Basics of fire compartment modelling by Computational Fluid Dynamics

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Note: this presentation is based on the original presentation made by Sylvain Desanghere (CSTB)

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1. Computational Fluid Dynamics - Generalities

Aims at modelling the movements of fluids in a volume.
Many various applications: weather predictions, combustion in motor cylinders, airflow around aircraft wings, wind penetration of cars, ….
and gaz movements in a fire.

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4 steps

1. Write the laws of physics in term of differential equations (conservation of mass, of energy, boundary conditions => Navier-Stokes equations).
2. Transform the D.E. into algebric equations (numerical schemes).
3. Solve the algebrix equations (solver)
4. Observe the results (graphic representation)

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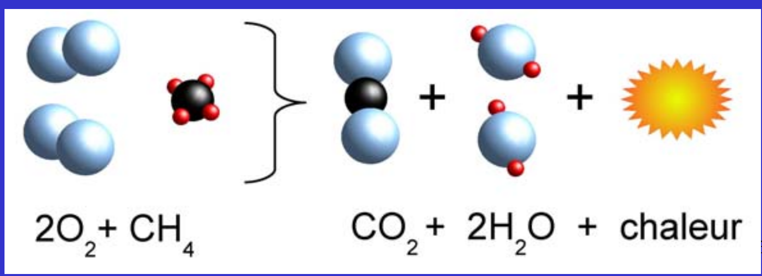
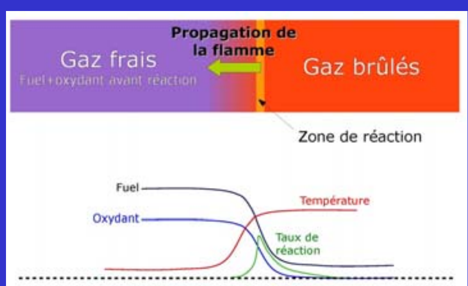
2. Combustion and turbulence

Fast oxydation of, e.g., methane.
High production of heat => Variation of density of the gaz
Thickness of the reaction zone ≅ 1 mm



Two types of flames:

1) Premix flames
Very fast propagation (10 m/s), backdraft



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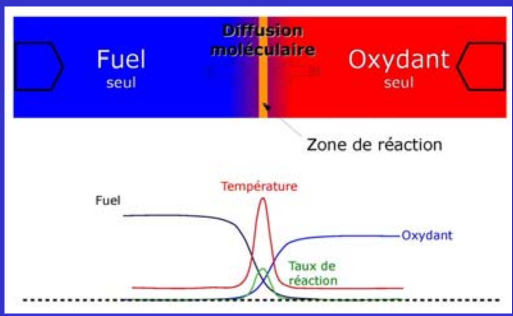
Two types of flames:

2) Diffusion flames

Fuel and oxygen separated before combustion

Representative of most fires



=> Conclusion: many different phenomena linked by strong coupling.

Chemical reaction ⇔ diffusion of chemical species ⇔ heat transfer ⇔ movements of fluids ⇔ turbulence

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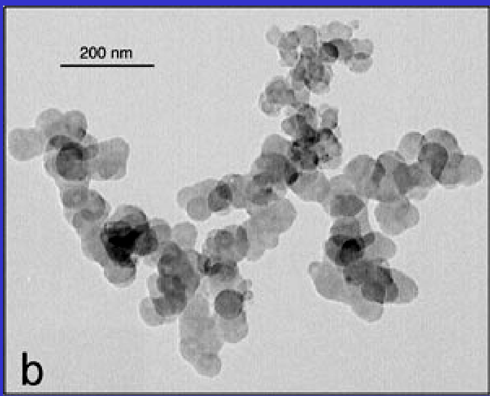
And, to make things more complex in a fire:

1. Heat exchange by radiation through the gaz
2. Production of soot that make the gaz non transparent



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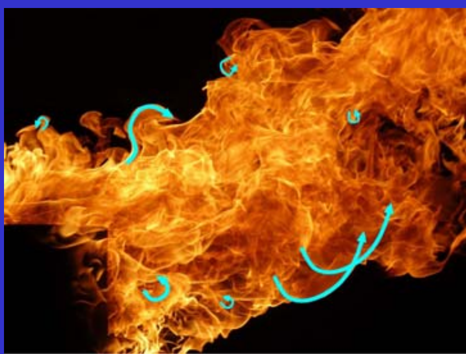
The flow in compartment fires is is not laminar; it is turbulent (with different scales, in space and in time).



=> The real flow (in detail) is unpredictable and, yet, the turbulence is essential for the mixing of chemical species and of hot and cold air masses.

Three different methods for modelling turbulence:

1. DNS (Direct Numerical Simulation). Modelling all scales exactly. Not possible.
2. RANS (Reynolds Average Navier Stokes). Modelling the « average » flow. Can be OK in some cases.
3. LES (Large Eddy Simulation). Modelling only the large scales. Is a compromise. Used by FDS.

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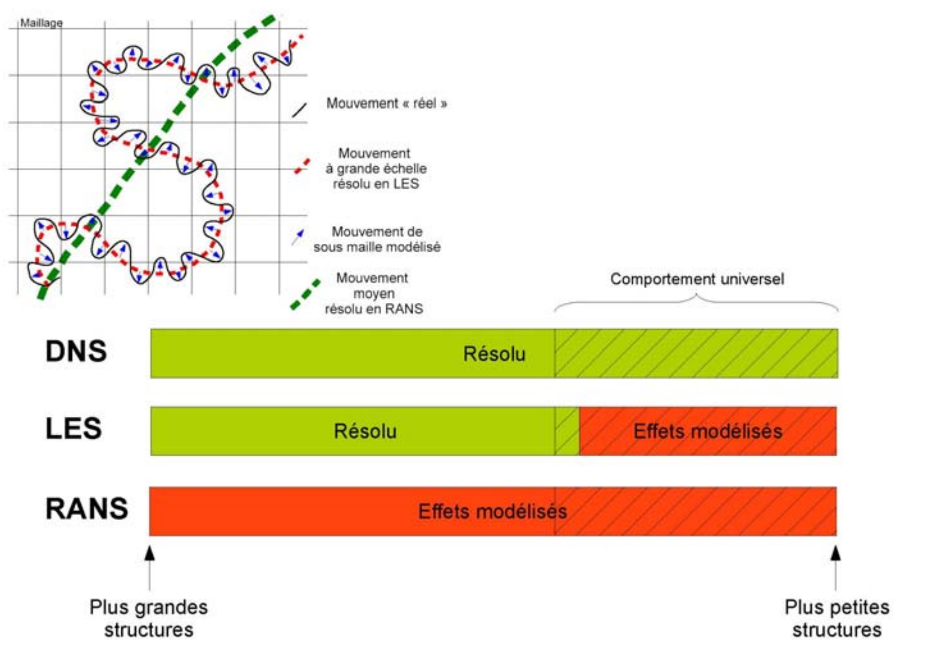
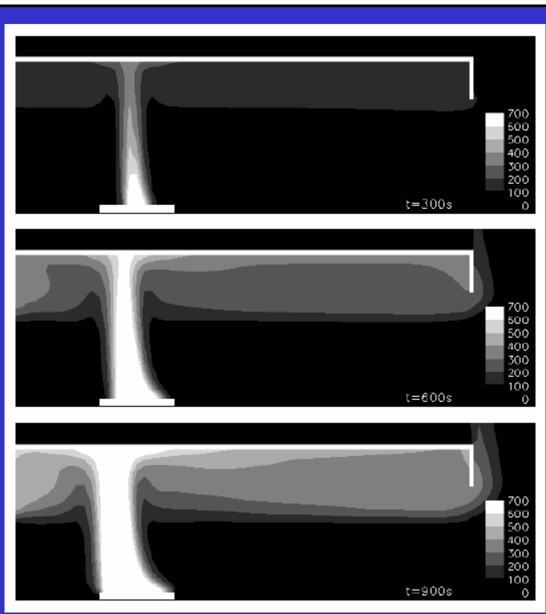
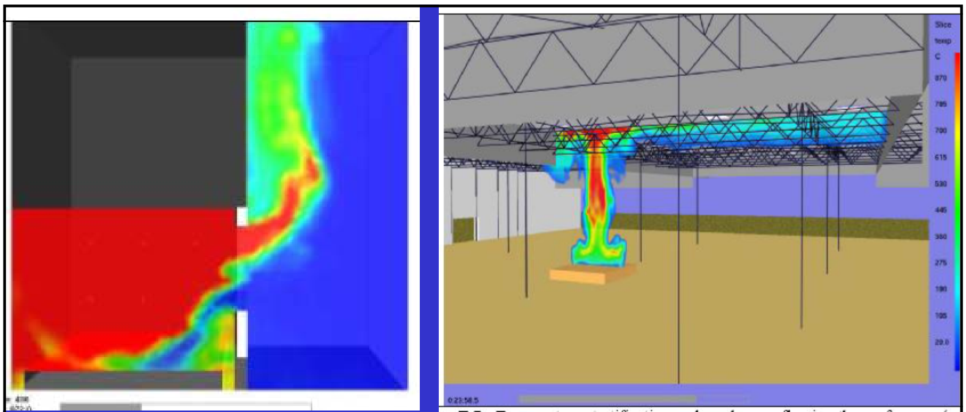




Typical RANS solution. The contour lines are regular.



Typical LES solutions. The eddies are visible. 14

3. Heat transfer

1. Conduction

Essential in solids. Negligable in gases.

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3. Heat transfer

2. Convection

Requires movements in the fluid.

Can be forced or natural, i.e. based on density gradients. In fire, the convection is mainly natural.

$$\phi = h\left(T_{gas} - T_{solid}\right)$$

In FDS:

$$h = \max\left[c\left|\Delta T\right|^{1/3}; \frac{k}{L} 0.037\,\mathrm{Re}^{4/5}\,\mathrm{Pr}^{1/3}\right]$$

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3. Radiation

Dominant in fires.

Based on electromagnetic waves. No need of material (exists also in void).

Emittance: power emitted by surface unit in all directions. Proportionnal to $T^{4.}$

Emissivity: ratio between the emittance of a body and the emmitance of a black body at the same temperature.

$$e_b = \sigma T^4 \quad \text{black body}$$
$$e_g = \sigma \varepsilon T^4 \quad \text{grey body}$$
$$\varepsilon \in [0;1]$$

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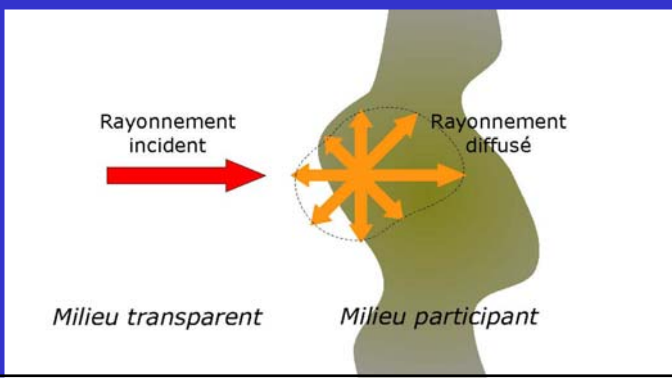
Ambiant air: virtually transparent to radiation.

Combustion products (smoke): participating medium.

⇒Absorption by some molecules (H_2O, CO_2,CH_4…) and by soot.

⇒ Diffusion by solid particles.



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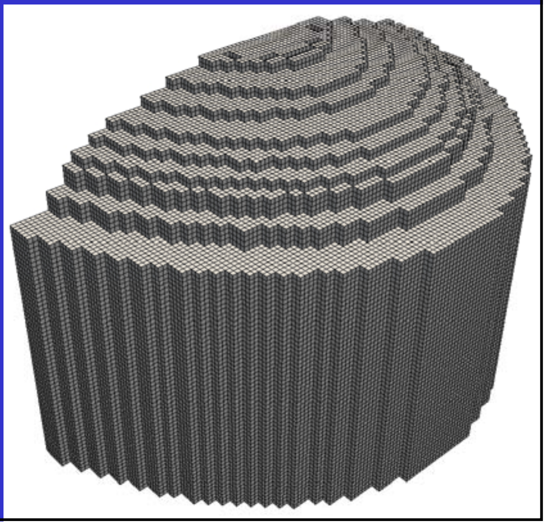
4. Numerical resolution of the equations

Discretisation of the volume into a large number of elementary cells.
In FDS, the cells are parallelipedic.



All variables have a uniform value in each cell.

The differential equations are written in each cell.
• Finite differences (FDS). Derivatives are approximated by series of Taylor. Easy to write, but work well only with regular meshes.
• Finite volumes. Flux between the cells. More difficult to write but works with any mesh.
• Finite elements. Similar to finite volumes, but the equations are multiplied by weigthing functions.

The integration on time of the equations is explicit in FDS.

Stability requires: $u \Delta t / \Delta x < CFL$

With: u velocity of the flow

Δt time step

Δx size of the cell

CFL control number.

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$u \Delta t / \Delta x < CFL$

Small cells require smaller time steps

High velocity requires smaller time steps.

=> Filter the acoustic waves (low mach model)

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5. Presentation of FDS

3D CFD software specifically written to model fire situations.
Written by NIST (USA)
Open code available at: http://fire.nist.gov/fds/

History
- System of equations written at the end of the 70's
- First 3D calculations in the 80's, crude meshes
- Turbulence introduced in the 90's
- Named « FDS » in 2000
- Possibility of parrallel solving

Hydrodynamic model: low mach Navier Stokes
Combustion model: one step chemistry based on the mixing fraction
Radiation: by finite volumne and calculation of the absorption coefficient based on the composition of the gases.
Meshing: cartesian (multi meshing is possible)

Advantages:

Free code (in FORTRAN), wide utilisation by the scientific community
Easy to use, well documented
Graphic output interface Smokeview
Runs on a normal laptop
Possibility to have exchange with the developers, active user's forum.

To be considered:
Not a commercial code (as is Fluent, for example). Support on a voluntary base.
Used for research and real applications. Validation?
Not a very advanced CFD code.
Vey robust. Very rarely breaks => It is necessary to analyse the results about their validity.
Risk of a mono-culture in the scientific community.
Unlike displacement based F.E., the solution does not converge toward the correct solution when the mesh is refined. => What is the optimum mesh?

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Documentation
See: http://fire.nist.gov/fds/documentation.html

Software to use:
See: http://code.google.com/p/fds-smv/downloads/list
Executable: fds5.exe
Creation of input files: either a text editor, or one of the software developed (e.g., Pyrosim, not free)
Viewing the results: Smokeview
EXCEL can be used to read some .CSV files
Various post-processors: Tecplot (not free), paraview (free), etc.

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6. How to run FDS?

- Create a folder
- Copy fds5.exe in the folder
- Copy the input file (e.g., cas01.fds) in the folder
- Open a command DOS window. For example, create a file named « start_FDS.bat » that contains only the instruction: CMD).
- In the dos window, type « fds5.exe cas01.fds »
- Some output appear in the DOS window. They can be redirected to a file with >.

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7. Input - Output

Input: ASCII file
Each line starts with « &WXYZ » and ends with « / » where WXYZ is a 4 characters key-word. Anything outside & and / is a comment.
In each line, the parameters are separated by « , », or by blank spaces.
Blank lines are possible.
The last line of the file is: &TAIL /

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&MESH IJK=20,20,30 , XB=0,10,-5,5,0,3 /

20 cells in the X direction, from x=0 to x = 10
20 cells in the Y direction, from y=-5 to y = 5
30 cells in the Z direction, from z=0 to z = 3

Note: the number of cells must be $2^n 3^p 5^q$

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&SURF

Defines a type of surface with different possible characteristics such as color, adiabatic condition, emissivity, HRR per unit area, front surface temperature, velocity of the gas flow through the surface.
Note: the type of surface does not have any coordinate.

HRR per unit area => the user must define the fire.

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&OBST

Defines a parrallelipedic volume with different posible characteristics such as color, associated surface types, and coordinates.

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&VENT

Defines a surface with coordinates, associated surface type

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OUTPUT

&DEVC: device, e.g., a thermocouple at a precise location
&PROF: profile, e.g., temperature in a solid
&SLCF: slice in the volume with animation of the result, for example the temperature.
&BNDF: animated result on a surface
&ISOF: animated iso-surface

Utilisation of Smokeview

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7. Other considerations

The equations are always the same. Only the boundary conditions (and the geometry), make the solution unique.
In a compartment fire, the boundary conditions are essential.
Precision on losses to the walls are especially important in powerful fires.
By default, solids and surfaces at the limits of the domain are isotherms at ambiant temperature.

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On the surfaces, it is possible to have adiabatic condition, isotherm condition, imposed net heat flux, imposed convective flux, fixed coefficent of convection…

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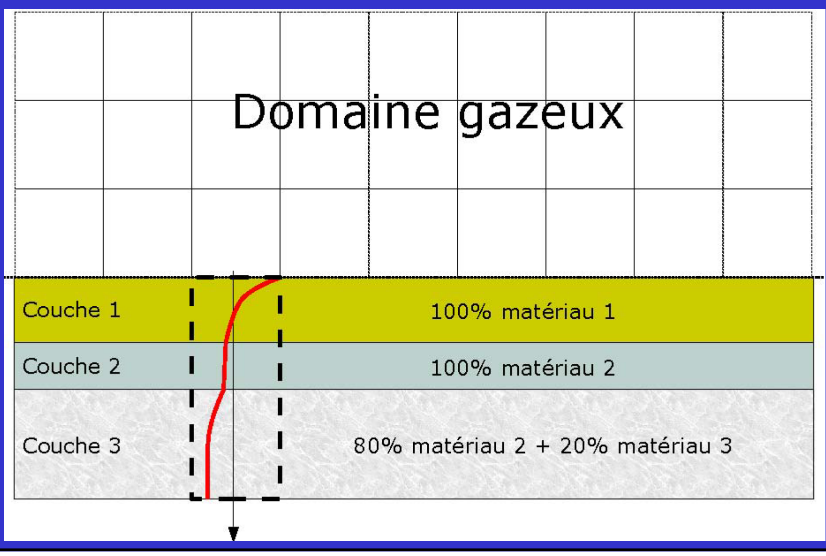
The walls can have different layers, with different materials. The heat transfer in the walls is uniaxial.



Not recommended to refine the mesh near the walls in the hope of improving precision of the heat exchanges.
Inclined surface approximated by steps. Don’ try to reproduce exactly the mass flow around the obstacles, even with SAWTOOTH=.FALSE.

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Mass flow through the openings governed by Bernoulli.
An opening requires at least 4 cells in both directions. Small openings (gap under a closed door) must be smeared.

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Combustion model is rather simple.
• Not realistic in underventilated fires
• Extinction model is simple (based on O_2 concentration and temperature).

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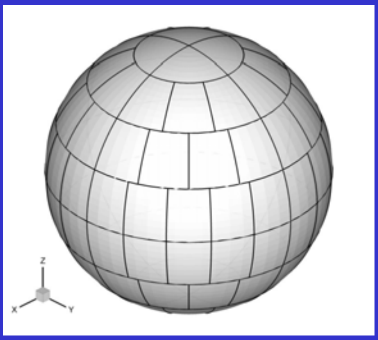
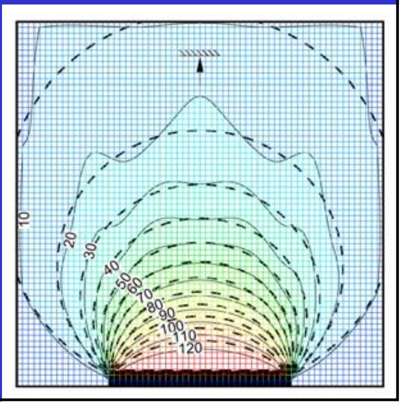
Radiation

• Hypothesis of grey gas (soot concentration is dominant, diffusion is neglegted in smoke)
• Discretisation of the spheric solid angle in about 100 finite solid angles => some directions are given particular attention.





7. « Quality of a simulation »

Use regular cell shape, as cubic as possible.
Use odd dimensions (0.20 rather than 0.19275).
Check that the maps of the resulyts don't match the mesh.
Make a first model with a crude mesh (200.000 cells)
Ideally, make several models with different mesh refinement.
Beware of multi meshes (problems at the interface).
A finer mesh is required near the fire.
As a rule of thumb, cells of 10 cm seem appropriate for ordinary fire compartments.
Use symetries when possible.
Avoid very thin solids.

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7. « Quality of a simulation »

Use the default chemical fire reaction if not an expert.
Use predefined RHR curves for your first examples.
Model the fire in a simple way (solid with RHR on the top surface).
Make a first run with full power from the beginning to check the model (gives quickly an idea of the steady state solution).
Look with Smokeview whether the flames are realistic.
Don't « play » with the parameters if you don't know exactly their role and meaning.
Be aware of default values.
Compare your results with similar cases, or experimental test, or more simple models (OZone).

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Thank you.