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2017 J. Phys.: Conf. Ser. 796 012035

(http://iopscience.iop.org/1742-6596/796/1/012035)

IOP Conf. Series: Journal of Physics: Conf. Series **796** (2017) 012035 doi:10.1088/1742-6596/796/1/012035

Comparative CFD simulations of a hydrogen fire scenario

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Abstract. Hydrogen leakage and fire ignition and propagation are safety concerns in several industrial plants. In a nuclear fusion power plants the separation of hydrogen and tritium takes place in different steps, among which one or more electrolyzers are foreseen. A fire scenario could take place in case of leakage of hydrogen. In such cases, it is important to prevent the spreading of the fire to adjacent rooms and, at the same time, to withstand the pressure load on walls, to avoid radioactivity release in the surrounding environment. A preliminary study has been carried out with the aim of comparing CFD tools for fire scenario simulations involving hydrogen release. Results have been obtained comparing two codes: ANSYS Fluent© and FDS. The two codes have been compared both for hydrogen dispersion and hydrogen fire in a confined environment. The first scenario is aimed to obtaining of volume fraction 3D maps for the evaluation of the different diffusion/transport models. In the second scenario, characterized by a double-ended guillotine break, the fire is supposed to be ignited at the same time of the impact. Simulations have been carried out for the first 60 seconds. Hydrogen concentration, temperature and pressure fields are compared and discussed.

1. Introduction

This paper summarises the calculations carried out to compare two different computer codes, Fire Dynamics Simulator (FDS) and ANSYS Fluent in the simulation of the release and the ignition of hydrogen after the break of a pressurised pipeline.

Fire Dynamics Simulator [1] is a computational fluid dynamics model of fire-driven fluid flow. The software solves numerically a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow, with the emphasis on smoke and heat transport from fires. The core algorithm is an explicit predictor-corrector scheme, second order accurate in space and time. Turbulence is treated by means of Smagorinsky form of Large Eddy Simulation. FDS uses, in its default configuration, a single step chemical reaction whose products are tracked via a two-parameters mixture fraction model. By default, two components of the mixture fraction are explicitly computed, the mass fraction of the unburnt fuel and the mass fraction of the burnt fuel. The code solves the radiative heat transfer using the radiation transport equation for grey rays with a technique similar to finite volumes method for convective transport.

ANSYS Fluent is a well-known commercial CFD code [2] and its main characteristics will not be reported here due to the large amount of selectable tools, schemes and models.

The simulations assume the rupture of a hydrogen pressurized line and the release of the gas in a closed environment in which several electric equipment can lead to safety issue for fires and explosions. It has been assumed that the room is provided with an operating HVAC system and the first 60 seconds after the break have been analysed.

2. Release conditions and geometry description

The hydrogen leakage takes place without the intervention of safety system for at least one minute. The accident is postulated to occur in a pressurized line with a nominal flow rate of 150 Nm^3/h. In normal operation P-T conditions in the rupture section are 7 bar and 40°C.

The release rate in the first milliseconds has been evaluated according to [3], considering the system as a vessel with a hole in the wall. The simplification is safety oriented because it overestimates the release, neglecting the pressure drops of the circuit. The calculated initial release rate is 0.555 kg/s and it drops to the nominal flow rate after 220 milliseconds.

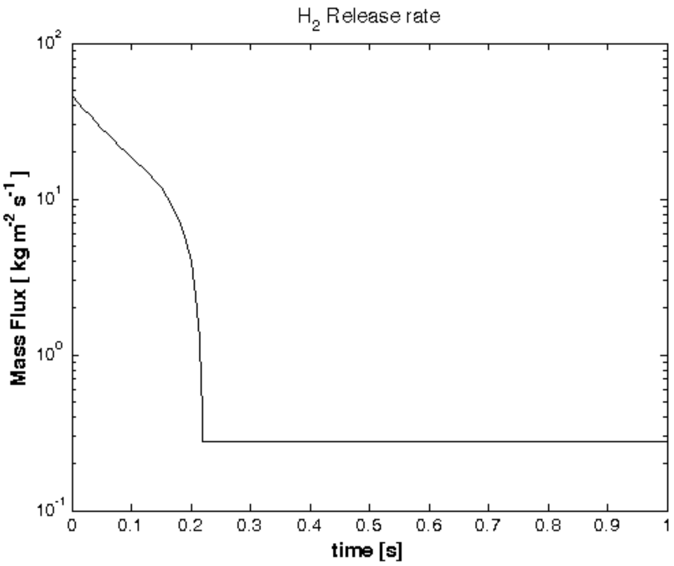


Figure 1. Mass Flow Inlet profile

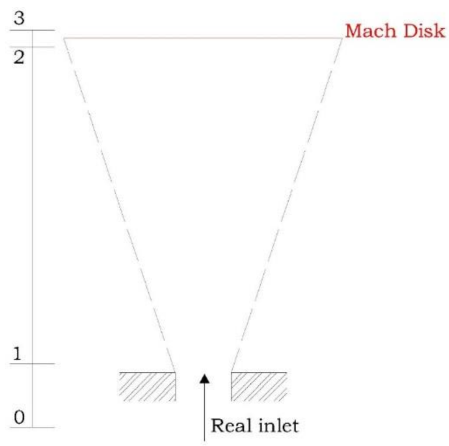


Figure 2. Schematic representation of the single Mach disk model approach

Being the line pressurized at 7 bar, the accidental break results in a critical flow of hydrogen. An ideal single Mach disk model [4] was applied to obtain the inlet dimensions in subsonic conditions. The chocked flow at the real inlet expands isentropically to a location where a single Mach disk forms. All the hydrogen is assumed to flow through the disk and, due to the isentropic expansion, the gas is in supersonic condition just upstream of the Mach disk but it is in subsonic state, but still compressible, at the downstream location. Across the Mach disk the Shapiro's normal shock relations are valid and they allow to calculate the flow conditions and the Mach disk dimensions.

Starting from the stagnation condition in section 0, the following relations allow to calculate the new inlet dimension.

$$P_{1t} = P_0 \left(\frac{2}{\gamma+1} \right)^{\frac{\gamma}{\gamma-1}} \quad P_{2t} = P_{1t} \quad P_2 = P_{2t} \left(1 + \frac{\gamma-1}{2M_2^2} \right)^{-\frac{\gamma}{\gamma-1}} \quad P_3 = P_{3t} \left(1 + \frac{\gamma-1}{2M_3^2} \right)^{-\frac{\gamma}{\gamma-1}}$$

$$T_{1t} = T_0 \left(\frac{2}{\gamma+1} \right) \quad T_{2t} = T_{1t} \quad T_2 = \frac{T_{20}}{1 + \frac{\gamma-1}{2M_2^2}} \quad M_3 = \left(\frac{\frac{M_2^2+2}{\gamma-1}}{\frac{2\gamma}{\gamma-1} M_2^2 - 1} \right)^{0.5} \tag{1}$$

Where the subscript t indicates the *total* quantities. The position of the disk cannot be determined by this model, but it is reasonable to consider this virtual inlet in the position of the real one, with a negligible error. FDS imposes to use square surfaces and with this limitation the virtual inlet has the dimension of 0.11 × 0.11 m^2, while the real pipe has an internal diameter of 0.04 m.

2.1. Computational grids
The assumed dimensions of the room are 5 m (width), 6 m (length) and 3 m (height). Grid size, for both FDS and ANSYS Fluent, has been differentiated according to preliminary considerations on velocity and temperature gradients. In Table 1 the principal features of both grids are summarized.

Table 1. Mesh main features.

	Minimum size	Maximum size	Elements number
FDS	1 cm × 1 cm × 2.5 cm	10 cm × 10 cm × 10 cm	926640
ANSYS Fluent	1 cm × 1 cm × 2.5 cm	10 cm × 10 cm × 10 cm	1569921

In figure 3 and 4 the two computational grids and their details are shown.

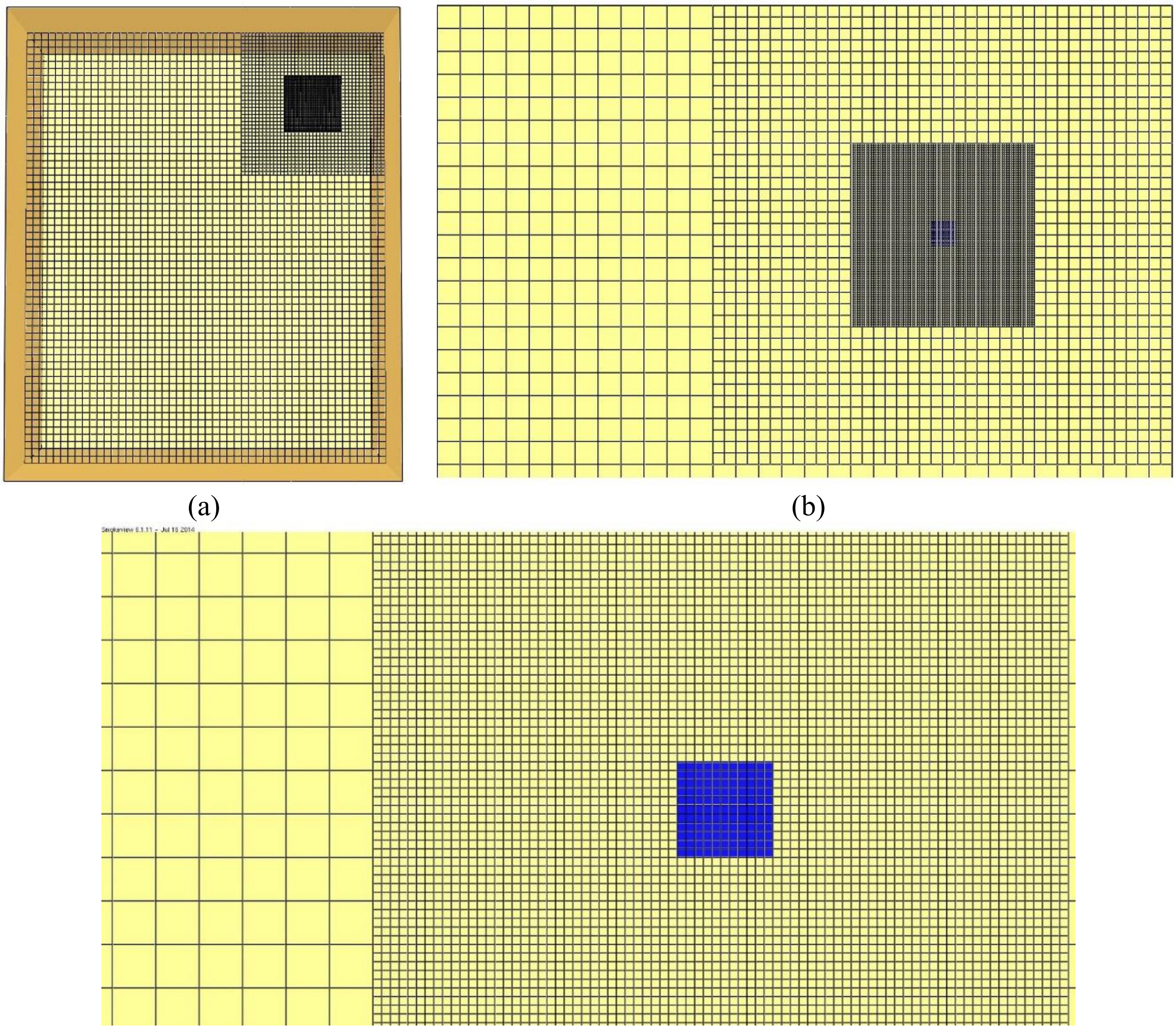
Figures 3a, 3b and 3c show FDS mesh and its details and it can be seen that with this code, the domain is made up of rectilinear volumes. Limitations on elements shape is compensated by a greater flexibility on mesh alignment. ANSYS Fluent mesh was obtained with Gambit 2.4 and it is made of both hexahedral and tetrahedral mesh elements. Gambit does not have the possibility to switch from a finer regular mesh to a coarser regular mesh, so the transition needs a mix of hexahedral and tetrahedral elements. This different approach motivates the difference in the elements total number. To maintain the same grid size in the inlet zone, the transition to the outer zone requires a larger number of elements in the Gambit mesh.

3. Results
The codes comparison has been performed in two different situations:

1) Release and dispersion of hydrogen from the break in the pressurized line, without any trigger;
2) Release and early trigger of hydrogen leading to a fire scenario.

In both cases the initial condition of temperature and pressure in the room is 25°C and 1 atm. Wall, both parietal and equipment, are treated as adiabatic. The HVAC system was maintained operative during both the simulations, the inlet and outlet air velocity was 2 m/s.

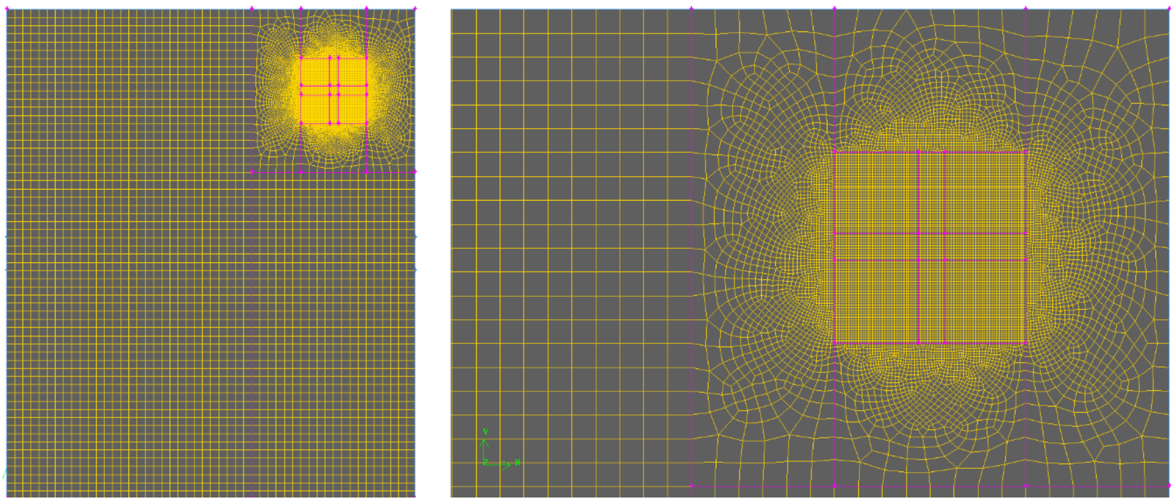
3.1. Hydrogen release
A hydrogen release from a tank in a closed environment may lead to dangerous concentrations that can cause fast deflagration or even detonation, jeopardizing the integrity of the structure.



(a) (b)

(c)

Figure 3. (a) FDS rectangular grid (b) detail of the intermediate zone (c) Finer zone and inlet mesh



(a) (b)

Figure 4. (a) ANSYS Fluent grid (b) detail of the intermediate and inlet mesh

In some cases, such as nuclear industry, this is a main safety issues due to the potential uncontrolled release of radionuclides.
At 1 bar the minimum concentration necessary to support the combustion, *lower explosive limit LEL*, is about 4.19% in volume and the correspondent *upper explosive limit UEL* is about 74.6% [5].
For this reason, the present CFD tools comparison is focused on the distribution of hydrogen in the room and in particular on the differences in volume concentration of the H_2-air mixture.

Five different parameters are presented to compare the two simulation tools:
1) Total amount of hydrogen in the room and within *LEL* and *UEL;*
2) Volume fraction time trend in 3 control points above the break;
3) Volume fraction along the vertical axis above the rupture, at the end of pressurized discharge (0.22 s);
4) Contours of volume fraction on a vertical plane at 0.1, 1.0 and 10.0 seconds.

3.1.1. Hydrogen total mass and hydrogen mass within flammability limits
Hydrogen flows within the room with the same mass flux in both calculations. The HVAC system removes part of this hydrogen through an outlet fan located at the centre of the ceiling. The comparison of the two calculations shows a greater ventilation effectiveness in the ANSYS Fluent calculations. It carries more hydrogen with the "fresh" air flow, and, initially, it keeps the flammable fraction below the value calculated by FDS. While maintaining a lower amount of fuel in the room, ANSYS Fluent calculation after few seconds foresees a higher mass within the flammability limits.

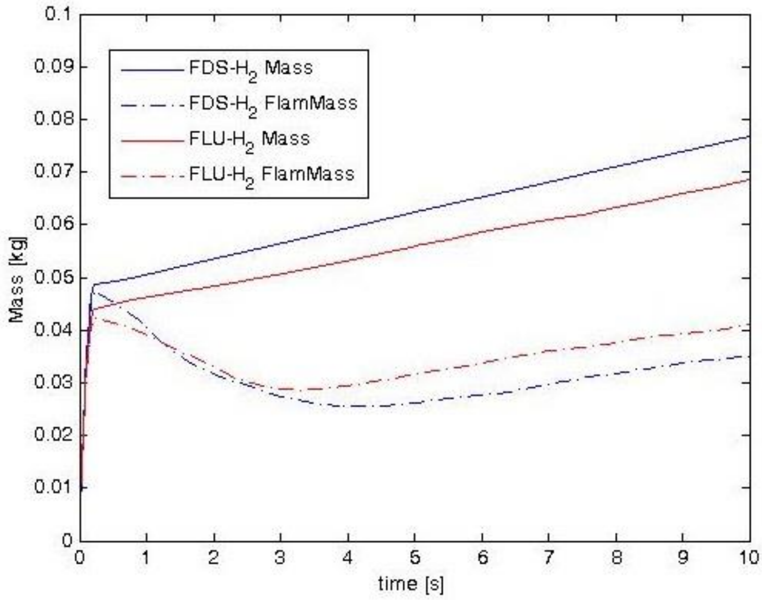
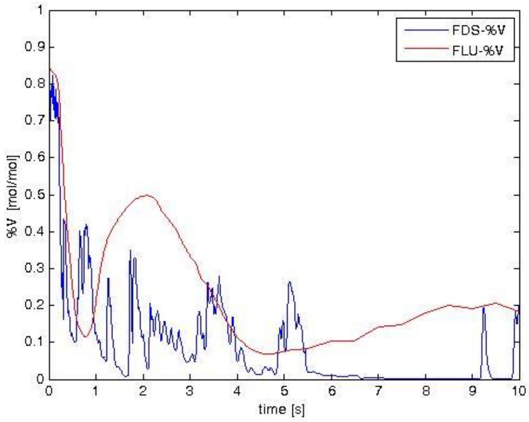
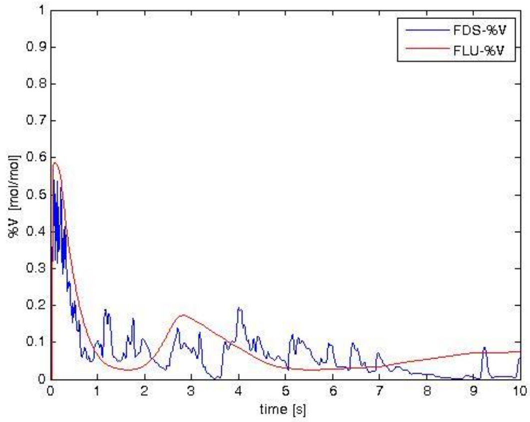


Figure 5. H_2 total mass and H_2 mass within flammability limits

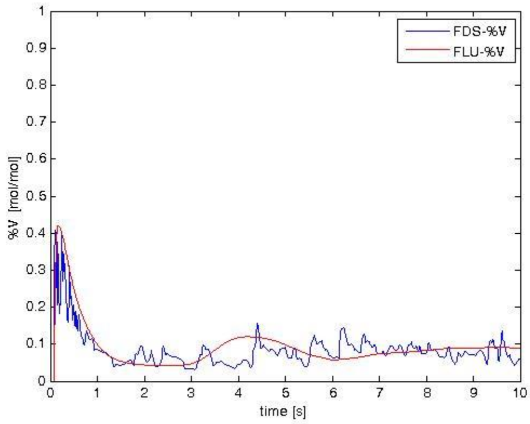
3.1.2. H_2 volume fraction
Time trends of hydrogen volume fraction have been plotted for three different point in the vertical direction, at 1, 2 and 3 meters above the break. Due to its turbulence treatment, the results of FDS calculations are more unstable, but the main trend is replicated by ANSYS Fluent analysis. Higher differences are in correspondence of the inversion in the flammable mass trend. Fluent overestimates the volume fraction at 1 meter along the axis in terms of both peak height and width. The gap between the two calculation for the lower control point is anyway significant and non-negligible. In case of the higher control points 2 and 3 instead, the results obtained with RANS calculation are in accordance with FDS results.



(a)



(b)



(c)

Figure 6. (a) H_2 %vol vs time at 1m along the inlet axis, (b) at 2m, (c) at 3m

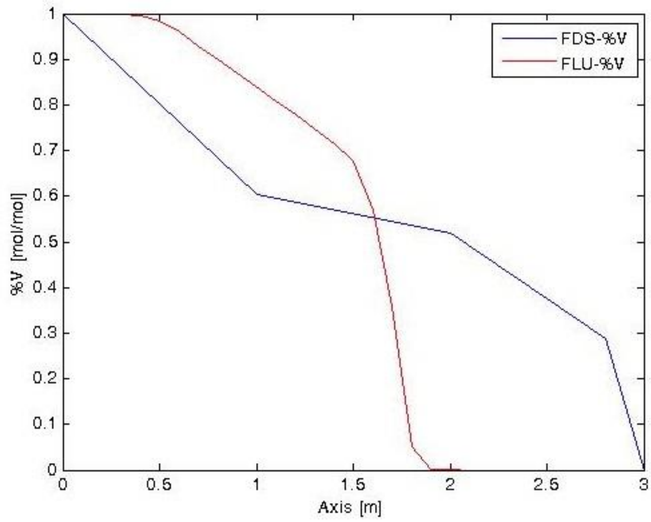
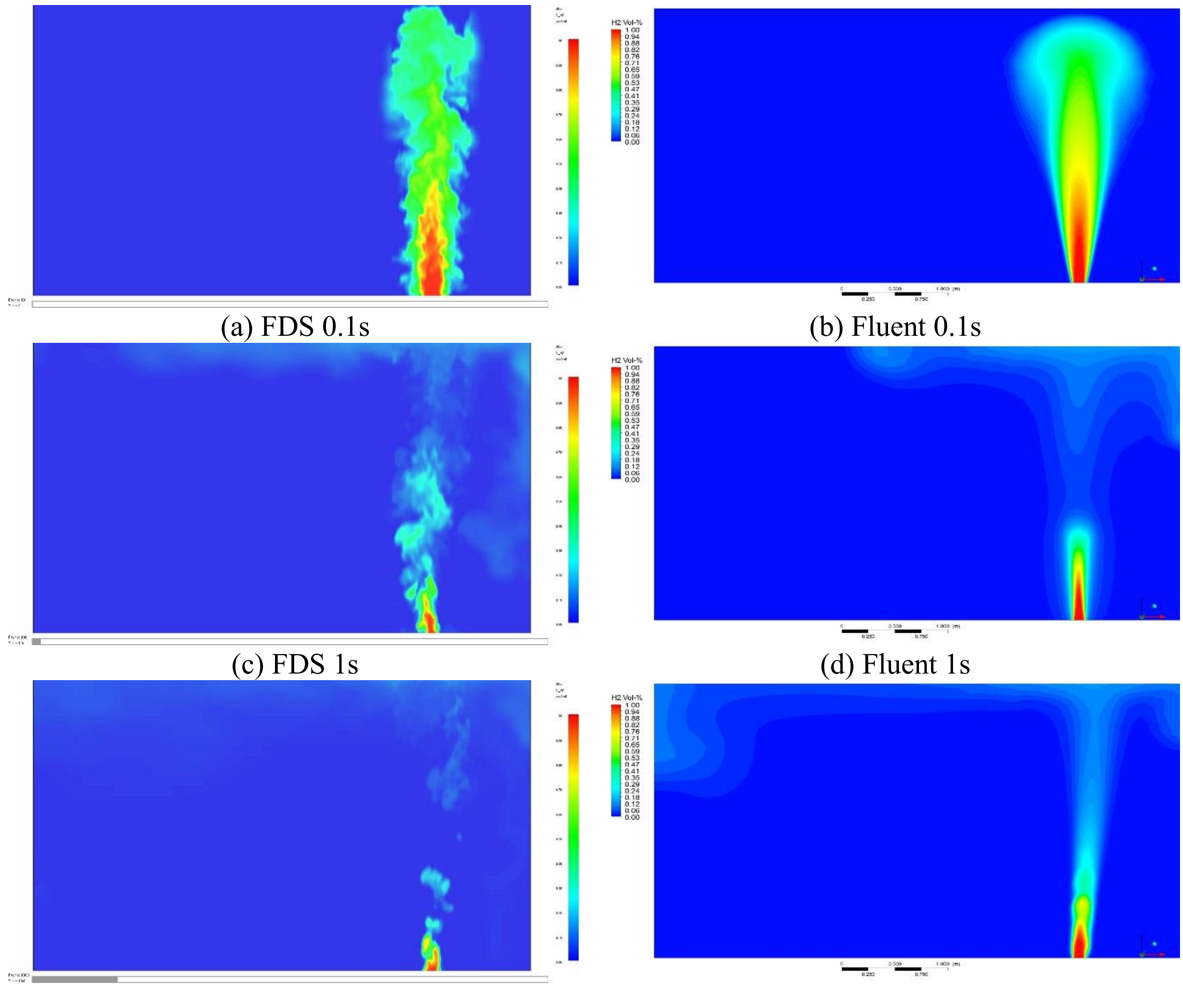


Figure 7 shows the comparison of the hydrogen volume fraction calculated along the vertical line in correspondence of the break, at the end of the pressurized release phase. At this time the hydrogen cloud shows an opposite behaviour in the two simulation. ANSYS Fluent results show a denser cloud in the lower zone and a rapid decrease at about 1.5 meters. FDS calculations lead to an almost linear behaviour, the volume fraction varies smoother between its maximum at the break level and its minimum at ceiling.

Figure 7. H_2 %vol along the inlet axis at 0.22s (end of pressurized phase)

3.1.3. H_2 volume fraction contour

The contours of the hydrogen volume fraction are shown at 0.1s, 1s and 10s on a XZ plane cutting the inlet section (Fig. 8). ANSYS Fluent results are not affected by diffusion near the break for the pressurized release phase, but the dimension of the hydrogen cloud appears overestimated. The shape of the cloud is similar to a typical jet-shape. The obtained contours are comparable with the experimental Rayleigh scattering images of unignited hydrogen leak provided in [6].



(a) FDS 0.1s (b) Fluent 0.1s

(c) FDS 1s (d) Fluent 1s

(e) FDS 10s (f) Fluent 10s

Figure 8. H_2 %vol contours in a vertical plane

3.2. Fire scenario

In this second comparison calculation, a triggering of fire at the beginning of the release is assumed to occur. Results have been compared with respect to the:

1) Maximum gas temperature in the room;
2) Temperature distribution along the inlet axis;
3) Temperature contours.

3.2.1. Maximum gas temperature vs Time

The results from ANSYS Fluent calculation show a higher peak at the beginning of the transient and, for the first 10 seconds, they overestimate the temperature with respect the FDS results. After an initial instability, the temperature trend calculated with Fluent is smoother, while FDS profile is susceptible of oscillations due to adopted LES turbulence formulation. The difference is constantly about 150°C, as shown in Fig. 9.

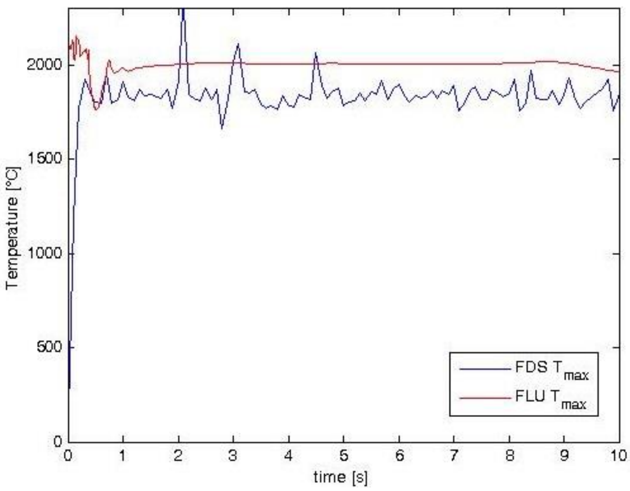
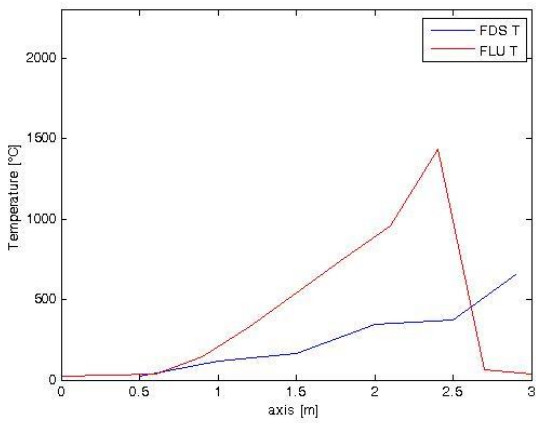


Figure 9. Maximum temperature in the fire flames

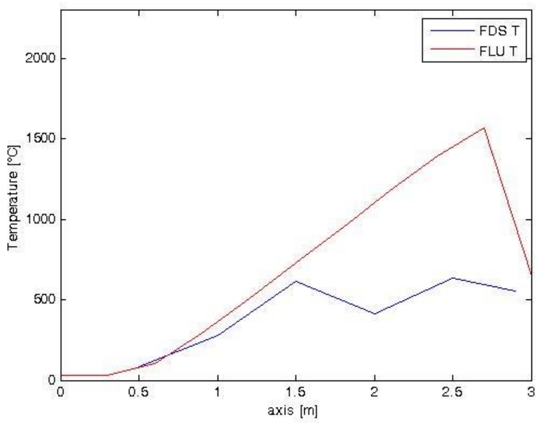
3.2.2. Temperature along the inlet axis for different times and temperature contours

The following figures show different temperature distributions along the inlet axis. Figure 10a and figure 10b refer to 0.1 and 0.22 seconds, respectively. During the pressurized discharge phase the temperature difference in the higher part of the flame is quite large, about 1000 °C. The punctual nature of these data sets increases the difference due to velocity fluctuations. The comparison for t=1s (Fig. 10c) shows a very different axial distribution. FDS results lead to an almost flat profile, describing a situation in which seems to be the absence of combustion in the central zone. ANSYS Fluent results show instead a different profile, with higher value in the central segment. It seems that in FDS simulation, at t=1s, the hydrogen cloud is spread in the room and the higher temperature peak are localized in different zones. At t=10s (Fig. 10d) the distributions along the axis is similar, higher temperature are reached around the break and near the ceiling, where higher gas concentrations are achieved.

These behaviours can be seen in the contour maps in Fig. 11.



(a)



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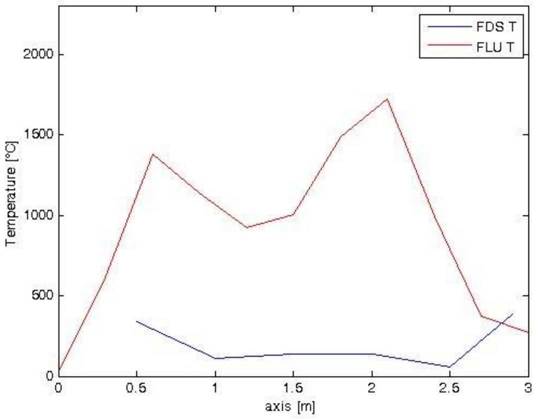
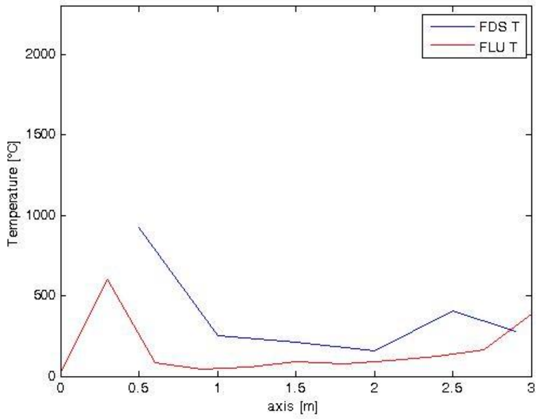
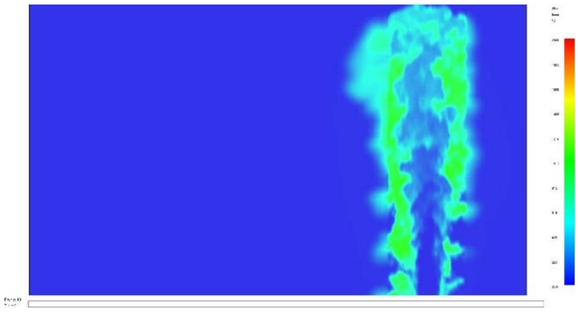


(c)

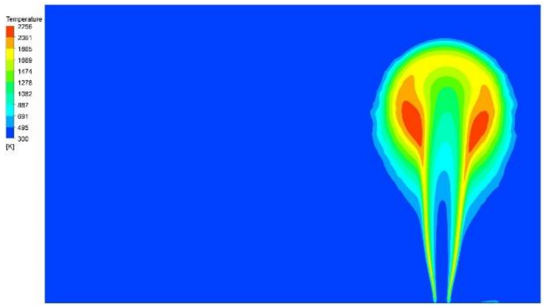


(d)

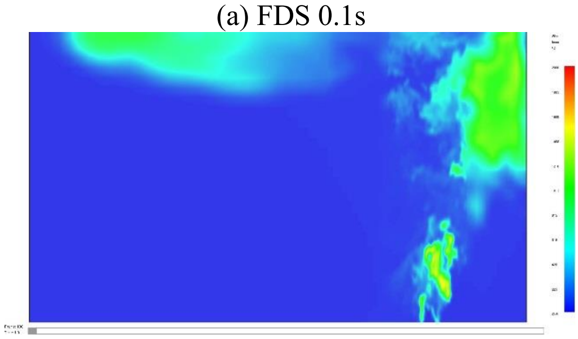
Figure 10. Gas Temperature along inlet axis – (a) 0.1s (b) 0.22s (c) 1s (d) 10s



(a) FDS 0.1s

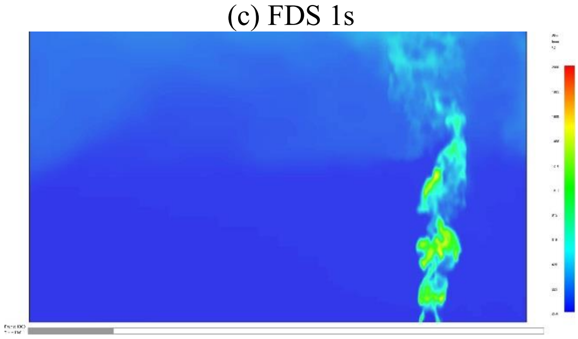


(b) Fluent 0.1s

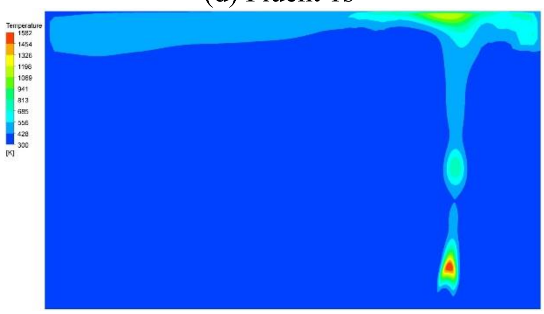


(c) FDS 1s

(d) Fluent 1s



(e) FDS 10s



(f) Fluent 10s

Figure 11. Temperature contours

4. Conclusions

FDS models and methods have been validated in the past over a large number of experimental results and test cases involving fire scenarios [7,8]. Even if a safety margin has to be taken into account due to unavoidable errors linked to numerical solutions, it has been proven to be a suitable code for safety analyses of fire accident. Its low flexibility and its high simplicity in geometry definition and mesh generation result in a higher computational speed, which allow to execute LES calculation of complex unstable phenomena in a reasonable time. On the other side, combustion models and LES turbulence treatment in ANSYS Fluent require a greater computational effort, which is mainly due to its adaptability. RANS models for turbulence are not, theoretically, suitable for highly unstable phenomena description and simulation, due to the averaging methods which tend to flatten the profiles and the fluctuations. In the present comparison these aspects have been clearly identified but, at the same time, a good match in some results have been obtained. Anyway, a deeper comparative analysis is needed and validation over experimental results for particular cases with clear boundary conditions are due, but in a first approximation the results from RANS based numerical simulation of fire accident can be considered quite reliable.

5. References

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