

FIRE DYNAMICS - COMPARATIVE ANALYSIS OF CFD SIMULATION TOOLS AND THEIR UTILIZATION

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Introduction

What is CFD ?

It is a field/discipline/area of simulation analysis, where a practitioner recreates and **visualizes** the process based on fundamental **mathematical relations** of physics, chemistry, biology, economics, social interactions etc.

Introduction

Simulation process is used increasingly as a performance based design tool to **support engineering analysis** and to **complement** experimental and testing programmes or even to substitute them.

The reasons for this are **economic** as the simulation techniques offer

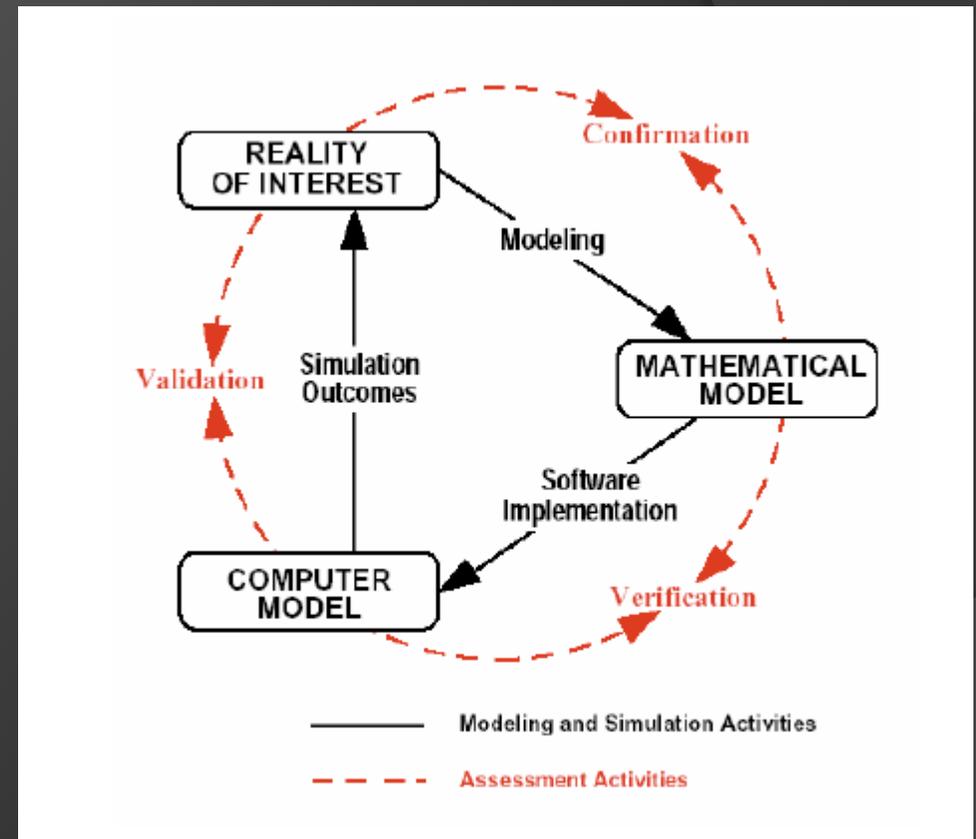
- greater flexibility in managing 'testing' environment
- a faster turn-around time
- more comprehensive post-processing options
- lower costs

In some cases, **safety considerations** make physical testing impractical all together (e.g. fire engineering, nuclear safety, space equipment design).

Introduction

Despite all these advantages, it is important to recognise that the simulation process is fundamentally **different** from physical experimentation and testing.

- In the world of numerical simulations, most of the effort is focused on recreating reality in a digital environment.
- Once the created virtual reality is representative of the analysed environment, capturing relevant data is often much simpler than during physical testing.



Concept relations in modelling analysis [1]

Fire dynamics and modelling principles

Fire (or 'a rapid oxidation of a material in the exothermic chemical process of combustion, releasing heat, light, and various reaction products' by Wikipedia) is a **complex process**:

- chemical reaction → reaction mechanism, change in composition
- release of heat → its convection, conduction and radiation
- external factors → supply of fuel and oxidiser, convective parameters (i.e. wind direction and strength), radiation emissivity/absorptivity, thermal far-field conditions

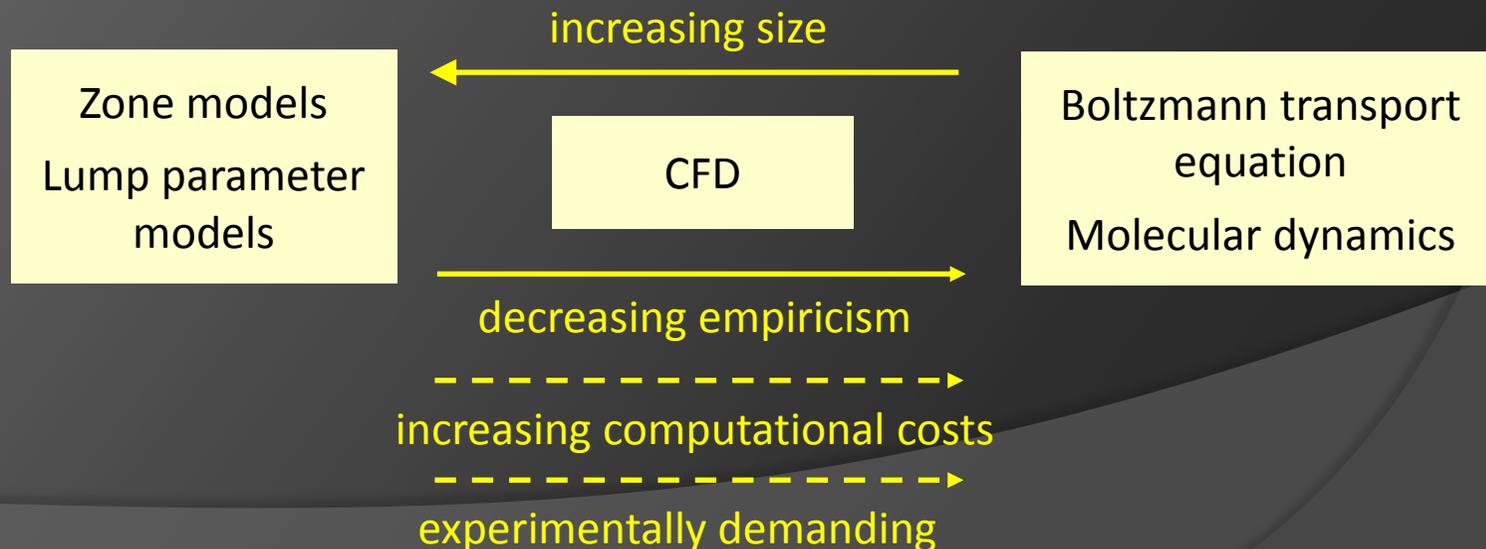
Due to complexity, **analytical tools are of limited applicability** → the required simplifications would be too large for the results to have practical value.

Fire dynamics and modelling principles

The solution is in **space discretisation** !

- Thermodynamic conditions in these discrete volumes are constant
- Exchange of mass and energy between these volumes is governed by the difference in temperature, pressure, velocity etc. → depends on the **model complexity and level of empiricism**

Larger the control volumes for which conservation equations are solved, larger is degree of empiricism.



Fire dynamics and modelling principles

Further domain discretisation and introduction of elementary physics leads to so-called 'field' or CFD models

and

more accurate results.

Computational Fluid Dynamics (CFD) is a group of methods and algorithms to solve discretized fluid flow and heat transport equations (and their derivations).

Validation and verification

As the complexity of models increase, how do we know that the models give correct and accurate results?

- To tick capability boxes in the software package is clearly not enough,
- Simulated problem needs to be well defined ,
- Analysis objectives need to understood,
- Performance parameters need to defined, and
- Quality acceptance criteria (e.g. modelling uncertainty, numerical errors, results variability and sensitivity) agreed.

Validation and verification

The correct way to control quality of the simulation analysis is through **validation** and **verification cases** [3]:

- geometrically simple
- contain representative and predominant 'physics'
- with available experimental and/or theoretical data

Such cases not only test the **methodology** and **toolset** (i.e. software), but also the **practitioner**.

Some of validation and verification activities are **generic** and can be conducted independently from project work, but part will be highly focused on a **specific project**.

Validation and verification

So what are typical **performance parameters** in fire modelling?

They are case dependent, but in general **conservation of mass, momentum and energy** has to hold:

- **Adiabatic temperature of combustion** shall not be exceeded
- **Released energy** shall not exceed the net reaction heat
- **Flame speed** shall not exceed experimentally published
- **Composition change** shall match the reaction rate over the simulated time interval
- **Far field heat flux** shall not exceed heat flux associate with fire irradiation
- Different correlations associated with **atmospheric dispersion and heat transfer** shall hold
- **Supersonic flow speeds** are rarely associated with fires

CFD analysis codes

From engineering prospective, fire dynamics is essentially a **fluid flow** and **heat transfer** problem.

A number of **general CFD simulation packages** are being used for fire dynamics simulations: ANSYS-CFX, ANSYS-Fluent, Star-CD, Numeca, Comsol, OpenFoam etc.

Specialized CFD simulation tools have been also developed: FDS, Flacs, KFX, Sophie, SmartFire etc.

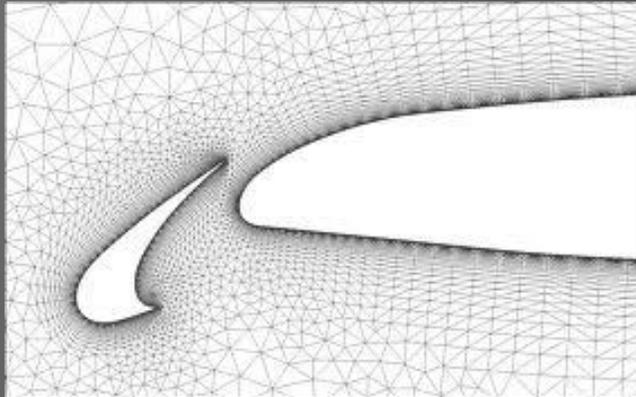
There are significant differences between these tools in **simulation approach**, **physics and chemistry models**, **user friendliness**, **support and business model**.

All these matters in selecting the right tool !

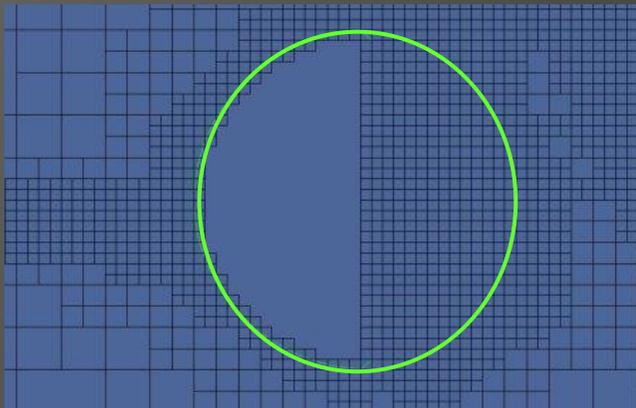
CFD analysis codes

Areas of differentiation:

- **Geometry resolution** : fully resolved geometry OR immerse solids

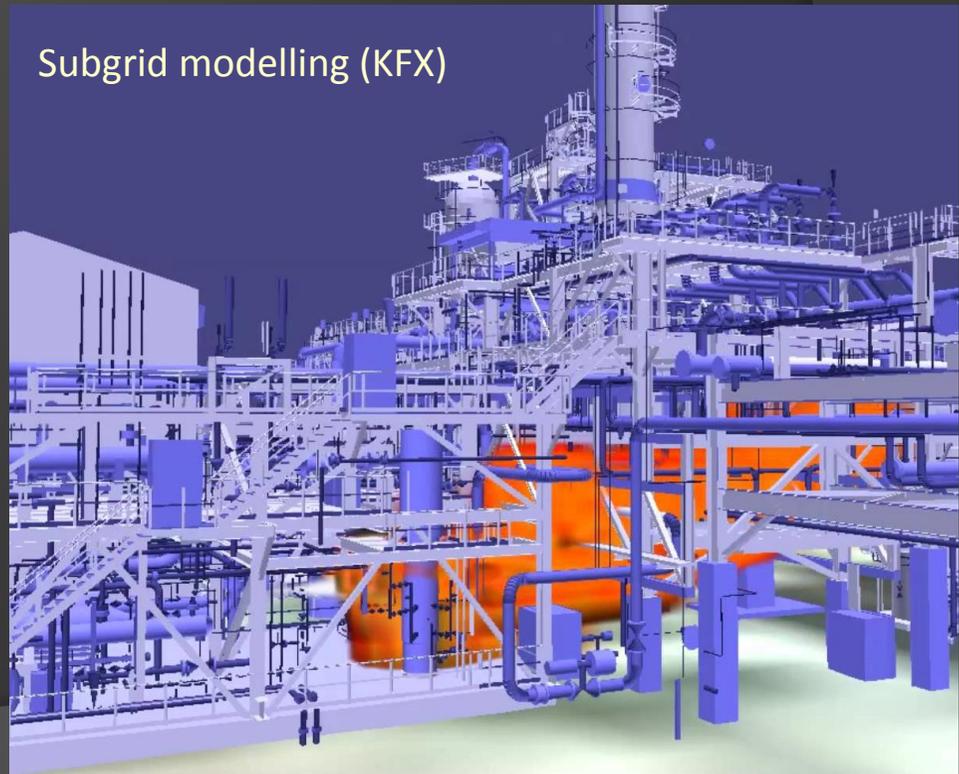


Fully resolved geometry (ANSYS CFX)



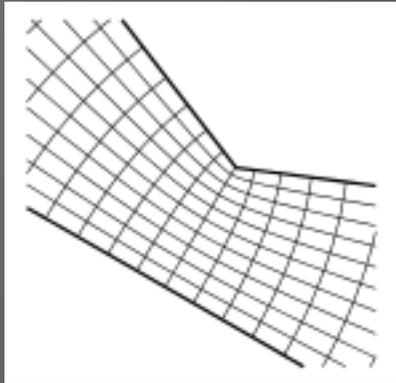
Immerse solid

Practitioner needs to understand which geometrical features **to resolve**, or **to represent** through subgrid models , or **to exclude**.

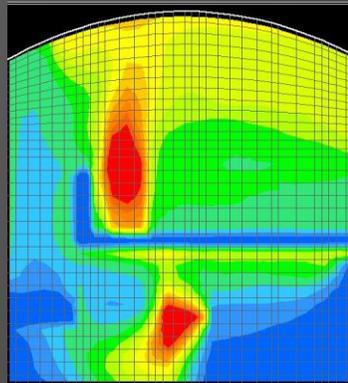


CFD analysis codes

- Grid type and generation method: body fitted, structured, unstructured (tetrahedral, hexahedral or polyhedral elements), nested meshes etc.



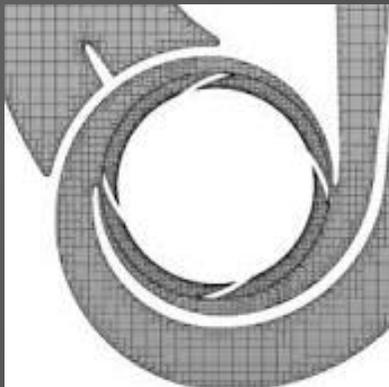
Body-fitted grid



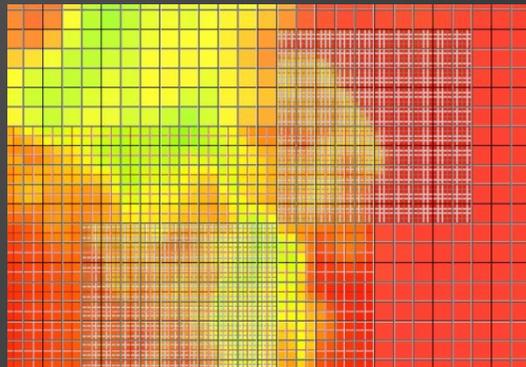
Structured grid
(SmartFire)



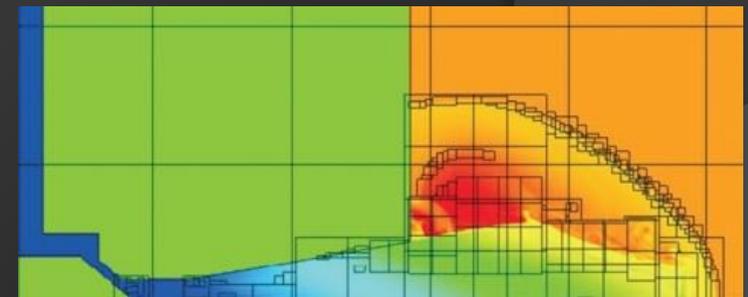
Unstructured polyhedral grid
(Star-CD)



Cartesian cut-cell grid
(Mentor Graphics)



Nested grid (FDS)



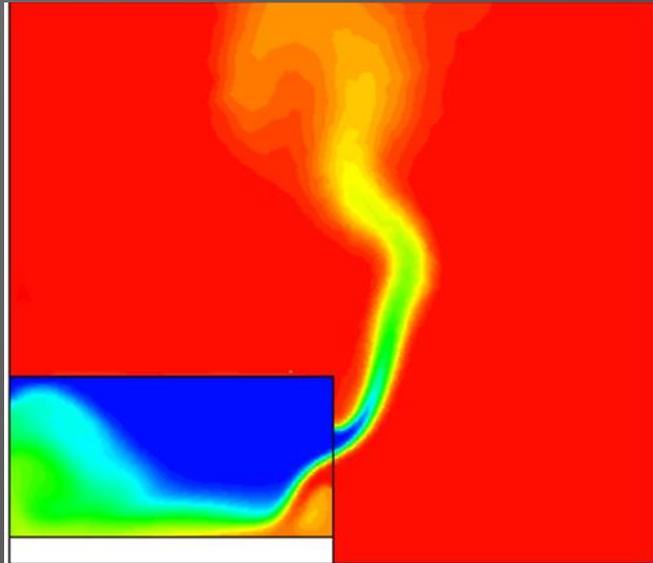
Dynamic nested grid

CFD analysis codes

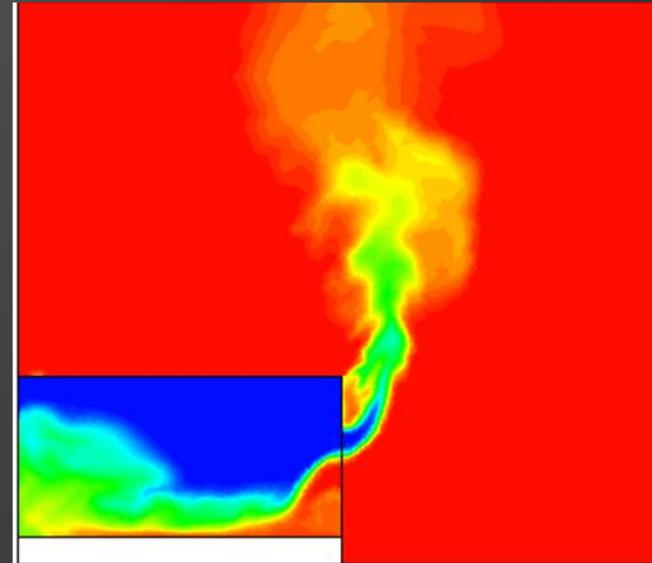
Numerical grid is the critical component - on one side it defines the quality of numerical results, on the other it provides foundation for any software development !

CFD analysis codes

- **Turbulence modelling:** algebraic turbulence mixing models, two-equation turbulence models, Reynolds stress modelling, Large-Eddy Simulation models



Backdraft - RANS turbulence model [4]

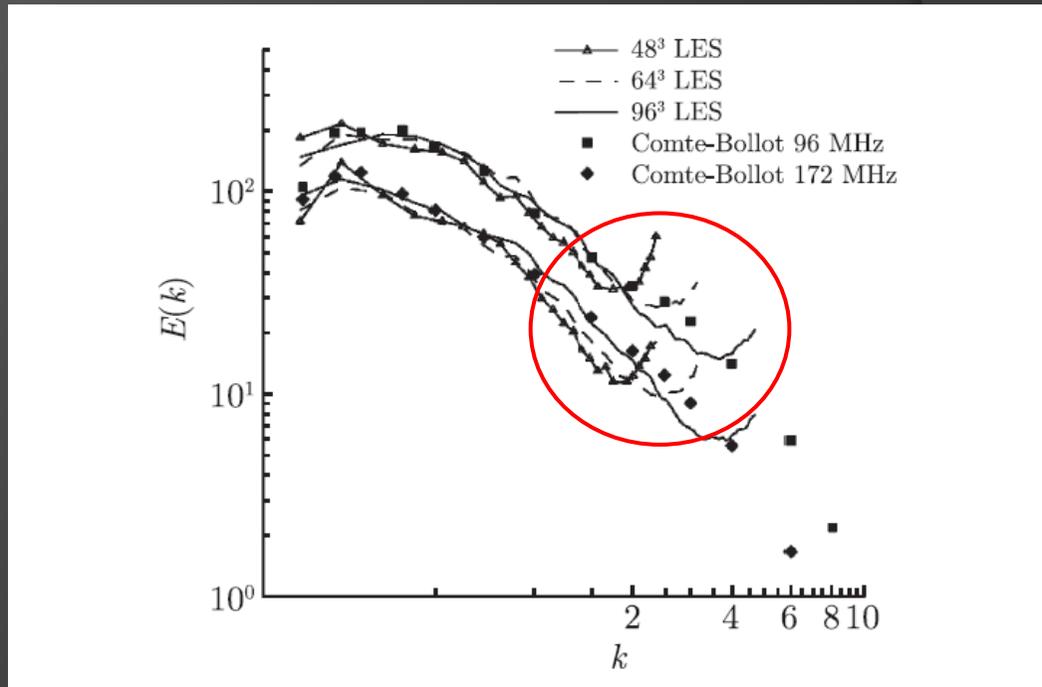


Backdraft - LES turbulence model [4]

Large-Eddy Simulation (LES) models **are capable** of resolving more flow details, therefore flow velocities, temperature, heat flow, composition can be predicted more accurately.

CFD analysis codes

Using LES models on the numerical grid that is **too coarse** may lead to **wrong results** especially if the combustion rate depends on the level of turbulence !



Turbulence energy cascade -
underresolved LES [5]

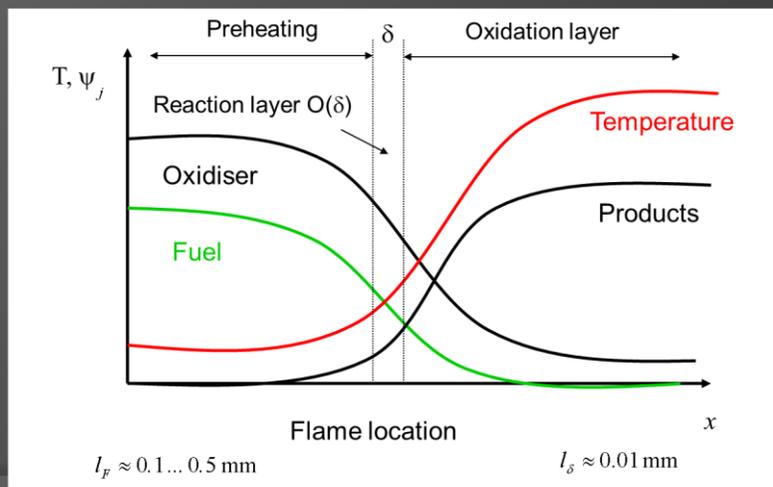
Reynolds Average Navier-Stokes (RANS) models are much more robust than the LES models, and require less dense numerical grids.

CFD analysis codes

- **Combustion modelling:** It can be represented via **heat sources**
 - information on chemical composition is lost
 - thermal loading is usually under-estimated

or with **reaction modelling**

- solving transport equations for composition
- chemical balance equation
- reaction rate model (eddy dissipation model, flamelet model, finite chemistry, burning velocity, mixed-is-burnt)

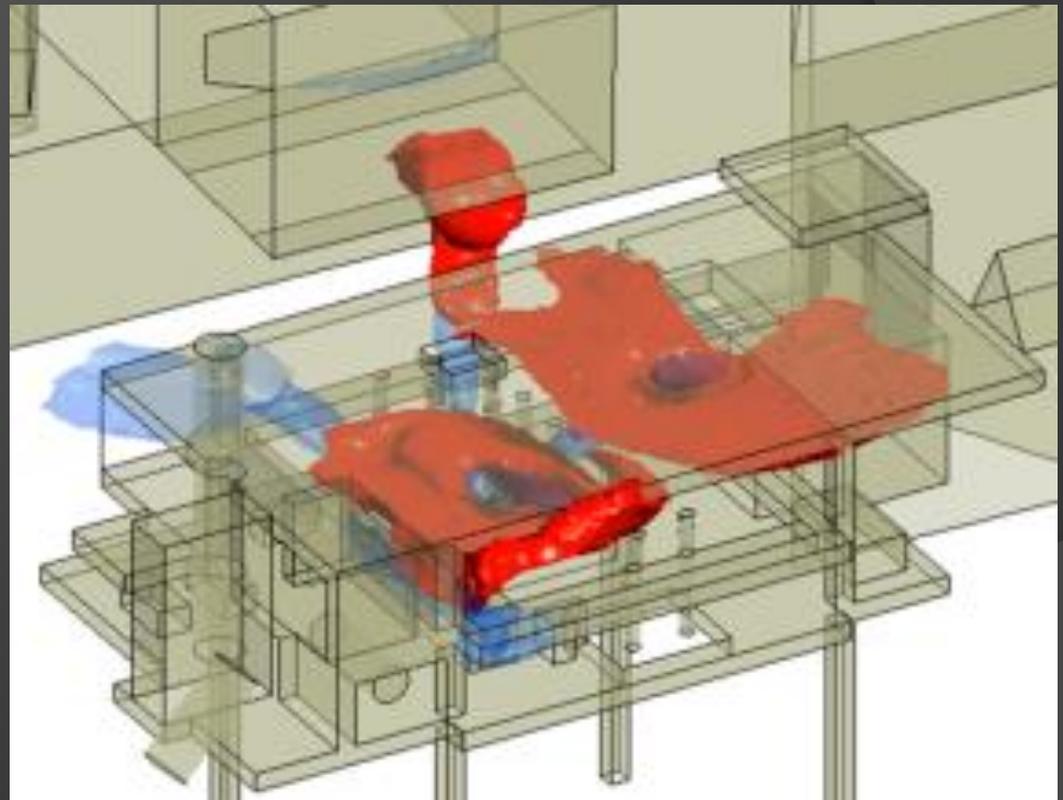


Premixed combustion [2]

CFD analysis codes

Modelling approach dictates the number of **additional transport equations** required.

The combustion model deficiencies are usually associated with extinction criteria (i.e. shear, temperature, local energy density, time of preheating etc).



Premixed combustion developing
into jet fire

CFD analysis codes

- **Thermal radiation:** 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)

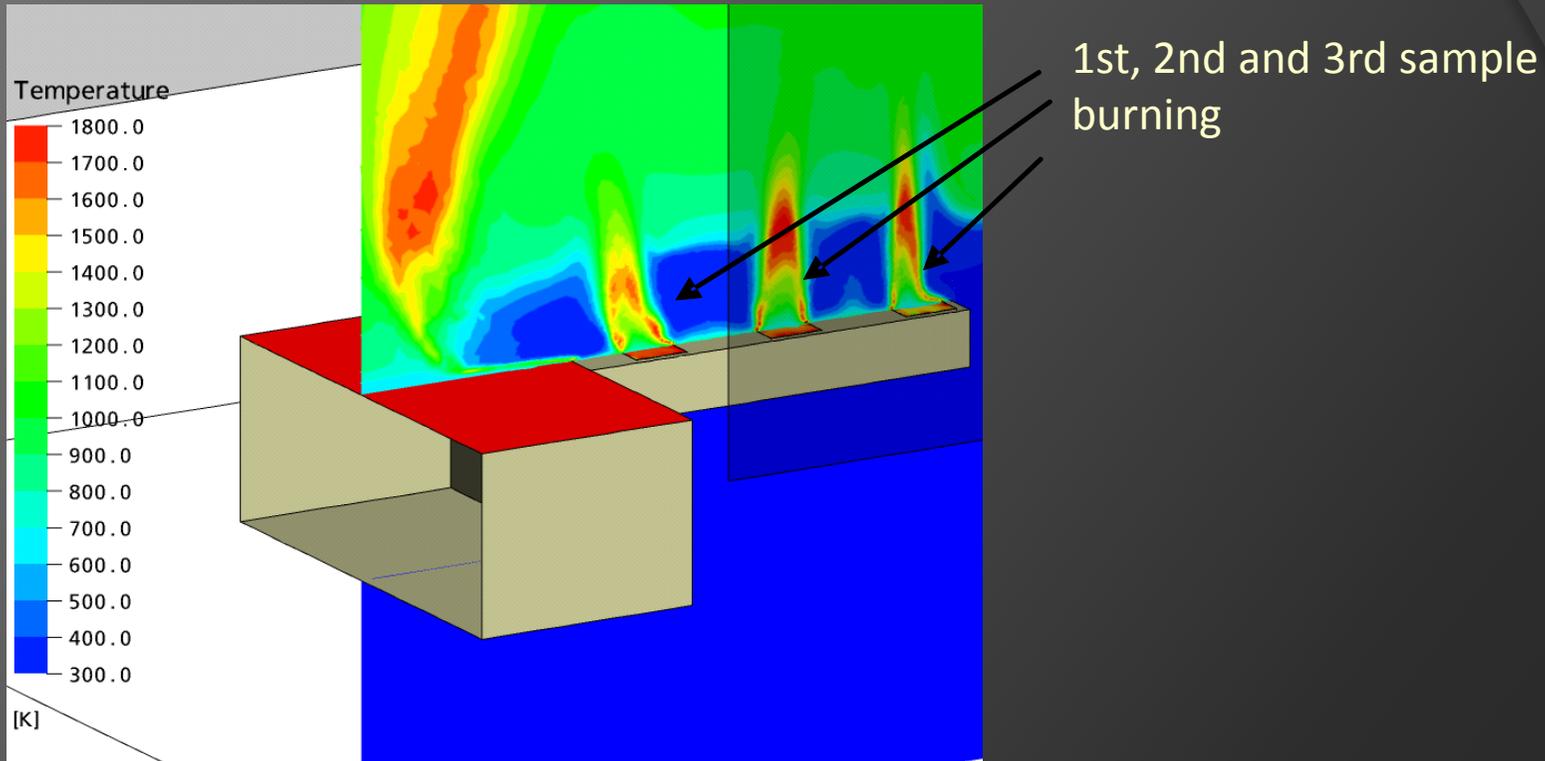
Modelling of thermal radiation - solving transport equation for radiation intensity
(challenging in optically thin environment)

$$\frac{dI_v(\Omega)}{ds} = -\underbrace{(K_{av} + K_{sv})I_v(\Omega)}_{\text{absorption and scattering}} + \underbrace{K_{av}I_{ev}}_{\text{emission}} + \underbrace{\frac{K_{sv}}{4\pi} \int_{4\pi} I_{sv}(\Omega') P_v(\Omega' \rightarrow \Omega) d\Omega'}_{\text{in-scattering}}$$

change of intensity

Probably the weakest feature in many CFD packages used in fire simulation.

CFD analysis codes



CFD simulation of
flashover experiment [6]

CFD analysis codes

- **User support:** It is essential to achieve high productivity of engineers and to utilize the software to its full capabilities
- **Business model:**
 - open source code
 - one-off or annual license fee
 - funding through governmental agency

Development cycles of engineering software are short; 6 to 12 months between major releases. The software is **constantly improved** and therefore maintenance is required.

Comparative analysis

The comparative analysis of **Fire Dynamics Simulator (FDS)** and **ANSYS simulation tools** was a part of the study conducted by ANSYS to evaluate performance of their simulation tools [7, 8].

Three different fire scenarios were studied

- **fire in an enclosure** (Ulster experiments)
- **fire in a tunnel under natural ventilation** (Memorial tunnel)
- **fire in a underground train station** (Kings' Cross accident)

These cases were selected due to their **transient behaviour**, importance of **convective vs radiative heat transfer**, heat transfer across the **walls** or in the last case, **complex geometry**.

Comparative analysis

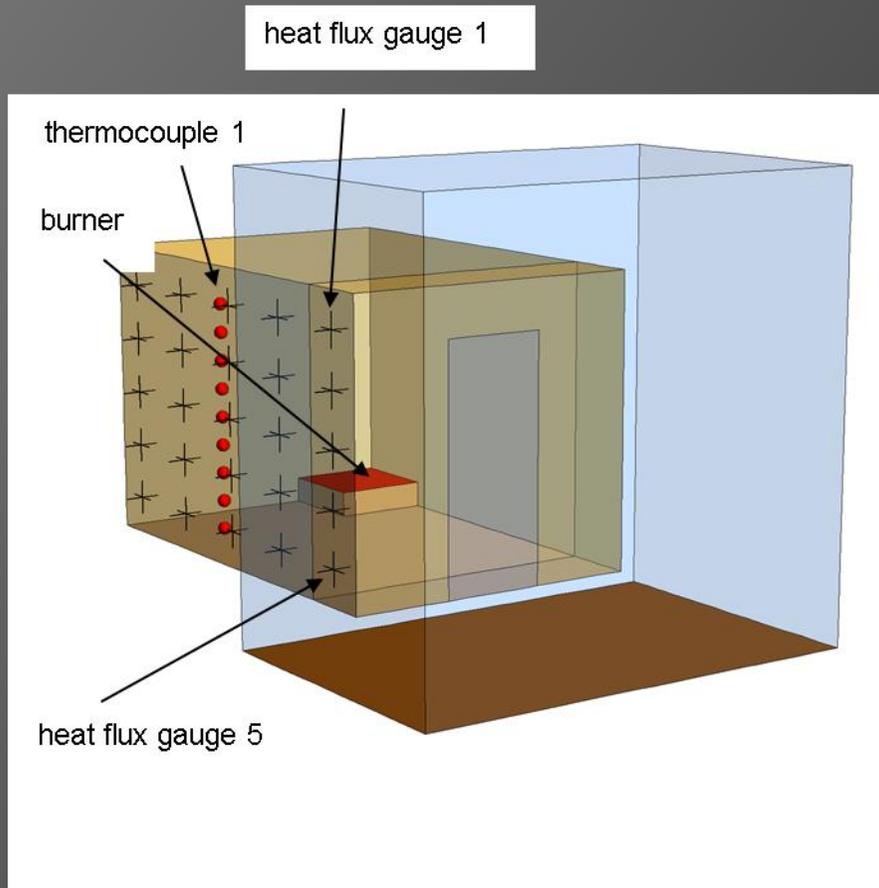
- **Fire Dynamics Simulator (FDS)** is a computational fluid dynamics (CFD) model for simulation of fire-driven fluid flow.
- **Smokeview (SMV)** is a visualization program that is used to display the output of FDS and CFAST simulations.
- **PyroSim** is a commercial graphical pre-processor from Thunderhead Engineering other preprocessing tools are also under development (e.g. BlenderFDS, FDS Designer) !

The FDS and Smokeview applications have been developed by the **National Institute of Standards and Technology (NIST)** of the United States Department of Commerce, in cooperation with **VTT Technical Research Centre** of Finland.

The software solves numerically a form of the Navier-Stokes equations appropriate for **low-speed, thermally-driven flow**, with an **emphasis on smoke and heat transport from fires**.

Comparative analysis

- Fire in an enclosure (Ulster experiments)



CFD simulation domain for the Ulster experiments [10]

The numerical model followed the experiments from at the University of Ulster [9]

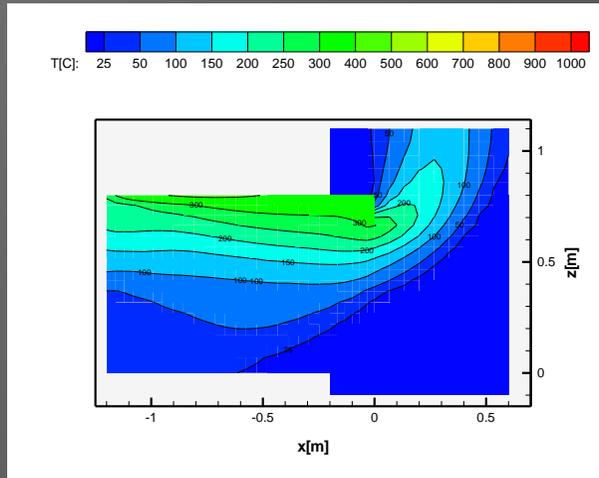
Transient fire (approx. 650 s) in a corner of an enclosure (80 cm long, 80 cm high, 120 cm wide):

- fuel (methanol) mass flow prescribed
- full combustion model
- radiation heat transfer
- heat transfer across the walls

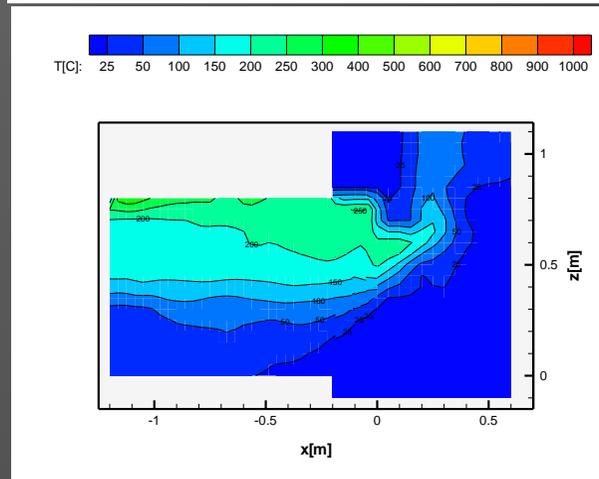
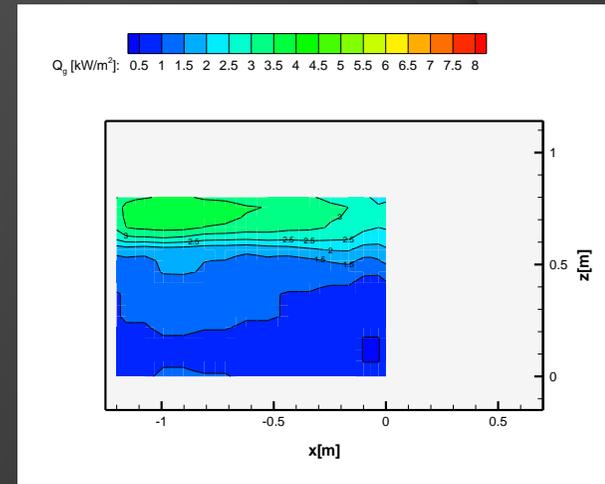
Temperature and **heat fluxes** were monitored on the wall

Comparative analysis

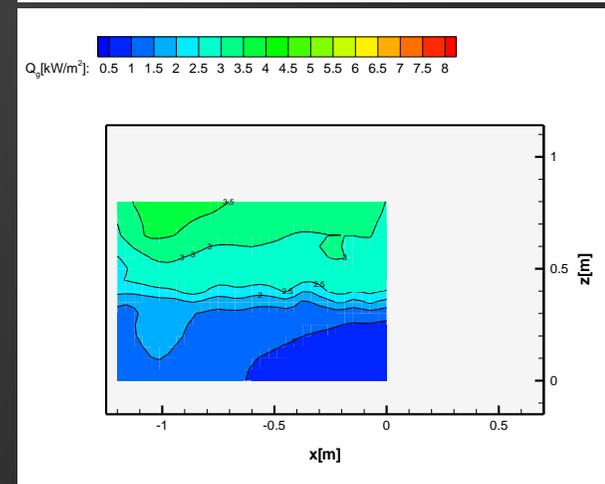
- Fire in an enclosure (Ulster experiments)



a)



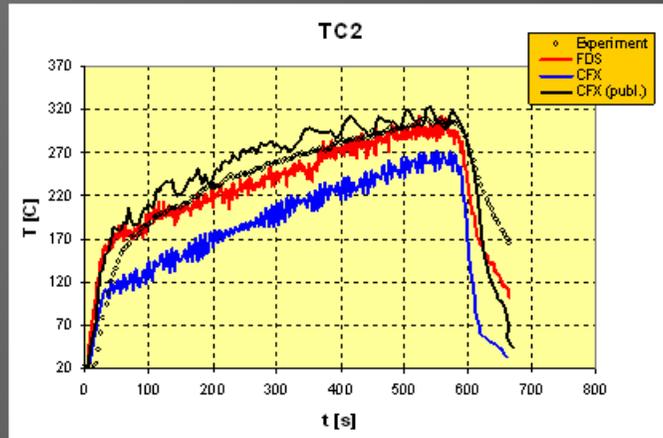
b)



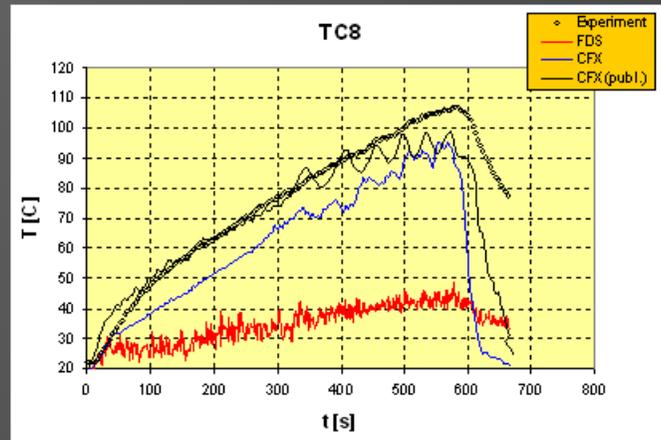
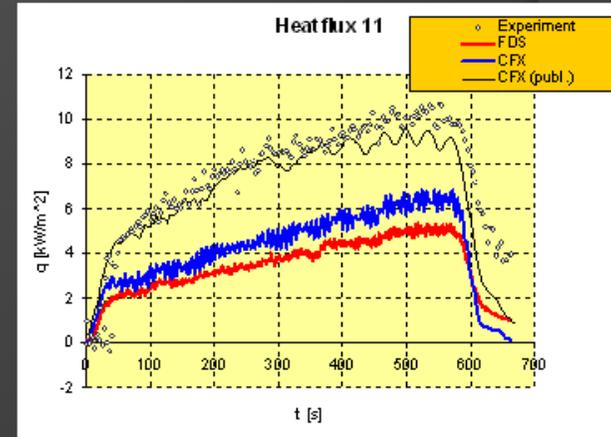
Temperature (left) and gauge heat flux (right) at 600.0 s and $y = 0$; a) CFX, b) FDS [8]

Comparative analysis

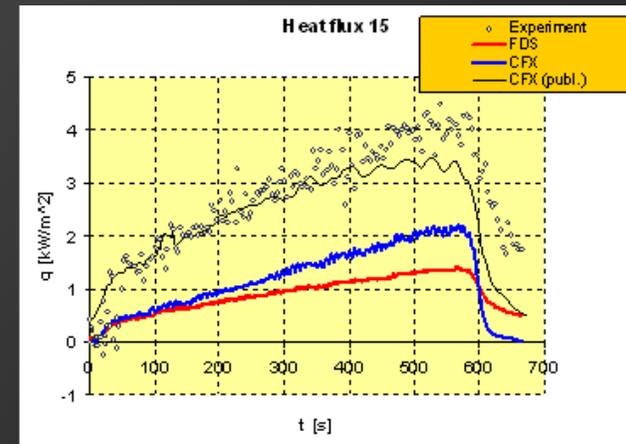
- Fire in an enclosure (Ulster experiments)



a)



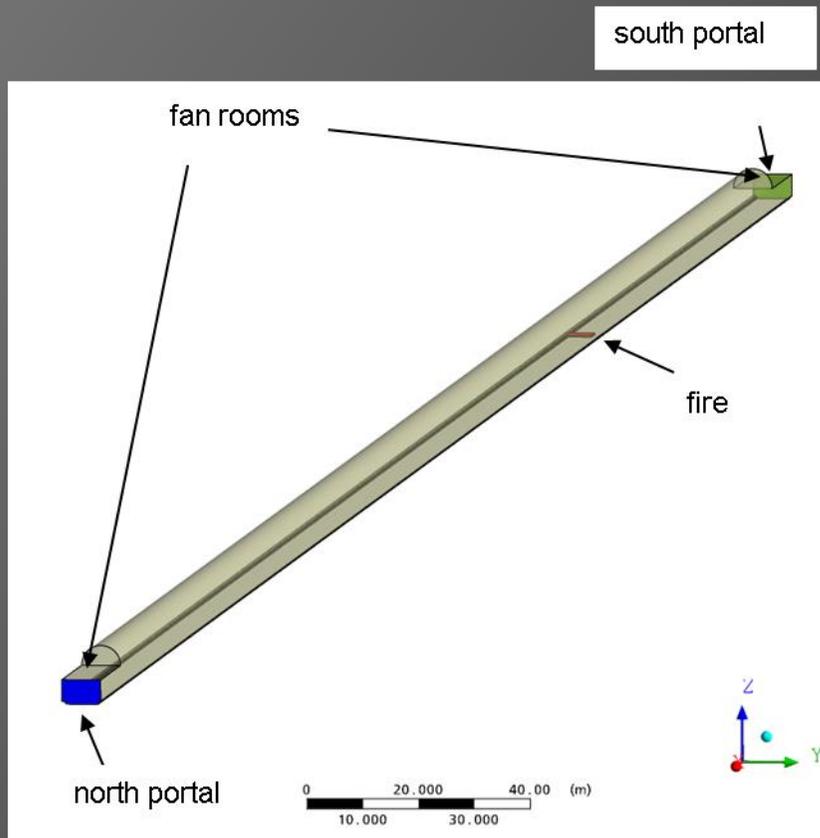
b)



Temperature (left) and gauge heat flux (right) time variations; a) hot layer, b) cold layer [8]

Comparative analysis

- Fire in a tunnel under natural ventilation (Memorial tunnel)



The numerical simulation of a **full scale fire** in a tunnel (Memorial Tunnel experiment, USA, 1995)

50 MW fire in a 853 m long road tunnel with 3.2% inclination from South to North:

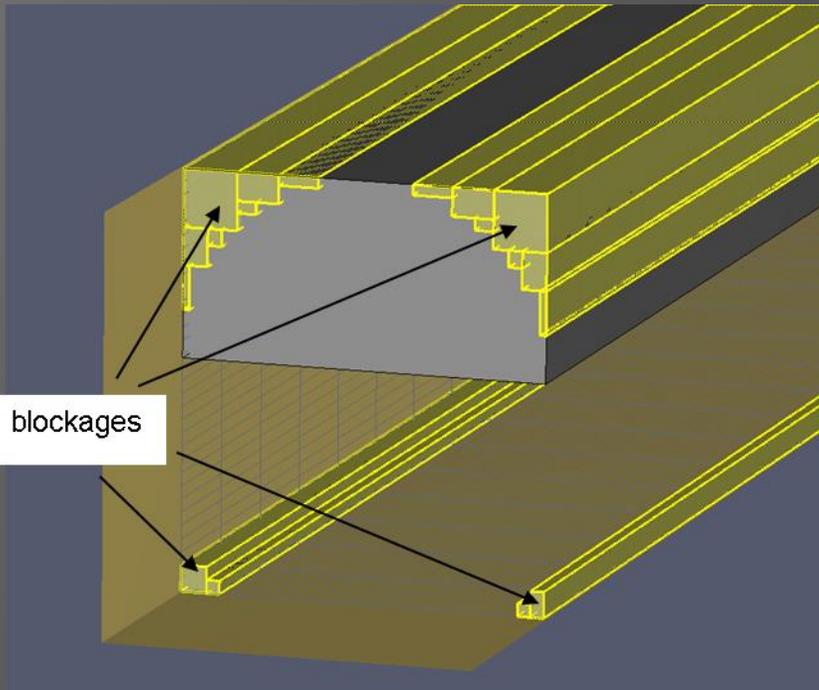
- propane as a fuel
- full combustion model
- radiation heat transfer
- prescribed wall heat transfer coefficient

Temperature comparison between the CFX and the FDS results, and comparison of **velocity profiles** with the experiment

CFD simulation domain for the Memorial tunnel experiment [7]

Comparative analysis

- Fire in a tunnel under natural ventilation (Memorial tunnel)



Geometry representation in FDS

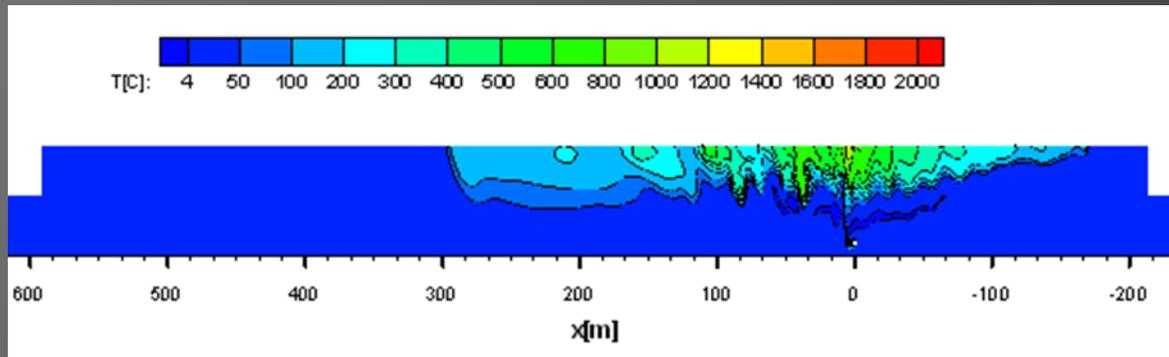
FDS uses structured mesh:

- the mesh needs to be defined as a simple rectangular volume
- non-rectangular (e.g. cylindrical) shapes needs to be carved from the initial rectangular volume using rectangular blockages
- due to rectangular blockages, curved walls are not smooth and a boundary layer is not approximated

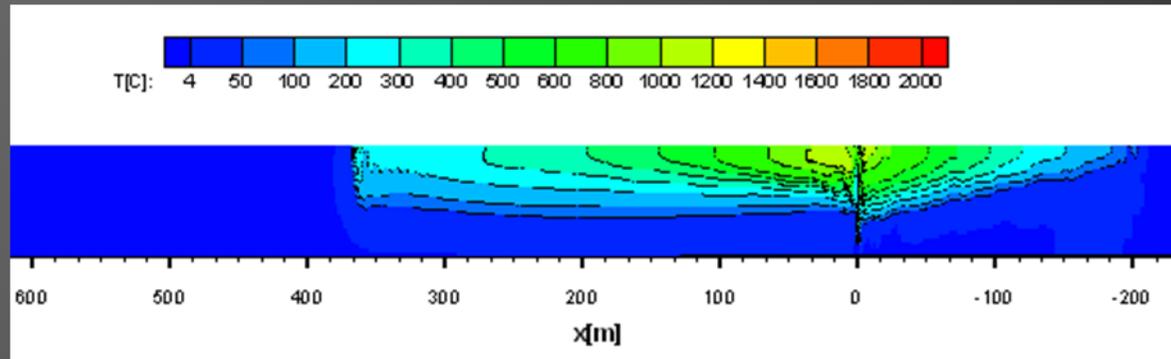
Recently, the process has been automated by **PyroSim** !

Comparative analysis

- Fire in a tunnel under natural ventilation (Memorial tunnel)



a)



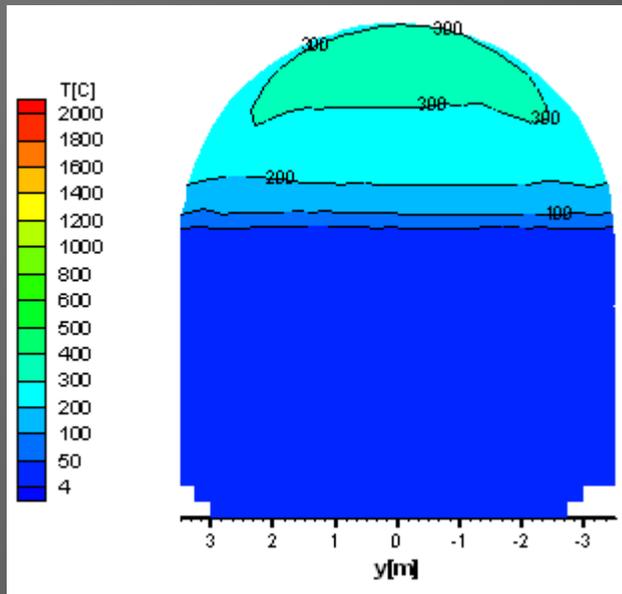
b)

Temperature at 120.0 s and $y = 0$; a) CFX, b) FDS

- In the CFX simulation, the hot upper layer resolves much more instabilities (K-H and R-T instability)
- Therefore, the progress of the hot layer is slower in the CFX simulation.

Comparative analysis

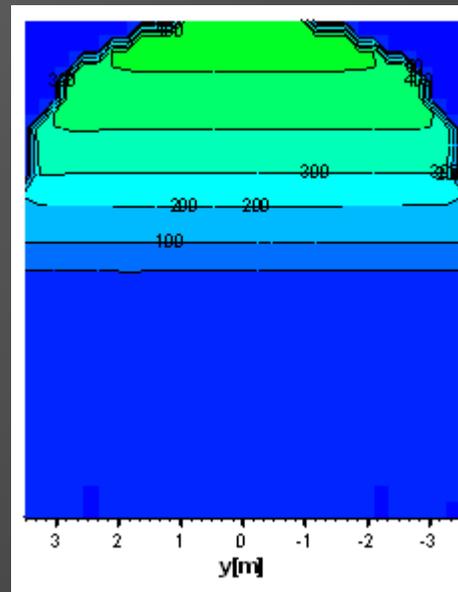
- Fire in a tunnel under natural ventilation (Memorial tunnel)



a)

Temperature (above) at 180.0 s and $x = -12.19$ m;

a) CFX, b) FDS [8]

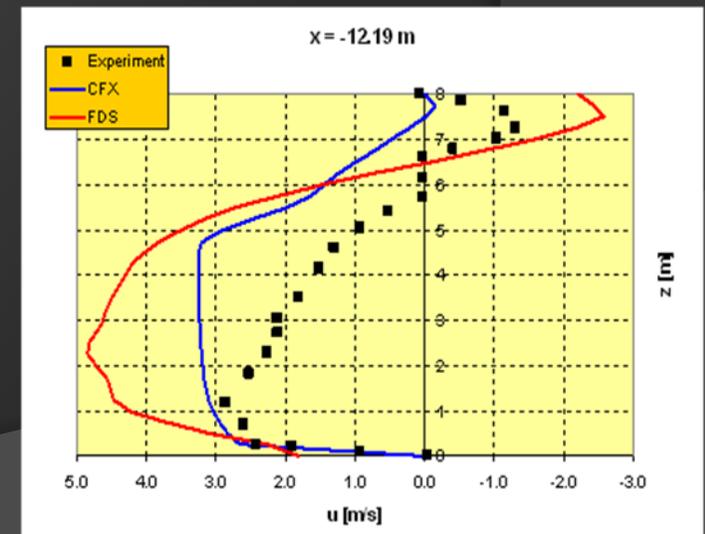


b)

Streamwise velocity (right) at 180.0 s and $x = -12.19$ m, $y = 0$ m;

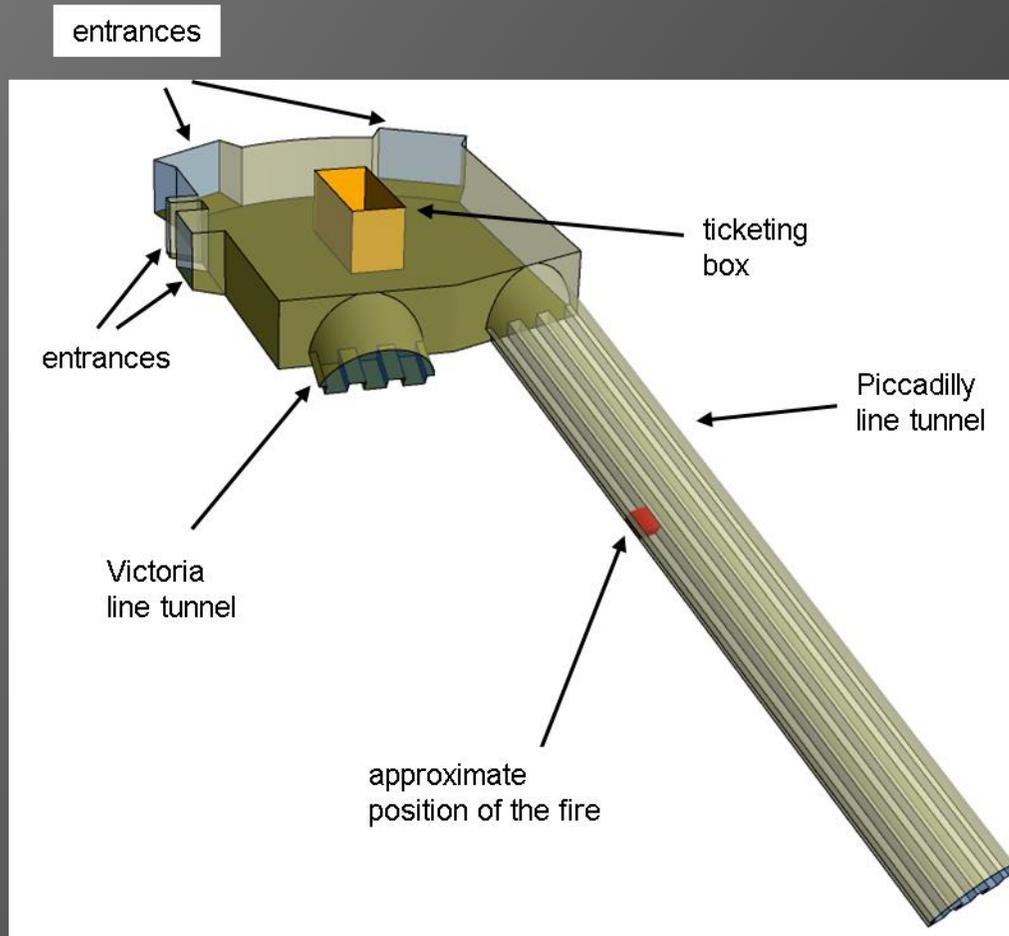
a) CFX, b) FDS [8]

- FDS predicts thicker hot layer than CFX - probably a result of different turbulence models used in the simulations



Comparative analysis

- Fire in a underground train station (King's Cross accident)



CFD simulation domain for the King's Cross accident simulation [8]

The numerical simulation of a fire in an escalator tunnel of an underground station (Kings' Cross accident, UK, 1987)

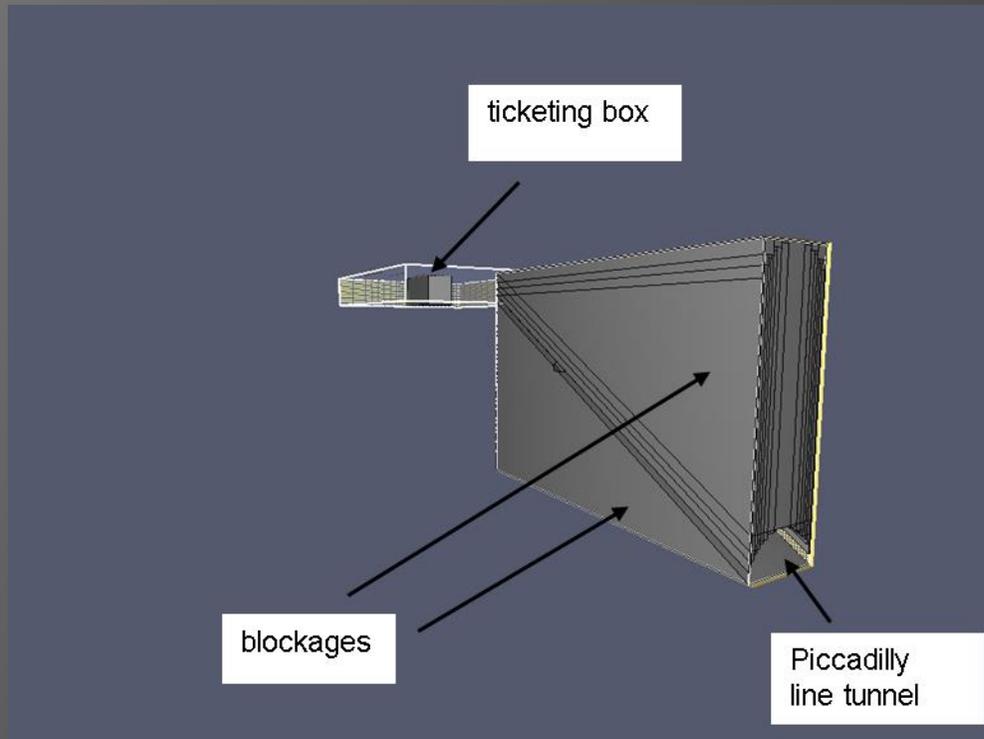
1.6 MW fire in a 45 m long Piccadilly line tunnel with inclination of almost 45° :

- transient fire modelling
- inert fire model in CFX
- full combustion model with radiation in the FDS simulation

Qualitative comparison of **temperature distribution**

Comparative analysis

- Fire in a underground train station (King's Cross accident)

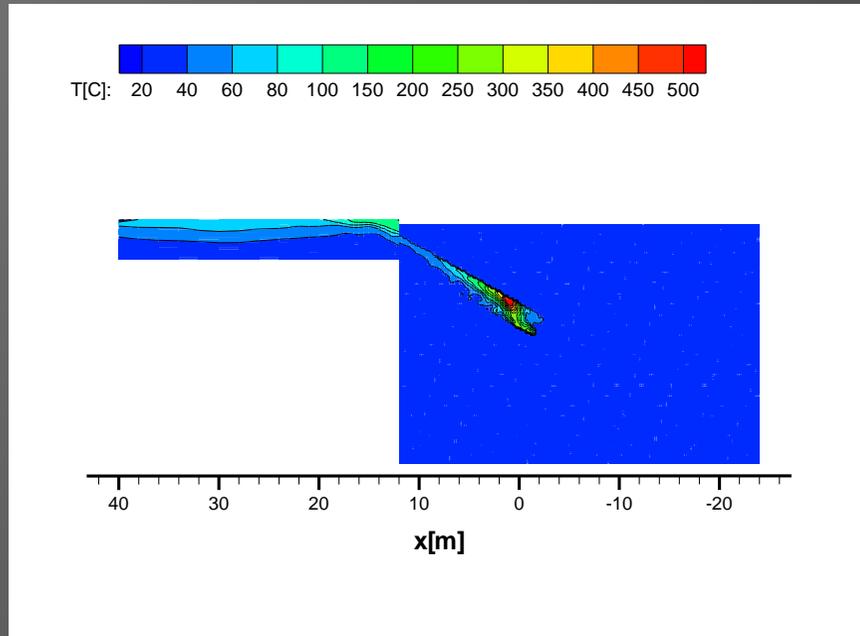


- The geometry was significantly simplified
- As the tunnel is not aligned with one of the coordinate axis, triangular blockages needs to be constructed in PyroSim (Thunderhead Eng.) - these are then transformed into rectangular blockages
- For this case, approx. 1850 rectangular blocks were needed

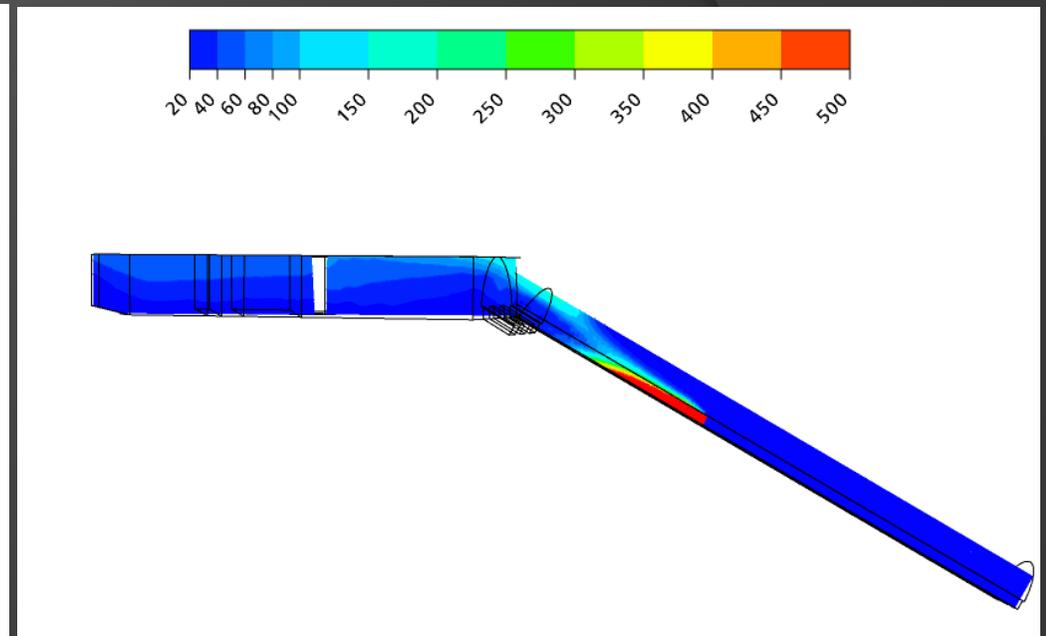
FDS model of the King's Cross station [8]

Comparative analysis

- Fire in a underground train station (King's Cross accident)



a)



b)

Temperature at 100.0 s: a) FDS, b) CFX [8]

Summary

- In the region where **thermal radiation is a dominant heat transfer mechanism** (lower – cold layer), FDS significantly under-predicts temperature.
- The **heat fluxes** on the walls are in general under-predicted by the FDS. This difference is small in the convection dominated region, but becomes larger (up to 40%) where thermal radiation is important.
- Beside possible modelling shortcomings of thermal radiation heat transfer, there are also more serious accuracy limitations related to **numerical grids**.

Summary

- As the rectangular structured mesh cannot describe an **arbitrary shape** of the simulation domain, FDS used rectangular blockages to suppress the numerical solution over a certain location.
- Representation of complex shapes with **blockages** is very time-consuming and often impossible. **PyroSim preprocessing software automates the geometry preprocessing and solves the problem.**
- Describing a curved surfaces with rectangular sections, produces a **step-like surfaces**, which often cannot adequately capture boundary effects.
- **Uniform grid resolution** may limit accuracy of numerical prediction as important local effects (i.e. boundary layer, wall heat transfer, mixing, combustion etc.) are under-represented.

Summary

- Fire Dynamics Simulator has an **explicit solver** for equidistant, structured numerical meshes.
- Due to its simplicity, the solver is at least **4 times faster** than the CFX solver, but its **parallel capabilities** are limited (MPI parallel simulations possible).
- **Interfaces** between different structured meshes are possible, but communication (interpolation) is performed only in one direction – from the first mesh in the command file onto the next.

Summary

- The only available turbulence model is **Large-Eddy Simulation (LES)**, which is not appropriate for a grid distance outside inertial subrange of turbulence.
- As standard, FDS offers a **mixing fraction combustion model**. Laminar flamelet model is also available, but has to be used with limitations.
- Solver parameters to **control accuracy** of the solution are not accessible to a user.
- Also **tracking the progress** of the numerical solution and its residuals (divergence) is available in command line mode.

Summary

The analysis software is constantly revised (**mistakes** are corrected and **features** are added). This requires continues effort and funding.

The **weakest point** in any analysis project is not the toolset, but the **analyst**.

Thank you !

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