – 1004 finite volumes

Grid 2 – 4016 finite volumes

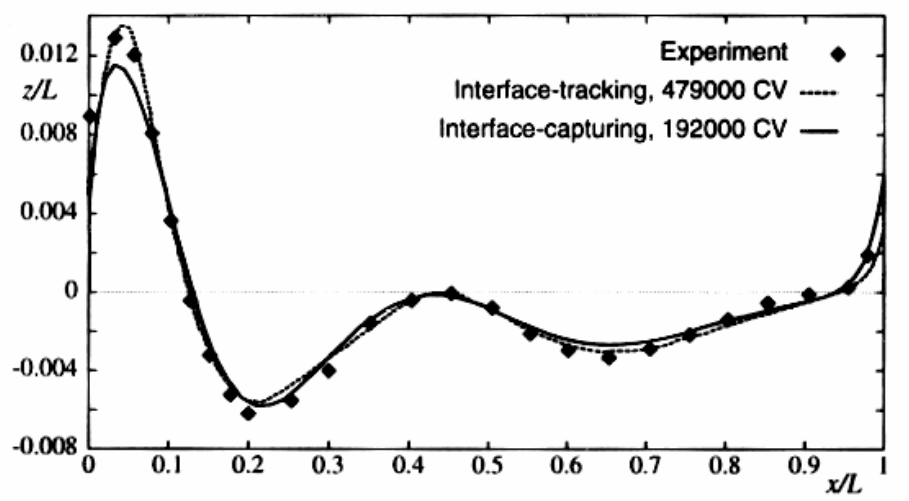
Grid 3 – 16064 finite volumes

Grid 4 – 64256 finite volumes

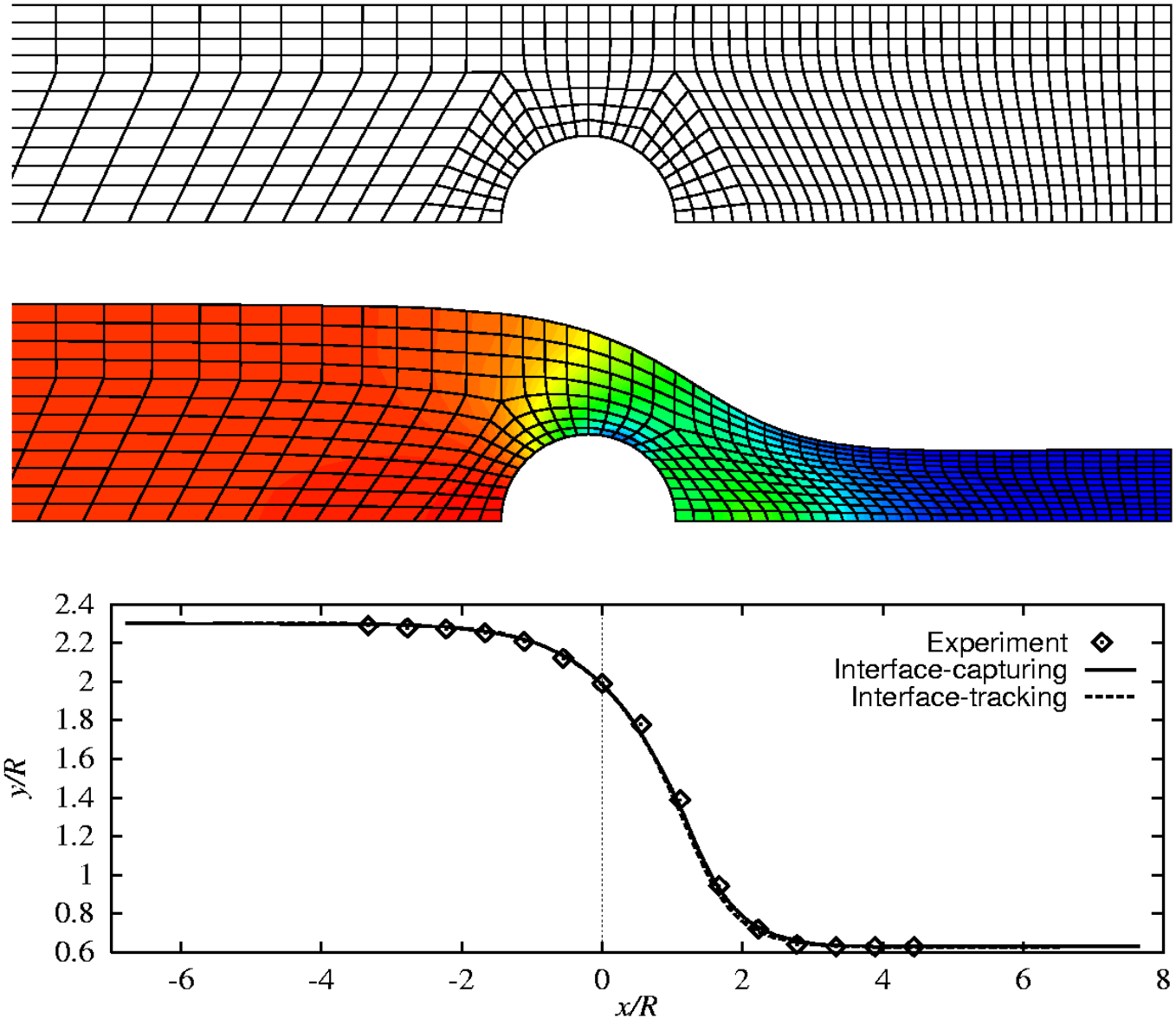
Comparison of the VOF and ITM methods on calculation of the wave system generated by a moving ship at Fr=0.267



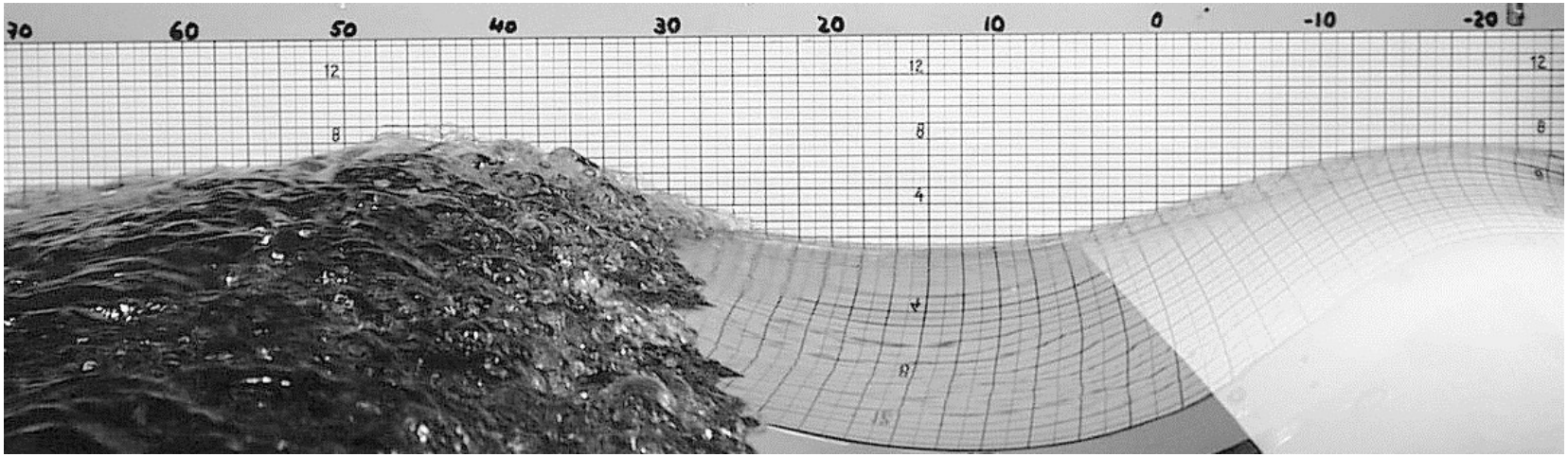
Calculated map of the wave system – upper part of the picture – VOF method, lower part of the picture – ITF method

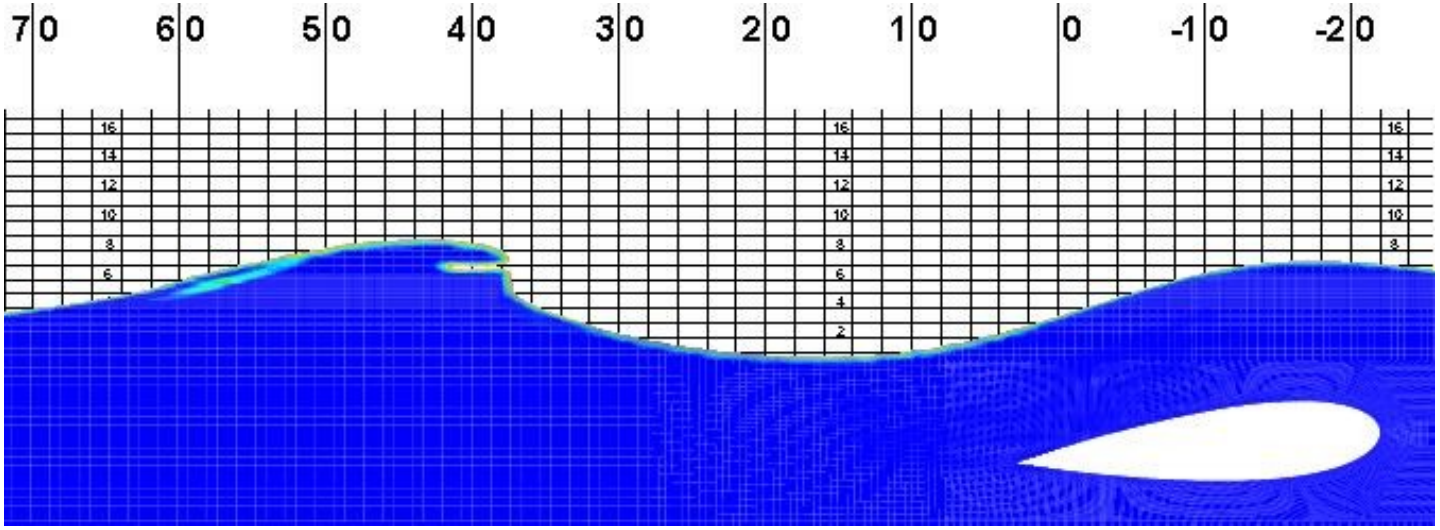


Comparison of the experimentally observed and calculated wave profile along the ship hull

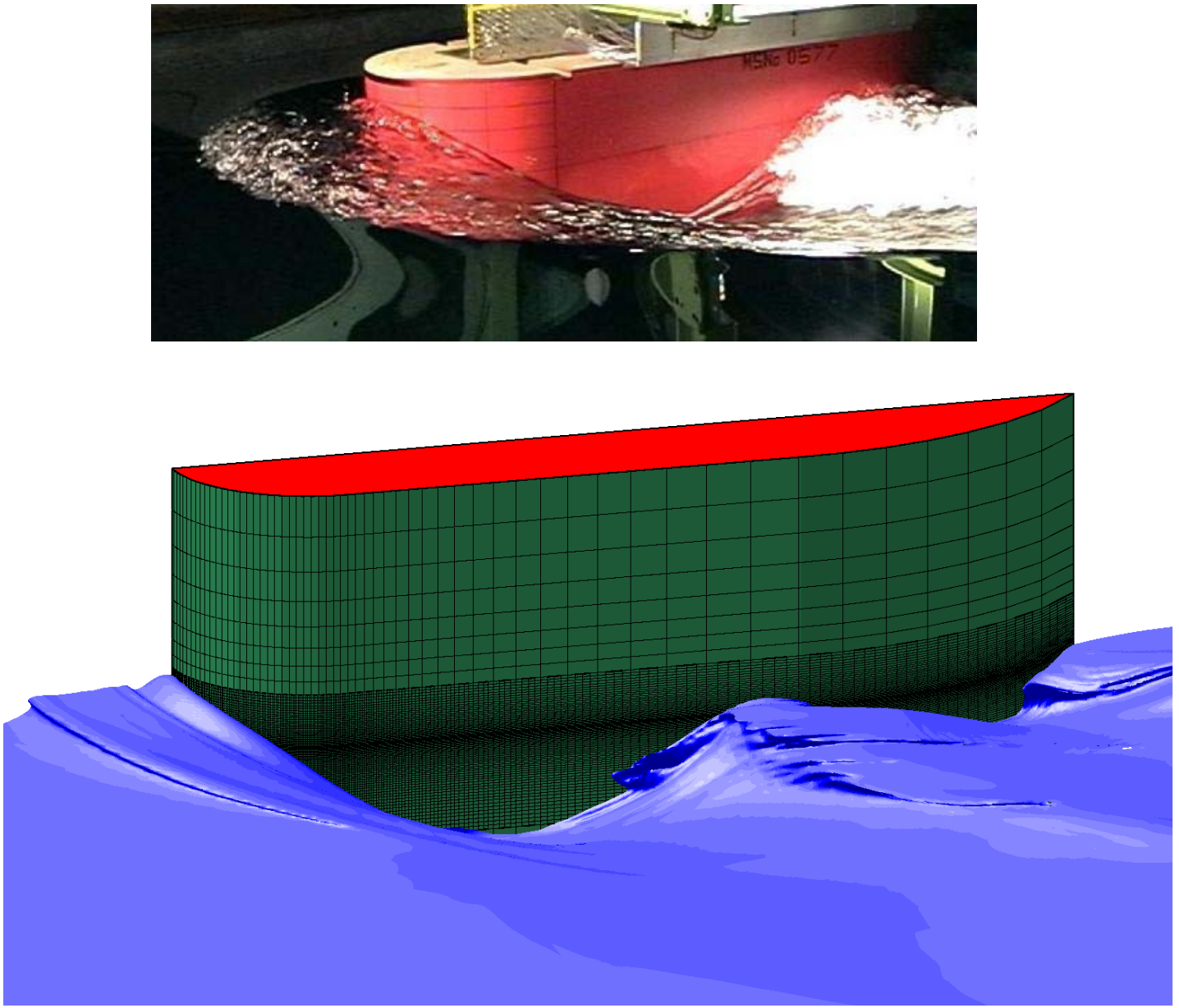


Supercritical free surface flow over a semi-cylindrical obstacle on the bottom

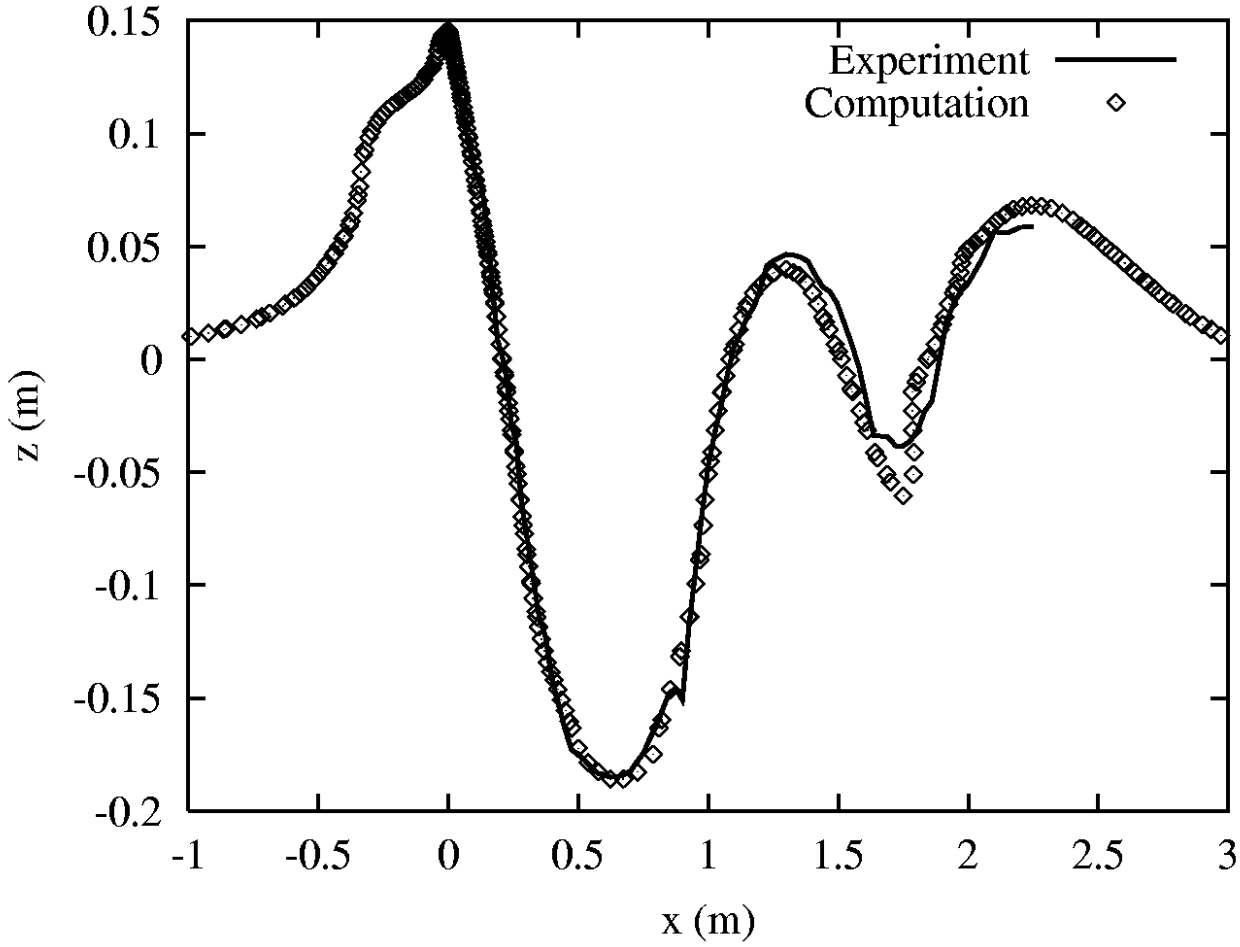




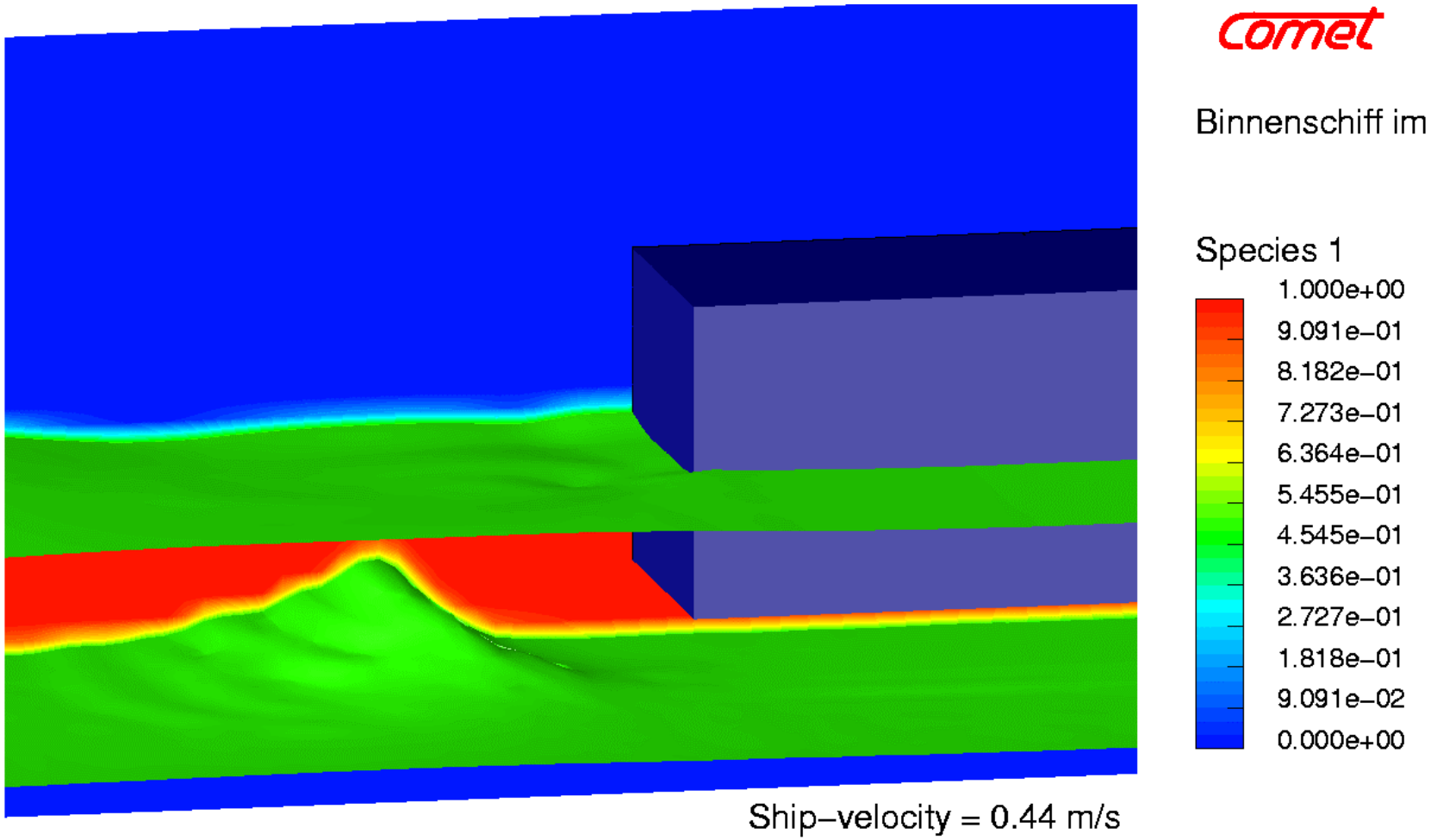
Free surface deformation over the moving submerged hydrofoil



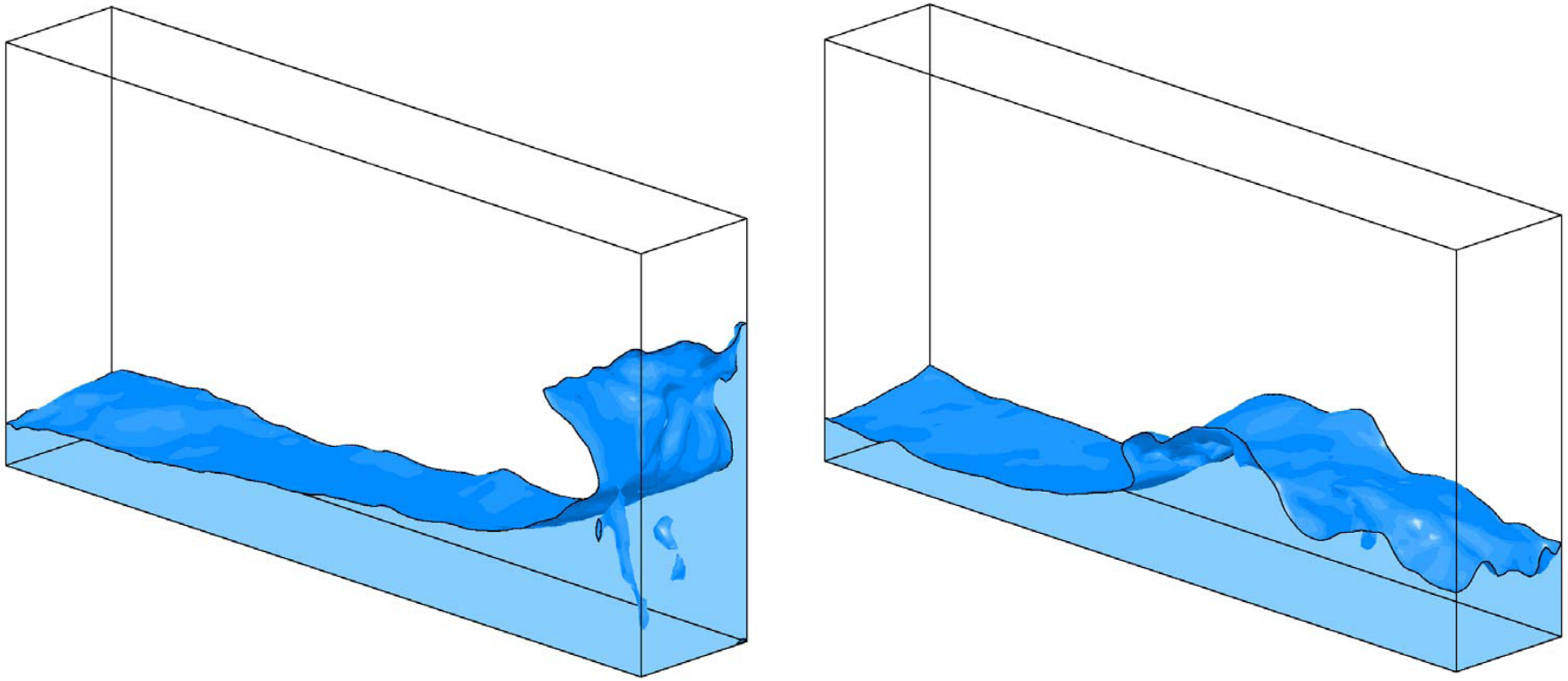
Free surface flow around a blunt ship hull



Comparison of observed and calculated free surface level along the blunt ship hull



Deformation of the muddy bottom due to ship motion in shallow water



Calculated phenomenon of liquid sloshing in the tank swaying horizontally

Appendix (free of charge): chemical reactions in flows – using the example of combustion

Combustion is a complicated chemical process: a common combustion of methane in air involves about 40 basic chemical reactions.

If we are interested only in the global results of the process , then a simplified approach may be applied, based on the following assumptions:

- chemical reactions develop with infinite speed

- combustion is a single stage reaction

- if one reactant is abundant, then the remaining reactants combine with each other in stoichiometric proportion, forming the products of the reaction:

1kg fuel + s kg oxidant = (1+s) kg products of reaction

$$CH_4 + 2 \cdot O_2 \rightarrow CO_2 + 2 \cdot H_2O$$

1kg methane + 64/16 kg oxygen = (1+64/16) kg products of reaction

The transport equations for the mass fractions of fuel and oxidant have the form:

$$\frac{\partial(\rho \cdot m_p)}{\partial t} + div(\rho \cdot m_p \cdot \bar{u}) = div(\Gamma_p \cdot gradm_p) + S_p$$

$$\frac{\partial(\rho \cdot m_u)}{\partial t} + div(\rho \cdot m_u \cdot \bar{u}) = div(\Gamma_u \cdot gradm_u) + S_u$$

where:

Γ – mass exchange coefficients

local variation+convection=diffusion+production

Assuming that transport coefficients are equal, we may introduce a function:

$$\varphi = s \cdot m_p - m_u$$

this allows us to combine both transport equations into one equation:

$$\frac{\partial(\rho \cdot \varphi)}{\partial t} + div(\rho \cdot \varphi \cdot \bar{u}) = div(\Gamma_\varphi \cdot grad\ \varphi)$$

Now the mixture coefficient *f* may be introduced : $$f = \frac{\varphi - \varphi_u}{\varphi_p - \varphi_u}$$

With such a definition of the mixture coefficient f its local value is 0 where there is only oxidant and the value is 1 where there is only fuel. Transport of the coefficient *f* in the flow is described by the equation:

$$\frac{\partial(\rho \cdot f)}{\partial t} + div(\rho \cdot f \cdot \bar{u}) = div(\Gamma_f \cdot gradf)$$

Solution of this equation together with the equations of mass conservation, momentum conservation, energy conservation and balance of entropy, using the appropriate boundary condition, leads to the distribution of *f* in the field of flow. This enables determination of the mass fractions of fuel and oxidant after the process of combustion.

with: $f_{st} \le f \le 1$ there is $m_p = \frac{f - f_{st}}{1 - f_{st}} \cdot m_{pw}$ $m_u = 0$

with: $0 \le f \le f_{st}$ there is $m_u = \frac{f_{st} - f}{f_{st}} \cdot m_{uw}$ $m_p = 0$

where: $f_{st} = \frac{m_{uw}}{s \cdot m_{pw} + m_{uw}}$ the value of *f* for the stoichiometric ratio

m_{pw} - mass fraction of fuel at inlet

m_{uw} - mass fraction of oxidant at inlet

The above simplified approach requires solution of only one additional differential equation, describing the transport of the coefficient *f* for determination of the concentrations of fuel oxidant and products of combustion in every point of the flow domain. Knowledge of *f* enables determination of temperature in the field of flow:

$T = \frac{h - m_p \cdot H_p}{\bar{C}_p}$ where: $\bar{C}_p = \frac{1}{T - T_0} \int_{T_0}^{T} C_p \, dT$

H_p - energy density of fuel

C_p - specific heat of the mixture

Transport equation for the specific enthalpy:

$$\frac{\partial(\rho \cdot h)}{\partial t} + div(\rho \cdot h \cdot \bar{u}) = div(\Gamma_h \cdot gradh) + S_h$$

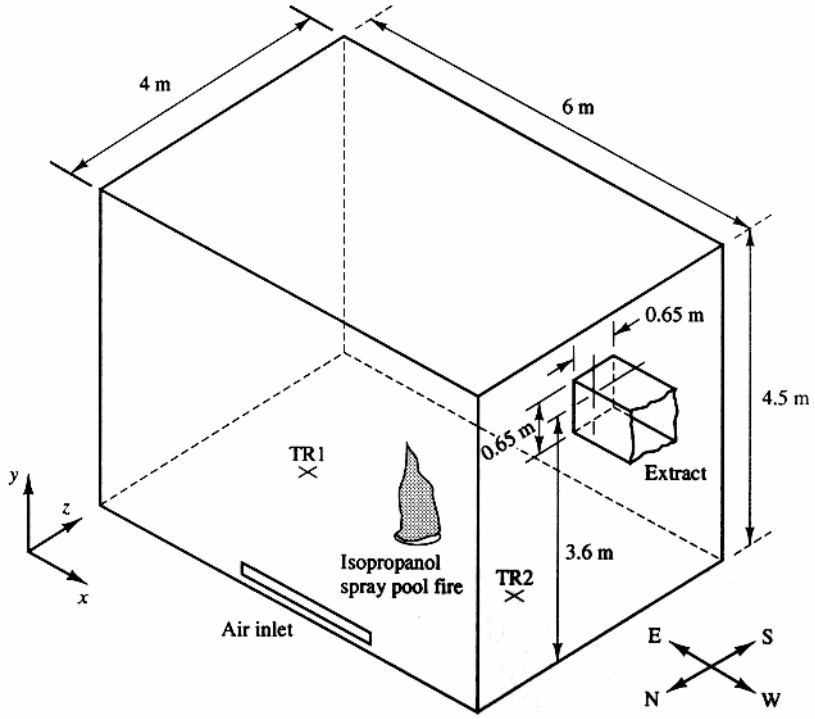
h – specific enthalpy

S_h - „source”of enthalpy

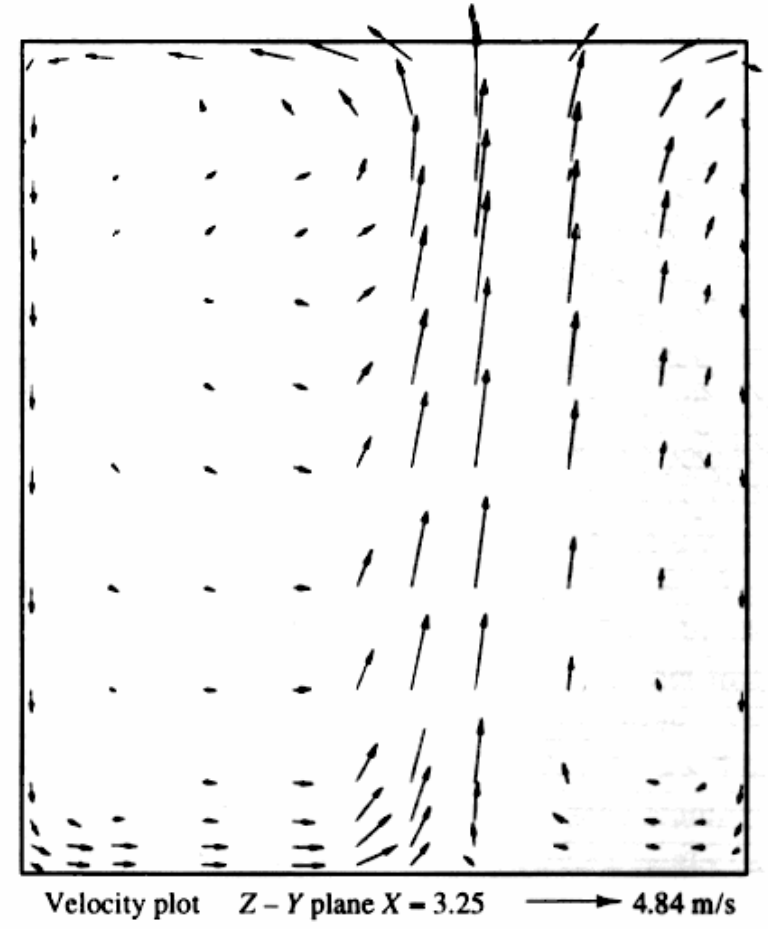
$$h = e + \frac{p}{\rho} = e + p \cdot \upsilon$$

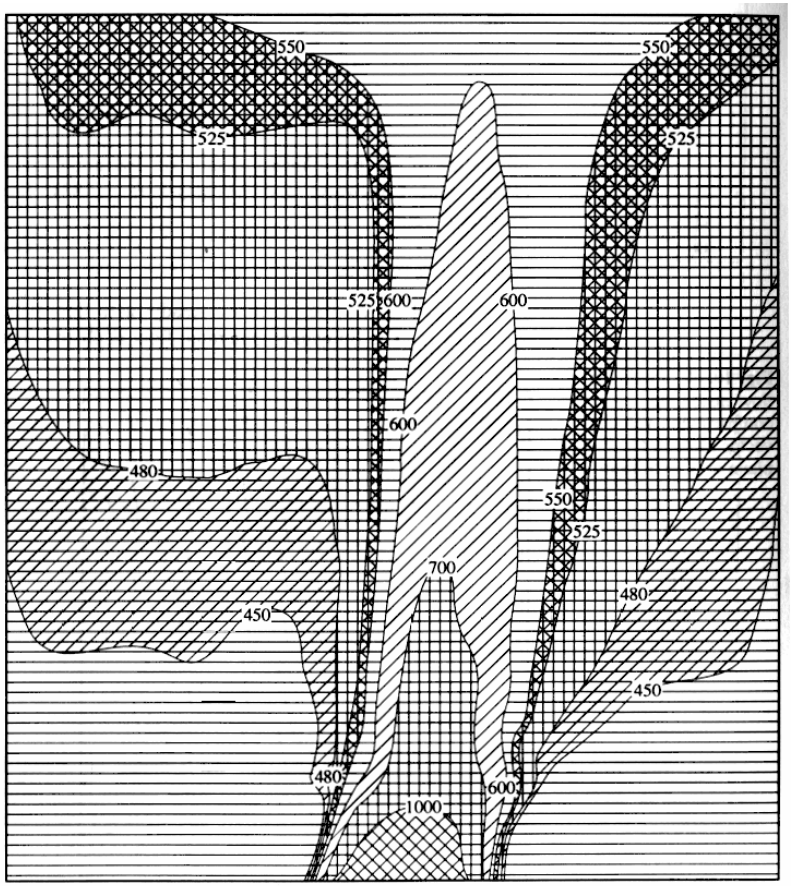
Example

Calculation of the velocity and temperature fields during a fire in the room. The finite volume grid 14*13*12=2688 was applied.



Velocity field calculated in the cross-section z-y for x=5,25 [m]→





←The calculated temperature field in the section z-y for x=3,00 [m]

Comparison of calculated and measured temperature distribution for the probes TR1 i TR2 →