4. Computational Fluid Dynamics

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The generic transport equation in differential form:

$$\frac{\partial \rho\phi}{\partial t} + \underbrace{\nabla\cdot(\rho\phi\vec{v})}_{\text{convective flux}} = \nabla\cdot\vec{S}_A + \overbrace{\nabla\cdot(\Gamma\nabla\phi)}^{\text{conductive flux}} + S_v$$

Transport equ.	ϕ
Continuity	1
x-momentum	u
y-momentum	v
z-momentum	w
Energy	e

Conservative form of the governing equations for single phase laminar flow:

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = S_m$$

$$\frac{\partial \rho u}{\partial t} + \nabla\cdot(\rho u\vec{v}) = -\frac{\partial p}{\partial x} + \nabla\cdot(\mu\nabla u) + \rho g_x + S_u$$

$$\frac{\partial \rho v}{\partial t} + \nabla\cdot(\rho v\vec{v}) = -\frac{\partial p}{\partial y} + \nabla\cdot(\mu\nabla v) + \rho g_y + S_v$$

$$\frac{\partial \rho w}{\partial t} + \nabla\cdot(\rho w\vec{v}) = -\frac{\partial p}{\partial z} + \nabla\cdot(\mu\nabla w) + \rho g_z + S_w$$

$$\frac{\partial \rho e}{\partial t} + \nabla\cdot(\rho e\vec{v}) = \nabla\cdot(-p\vec{v} + \underline{\underline{\tau}}\cdot\vec{v}) + \nabla\cdot(\lambda\nabla T) + S_e$$

$$\nabla\cdot(-p\underline{\mathrm{E}} + \underline{\tau})$$

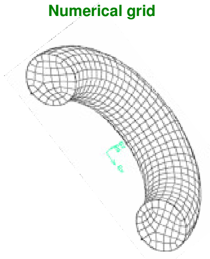
(Most turbulence models change only the transport coefficients λ and μ.)

Principles of CFD

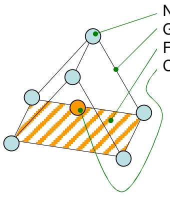
- Our aim is the approximate solution of the governing equations via numerical methods.
- Leading methods:
  - **Finite volume method**; - prevails in CFD
  - Finite difference method;
  - Finite element method.
- Some less widely spread methods:
  - Spectral methods;
  - Mesh-less methods;
  - Latice-Boltzmann.
- The domain is subdivided into smaller volumes (cells) in which the solution is approximated by simple functions (e.g. by linear functions). The process of subdivision is called: grid generation or meshing.
- The approximate solution is based on discrete values of the field variables stored in specific points of the numerical grid.
- The interaction between the meshed domain and the outer world is specified in the form of boundary conditions over the contour surface of the domain.

Numerical grid

Numerical grid



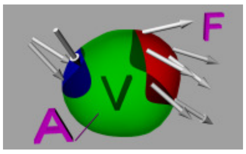
Elements of the numerical grid



Cell: Control volume. Field variables are (typically) defined in cell centroids.
Node: Grid geometry is defined by node positions.
Grid lines: Straight sections between neighboring nodes.
Facets: Cell sides defined by 3 or 4 nodes. A cell can have arbitrary number of sides.

Finite volume method

The generic transport equation



U: volume intensity of a conserved quantity

$$\frac{\partial}{\partial t}\int_V U\,dV + \oint_A \vec{F}\cdot d\vec{A} = \int_V S_V\,dV + \oint_A \vec{S}_A\cdot d\vec{A}$$

Conserved quantity per unit mass of fluid:

$$\Phi = U/\rho$$

Convective and conductive (diffusive) fluxes:

$$\vec{F}_C = \rho\Phi\vec{v} \qquad \vec{F}_D = -\Gamma\nabla\Phi$$

$$\frac{\partial}{\partial t}\int_V \rho\Phi\,dV + \oint_A \rho\Phi\vec{v}\cdot d\vec{A} = \oint_A (\Gamma\nabla\Phi + \vec{S}_A)\cdot d\vec{A} + \int_V S_V\,dV$$

Characteristics of the Finite Volume Method (FVM)

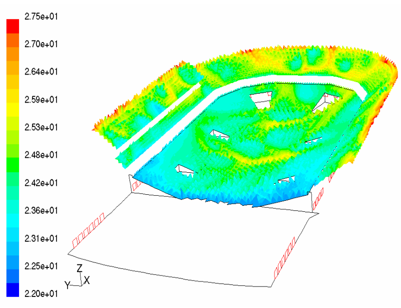
- The governing equations are used in **integral form**. (Integrated over cell volumes.)
- Divergence terms are converted into **surface integrals** over the facets enclosing the cells. The numerical approximation of the flux integral for one facet depends only on two unknown ϕ values stored in the centers of the two neighboring cells adjacent to the facet.
- As a result of this - so called discretization - process, every transport equation provides one (non-linear) **algebraic equation per cell**, e.g. if we have 5 transport equations and 1 000 000 cells, then we obtain a system of 5 000 000 non-linear algebraic equations. In the case of time dependent problems, we have to solve this system of equations in every time step.
- Each algebraic equation contains unknown ϕ values for one particular cell and for all of its neighboring cells. This is e.g. 5 unknowns per equations for tetrahedral grids.
- Due to the large number of unknowns and the non-linearity of the system of equations, **iterative** methods have to be used. The solution is first **initialized**, and then iteratively refined, thus **converging** towards the final solution.
- Integrals of fluxes over the boundary facets need to be defined in consistence with the physical characteristics of the region outside of the boundary, done by imposing additional mathematical conditions: **boundary conditions**.
- Surface integrals are numerically evaluated for every small facet, such as for that connecting two neighboring cells. These integrals express the flow rates of conserved quantities (mass, momentum, energy). When we calculate the integrals for such conserved quantities of the whole domain, the surface integrals for the internal facets are canceled, therefore the conservation equations for the whole domain are exactly fulfilled. This is called the **conservative behavior** of the finite volume method.

Overview of the process

1. Creation of model geometry,
2. Meshing,
3. Marking the boundary zones,
4. Selection of physical model, specification of material properties,
5. Parameterization of BC-s,
6. Adjustment of numerical controls
7. Initialization
8. Iteration
9. Visualization of the results

Development of User Defined Functions, if necessary.

Air temperature



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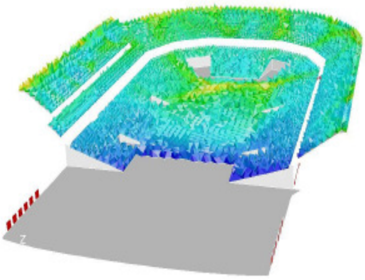
Application examples

Humidity

Moisture load: 0.0187 g/s/person



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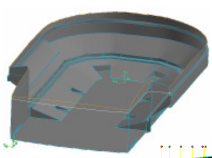
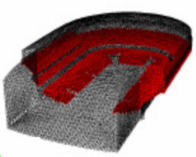
1. HV&AC analyses of a sport hall

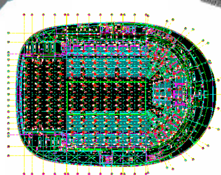
Papp László Sportaréna, Budapest, 2001.



Geometrical model



Mesh
40 k cells,
2m resolution



Air inlets (red dots)

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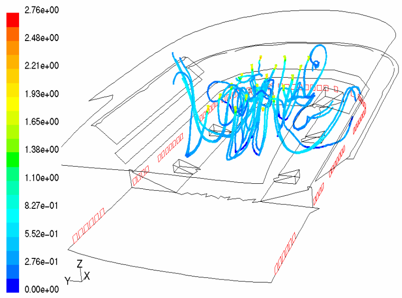
Streamlines in concert operation mode



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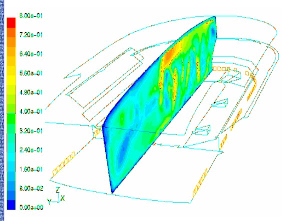
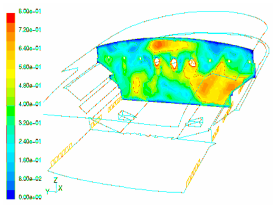
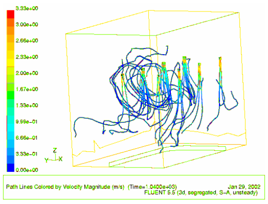
Contour plots of velocity magnitude

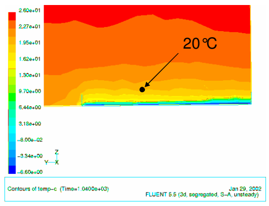




Fulfillment of a sports related technical requirement: temperature above the ice



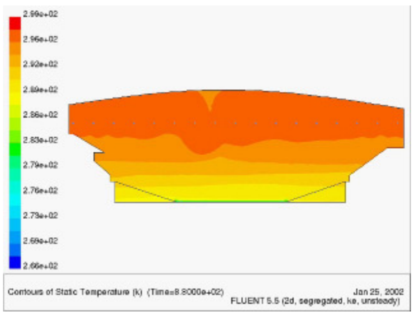
3 rows of air inlets
operating in jet mode



Temperature
distribution

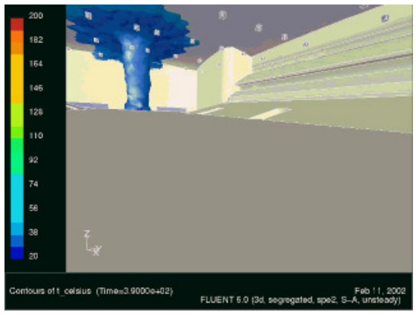
Temperature transient during start-up

Total time frame: 25 minutes



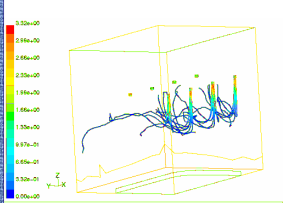
Smoke analyses

at 10 minutes

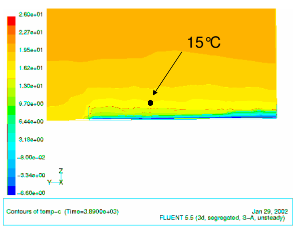


The fire spreads with time

Fulfillment of a sports related technical requirement: temperature above the ice



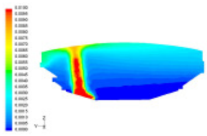
1 row of air inlets
operating in jet mode

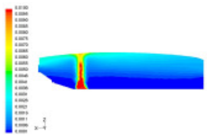


Temperature distribution

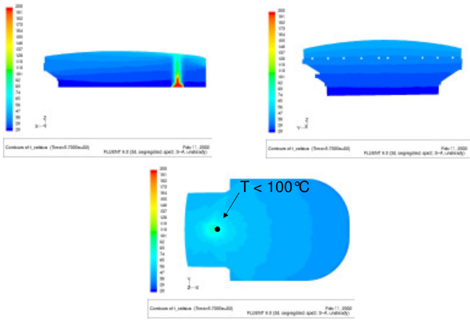
Different fire locations

CO_2 concentration





Temperature distribution



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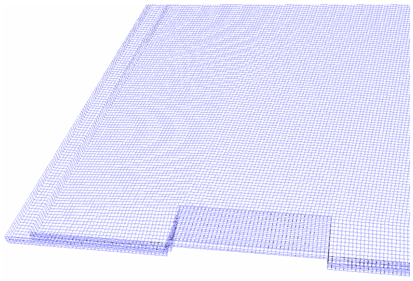
Numerical mesh



Spatial resolution: 0,14 x 0,14 x 0,14 m^3

Number of cells: 470 000

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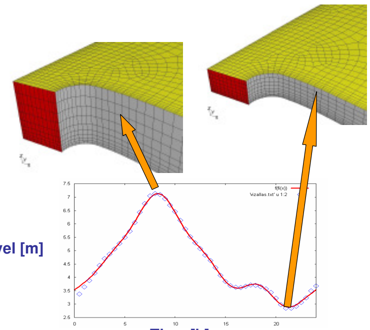
2. Guber József Water Reservoir CFD analyses (2007)

Deforming mesh (35.000 cells)

Water level [m]



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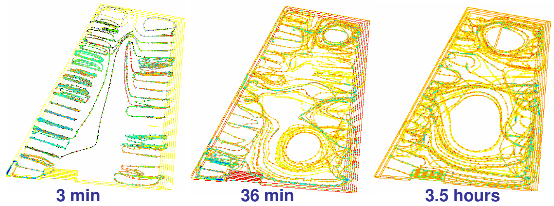
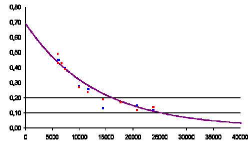
Flow structure





Modeled as a volume source:

$$S_{Cl} = \frac{c_{Cl}}{\tau}$$

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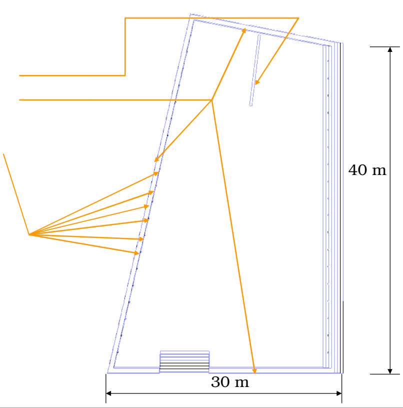
3. Thermal bath

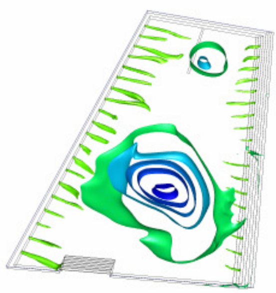
Floor outlet

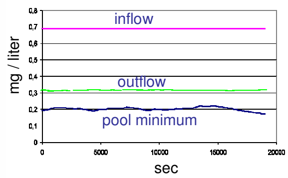
Weir outlet

Water inlets (38 jets)



Evolution of the active chlorine concentration





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5. Turbulence models

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February, 2009.

Characteristics of turbulent flows

1. Unsteady, chaotic.
2. Three-dimensional. (Even in 2D flow situations.)
3. Fluctuations are caused by the passing vortices. Advection velocity is the average flow velocity.
4. Turbulence depends not (only) on local flow field but also on the shear-rate history of the fluid parcel.
5. Turbulence causes intensive local mixing of any conserved property. From the point of view of the mean flow, it can be regarded as an increase in transport coefficients.
6. Due to the apparent viscous stresses the kinetic energy of the mean flow is being converted to (stochastic) turbulent kinetic energy and than to internal energy (heating).
7. The size of the largest eddies is close to (and proportional with) the characteristic size of the domain (l).
8. Eddy size cover a wide spectrum.
   $l/\eta = (Re_l)^{3/4}$ - 2..6 orders of magnitude.

Origin of turbulence

1) Wall shear;
2) Free shear;
3) Unstable stratification.

Turbulent kinetic energy

The most expressive quantity of turbulence is the turbulent kinetic energy: $k = \dfrac{\overline{u'^2 + v'^2 + w'^2}}{2}$ [m²/s²] (Measurable.)

Note that, the square root of k does have the dimension of **m/s**; therefore on the basis of k we can define the velocity scale of turbulence as:

$$V' = \sqrt{k}$$

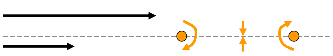
Isotropic turbulence can be characterized by a single scalar quantity ν_t (turbulent viscosity), which somehow needs to calculated: ν_t [**m²/s**].

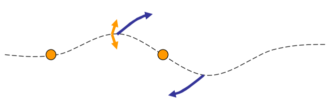
Purely from a dimension point of view, we need another turbulent quantity having a dimension other than (m/s)ⁿ.

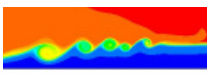
Free shear layers

Due to the existence of an inflexion point in the velocity profile, a free shear layer is unstable. This can be shown even for 2D flow of perfect fluid. (Kelvin-Helmholtz instability.)

We can model the shear layer with an infinite series of line vortices:



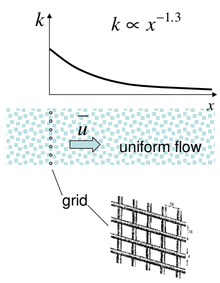




Large eddies create smaller eddies, they create even smaller eddies ...
This turbulent energy cascade is driving kinetic energy from the mean flow to the smallest eddies of η [m] size (dissipative level).

Dissipation rate of turbulent kinetic energy

This very fundamental experiment shows the behavior of isotropic turbulence in a „closed system" (without eg. turbulent production in the mean flow).



[From the measurements of Comte-Bellot and Corssin, 1966]

We can define the dissipation rate of turbulent kinetic energy in this experiment as:

$$\varepsilon := \frac{dk}{dt} \qquad [\mathrm{m^2 s^{-3}}]$$

Turbulent viscosity

Assuming that turbulence can be characterized by only 2 scalar parameters k and ε, we can define the necessary scales of turbulent motion:

$$T = \frac{k}{\varepsilon} \quad \text{[s]} \quad \longleftarrow \quad \varepsilon = \frac{dk}{dt}$$

$$V' = \sqrt{k} \quad \text{[m/s]} \quad \longleftarrow \quad k = \frac{\overline{u'^2 + v'^2 + w'^2}}{2}$$

$$L = \frac{k^{3/2}}{\varepsilon} \quad \text{[m]} \quad \longleftarrow \quad L = V'T$$

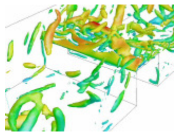
Now, we can calculate the turbulent viscosity (Kolmogorov-Prandtl formula) :

$$\nu_t = C_\mu LV' = C_\mu \frac{k^2}{\varepsilon}$$

From measurements:

$$C_\mu = 0.09$$

Characteristics of the Scale Resolving Models



[LES results from dr. Máté Lohász]

- Unsteady simulations, resulting in a fluctuating velocity field.
- Depending on model resolution, less (if any) turbulent viscosity is used.
- Rely much less on the accuracy of turbulent models.
- Usually give more accurate mean flow quantities.
- Synthetic turbulence must to be defined at the inlet.
- Application of special numerical schemes, which do not suppress fluctuations, is necessary.
- Steady field quantities can only be obtained after a long term averaging.

Evolution of *k*

A transport equation for turbulent kinetic energy in general flow situations can be analytically derived. We mention only the two most fundamental source terms below.

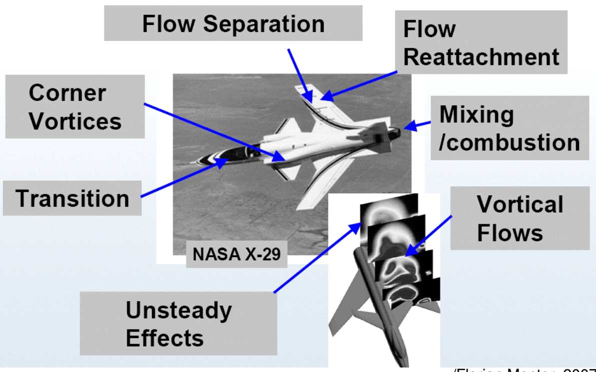
$$\frac{dk}{dt} = \underbrace{P}_{\text{production}} - \overbrace{\varepsilon}^{\text{dissipation}}$$

The turbulent production P is interpreted as: $P = \nu_t S^2$,

where S is the modulus of the mean rate-of-strain tensor: $S = \sqrt{2 S_{ij} S_{ij}}$ $\qquad S_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right)$

Unfortunately, we cannot derive a formula for ε.
Some further assumptions have to be made in order to achieve closure.

Modeling challenges



/Florian Menter, 2007/

Evolution of ε

According to the **standard *k-ε* model** proposed by Launder and Spalding (1972) ε can be described by a transport equation similar to the equation of *k*, because ε is also rooted in turbulent eddying.

$$\frac{d\varepsilon}{dt} = C_{1\varepsilon}\frac{\varepsilon}{k}P - C_{2\varepsilon}\frac{\varepsilon^2}{k}$$

(We need to correct the dimensions of the production and dissipation terms by multiplying them by ε / k.)

Model constants can be identified on the basis of measured data:

$$C_{1\varepsilon} = 1.44, \; C_{2\varepsilon} = 1.92$$

eg. $C_{2\varepsilon}$ is coming from grid turbulence experiments.

Classification of some well known turbulence models

Algebraic models - Local shear rate + length scale (eg. distance from wall). *Does not know about the flow history, wall distance cannot be defined in complex cases.*

Reynolds averaged (RANS) models based on transport equations:

Spalart-Allmaras	1 eq.	- Airfoils, nearly 2D flow, *Spreading rate of jets are predicted with 100% error.*
k-ε	2 eq.	- For general use 3D, isotropic.
k-ω	2 eq.	- Viscous sub-layer, transition.
RSM	7 eq.	- Anisotropy, eg. for secondary flow and for cyclones. *Up to 10 or 20 times more iterations can be necessary.*

Stabilization of the flow (steady flow) is not guaranteed by any RANS models.

Scale resolving models:

DNS	- Fully resolved turbulence. *Computational cost grows with $Re^{9/4}$. Huge amount of junk data is produced.*
LES,	- Only the large eddies are taken into account. Effect of sub-grid scale turbulence: SGS models. *Close to the wall a fine mesh is required.*
DES, SAS	- RANS model is used close to the wall (e.g.Spalart-Allmaras model), gradually changes to LES in the main flow.