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Practical LES Modelling of Jet Fires: Issues and Challenges

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Jet fires represent a major risk in the process industry and it is a growing trend to use Computational Fluid Dynamics (CFD) models to achieve a better description in realistic scenarios. In this work, a process of validation was undertaken to investigate the capabilities of Fire Dynamic Simulator (FDS) in representing a jet fire. In particular, a medium scale subsonic propane jet fire was simulated with the purpose of analysing two main parameters (mesh dependency and initial unmixed fraction of the reactants).
Results of different simulations were compared with the experimental data to highlight model performance and limitations.

1. Background

A jet fire in a congested environment can rapidly lead to major consequences; even short time exposures to jet fire effects can generate catastrophic outcomes due to the high temperatures and heat transfer rates which can easily lead to the failure of other vessels or equipment. Jet fire research is still an open problem because even if a certain number of correlations are available in literature (Lees, 2004), better estimations are always required for different aspects. An example is represented by Boot (2016), who found radiation correlations still requiring improvements and validation.
One of the fundamental aspects to consider when evaluating a jet fire is the impinging phenomenon, which consists of the modification of the free flame behavior due to the interaction with obstacles, barriers, or equipment (Casal et al., 2012). That said, flame impingement is strongly affected by environmental conditions, plant layout and geometric factors. Consequently, to perform a correct risk assessment in real scenarios neither semi-empirical correlations nor integral models are sufficient because they refer to non-impinged conditions. Therefore, CFD modelling is a suitable tool to be used in the decision-making procedure for loss prevention when jet fires are involved.

1.1 FDS development and extended applications

In the last years, FDS has been increasingly used as a fire engineering tool. In parallel with the spreading of the software, a deep knowledge of the physical behaviour of fire and smoke and of its computational limits is required (Tavelli et al., 2013; Johansson & Ekholm, 2018). As a direct consequence of this, before it is possible to use FSD to model new phenomena (such as jet fires), it is necessary to perform a specific validation of the software. Validation and extension of the fields of applicability of FDS has been addressed in recent works such the one of Sellamy et al. (2018) in which a modelling of BLEVE phenomena is proposed, or by Sun et al. (2017) who performed a preliminary validation of FDS for impinging jet fires.
Different aspects concur in the simulation of jet fires; first of all, the combustion model, even if extremely simplified needs to be adequate to the purpose of describing the combustion in the flame region. Maragkos & Merci (2017) reported the good agreement achieved using FDS in modelling the combustion of a fire plume. Other critical aspects are related to the description of high momentum jets, but as reported in Ferreira & Vianna (2016) FDS appears to be able to deal with high velocity gaseous dispersions and good agreement can be expected. Several studies have been performed to understand high velocity jet flames but usually they present two main limitations: steady state conditions and low dimensions of the domain. Simulating a stationary flame is a limitation because change in shape can happen rapidly and can be not well described by a steady solution: the case of vortexes or periodically steady solutions is representative of this limitation. Low dimensions of the domain are the price payed to implement a detailed combustion model. Unfortunately, the

high computational cost required to implement those models prevent them from being extended to real scale scenarios.

2. Case study

The selected propane jet fire was chosen from the work of Palacios et al. (2009). In order to have a Mach number adequate to FDS limitations, a small jet fire was selected, with a source diameter of 12.5 mm and a mass flow-rate of 0.014 kg/s. Reported values indicate an average experimental value of the total flame length of 2.1 m. In Table 1, the main characteristics of the selected jet fire are reported. It is possible to notice that the mass flow rate of the selected jet fire can be modelled in FDS, because the corresponding Mach number is less than 0.3 (which is the Mach number constraint to be in the incompressibility region).

Table 1: jet fire parameters

-	Diameter	Mass flow rate	velocity	Sound velocity	Mach number	Flame length
	12.75 mm	0.014 kg/s	59.5 m/s	277.45 m/s	0.214 -	2.1 m

3. CFD modelling

In this work FDS version 6.5.3 was used. FDS is a Large Eddy Simulation (LES) solver, developed by NIST (National Institute of Standards and Technology), for the simulation of turbulent reactive flows. Its main characteristics are the use of an orthogonal grid and the compressibility limit (Mach number has to be lower than 0.3). FDS presents a short computational time and an excellent heat transportation description, extensively validated for pool fire scenarios (Tavelli et al., 2013, 2014; Borghetti et al., 2017).
Due to these characteristics, it is worth investigating as a suitable tool to study and perform safety assessments related to jet fires. In this complex framework, two mayor parameters have been investigated: mesh effects and initial unmixed fraction dependency.

3.1 Selected meshes

In practical simulations, usually it is not possible to reach the grid independency. In this work, two meshes have been used and compared. Both meshes are coarse enough to allow simulations to be done without supercomputers.
Mesh A is the coarser mesh that allows the experimental velocity of the jet to be reproduced; this is obtained with a single cell whose side area is equal to the experimental nozzle area. The domain is meshed with uniform cell dimensions. Mesh B is a fine mesh with cell dimensions equal to half of the dimensions of Mesh A. In this case, to reduce the computational efforts, a non-uniform mesh strategy was used, with smaller cells in the region of the nozzle, and larger cells in the zone far from the nozzle.
In Table 2, a summary of the mesh characteristics is reported. It is interesting to notice that even if the total number of cells is of the same magnitude, computational times are completely different. This is related to the Courant–Friedrichs–Lewy condition used by FDS to determine the time step length. When the characteristic length of the cells halved, the time is halved equally. The domain dimensions are equal in the two meshes and are 2.034 m (W) x 2.034 m (L) x 5.424 m (H).

Table 2: Mesh characteristics

-	Minimum cell dimension	Maximum cell dimension	Total number of cells	Time to simulate 1s with 20 cores
Mesh A	11.300 mm	11.300 mm	15552000	~20 h
Mesh B	5.655 mm	22.600 mm	17820000	~3.5 d

3.2 Initial unmixed fraction

The other parameter studied is the initial unmixed fraction (UF). In FDS a “mixed is burnt” combustion mechanism is implemented, if the chemical reaction is infinitely faster than the mixing process. FDS implements a characteristic time as well to properly estimate the mixing time in case the mesh is not fine to allow to describe the diffusion processes. Further details can be found in FDS technical guide (McGrattan et al., 2013) while mixture fraction details are reported by McDermott et al (2011).
Imposing a UF equal to 0 means that at the starting of each time step the fuel in each cell is completely mixed with the oxidizer. This assumption reduces the combustion model to a perfect “mixed is burnt” model, which is

indicated only for really fine meshes in which the mixing is well resolved. On the other hand, a UF equal to 1 assumes that at the starting point of each time step, fuel and oxidizer in each cell are completely separated, and the time before the reaction completion is computed by FDS using different constants.
In this work, the effect of three different UF values (0.2, 0.6, 1.0) was investigated.

4. Data analysis and processing

The main interest of this work is to understand the ability of FDS to reproduce the geometry of the flame, so a method to evaluate the flame length was required. The same approach proposed by the experimental work was adopted: flame length is obtained from image analysis.
Images representing the Heat Release Rate Per Unit Volume over the threshold of 200 kW/m^2 were saved with a frequency of 100 Hz. In Figure 1 is reported an example of the image used. These images are supposed to give a 3D representation of the reaction geometry, allowing an evaluation coherent with the experiment. The original images (Figure 1) were then cropped, adapted to be imported in Matlab, and transformed in matrices (Figure 2). A sensitivity study was done to find the proper agreement between original images and the transformed matrices.

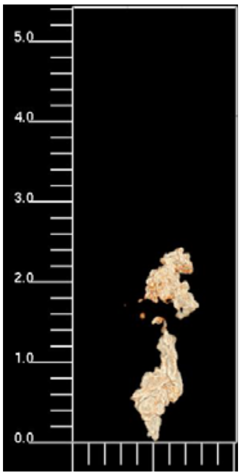

Figure 1: FDS results: flame visualization for Heat Release Rate Per Unit Volume >200 kW/m^2

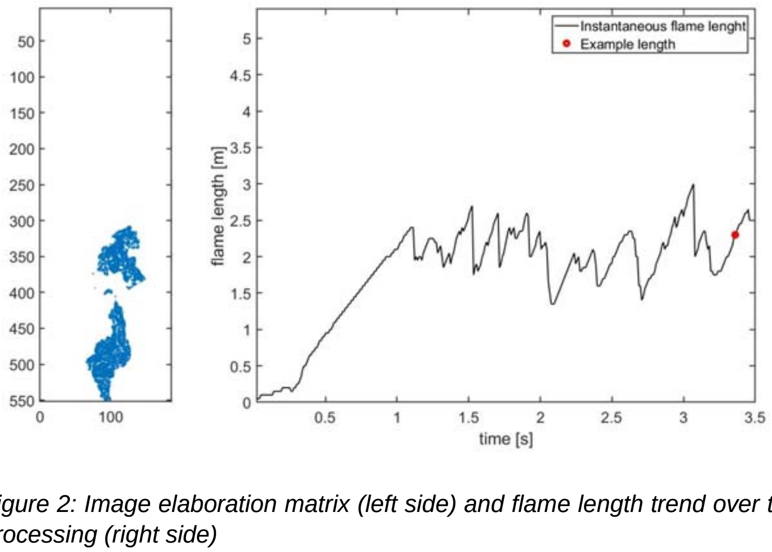

Figure 2: Image elaboration matrix (left side) and flame length trend over time obtained from the images post-processing (right side)

To obtain the flame profile, the Red component of the RGB file was selected and only values over 200 were considered. The sequence of images elaborated were then used to calculate the instantaneous flame length trend. As an example, the plot of Figure 2 highlights the point (red symbol) derived from the image matrix (left side of Figure 2) on the flame length trend.

5. Results and discussion

Results are reported with flame length as a function of time. Due to the lack of further information about flame behaviour, it was not possible to analyse other features such as width or frequency. Moreover, it has to be considered that the visible flame in FDS is equal to the sum of lift-off and real flame length. This is due to the impossibility of FDS to properly reproduce the lift-off region because of the combustion model used (combustion happens every time mixture is in the flammable region, regardless to other physical considerations).

5.1 Mesh effects

To evaluate the effects due to different meshes, in Figure 3 are reported two examples of the flame behaviours observed (results obtained for the same UF value). While Mesh B (fine) allows for a more stable and thin flame, Mesh A (coarse) produces a strongly unstable flame resulting in a much larger and shorter flame. Starting from Figure 4 (UF = 0.2), it is possible to appreciate quantitatively the effect presented in Figure 3: Mesh A generates greater oscillations with a lower frequency with respect to Mesh B. Time trends are reported for the last two seconds of each simulation, which were assumed to be representative of steady state conditions.

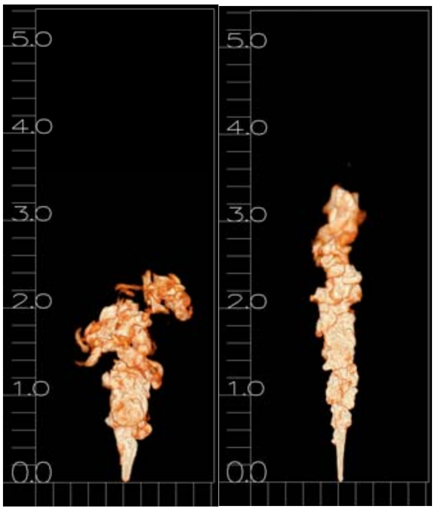

Figure 3: FDS visualization of flame shape for Mesh A (left side) and Mesh B (right side), respectively

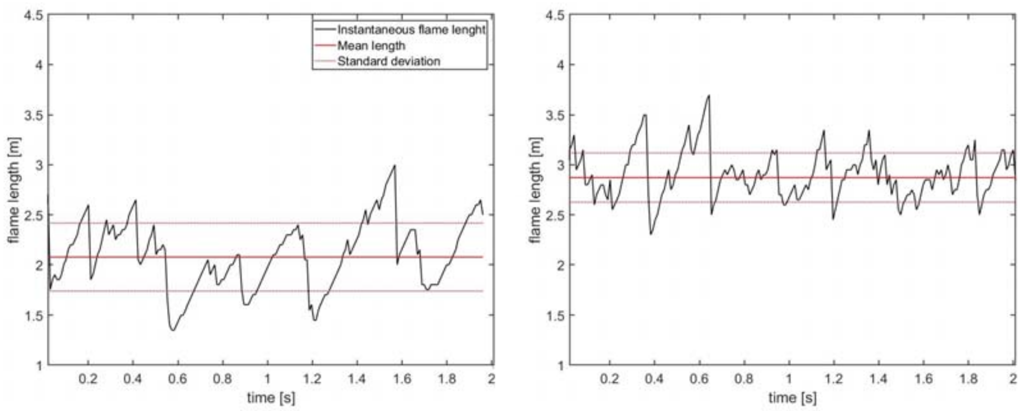

Figure 4: Flame length with initial Unmixed Fraction UF=0.2: Mesh A (left-side); Mesh B (right side)

The same effect is confirmed both in Figure 5 and Figure 6 for UF=0.6 and UF=1.0, respectively. The different stability behaviour is well pointed out both by the oscillations frequency, both by the different lengths reached, with Mesh A flames being noticeably shorter than Mesh B flames.

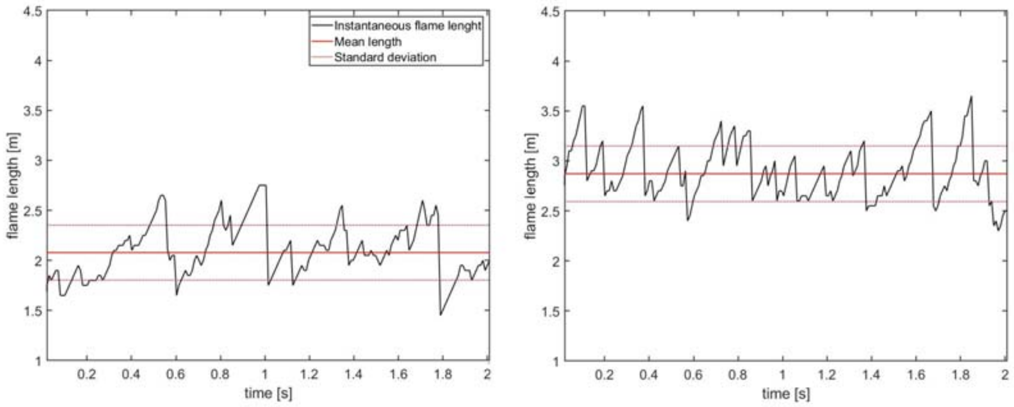

Figure 5: Flame length with initial Unmixed Fraction UF=0.6: Mesh A (left-side); Mesh B (right side)

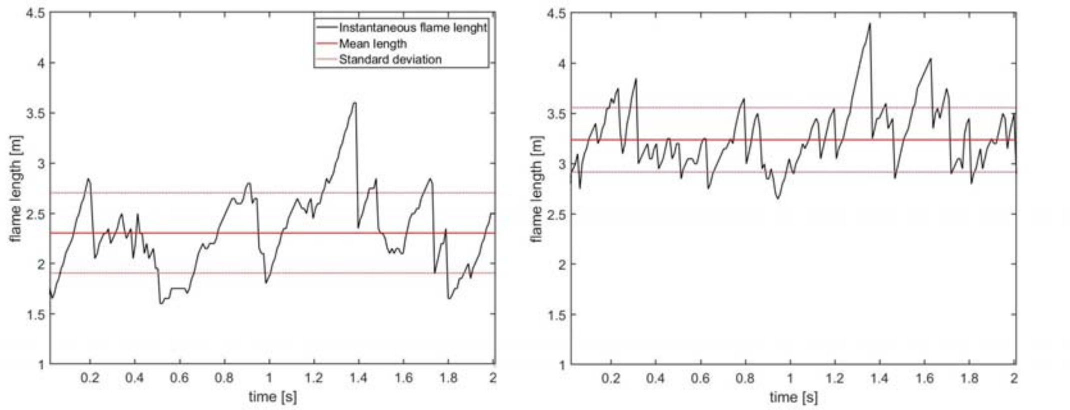

Figure 6: Flame length with initial Unmixed Fraction UF=1.0: Mesh A (left-side); Mesh B (right side)

5.2 Initial Unmixed Fraction effects

To highlight the effect of the initial unmixed fraction, an aggregated plot of flame lengths is reported (Figure 7).

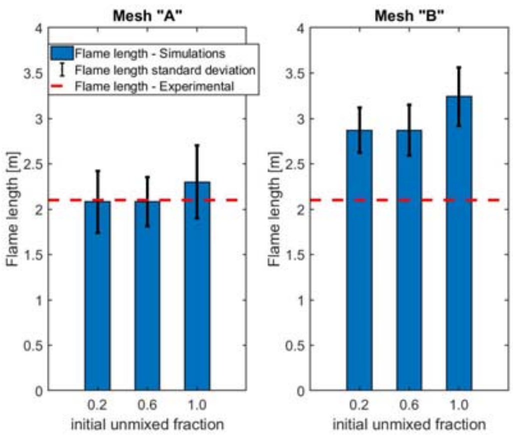

Figure 7: Comparison among the average experimental flame length and those obtained from different simulations

It is possible to notice that UF does not appear to have effects on the flame length except when its value is equal to UF=1.0. Similarly, it was found that the shape and the stability of the flame appear to be unaffected by the UF value.

6. Conclusions

In this study, the capacity of FDS to represent jet fires was investigated. It was found that the computational mesh can have strong effects on the flame stability, altering the flame behavior and length. It is possible to evaluate this dependency by analyzing the characteristic standard deviation as a percentage of the flame length.

As presented in Table 3, Mesh A (coarse) presents percent deviations which are about 15% of the flame length, while the fine mesh presents deviations of about 9%. This can be related to the instability of the flame: when the flame is unstable, its main axis is not constant; this induces some plumes to detach from the flame, resulting in flame length oscillations. On the other hand, Mesh B has a higher frequency of plume detachment, but since the main axis of the flame is stable, this frequency doesn't affect the flame length very much.

Table 3: Flame length results in the different simulations. Mean length, standard deviation and percent deviation with respect of the total flame length are reported.

	UF = 0.2		UF = 0.6		UF = 1.0	
Mesh A	2.076 ± 0.341	(16.4%)	2.077 ± 0.274	(13.2%)	2.305 ± 0.401	(17.4%)
Mesh B	2.872 ± 0.246	(8.6%)	2.871 ± 0.278	(9.7%)	3.238 ± 0.320	(9.9%)

In conclusion, it should be noticed that all the simulations present limitations. Adopting the Mesh A strategy introduces an undesired instability in the flame, suggesting that a finer mesh is required. While the Mesh B strategy solves the instability, it appears to overestimate the experimental data.

General conclusion is that FDS appears to be able to deal with the jet fire phenomena, but additional analyses are required before it could be considered as a tool for evaluating risks related to jet fires.

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