

CFD Modelling of Vertical Sonic Jet Fires

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ABSTRACT

The use of Computational Fluid Dynamics (CFD) models can contribute to prevent jet fire accidents in facilities. Despite their great potential, validation analysis must be performed before their use in real applications to examine the accuracy of the results obtained. The paper examines the predictive capabilities of the FDS, FireFOAM and FLACS-Fire codes when modelling the expanded regions of vertical sonic jet fires of propane in an open environment. To comply with the low Mach number limitation of the CFD codes used, the pseudo-diameter approach has been applied to simulate the equivalent exit conditions of the jet after the expansion. Predictions of the flame temperatures, the emitted radiative heat fluxes, and the flame-geometry descriptors are compared with experimental data. The promising results indicate the suitability of the technique used to predict the hazardous effects of sonic flows, especially in FDS and FLACS-Fire.

KEYWORDS: CFD, fire modelling, jet fires, sonic flow.

NOMENCLATURE

A	flame area (m ²)	S	lift-off distance (m)
c	speed of sound (m/s)	T	temperature (K)
D	diameter (m)	u	gas velocity (m/s)
k	turbulent kinetic energy (m ² /s ²)	Greek	
L	flame length (m)	ε	dissipation rate (m ² /s ³)
\dot{m}	mass flow rate (kg/s)	ρ	density (kg/m ³)
M_a	Mach Number	Subscripts	
M_w	molecular mass of fuel (g/mol)	eq	equivalent exit conditions
R	constant of ideal gases	F	flame
Re	Reynolds number	or	orifice
		∞	ambient conditions

INTRODUCTION

Onshore and offshore facilities, involving chemical process industries or refineries, are continuously exposed to the risk of industrial accidents (fires, explosions and toxic releases) [1]. In particular, explosions and toxic releases may injure people within a large damage radius. However, fires are the most common events (41.5%) as reported from a MHIDAS (Major Hazard Incident Data Service) survey involving 6,099 accidents [2]. Most hydrocarbon fires originate from a loss of containment. However, the final type of fire can be different, depending on the fuel properties and their state [3]. When a pipe is broken, when a hole forms in a tank, when gas leaks from a flange, or

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when a safety valve is opened, a high-velocity leak of gas, or two-phase flow, can be immediately ignited creating a jet fire [4]. For most gases, the sonic velocity is reached if the source pressure exceeds 1.9 bar, which is common in many storage tanks and pipelines [5].

In general, sonic jet fires are smaller than other accidental fires; nevertheless, the high probability of flame engulfment and the high heat flux can in turn affect other equipment within a very short period of time, leading to a significant escalation of the accident, known as the domino effect [6]. In this context, active protection systems as well as inherently safer design measures are commonly applied, such as effective separation distances, in order to prevent the chain of accidents possibly caused by jet fires [7]. Specifically, international standards provide safe distances that should be attained between potential ignition sources and flammable materials, to restrict the occurrence of jet fires. However, these are based on empirical and statistical data, and do not cover the overall characteristics of the fire behaviour, and are restricted to certain fire scenarios [8]. In addition, the continuous developments of the processes performed in these facilities may affect the geometrical distribution of the plant, the fuel inventory, and the location of the ignition sources. Therefore, separation distances could be unfeasible due to the high costs involved and the operability restrictions.

Given the difficulties in establishing reliable separation distances by traditional methods, alternative techniques should be used, such as Computational Fluid Dynamics (CFD) modelling. CFD codes solve the fundamental conservation equations governing fluid dynamics coupled with additional sub-models (i.e. turbulence, combustion, radiation) to describe the processes occurring during a fire. By this, an in-depth understanding of the phenomena associated with accidental jet fires can be attained, combined with the implementation of reliable safety distances. Despite the great potential of CFD codes, validation analysis must be performed before their use in real applications to examine the accuracy of the results obtained. The fundamental strategy is to compare computational estimations with experimental data.

This paper assesses the predictive capabilities of the Fire Dynamics Simulator v6.6.0 (FDS), the fire solver of OpenFOAM v6.0 (FireFOAM 2.2.x) and the Flame Accelerator Simulator Fire v10.7 (FLACS-Fire) when modelling the expanded regions of experimental vertical sonic jet fires. The pseudo-diameter approach is used to convert the sonic flow compressible conditions to subsonic expanded conditions as function of different Mach numbers. Predictions of the mean flame temperatures, mean heat fluxes, mean flame lengths, and mean flame areas are qualitatively and quantitatively compared against experimental data.

EXPERIMENTAL DATASET

CFD simulations are aimed at reproducing five vertical sonic experimental propane jet fires in an open environment, designated D10_0.09, D12.75_0.13, D15_0.18, D20_0.27 and D25.5_0.34 [9]. The first figure corresponds to the diameter of the jet orifice in mm and the second figure the mean mass flow rate of the gas through the exit orifice in kg/s. During the experiments, a wide-angle radiometer was located at 5 m distance from the fire origin and 1 m above the exit orifice to record the heat flux. Also, a B-type (0.35 mm-diameter) uncoated thermocouple was located 3.2 m above the orifice to register the flame axis temperature. Moreover, jet fires were filmed using a VHS camera, which registered visible images, and a thermographic IR camera, which indicated the apparent temperature distributions of the flames, defining the jet flame contour by the isotherm of 525 °C [9] (Fig. 1).

For each test, the recorded IR images corresponding to the stationary state of the fires were subsequently treated with an in-house MATLAB® algorithm [10]. The stationary state is that of a fully developed flame, stabilized with a lift-off distance from the jet exit. The main goal of the

image treatment was to separate the flame region from the background of the IR images, by comparing the temperature at each pixel element. Pixels with greater apparent temperatures than $525\text{ }^{\circ}\text{C}$ were considered as flame, while the rest were considered as background. Mean values of the flame-geometry descriptors were obtained by averaging the segmented images. The flame length was defined as the orthogonal distance between the fire base and the highest pixel element; and the flame area was determined by multiplying the number of pixel elements by the area occupied for each one.

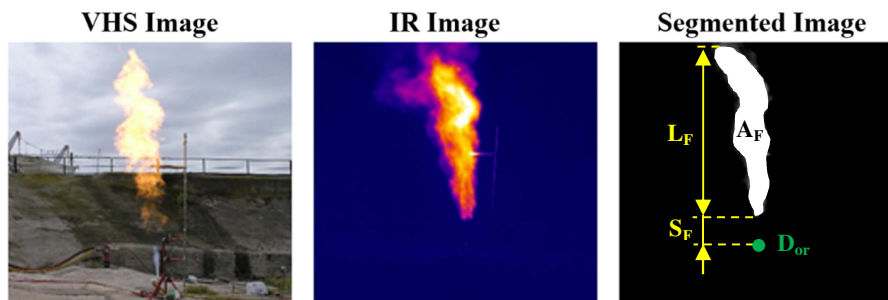


Fig. 1. Example of images recorded from the D25.5_0.34 sonic jet fire experiment by means of a VHS camera, an IR camera, and the corresponding segmented image.

NUMERICAL MODELLING

CFD codes

FDS is an open source code developed by the National Institute of Standards and Technology (NIST) that numerically solves a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow. FireFOAM is another open code developed between CFD Direct and FM Global, based on a set of object-orientated CFD toolboxes written in C++. FLACS-Fire is a commercial CFD code especially designed for fire hazard applications in the process industry.

Due to the high-turbulent flows occurring in sonic jet fires, the exact solution of the governing equations is beyond the capabilities of the most powerful computers. Alternatively, numerous turbulent models are available to figure out the flow structures in a sub-grid scale stress accounting for the important small-processes that cannot be directly resolved. In particular, the $k - \varepsilon$ two-equation eddy viscosity model is implemented in FLACS-Fire to ensure the closure the Reynolds-averaged Navier–Stokes equations (RANS). It is one of the least computational expensive turbulence models as it solves the Navier-Stokes equations for the mean flow variables. On the other hand, FDS and FireFOAM represent the flow motion via Large Eddy Simulations (LES). Additional equations are not required and a more realistic flow field is rendered; however, LES are more computationally expensive than RANS. In both codes the sub-grid scale turbulent viscosity is dynamically solved as a function of the sub-grid kinetic energy, the LES filter size, and a model constant.

The chemical reaction of fuel and oxidant is computed in the codes used by means of the Eddy Dissipation Concept (EDC), which simplifies the chemistry and neglects the kinetic effects derived. Specifically, the differences between codes lie in the way of solving the mixing time scales between fuel and oxidizer. For example, in FLACS-Fire, these depend on the mass fractions and the reacting fractions of fine structures. Differently, the mixing scale times in FireFOAM are calculated as a function of two model constants, the LES filter size, and the sub-grid kinetic energy. Otherwise, FDS uses a more detailed reaction time scale model, based on the fastest physical process of the local state of the flow field.

Moreover, the Discrete Transfer Model approach is used to compute the radiation transport equation in FLACS-Fire, whose spatial discretization notably depends on the number of solid angles, and the ambient emissivity. Particularly, 100 solid angles were set-up to solve the radiation field in FLACS-Fire. On the other hand, FDS and FireFOAM use the Discrete Ordinate Model to estimate the radiation heat transfer. The main difference between both codes is that FDS incorporates a correction factor. A total of 48 solid angles have been proven sufficient for an accurate angular discretization for the solution of the radiative transport equation in FireFOAM [11], whereas 100 were set-up for FDS, as defined by default. More technical details about the sub-models solved and the model's constants can be found in [12] for FDS, in [13] for FireFOAM, and in [14] for FLACS-Fire.

Measuring devices

Different virtual sensors were located, as described in the experimental dataset within the computational domain for each jet fire simulation, to estimate the flame temperatures and heat fluxes. The flame-geometry descriptors were calculated by means of a 2D slice file (SF) that recorded the temperatures evolution on the centreline axis of the jet. Then, different post-processors were used to convert the slice files into spreadsheets containing the mean temperatures gathered at each cell for the different simulated times: fds2ascii for FDS, ParaView v5.4 for FireFOAM and Flowvis v5 for FLACS-Fire. As performed with the IR segmented images, the flame regions for each simulation were separated from the background by applying the defined threshold temperature.

Mach number constraint

Sonic jet fires are usually divided into three zones, which are related to different Mach numbers: (i) the nearfield or under-expanded zone ($M_a \geq 1.0$); (ii) the transition zone ($0.3 \leq M_a \leq 1.0$); and (iii) the farfield or expanded zone ($M_a \leq 0.3$) [15]. Within the nearfield zone, the sonic velocity is established at the nozzle exit ($M_a = 1.0$) with a gas pressure greater than the ambient. Then, the released flow undergoes rapid expansion and quickly accelerates to supersonic expansion ($M_a \gg 1.0$) with the decrease in pressure and density. Consequently, the outflowing gas is governed by compressible and viscous effects, which avoids its mixture with the ambient flow. As the supersonic flow crosses the Mach disk, better mixing occurs in the transition zone, due to an abrupt decrease in velocity to subsonic speeds and increases in pressure and density. Both flameless zones are surrounded by a supersonic flow and coincide with the lift-off distance, defined as the distance between the outlet orifice and the base of the flame. Figure 2 shows the schematic representation of the under-expanded structure of sonic jet fires and the Mach number distribution [16]. As the distance from the gas release orifice increases, the velocity of the flow and the Mach number decrease progressively, until the air-fuel mixing is completed and the jet flame occurs. At this point, at the farfield zone, the jet is totally expanded, the subsonic regime is achieved and the flow becomes incompressible.

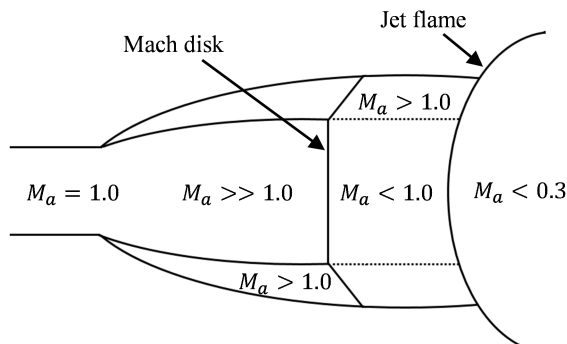


Fig. 2. Schematic representation of the under-expanded structure of sonic jet fires [16].

The CFD tools used consider the low Mach number formulation of the Navier-Stokes equations to reduce the number of equations solved, hence improving the numerical stability and reducing the computational times. Therefore, these CFD codes are only able to simulate the farfield zones, where the jet is in pressure equilibrium with the ambient fluid. In this context, the pseudo-diameter approach is used to scale the compressible initial conditions of the sonic jet at the exit orifice (i.e. temperature, velocity, diameter and velocity) to the expanded zone (Fig. 3) [17]. The method relies on mass conservation, and prevents air entrainment within the compressible region. Also, the equivalent pressure and temperature are assumed to be the same as the ambient fluid: (i) $\dot{m}_{eq} = \dot{m}_{or}$; (ii) $T_{eq} = T_{\infty}$; (iii) $P_{eq} = P_{\infty}$. Given that $u_{eq} = M_a c$, the equivalent diameter of the sonic jet fire can be determined as a function of M_a as follows: $D_{eq} = \sqrt{4\dot{m}_{eq}/\pi\rho_{eq}M_a c}$.

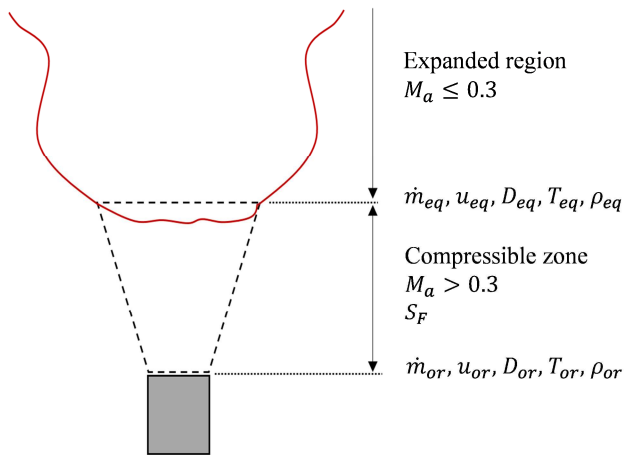


Fig. 3. Sketch of the pseudo-diameter approach used to scale the initial conditions of the sonic jet fires [17].

Table 1. Equivalent diameters of the jet fire experiments as a function of the Mach number

Mach number	-	0.01	0.025	0.05	0.10	0.20
Experiment	d_{or} (mm)	d_{eq} (mm)				
D10_0.09	10	140	90	60	40	30
D12.75_0.13	12.75	160	100	70	50	40
D15_0.18	15	190	120	90	60	40
D20_0.27	20	240	150	110	70	50
D25.5_0.34	25.5	260	170	120	80	60

The equivalent diameter approach proposed for this analysis neglects some of the real physical effects. First, the amount of ambient air entrained into the base of the flame that mixes with the fuel is not accounted. Also, the flameless distance between the exit orifice and the flame base is not estimated. Instead, an equivalent diameter of the flame base is directly assumed as a function of a Mach number, whose value is unknown. In this sense, five different Mach numbers have been considered for the analysis, to identify the most appropriate one: 0.01, 0.025, 0.05, 0.10 and 0.20 (Table 1). As observed, the greater the Mach number, the smaller the equivalent diameter of the jet after the expanded region. Even if $M_a = 0.3$ typically represents the threshold accounting for flow compressibility, this value has not been considered due to the very small diameters that would imply. Indeed, the equivalent diameter values would be very similar to the experimental ones, hence significantly increasing the computational times due to the very thin cell sizes required.

Mesh resolution

The size of the cells modelled may probably represent the most important numerical parameter defined by the user in CFD simulations. The grid sizes, coupled with the numerical methods, often determine the accuracy of the results reached and the computational times: the thinner the cell size, the better the computational resolution and the greater the simulation time. Consequently, it is necessary to provide a good balance between low grid resolution and reasonable computational costs. Cell sizes of buoyant plume simulations are commonly based on the characteristic diameter of the fire [18]. However, this approach cannot be used in sonic jet fires due to its momentum-dominated nature and the high flow velocities achieved. Furthermore, the equivalent diameters of the jets are the only geometrical constraints that define the minimum cell size. Consequently, the cell size of each jet fire scenario (in m^3) has been defined as the cubic root of its equivalent diameter (in m). For example, the D10_0.09 ($M_a = 0.01$) scenario has been modelled with a cell size of $0.14 \times 0.14 \times 0.14 \text{ m}^3$, and the D12.75_0.13 ($M_a = 0.05$) with a cell size of $0.07 \times 0.07 \times 0.07 \text{ m}^3$.

Simulations were run for 60 s to achieve long-duration steady states. The mass loss rates were prescribed according to the experimental data. A soot fraction of 0.09 kg/kg was assumed for the combustion of propane [19]. Apart from that of the ground, the rest of the boundaries were open.

RESULTS AND DISCUSSION

Experimental results

Figure 4 depicts the scatter plots of the variables experimentally measured for the different sonic jet fires as function of the Reynolds number: the flame temperature obtained with the thermocouple, the heat flux, the flame length, and the flame area. These values correspond to the mean values obtained by averaging the variables evolutions over 30 s during the steady state. Also, vertical bars are added to represent the standard deviation around their mean values.

The mean flame temperatures oscillate considerably between 1100 and 1600 °C due to the continuous thermocouple reading fluctuations along the jet axis, as a result of the high-velocity flow driven forces. Also, some temperatures measuring errors could be induced due to the type of thermocouple used. So, discrepancies between simulated and measured temperatures may be found, given the difficulties of reaching stable values of the mean flame temperature. On the other hand, the measured heat fluxes slightly increase with Reynolds number, i.e. higher flow velocities lead to greater heat fluxes received at a certain distance from the jet flame. Then, the dimensionless flame-geometry descriptors behave similarly: their mean values decrease as the Reynolds number increases. In particular, the non-dimensional flame areas constantly decrease, while the dimensionless flame length variations become more evident when $Re > 3 \cdot 10^6$. Consequently, it is deduced that sonic jet flames become thinner and longer as the Re increases until achieving maximum lengths at a certain experimental conditions.

CFD modelling results

Figure 5 qualitatively compares the previous experimental measurements against the mean predictions obtained with the CFD codes used by averaging the steady evolutions computed during 30 s. The solid diagonal line indicates perfect agreement between predictions and measurements, while dotted lines and long-dashed lines represent the $\pm 25\%$ and $\pm 50\%$ prediction error, respectively, compared to the experimental measurement. All graphs include vertical and horizontal bars that represent the standard deviation of the simulation results and the experiments, respectively.

Prior to the analysis, it is worth noting that FLACS-Fire could not perform simulations with cell sizes smaller than 0.06 m, which occurred in those tests with Mach numbers of 0.10 and 0.20. The use of very thin grids under RANS turbulence model creates convergence problems in the near

boundary surfaces of the domain leading to numerical instabilities. On the other hand, when FireFOAM simulations were run with cell sizes greater than 0.15 m (Mach numbers of 0.01 and 0.025), jet flames are represented as “columns of fire” ranging from their bases to the upper boundary layer. In that case, the coarse grids cannot accurately resolve the rate of fuel/oxidant mixing.

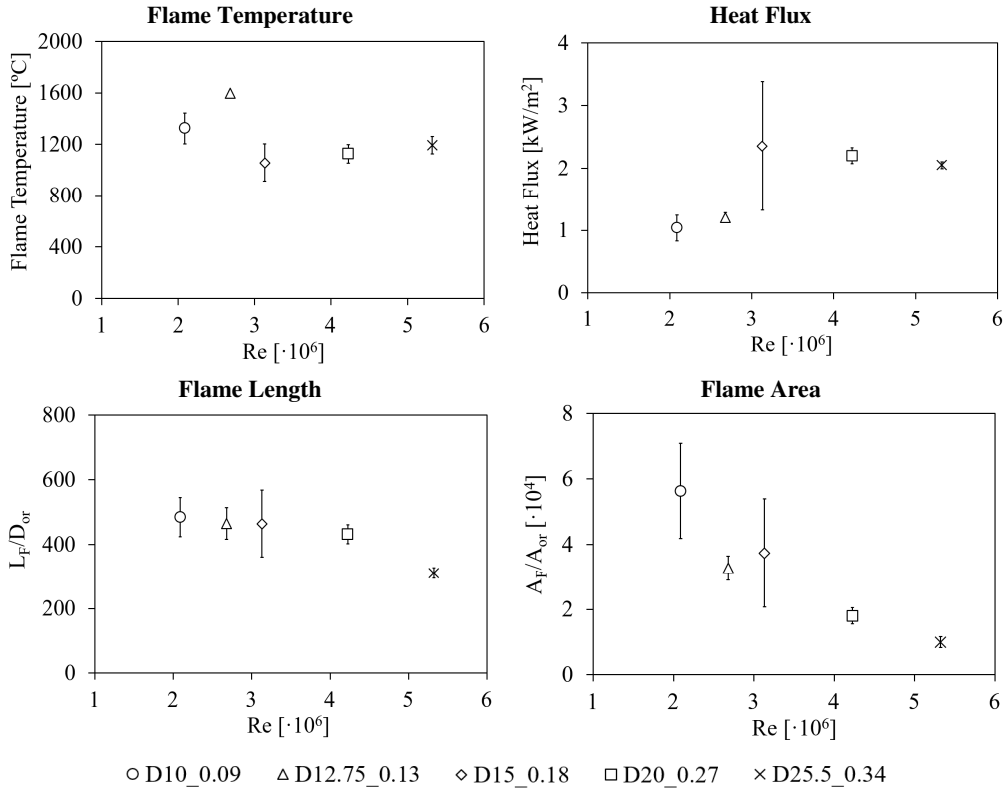


Fig. 4. Flame temperatures, heat fluxes, flame lengths, and flame area measurements obtained for the different sonic jet fires analysed.

In general, flame temperatures are often under-predicted in the CFD codes used. FDS estimations lead to an error estimation that ranged between 25% and 50%, where better agreement is often found when jet fires are modelled at smaller Mach numbers. In the case of FireFOAM, a lack of agreement is clearly observed, as an error estimation higher than 50% is reached in most cases. The maximum simulated temperatures are 650 °C, while the measured values notably exceeded 1000 °C. The lower accuracy obtained in this code could be mainly due to the model constants implemented within the combustion approach, as well as the simplicity of the mixing scale time calculation method. On the other hand, FLACS-Fire appears to be the most precise CFD model to predict the temperatures of the flame, as most of the values lead to an error estimation lower than 35%. This highlights the suitability of the $k - \epsilon$ turbulence model, and the methodology used to compute the mixing scale times within the EDC approach.

Concerning the heat flux predictions, each code behaves differently. For example, over/under estimations are obtained in FDS, with an error estimation often lower than 50%. In contrast, heat fluxes are largely over-estimated in FireFOAM, with an averaged error estimation greater than 50%. The implementation of a model constant able to correct the emission term in the DOM equation,

such as this applied in FDS, could improve agreement. Also, a better agreement may be reached in both codes by increasing the number of solid angles. Furthermore, the FLACS-Fire results reasonably match the experimental measurements, as occurs with the predicted flame temperatures. The promising results obtained in FDS and in FLACS-Fire could be also used in further analysis to determine the surface emissive power of the jets by considering the atmospheric transmissivity (often assumed to be 1) and the corresponding view factor.

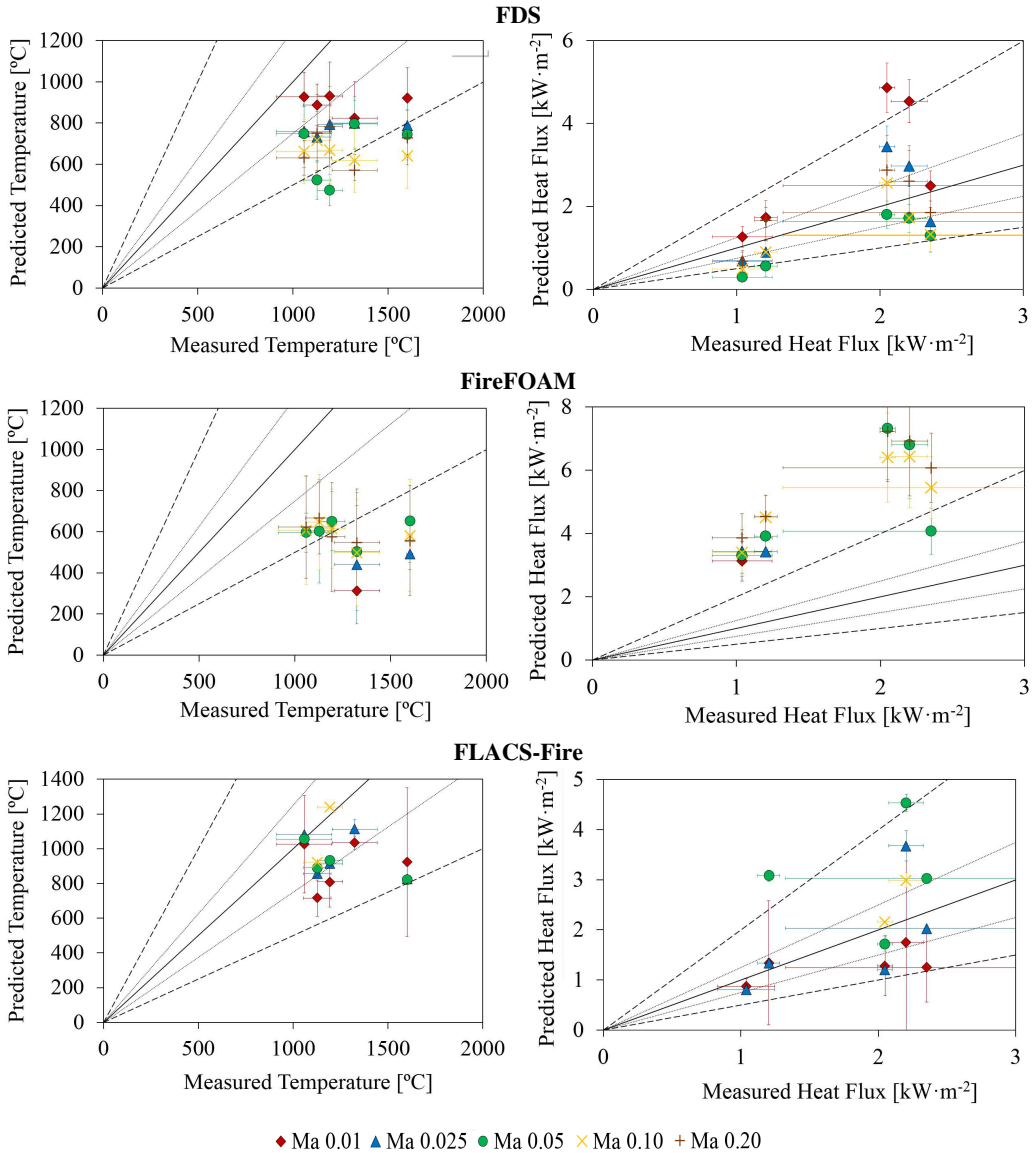


Fig. 5. Predicted values of the mean flame temperatures (left) and the mean radiative heat fluxes (right) estimated in FDS, FireFOAM and FLACS-Fire.

Furthermore, very good agreement is reached in FDS when calculating the mean flame lengths, with error estimations always lower than 25%, whereas less accurate predictions are obtained in FireFOAM and FLACS-Fire (Fig. 6). In general, the lower the Mach number, the more precise the

estimations found in FLACS-Fire. On the other hand, flame areas are reasonably predicted in FDS, with better agreement reached under smaller cells. Contrarily, these are remarkably under-estimated in FireFOAM and in FLACS-Fire, regardless of the cell size. Therefore, both codes simulate very thin flames, hence demonstrating that the air entrained into the domain mixes with the released fuel much faster than in reality.

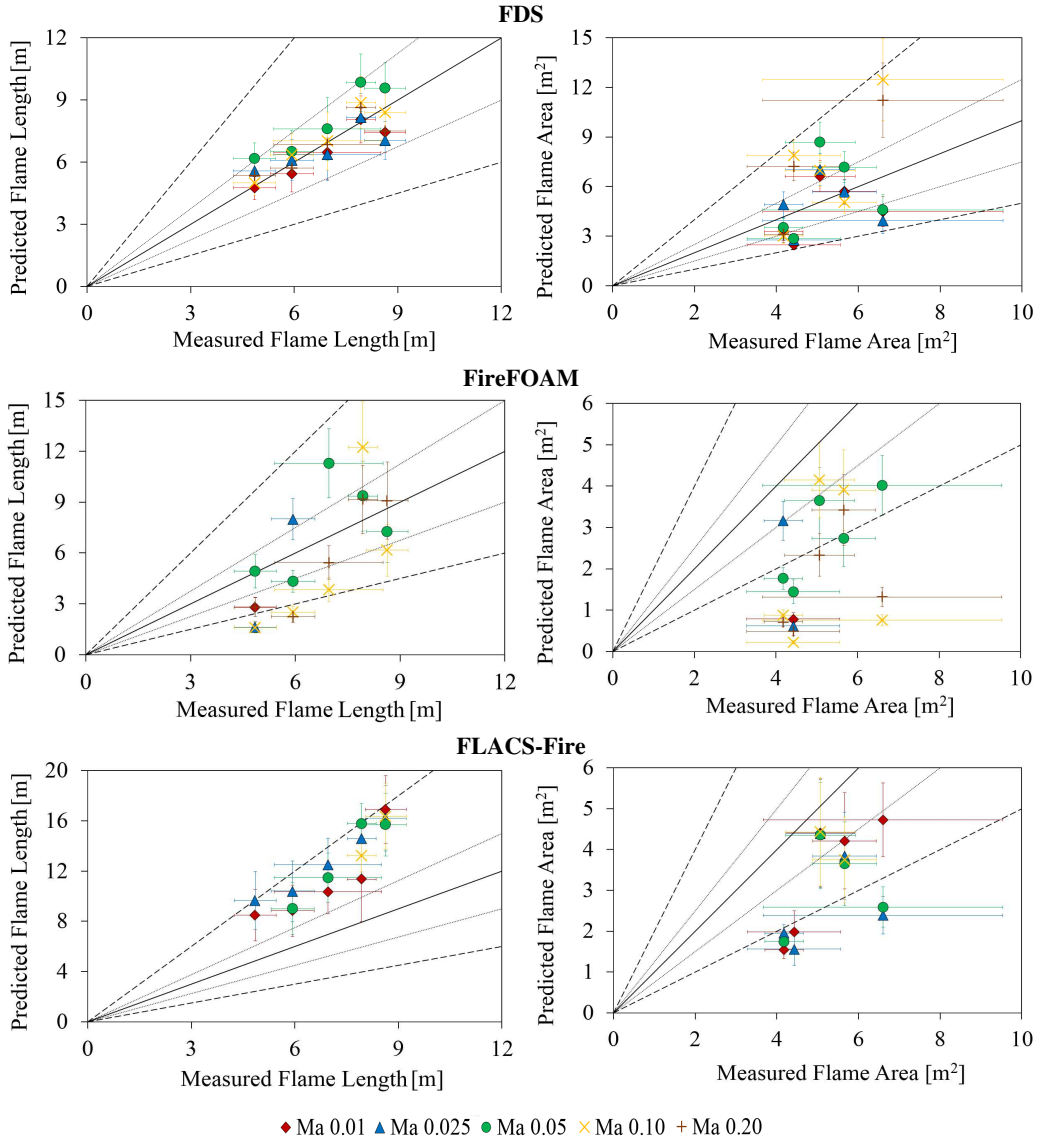


Fig. 6. Predicted values of the mean flame lengths (left) and the mean flame areas (right) estimated in FDS, FireFOAM and FLACS-Fire.

Quantitative error estimation

Qualitative comparisons are of high interest to quickly determine the suitability of a code to predict a variable of interest. However, when using this approach, there is no quantification of either the computational uncertainties or the agreement reached over time. Alternatively, the fractional bias

(FB) and the normalized mean square error (NMSE) quantitative performance measures have been calculated (Table 2) [20]. Although a perfect model would have FB and NMSE values of 0, it is to be noted that for research-grade field experiments, “acceptable” performing models must be within the performance criteria (PC): $NMSE \leq 0.5$ and $-0.3 \leq FB \leq 0.3$ [21].

Table 2. FB and NMSE values for the main variables of interest obtained with the different CFD codes as a function of the Mach number. Bold italic values indicate that the metric is within the established PC

CFD	Mach Number	Temperature		Heat Flux		Flame Length		Flame Area	
		FB	NMSE	FB	NMSE	FB	NMSE	FB	NMSE
FDS	0.01	0.32	<i>0.14</i>	-0.42	<i>0.30</i>	<i>0.06</i>	<i>0.01</i>	<i>0.18</i>	<i>0.13</i>
	0.025	0.47	<i>0.25</i>	<i>0.05</i>	<i>0.15</i>	<i>0.02</i>	<i>0.01</i>	<i>0.10</i>	<i>0.13</i>
	0.05	0.63	<i>0.49</i>	<i>0.26</i>	<i>0.39</i>	<i>-0.15</i>	<i>0.03</i>	<i>0.04</i>	<i>0.14</i>
	0.10	0.61	<i>0.46</i>	<i>0.30</i>	<i>0.23</i>	<i>-0.04</i>	<i>0.00</i>	<i>-0.21</i>	<i>0.20</i>
	0.20	0.57	<i>0.40</i>	<i>-0.03</i>	<i>0.10</i>	<i>0.00</i>	<i>0.01</i>	-0.63	1.09
FireFOAM	0.05	0.70	0.60	-0.96	1.33	<i>-0.03</i>	<i>0.08</i>	0.67	0.62
	0.10	0.71	0.65	-1.01	1.44	0.32	<i>0.47</i>	1.05	5.56
	0.20	0.71	0.64	-1.07	1.65	0.36	<i>0.28</i>	1.12	3.06
FLACS-Fire	0.01	0.33	0.62	<i>0.27</i>	0.38	-0.47	<i>0.26</i>	0.49	1.02
	0.025	<i>0.27</i>	<i>0.13</i>	<i>0.06</i>	<i>0.13</i>	-0.60	<i>0.39</i>	0.63	0.62
	0.05	<i>0.28</i>	<i>0.14</i>	<i>-0.28</i>	<i>0.40</i>	-0.65	<i>0.32</i>	0.57	0.51

Concerning the FDS estimations, it is observed that most of these are within the criteria established. Nevertheless, the notable under-predictions of the flame temperatures lead to fractional bias values greater than 0.30 for all the Mach numbers modelled. Also, non-acceptable values of the statistical metrics are obtained for flame areas and for heat fluxes when simulations are performed with very thin and coarse cell sizes, respectively. Apart from the predictions of the flame temperatures, whose deviations may be caused for multiple reasons (i.e. sub-models implemented, models constants, numerical schemes, etc.), the rest of the variables are reasonably well estimated. In particular, the sonic jet fire simulations performed in the current study are recommended to be run with equivalent diameters obtained with Mach number ranged between 0.025 and 0.10 in FDS. The numerous Mach numbers suggested for FDS allows simulations with multiple cell sizes, which could be of great interest when modelling complex geometries. Moreover, the favourable predictions of the heat fluxes and the flame lengths, make FDS a suitable candidate for determining hazardous effects of sonic jet fires.

Differently, notorious errors are found in the FireFOAM predictions, hence highlighting the need for further improvement before its application when modelling real sonic jet fires. Specifically, a sensitivity analysis of the modelling parameters previously discussed (i.e. model’s constants, mixing scale times, number of solid angles, etc.) could be performed to determine the most suitable ones. Furthermore, FLACS-Fire is revealed as the most suitable among the CFD codes used to determine the flame temperatures of expanded jet fires. Also, the heat fluxes found are in accordance with the performance criteria. However, neither the flame lengths nor the flame surfaces are accurately calculated. Despite this, reliable results can be obtained in FLACS-Fire when the equivalent diameter of the jets is obtained with a Mach number ranged between 0.025 and 0.05.

According to the different levels of agreement in the CFD codes when varying the Mach number, it is deduced that the unconventional boundary condition at inflow have a strong impact on the final

results. Despite the highlighted discrepancies when comparing simulation results with experimental measurements, promising results were often found under very low Mach numbers (≤ 0.05), especially in FDS and in FLACS-Fire. In consequence, reasonable estimations of the main hazardous effects of sonic jet fires can be obtained under cell sizes and equivalent diameters of at least 5 times higher than the exit orifice. In short, the pseudo-diameter approach is noted as a worthwhile technique for modelling sonic flows in CFD.

CONCLUSIONS

1. FDS, FireFOAM and FLACS-Fire codes were used to predict the flame temperatures, the heat fluxes and the flame-geometry descriptors of five propane jet fire experiments in an open environment. Due to the low Mach number formulation of the CFD codes used, the pseudo-diameter approach was used to determine the conditions of the jets after the expansion of the released gas. The equivalent properties of these (temperature, velocity and diameter) were simulated as a function of five Mach numbers proposed for analysis for each jet fire experiment.
2. Simulations and measurements were qualitatively and quantitatively compared in order to reveal the level of agreement reached in each CFD code. Temperatures were only accurately estimated in FLACS-Fire, while FDS and FireFOAM provided notable under-estimations. On the other hand, the radiative heat fluxes were reasonably calculated in FLACS-Fire and in FDS, whereas important over-estimations were achieved in FireFOAM. Also, acceptable predictions of the flame-geometry descriptors were obtained in FDS, while significant discrepancies were achieved in FLACS-Fire and FireFOAM. Indeed, these two codes predicted very thin flames as the air entrained into the domain mixed with the released fuel much faster than in reality.
3. The notorious discrepancies found in FireFOAM suggest that further improvement of the constants, as well as the mixing scale times calculation method within the combustion sub-model should be re-examined. Also, a higher number of solid angles, and the implementation of a correction factor to solve the DOM equation could deliver more accurate radiative heat fluxes predictions. Otherwise, FDS and FLACS-Fire are able to predict reasonably the hazardous effects of sonic jet fires under cell sizes of at least 5 times higher than the exit orifices.
4. This paper has demonstrated the capabilities of CFD tools to predict sonic jet fires by considering the equivalent conditions after expansion. Given the promising results found, especially in FDS and in FLACS-Fire, the pseudo-diameter approach may be used when modelling sonic flows in further analyses. In particular, additional sonic jet fire experiments could be simulated and compared with the main findings highlighted in the present paper.

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REFERENCES

- [1] R. Benintendi, A. Deisy, S. Marsh, A risk-based approach to safety distance determination in the process industry, in: 24th Inst. Chem. Eng. Symp. Hazards, 2014.
- [2] E. Palazzi, B. Fabiano, Analytical modelling of hydrocarbon pool fires: Conservative evaluation of flame temperature and thermal power, *Process Saf. Environ. Prot.* 90 (2012) 121–128.

doi:10.1016/j.psep.2011.06.009.

- [3] J. Casal, Evaluation of the Effects and Consequences of Major Accidents in Industrial Plants, 2nd ed. Elsevier, Amsterdam, 2017.
- [4] M. Gómez-Mares, M. Muñoz, J. Casal, Axial temperature distribution in vertical jet fires., *J. Hazard. Mater.* 172 (2009) 54–60. doi:10.1016/j.jhazmat.2009.06.136.
- [5] A. Palacios, A. Muñoz, J. Casal, Jet fires: An experimental Study of the Main Geometrical Features of the Flame in Subsonic and Sonic Regimes, *AIChE J.* 55 (2008) 256–263. doi:10.1002/aic.
- [6] M. Masum, A. Rahman, S. Ahmed, F. Khan, LNG pool fire simulation for domino effect analysis, *Reliab. Eng. Syst. Saf.* 143 (2015) 19–29. doi:10.1016/j.res.2015.02.010.
- [7] M. Tanabe, A. Miyake, Effective implementation of inherently safer design during design phase of modularized onshore LNG projects, *Chem. Eng. Trans.* 48 (2016) 535–540. doi:10.3303/CET1648090.
- [8] C. Azzi, L. Rogstadkjenet, Use of CFD in the Performance-Based Design for Fire Safety in the Oil and Gas Sector, in: 11th Conf. Performance-Based Codes Fire Saf. Des. Methods, 2016.
- [9] A. Palacios, M. Muñoz, R.M. Darbra, J. Casal, Thermal radiation from vertical jet fires, *Fire Saf. J.* 51 (2012) 93–101. doi:10.1016/j.firesaf.2012.03.006.
- [10] C. Mata, E. Pastor, B. Rengel, M. Valero, E. Planas, A. Palacios, J. Casal, Infrared Imaging Software for Jet Fire Analysis, *Chem. Eng. Trans.* 67 (2018) 877–882. doi:10.3303/CET1867147.
- [11] P. Chatterjee, Y. Wang, K. V. Meredith, S.B. Dorofeev, Application of a subgrid soot-radiation model in the numerical simulation of a heptane pool fire, *Proc. Combust. Inst.* 35 (2015) 2573–2580. doi:10.1016/j.proci.2014.05.045.
- [12] K. McGrattan, S. Hostikka, R. McDermott, J. Floyd, C. Weinschenk, K. Overholt, *Fire Dynamics Simulator User’s Guide*, 2017. doi:10.6028/NIST.SP.1019.
- [13] Y.Z. Li, C. Huang, J. Anderson, R. Svensson, H. Ingason, B. Husted, M. Runefors, J. Wahlqvist, Verification , validation and evaluation of FireFOAM as a tool for performance design, (2017) 84.
- [14] G. AS, *FLACS v10.7 User’s Manual*, 2017.
- [15] E. Franquet, V. Perrier, S. Gibout, P. Bruel, Free underexpanded jets in a quiescent medium: A review, *Prog. Aerosp. Sci.* 77 (2015) 25–53. doi:10.1016/j.paerosci.2015.06.006.
- [16] V.G. Dulov, G.A. Lukyanov, *Gas Dynamics of the Outflow Processes*, Novosibirsk (Russia), 1984.
- [17] A.D. Birch, D.R. Brown, M.G. Dodson, The Structure and Concentration Decay of High Pressure Jets of Natural Gas, *Combust. Sci. Technol.* 5 (1984) 249–261.
- [18] C. Lin, Y. Ferng, W. Hsu, N.T. Hua, Investigations on the Characteristics of Radiative Heat Transfer in Liquid Pool Fires, *Fire Technol.* 46 (2010) 321–345. doi:10.1007/s10694-008-0071-7.
- [19] J.H. Kent, A quantitative relationship between soot yield and smoke point measurements, *Combust. Flame.* 63 (1986) 349–358.
- [20] P. Rew, D. Deaves, The validation and application of pool fire models, in: *Saf. Eng. Risk Anal.*, 1995: pp. 57–65.
- [21] S.R. Hanna, O.R. Hansen, S. Dharmavaram, FLACS CFD air quality model performance evaluation with Kit Fox, MUST, Prairie Grass, and EMU observations, *Atmos. Environ.* 38 (2004) 4675–4687. doi:10.1016/j.atmosenv.2004.05.041.