Fire Modelling in Computational Fluid Dynamics (CFD)

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  - influence of convection, diffusion, volumetric (buoyancy) force
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  - influence of averaging on zone and field models
  - solution methods
- CFD modelling
  - turbulence models (k-epsilon, k-omega, Reynolds stress, LES)
  - combustion models (mixture fraction, eddy dissipation, flamelet)
  - thermal radiation models (discrete transfer, Monte Carlo)
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Introduction

- Today, CFD methods are well established tools that help in design, prototyping, testing and analysis
- The motivation for development of modelling methods (not only CFD) is to reduce cost and time of product development, and to improve efficiency and safety of existing products and installations
- Verification and validation of modelling approaches by comparing computed results with experimental data is necessary
- Experimental investigation of fire in a realistic environment is in many situations impossible. In such cases, CFD is the only viable analysis and design tool.

Introduction

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- Fire modelling is an area of computational modelling which aims to predict fire behaviour in different environmental conditions.
- Therefore, these computational models need to take into account fluid dynamics, combustion and heat transfer processes.
- The complexity of the fire modelling arises from significantly different time scales of the modelled processes. Also, not completely understood physics and chemistry of fire adds the uncertainty to the modelling process.

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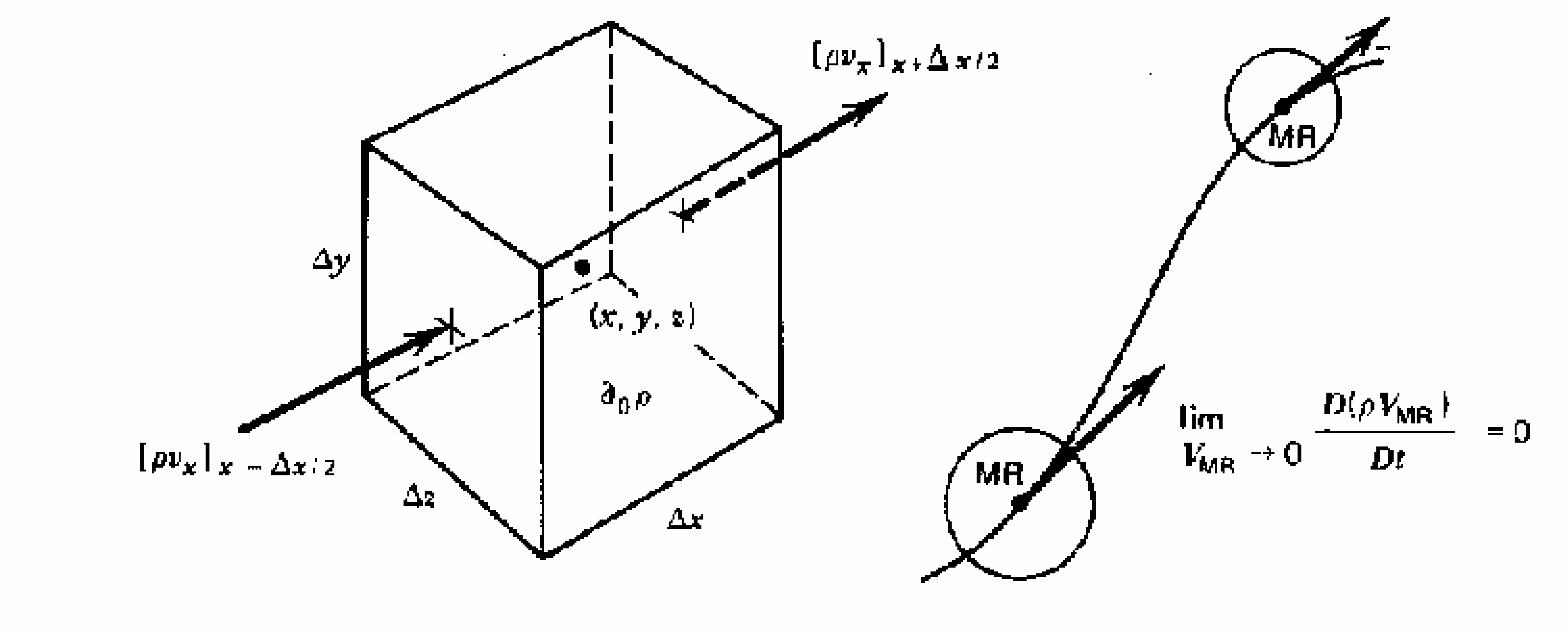
Overview of fluid dynamics

transport equations

Transport equations

- Eulerian and Lagrangian description

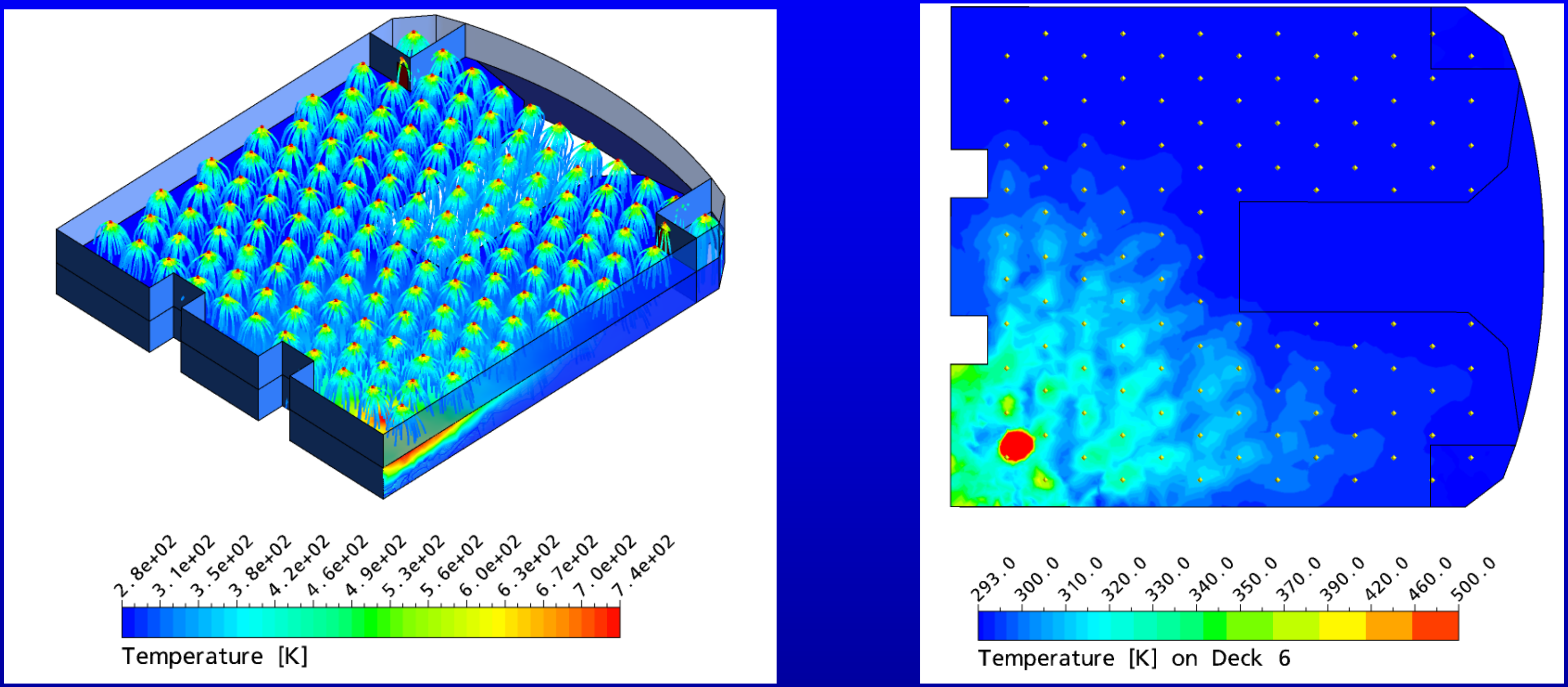


- **Eulerian description** – transport equations for mass, momentum and energy are written for a (stationary) control volume
- **Lagrangian description** – transport equations for mass, momentum and energy are written for a moving material particle

Transport equations

- Majority of the numerical modelling in fluid mechanics is based on the Eulerian formulation of transport equations
- Using the Eulerian formulation, each physical quantity is described as a mathematical field. Therefore, these models are also named field models
- Lagrangian formulation is a basis for particle dynamics modelling: bubbles, droplets (sprinklers), solid particles (dust) etc.

Transport equations



Droplets trajectories from sprinklers (left), gas temperature field during fire suppression (right)

Transport equations

- The following physical laws and terms also need to be included

- Newton's viscosity law
- Fourier's law of heat conduction
- Fick's law of mass transfer

diffusive terms - flux is a linear function of a gradient

- Sources and sinks due to thermal radiation, chemical reactions etc.

Transport equations

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- Transport of mass and composition

$$\underline{\partial_t\rho}+\underline{\partial_i(v_i\rho)}=M$$

$$\underline{\partial_t(\rho\xi_j)}+\underline{\partial_i(v_i\rho\xi_j)}=\underline{\partial_i(\rho D\partial_i\xi_j)}+\underline{M_j}$$

- Transport of momentum

$$\underline{\partial_t(\rho v_j)}+\underline{\partial_i(v_i\rho v_j)}=-\partial_j p+\underline{2\partial_i(\mu S_{ij})}+\underline{\rho g_j+F_j}$$

$$S_{ij}=\frac{1}{2}(\partial_j v_i+\partial_i v_j)$$

- Transport of energy

$$\underbrace{\partial_t(\rho h)}_{\text{change in a control vol.}}+\underbrace{\partial_i(v_i\rho h)}_{\text{flux difference (convection)}}=\underbrace{\partial_i(\lambda\partial_i T)}_{\text{diffusion}}+\underbrace{Q}_{\text{volumetric term}}$$

Transport equations

- Lagrangian formulation is simpler

- particle location equation $d\vec{x}/dt=\vec{u}$

- mass conservation eq. for a particle $dm/dt=M$

- momentum conservation eq. for a particle

$$m\left(d\vec{u}/dt\right)=\underbrace{\vec{F}_D}_{\text{drag}}+\underbrace{\vec{F}_L}_{\text{lift}}+\underbrace{\vec{F}_V}_{\text{volumetric forces}}$$

- thermal energy conservation eq. for a particle

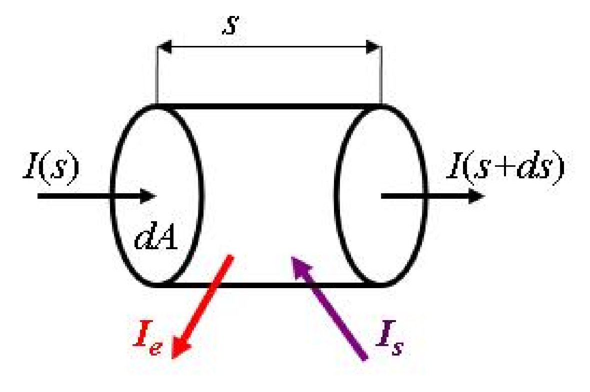
$$mc_p\left(dT/dt\right)=\underbrace{Q_C}_{\text{convection}}+\underbrace{Q_L}_{\text{latent heat}}+\underbrace{Q_R}_{\text{thermal radiation}}$$

Transport equations of the Lagrangian model need to be solved for each representative particle

Transport equations

- Thermal radiation

Equations describing thermal radiation are much more complicated



- spectral dependency of material properties
- angular (directional) dependence of the radiation transport

$$\underbrace{\frac{dI_\nu(\Omega)}{ds}}_{\text{change of radiation intensity}} = \underbrace{-(K_{a\nu}+K_{s\nu})I_\nu(\Omega)}_{\text{absorption and out-scattering}} + \underbrace{K_{a\nu}I_{e\nu}}_{\text{emission}} + \underbrace{\frac{K_{s\nu}}{4\pi}\int_{4\pi} I_{s\nu}(\Omega')P_\nu(\Omega'\to\Omega)\,d\Omega'}_{\text{in-scattering}}$$

Averaging and simplification of transport equations

Averaging and simplification of transport equations

- The presented set of transport equations is analytically unsolvable for majority of cases

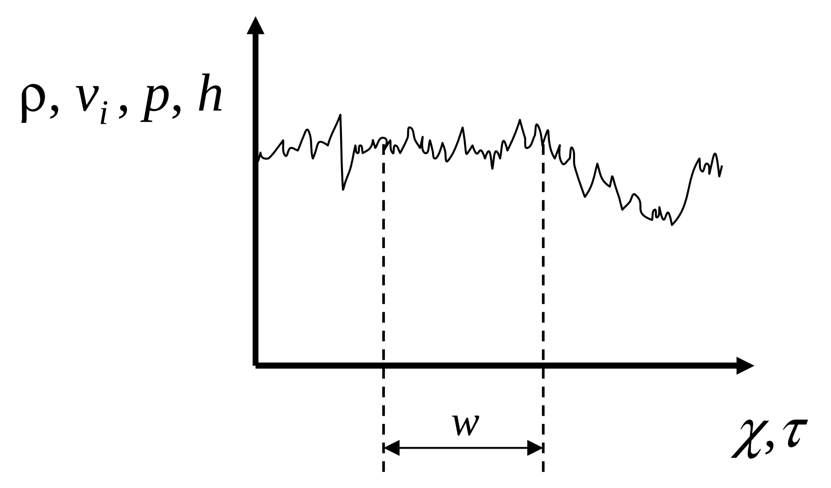
- Success of a numerical solving procedure is based on density of the numerical grid, and in transient cases, also on the size of the integration time-step

- Averaging and simplification of transport equations help (and improve) solving the system of equations:

- derivation of averaged transport equations for turbulent flow simulations
- derivation of integral (zone) models

Averaging and simplification of transport equations

- Averaging and filtering



The largest flow structures can occupy the whole flow field, whereas the smallest vortices have the size of Kolmogorov scale

$$\eta = \left(\nu^3/\varepsilon\right)^{\frac{1}{4}}$$

$$u_\eta = \left(\varepsilon\nu\right)^{\frac{1}{4}}$$

$$\tau_\eta = \left(\nu/\varepsilon\right)^{\frac{1}{2}}$$

Averaging and simplification of transport equations

- Kolmogorov scale is (for most cases) too small to be captured with a numerical grid

- Therefore, the transport equations have to be filtered (averaged) over:

  - spatial interval → Large Eddy Simulation (LES) methods
  - time interval → k-epsilon model, SST model, Reynolds stress models

Averaging and simplification of transport equations

- Transport equation variables can be decomposed onto a filtered (averaged) part and a residual (fluctuation)

$$\rho = \overline{\rho} + \rho'$$

$$p = \overline{p} + p'$$

$$v_i = \overline{\rho v_i} / \overline{\rho} + v_i^* = \tilde{v}_i + v_i^*$$

$$\xi_i = \tilde{\xi}_i + \xi^*$$

$$h_i = \tilde{h} + h^*$$

- Filtered (averaged) transport equations

$$\partial_t \overline{\rho} + \partial_j (\overline{\rho}\, \tilde{v}_j) = \underline{\overline{M}}$$

$$\partial_t \left(\overline{\rho} \tilde{\xi}_j\right) + \partial_i \left(\overline{\rho} \tilde{v}_i \tilde{\xi}_j\right) = \underline{\overline{M}_j} - \underline{\partial_i \left(\overline{\rho} \Gamma_j\right)}$$

turbulent mass fluxes

$$\partial_t \left(\overline{\rho}\, \tilde{v}_j\right) + \partial_i \left(\overline{\rho}\; \tilde{v}_i\, \tilde{v}_j\right) = -\partial_j \overline{p} + 2\partial_i \left(\mu \overline{S}_{ij}\right) + \overline{\rho} g_j + \underline{\overline{F}_j} - \underline{\partial_i \left(\overline{\rho} \Pi_{ij}\right)}$$

sources and sinks represent a separate problem and require additional models

$$\partial_t \left(\overline{\rho}\, \tilde{h}\right) + \partial_i \left(\overline{\rho} \tilde{v}_i\, \tilde{h}\right) = \partial_i \left(\lambda \partial_i \tilde{T}\right) + \underline{\overline{Q}} - \underline{\partial_i \left(\overline{\rho} \Omega_i\right)}$$

- turbulent stresses
- Reynolds stresses
- subgrid stresses

turbulent heat fluxes

Averaging and simplification of transport equations

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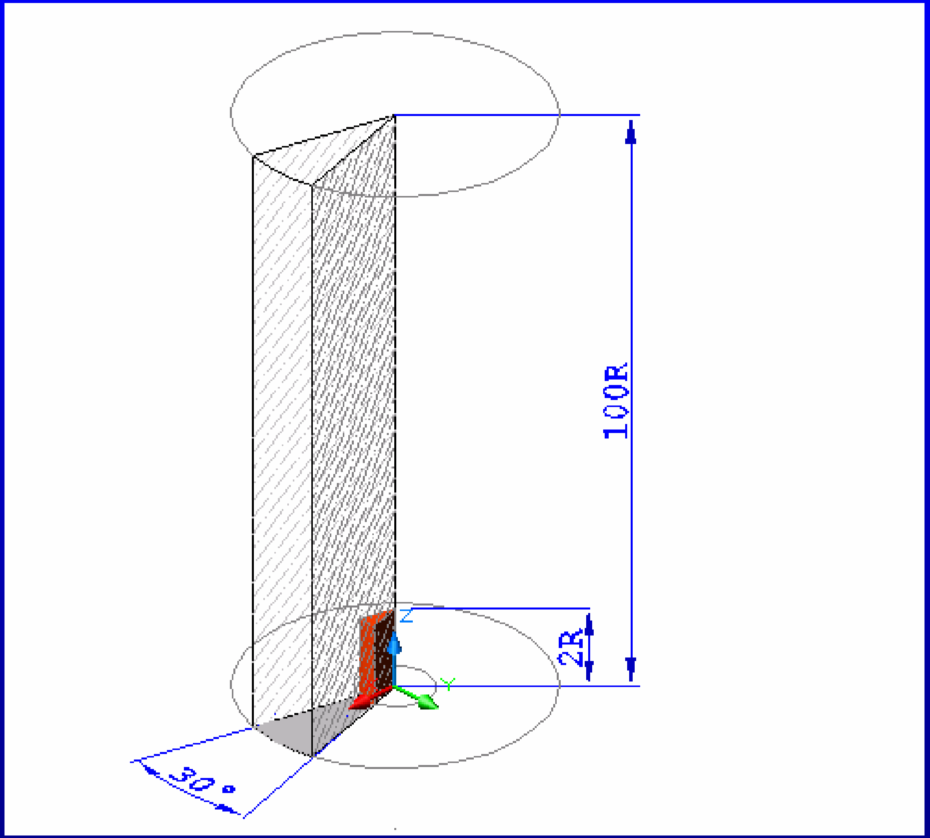
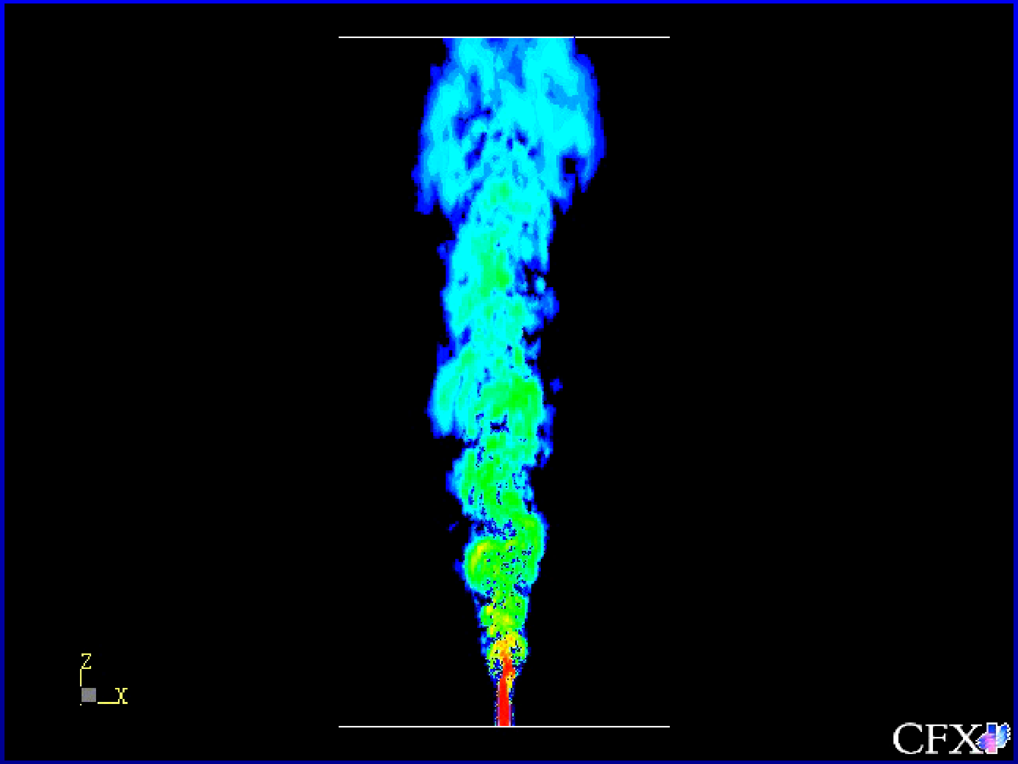


Buoyancy induced flow over a heat source (Gr=10e10); inert model of fire

Averaging and simplification of transport equations



LES model; instantaneous temperature field

Averaging and simplification of transport equations

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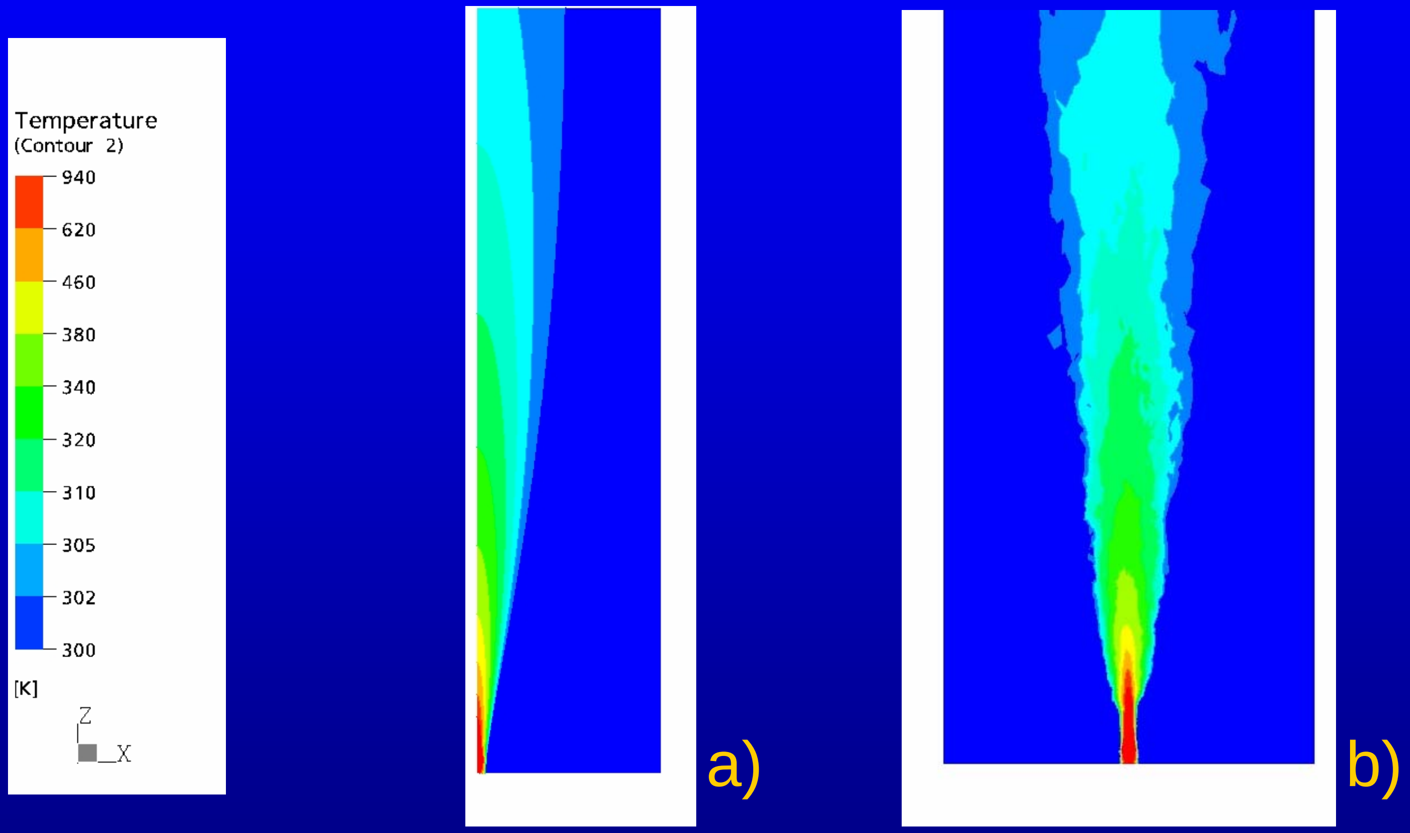


Temperature field comparison:
a) steady-state RANS model, b) averaged LES model results

Averaging and simplification of transport equations

- Additional simplifications

- flow can be modelled as a steady-state case → the solution is a result of force, energy and mass flow balance taking into consideration sources and sinks

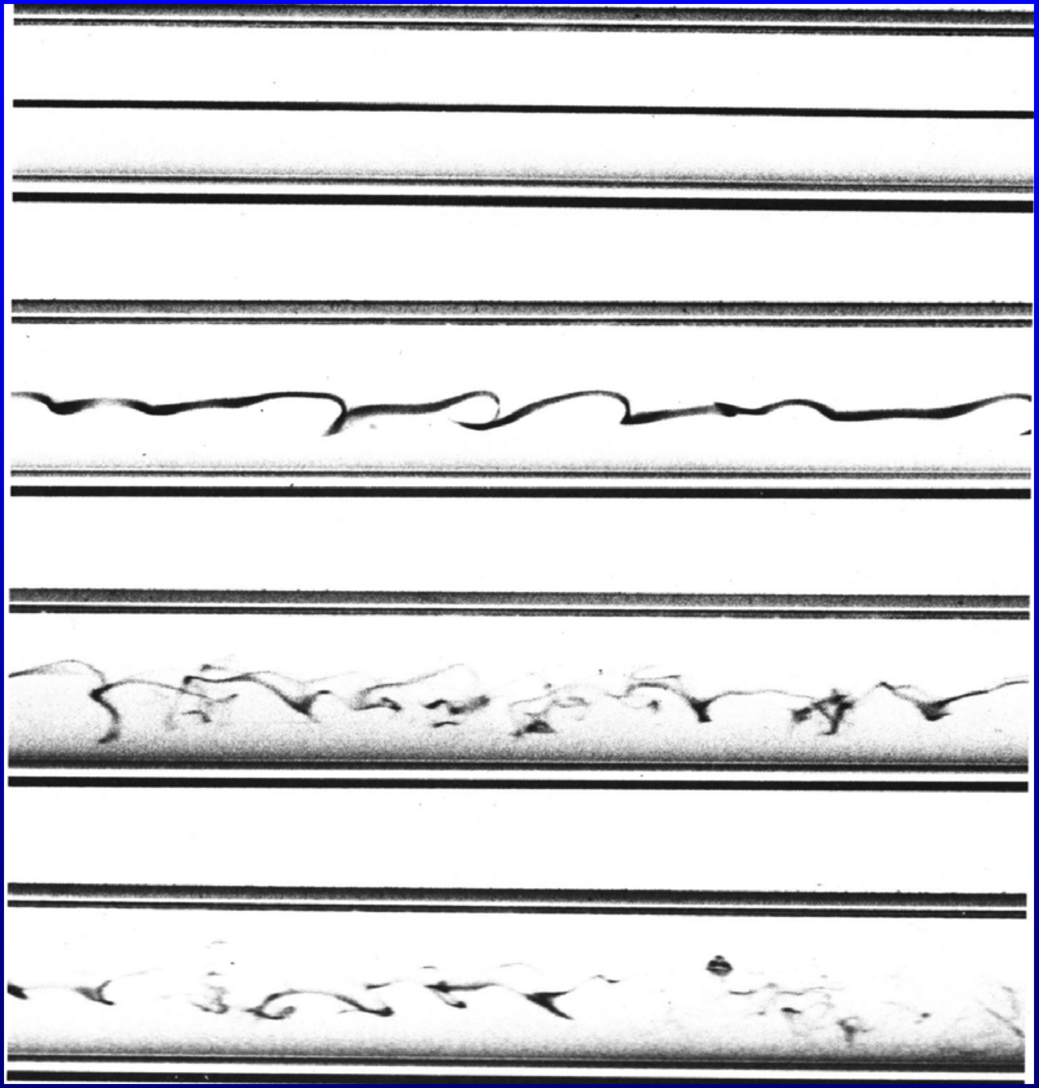
- fire can be modelled as a simple heat source → inert fire models; do not need to solve transport equations for composition

- thermal radiation heat transfer is modelled as a simple sink of thermal energy → FDS takes 35% of thermal energy

- control volumes can be so large that continuity of flow properties is not preserved → zone models

CFD Modelling

Turbulence models



laminar flow

transitional flow

turbulent flow

van Dyke, 1965

Turbulence models

- Turbulence models introduce additional (physically related) diffusion to a numerical simulation
- This enables :

- RANS models to use a larger time step (Δt >> Kolmogorov time scale) or even a steady-state simulation
- LES models to use a less dense (smaller) numerical grid (Δx > Kolmogorov length scale)

The selection of the turbulence model fundamentally influences distribution of the simulated flow variables (velocity, temperature, heat flow, composition etc)

Turbulence models

- In general, 2 kinds of averaging (filtering) exist, which leads to 2 families of turbulence models:

  - filtering over a spatial interval → Large Eddy Simulation (LES) models
  - filtering over a time interval → Reynolds Averaged Navier-Stokes (RANS) models: k-epsilon model, SST model, Reynolds Stress models etc

- For RANS models, size of the averaging time interval is not known or given (statistical average of experimental data)

- For LES models, size of the filter or the spatial averaging interval is a basic input parameter (in most cases, it is equal to grid spacing)

Turbulence models

- Reynolds Averaged Navier-Stokes (RANS) models

For two-equation models (e.g. k-epsilon, k-omega or SST), 2 additional transport equations need to be solved:

- for kinetic energy of turbulent fluctuations $k = 1/2\,\Pi_{ii}$

- for dissipation of turbulent fluctuations $\bar{\rho}\varepsilon = \mu(\overline{\partial_j v_i^{*}\ \partial_j v_i^{*})}$

or

- for frequency of turbulent fluctuations $\omega \sim \varepsilon / k$

These variables are then used to calculate eddy viscosity:

$$\mu_t = C_\mu\, \rho \frac{k^2}{\varepsilon} = \rho \frac{k}{\omega}$$

Turbulence models

- Reynolds Averaged Navier-Stokes (RANS) models

  - from eddy viscosity, Reynolds stresses, turbulent heat and mass fluxes are obtained

$$\overline{\rho}\Pi_{ij} - \frac{1}{3}\overline{\rho}\Pi_{ll}\delta_{ji} = -2\mu_t S_{ij} + \frac{2}{3}\mu_t(\partial_l \tilde{v}_l)\delta_{ji}$$

$$\overline{\rho}\Omega_j = -\frac{\mu_t}{Pr_t}\partial_j \tilde{h}$$

$$\overline{\rho}\Gamma_j = -\frac{\mu_t}{Sc_t}\partial_j \tilde{\xi}$$

  - model parameters are usually defined from experimental data e.g. dissipation of grid generated turbulence or flow in a channel

  - transport equation for k is derived directly from the transport equations for Reynolds stresses Π_{ij}

  - transport equation for ε is empirical

Turbulence models

- Large Eddy Simulation (LES) models

  - Large Eddy Simulation (LES) models are based on spatial filtering (averaging)

  - many different forms of the filter exist, but the most common is "top hat" filter (simple geometrical averaging)

  - size of the filter is based on a grid node spacing

Basic assumption of LES methodology:

Size of the used filter is so small that the averaged flow structures do no influence large structures, which do contain most of the energy.

These small structures are being deformed, disintegrated onto even smaller structures until they do not dissipate due to viscosity (kinetic energy → thermal energy).

Turbulence models

- Large Eddy Simulation (LES) models

- eddy (turbulent) viscosity is defined as

$$\mu_t \sim \rho\, l^{4/3}\varepsilon^{1/3}$$

where

$$l \sim C_s\underline{\Delta}$$

grid spacing

- using the definition of turbulence (subgrid) stresses

$$\bar{\rho}\Pi_{ji} - \frac{2}{3}\bar{\rho}k\,\delta_{ji} = -2\mu_t S_{ij} + \frac{2}{3}\mu_t\,(\partial_l \tilde{v}_l)\,\delta_{ji}$$

and turbulence fluxes

$$\bar{\rho}\Omega_j = -\frac{\mu_t}{Pr_t}\partial_j \tilde{h}$$

the expression for eddy viscosity can be written as

$$\mu_t = \bar{\rho}\left(C_s\Delta\right)^2\left(2S_{ji}S_{ij} + G\right)^{1/2}$$

where the contribution due to buoyancy is

$$G \sim \frac{g_i\partial_i \tilde{h}}{Pr_t\,\tilde{h}}$$

Turbulence models

- Large Eddy Simulation (LES) models

  - presented Smagorinsky model is the simplest from the LES models

  - it requires knowledge of empirical parameter C_s, which is not constant for all flow conditions

  - newer, dynamic LES models calculate C_s locally - the procedure demands introduction of the secondary filter

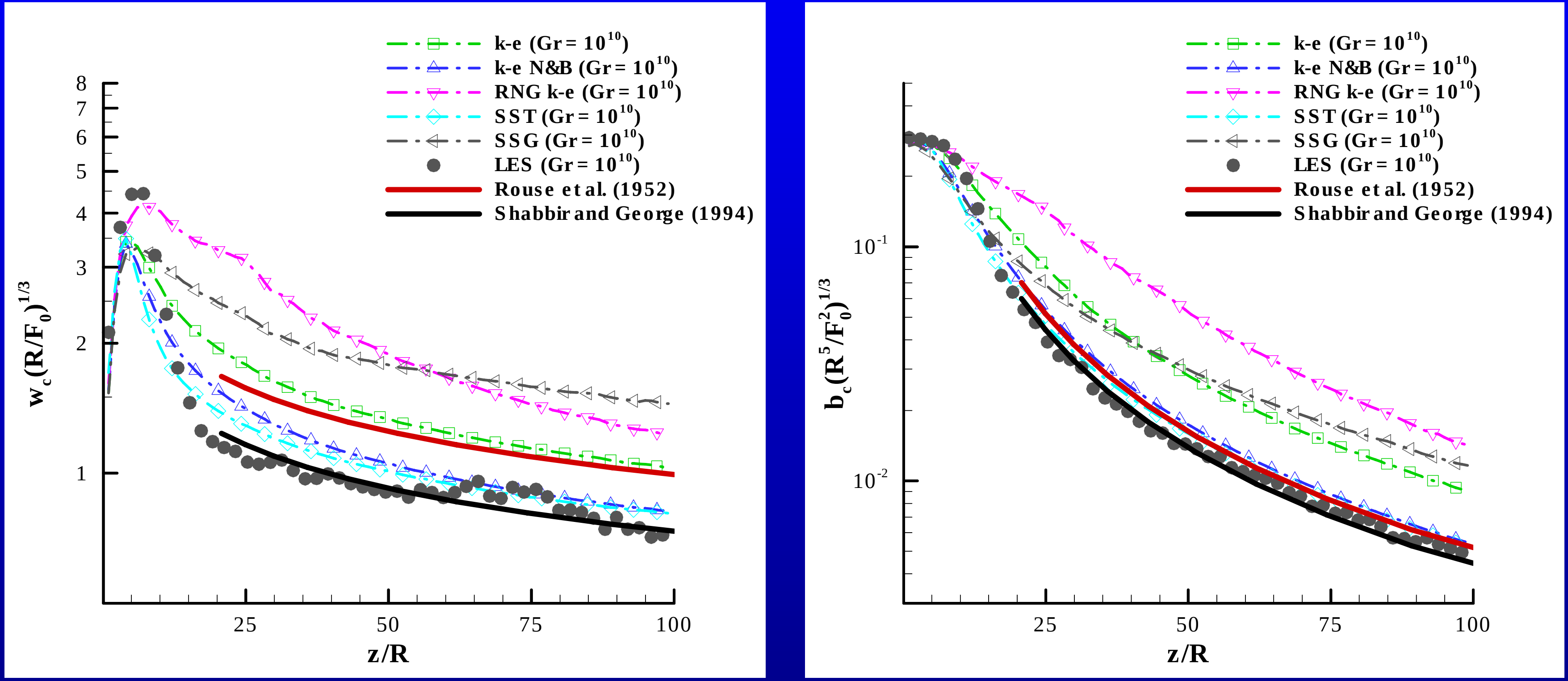
  - LES models demand much denser (larger) numerical grid

  - they are used for transient simulations

  - to obtain average flow characteristics, we need to perform statistical averaging over the simulated time interval

Turbulence models

- Comparison of turbulence models

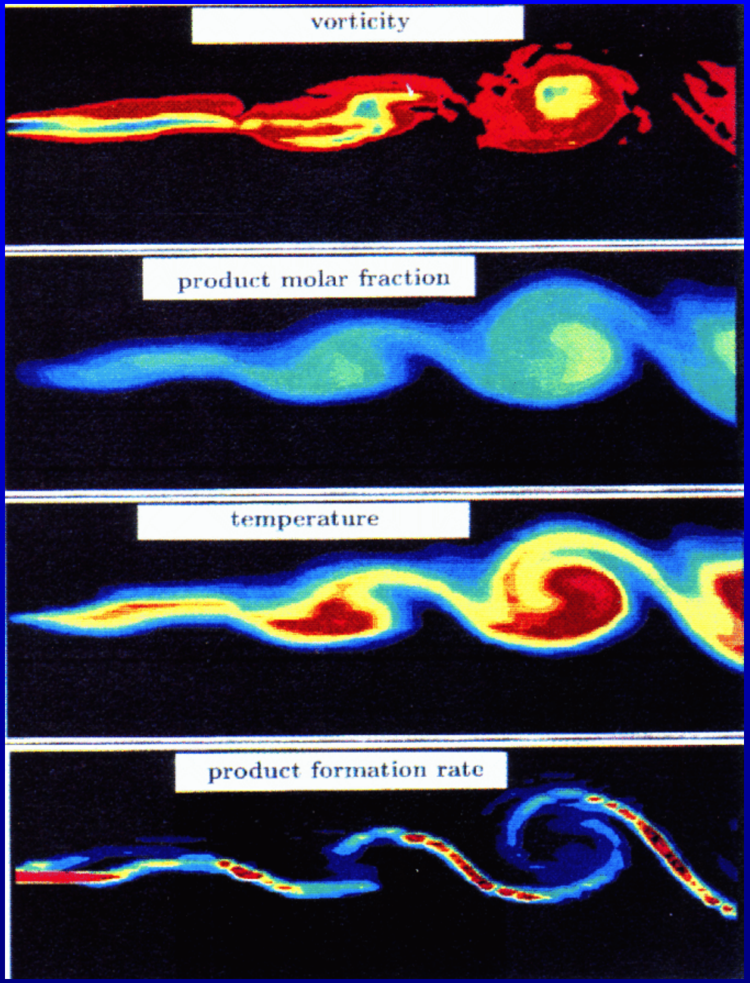


a) b)

Buoyant flow over a heat source: a) velocity, b) temperature*

Combustion models

Chen et al., 1988



Grinstein,
Kailasanath, 1992

Combustion models

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- Combustion can be modelled with heat sources
  - information on chemical composition is lost
  - thermal loading is usually under-estimated

- Combustion modelling contains
  - solving transport equations for composition
  - chemical balance equation
  - reaction rate model

- Modelling approach dictates the number of additional transport equations required

Combustion models

- Modelling of composition requires solving n-1 transport equations for mixture components – mass or molar (volume) fractions

$$\partial_t\left(\bar{\rho}\tilde{\xi}_j\right)+\partial_i\left(\bar{\rho}\tilde{v}_i\tilde{\xi}_j\right)=\partial_i\left(\left(\frac{\mu}{Sc}+\frac{\mu_t}{Sc_t}\right)\partial_i\tilde{\xi}_j\right)+\overline{M}_j$$

- Chemical balance equation can be written as

$$\nu'_A\,A+\nu'_B\,B+\nu'_C\,C\ldots.. \leftrightarrow \nu''_A\,A+\nu''_B\,B+\nu''_C\,C\ldots..$$

or

$$\sum_{I=A,B,C....}^{N}\nu'_I I \leftrightarrow \sum_{I=A,B,C....}^{N}\nu''_I I$$

Combustion models

- Reaction source term is defined as

$$\overline{M}_j = W_j\left(\nu''_j - \nu'_j\right)R$$

or for multiple reactions

$$\overline{M}_j = W_j \sum_k \left(\nu''_{k,j} - \nu'_{k,j}\right) R_k$$

where R or R_k is a reaction rate

- Reaction rate is determined using different models

- Constant burning (reaction) velocity
- Eddy break-up model and Eddy dissipation model
- Finite rate chemistry model
- Flamelet model
- Burning velocity model

Combustion models

- Constant burning velocity s_L

$$s_F = \frac{\rho_c}{\rho_h} s_L$$

speed of flame front propagation is larger due to expansion

- values are experimentally determined for ideal conditions

- limits due to reaction kinetics and fluid mechanics are not taken into account

- source/sink in mass fraction transport equation $\overline{M}_j \sim \rho_f s_L / l$

- source/sink in energy transport equation $\overline{Q} \sim M_j \Delta h_c$

- expressions for s_L usually include additional models

Combustion models

- Eddy break-up model and Eddy dissipation model

  - is a well established model that can be used for simple reactions (one- and two-step combustion)

  - in general, it cannot be used for prediction of products of complex chemical processes (NO, CO, SOx, etc)

  - it is based on the assumption that the reaction is much faster than the transport processes in flow

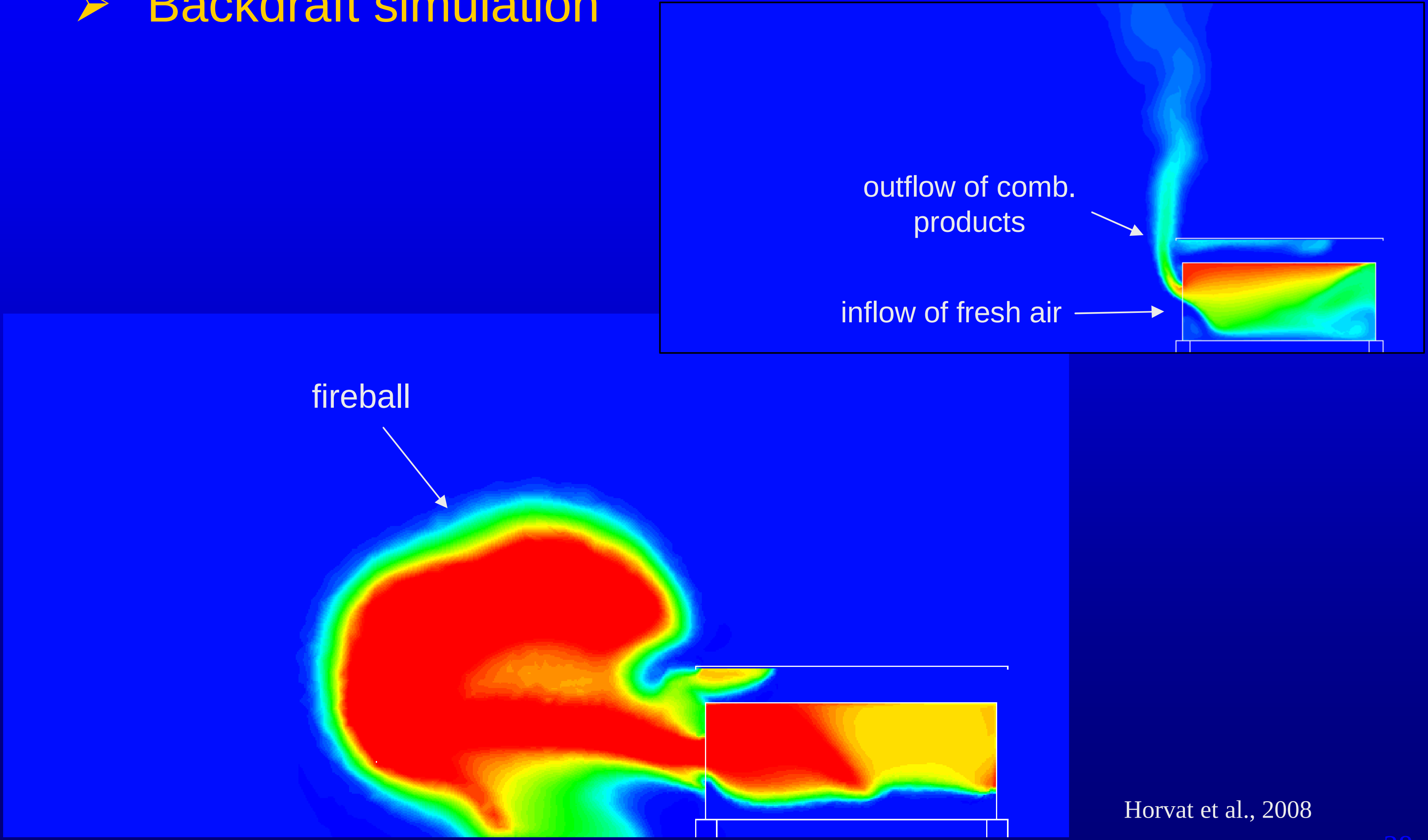
  - reaction rate depends on mixing rate of reactants in turbulent flow $s_L \sim \varepsilon / k$

  - Eddy dissipation model reaction rate

$$R = C_A \rho \frac{\varepsilon}{k} \min\left(\tilde{\psi}_f , \frac{\tilde{\psi}_o}{s} , C_B \frac{\tilde{\psi}_p}{(1+s)} \right)$$

Combustion models

- Backdraft simulation



Horvat et al., 2008

Combustion models

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➢ Finite rate chemistry model

- it is applicable when a chemical reaction rate is slow or comparable with turbulent mixing
- reaction kinetics must be known

$$R = A\tilde{T}^{\beta}\,exp\left(\frac{-E_a}{R\tilde{T}}\right)\prod_{I=A,B,C\ldots}\tilde{\psi}_I^{\nu'_I}$$

- for each additional reaction the same expression is added
- the model is numerically demanding due to exponential terms
- often the model is used in combination with the Eddy dissipation model

Combustion models

- Flamelet model

  - describes interaction of reaction kinetics with turbulent structures for a fast reaction (high Damköhler number)

  - basic assumption is that combustion is taking place in thin sheets - flamelets

  - turbulent flame is an ensemble of laminar flamelets

  - the model gives a detailed picture of the chemical composition - resolution of small length and time scales of the flow is not needed

  - the model is also known as "Mixed-is-burnt" - large difference between various implementations of the model

Combustion models

- Flamelet model

  - it is based on definition of a mixture fraction

Z kg/s fuel

A

1-*Z* kg/s oxidiser

B

mixing proces

1 kg/s mixture

M

$$Z\beta_A + (1-Z)\beta_B = \beta_M$$

or

$$Z = \frac{\beta_M - \beta_B}{\beta_A - \beta_B}$$

where

$$\beta = \xi_f - \xi_o / i$$

- the conditions in vicinity of flamelets are described with the respect to Z; $Z=Zst$ is a surface with the stoihiometric conditions
- transport equations are rewritten with Z dependencies; conditions are one-dimensional $\xi(Z)$, $T(Z)$ etc.

Combustion models

➢ Flamelet model

- for turbulent flow, we need to solve an additional transport equation for mixture fraction Z

$$\partial_t\left(\bar{\rho}\tilde{Z}\right)+\partial_i\left(\bar{\rho}\tilde{v}_i\tilde{Z}\right)=\partial_i\left(\left(\frac{\mu}{Sc}+\frac{\mu_t}{Sc_t}\right)\partial_i\tilde{Z}\right)$$

- and a transport equation for variation of mixture fraction Z''

$$\partial_t\left(\bar{\rho}\,\widetilde{Z''^2}\right)+\partial_i\left(\bar{\rho}\,\tilde{u}_i\,\widetilde{Z''^2}\right)=\partial_i\left\{\left(\bar{\rho}\,D+\frac{\mu_t}{Sc_t}\right)\partial_i\,\widetilde{Z''^2}\right\}+2\frac{\mu_t}{Sc_t}\left(\partial_i\,\tilde{Z}\right)^2-\bar{\rho}C_\chi\frac{\varepsilon}{k}\widetilde{Z''^2}$$

- composition is calculated from preloaded libraries

$$\tilde{\psi}_j=\int_0^1\psi_j(Z)\,\underline{PDF(Z)}\,dZ$$

$$\tilde{\psi}_j=\int_0^1\int_0^\infty\psi_j(Z,\chi)\,\underline{PDF(Z)}\,\underline{PDF(\chi)}\,dZ\,d\chi$$

these PDFs are tabulated for different fuel, oxidiser, pressure and temperature

Thermal radiation

- It is a very important heat transfer mechanism in fires
- In fire simulations, thermal radiation should not be neglected
- The simplest approach is to reduce the heat release rate of a fire (35% reduction in FDS)
- Modelling of thermal radiation - solving transport equation for radiation intensity

$$\underbrace{\frac{dI_\nu(\Omega)}{ds}}_{\text{change of intensity}} = \underbrace{-(K_{a\nu}+K_{s\nu})I_\nu(\Omega)}_{\text{absorption and scattering}} + \underbrace{K_{a\nu}I_{e\nu}}_{\text{emission}} + \underbrace{\frac{K_{s\nu}}{4\pi}\int_{4\pi} I_{s\nu}(\Omega')P_\nu(\Omega'\to\Omega)\,d\Omega'}_{\text{in-scattering}}$$

Thermal radiation

- Radiation intensity is used for definition of a source/sink in the energy transport equation and radiation wall heat fluxes
- Energy spectrum of blackbody radiation

$$E_\nu(T) = \pi I_\nu(T) = \frac{2\pi\nu^2}{c^2}\frac{n^2 h\nu}{exp(h\nu/k_B T) - 1} \quad [\mathrm{Wm^{-2}Hz^{-1}}]$$

ν - frequency
c - speed of light
n - refraction index
h - Planck's constant
k_B - Boltzmann's constant

integration over
the whole spectrum

$$E(T) = n^2\sigma T^4 = \int_0^\infty E_\nu(T)\,d\nu \quad [\mathrm{Wm^{-2}}]$$

Thermal radiation

- Discrete Transfer

- modern deterministic model
- assumes isotropic scattering, homogeneous gas properties
- each wall cell works as a radiating surface that emits rays through the surrounding space (separated onto multiple solid angles)
- radiation intensity is integrated along each ray between the walls of the simulation domain

$$I_\nu(r,s) = I_{0\nu}\mathrm{e}^{-(K_{a\nu}+K_{s\nu})s} + I_{e\nu}\left(1-e^{-K_a s}\right) + K_{s\nu}\bar{I}_\nu$$

$$q^{rad}_{\nu,j} = \int_{4\pi} I_\nu(r,s)\cos\varphi_j \cos\theta \, d\Omega$$

- source/sink in the energy transport equation

$$\overline{Q}^{rad} = -\partial_i q_i^{rad}$$

Thermal radiation

➢ Monte Carlo

- it assumes that the radiation intensity is proportional to (differential angular) flux of photons
- radiation field can be modelled as a "photon gas"
- absorption constant $K_{a\nu}$ is the probability per unit length of photon absorption at a given frequency ν
- average radiation intensity I_ν is proportional to the photon travelling distance in a unit volume and time
- radiation heat flux q^{rad} is proportional to the number of photon incidents on the surface in a unit time
- accuracy of the numerical simulation depends on the number of used "photons"

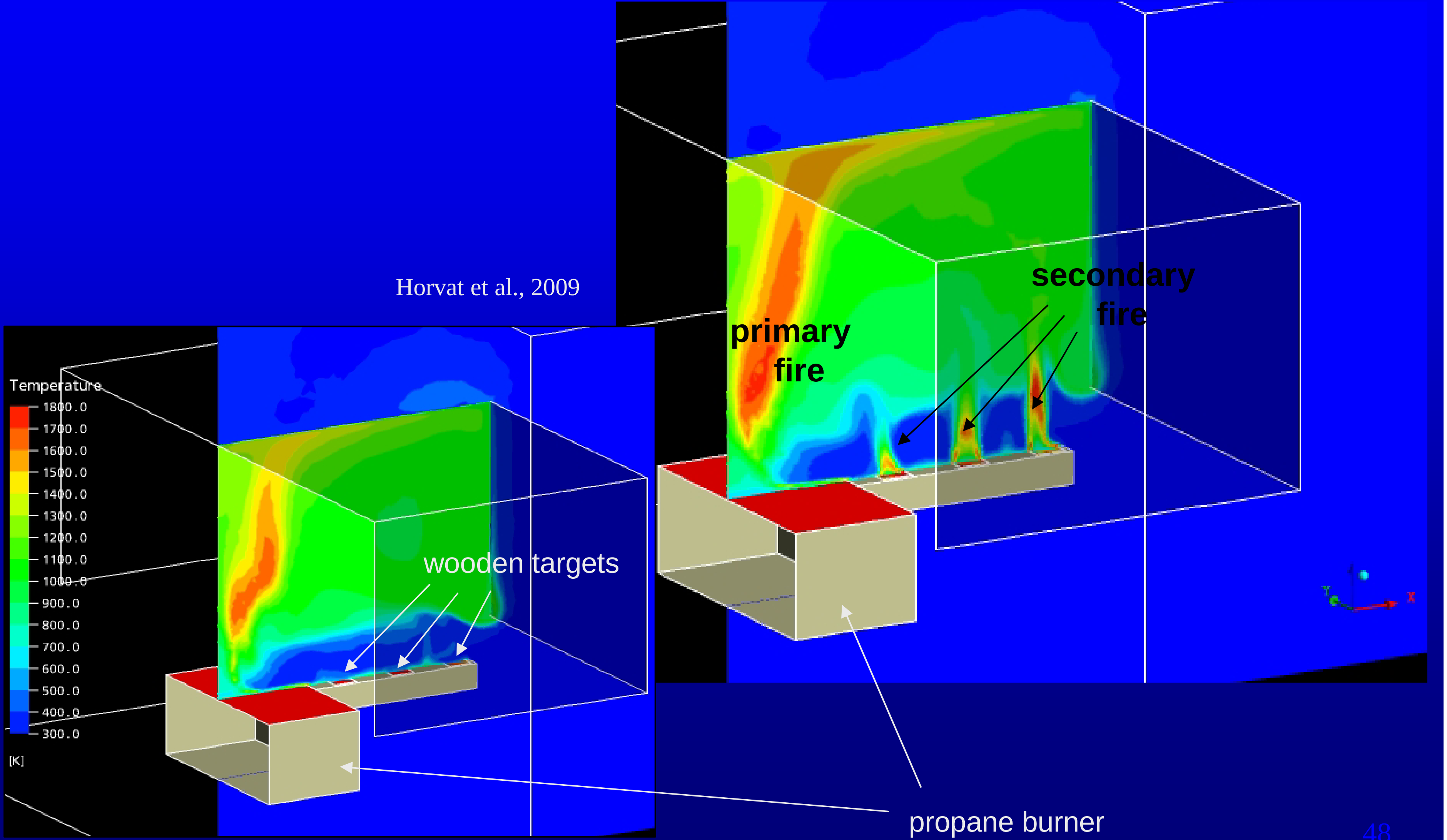
Thermal radiation

- These radiation methods can be used:

- for an averaged radiation spectrum - grey gas
- for a gas mixture, which can be separated onto multiple grey gases (such grey gas is just a modelling concept)
- for individual frequency bands; physical parameters are very different for each band

Thermal radiation

- Flashover simulation



Horvat et al., 2009

Conclusions

Conclusions

- The webinar gave a short (but demanding) overview of fluid mechanics and heat transfer theory that is relevant for fire simulations
- All current commercial CFD software packages (ANSYS-CFX, ANSYS-Fluent, Star-CD, Flow3D, CFDRC, AVL Fire) contain most of the shown models and methods:
  - they are based on the finite volume or the finite element method and they use transport equations in their conservative form
  - numerical grid is unstructured for greater geometrical flexibility
  - open-source computational packages exist and are freely accessible (FDS, OpenFoam, SmartFire, Sophie)

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