

Computational Analysis of Vertical Subsonic Propane Jet Fires: A Comparative Study of Commercial (COMSOL) and Open Source (FDS) Software

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Abstract—Jet fires can represent a great potential risk in the industry because they can lead to domino effects. Estimating specific semi-empirical correlations of the behavior of the flame such as thermal radiation, shape, and size can help to minimize or prevent the dangerous effects that a significant accident produced by a jet fire can have, regarding environmental consequences, human and financial losses. Computational Fluid Dynamics (CFD) is a technological tool that helps enterprises prevent major accidents through the simulation of possible scenarios. This paper compares the data obtained through the simulation of propane jet fires with the open-source Fire Dynamics Simulator software and the commercial software COMSOL Multiphysics v5.6 with the experimental data. The different correlations compared consist of flame length, flame area, and equivalent diameter, the results indicated that the jet fires of 12.75 and 20 mm and mass flows of 0.007, 0.016 and 0.020 kg/s were the ones with better correlations to the experimental data and two software programs employed.

Keywords—computational fluid dynamics, propane jet fires, COMSOL Multiphysics v5.6, fire dynamic simulator

I. INTRODUCTION

The production, manipulation, and transportation of hydrocarbon fuels (i.e., propane, methane, among others) imply security, environmental, and financial losses in case of an accident produced by human error, equipment malfunction, uncontrollability of properties—pressure, temperature, wind or the combination of various causes. Various types of accidents can occur in industrial and chemical facilities, such as: pool fires, flash fire, fireball, and jet fires. A special type of event is the jet fire that even though their damage radius is relatively low, they possess high heat fluxes [1], and depend on the fuel discharge rate [2].

Jet fires are turbulent diffusion flames resulting from the combustion of a fuel continuously released with some significant momentum in a particular direction or directions [3]. Jet fires are of particular interest due to the high momentum flame lifted above the mouth of the duct from which the fuel—often gas—is flowing, at a high pressure [2]. The dangerous effects provoked by jet fire explosions or toxic clouds can lead to the domino effect, which is a series of continuous events that aggravate the primary situation [4]. Example of this is the explosion of a pipe that impregnates in nearby equipment leading to injuries, costs per accident, and even deaths [5].

Even though jet fires can occur accidentally, there are some that are voluntary. A clear example is the industrial flare, in which industrial residues of certain processes usually combustible components, mostly hydrocarbons, are burned or thermally destroyed in mass quantities [6]. Regardless, the low damage radius but high thermal fluxes, it is important to be able to predict the size and shape of the flames and the thermal radiation produced [7]. In order to properly study the jet fires, it is necessary to know the parameters to examine.

Experimental jet fires of various sizes have been previously studied by diverse authors implying semi-empirical correlations providing rapid estimations. The results found can only be validated only if the fire scenarios studies are identical to the tests developed [5]. Therefore, recent research has conducted alternative modelling approaches using Computational Fluid Dynamics (CFD) used to estimate the harmful effects of hydrocarbon fires in a wide scope of layouts. CFD techniques can help chemical industries predict and assess fire hazards considering equipment, different types of fuels, location, environmental conditions, and even calculate variables of the user interest.

CFD simulations require input data and expertise within solving codes that can lead to high computational resources. Nowadays, there are main CFD fire codes developed by different research institutes, organizations, and private companies [5]. Consequently, there are commercial codes such as COMSOL Multiphysics that require a license, while others such as Fire Dynamics Simulator (FDS) that is an open source freely available for everyone to use. For that reason, numerous present-day investigations involving jet fires are done using primarily FDS. However, to the best of our knowledge, little or no simulations have been made using COMSOL Multiphysics.

The present paper first carries out a validation of numerical codes, consisting in a comparison process between experimental and predicted data [5], to then contrast the subsonic propane jet fires at different semi-empirical correlations using two different flame modelling software—Fire Dynamics Simulator (FDS) and COMSOL Multiphysics 5.6 to verify their correlation between one and other. The jet fires presented are compared in flame length (L_f), flame area (A_f), and equivalent diameter (D_{eq}).

II. LITERATURE REVIEW

FDS and COMSOL are software used to help simulate and compare fire dynamics in order to prevent an industrial hazard. However, each software encounters advantages and disadvantages presented either from the interface, programming, and show of results. On one hand, FDS is an open-source tool freely available developed by the National Institute of Standards and Technology (NIST). On the other hand, there are commercial codes such as COMSOL Multiphysics v5.6 that require a license to be used. All these are under the CFD domain, which require input data, expert knowledge of the sub-models solved within the codes and most of the time high computational resources.

Both software's allow for more cost-effective fire protection system design through better fire scenario prediction accuracy. FDS solves well-all-important fire mechanisms. Is a program structure that requires commands and the user to understand the programming language in order for the simulations to run, therefore users must understand the mechanism prior to the development of the equations. There is also plenty of information available and ready for the user to understand the interface, since it is the most commonly used CFD model for fire applications. In spite of that, FDS simulation time depends deeply on the mesh and the event simulated. A simple jet fire can run from either minute to days depending on the computer characteristics and input data.

On the contrary, COMSOL Multiphysics software makes it possible for simulation specialists to create easy-to-use simulation scenarios. Conversely to FDS, COMSOL enables the user to simulate all in one program electromagnetic, structural mechanics, fluid flow, heat transfer, and chemical phenomena in one environment [8]. It is also widely used because it is easy to understand the product behavior, since COMSOL provides the user with equations and all the input data depending on the interface using (e.g., Chemical Reaction gives the Arrhenius equation). It also provides answers quickly not depending on the fine-tuned mesh, solver, or other conditions. Nonetheless, in the fire industry COMSOL has not been extensively used making it harder to understand the software and finding information regarding jet fires.

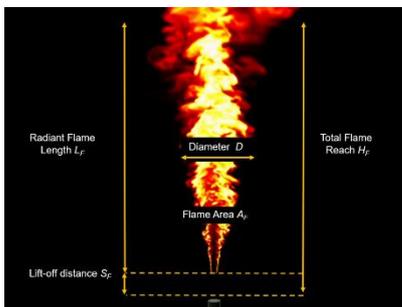


Fig. 1. Jet fire descriptors.

To prevent the most severe effects and consequences in the event of a jet fire, it is fundamental to assess the characteristics of the flame. For that cause, the flame-geometry descriptors need to be estimated. Fig. 1 identifies the most common jet fire descriptors. These are defined as: (i) radiant flame length (L_f), as the distance from the base of the fire to the fire tip of the visible flame; (ii) the total flame reach, (H_f), as the distance from the exit orifice to the tip of the

visible flame; (iii) flame area (A_f), flame surface defined by a given isothermal or by the visible flame; (iv) lift-off distance (S_f), distance from the exit orifice to the base of the flame, and (v) diameter (D), mean width occupied by the flame [7]. However, during the present paper, only the flame length, flame area, and diameter will be further evaluated.

Due to the high-turbulent flows occurring in accident fires, the exact solution of the governing equations is beyond the capabilities of the most powerful computers [5]. Numerous turbulence models have been developed. FDS utilizes the Large Eddy Simulations (LES) turbulent model equations. LES emphasizes spatial filtering by considering the structures smaller than the grid cell. In addition, LES does not require any additional equations, hence rendering a more realistic-looking flow field. The hydrodynamic model of FDS solves numerically the Navier Stokes equations that correspond to the low velocity flow that has thermal impulse for the transportation of smoke and heat from fires. The turbulence is treated through the LES; it creates with great accuracy turbulent flows and the calculation times are significantly lower than those from a Direct Number Simulation (DNS). To model the turbulence in the LES simulations there is an added viscosity called the turbulent Eddy viscosity (ν_t), given by Eq. (1):

$$\nu_t = C^2_x \Delta^2_x \bar{\omega} \quad (1)$$

Up until now, FDS has been revealed as the most appropriate code able to reasonably predict fire hazards of different types of hydrocarbon fires [5]. Under the use of CFD simulations, the cell size represents the most important numerical parameter user-defined. Hence, the smaller the cell size, the better the computational resolution and the larger the simulation time [9]. Therefore, the selection of the suitable cell sizes mostly depends on the fire regime. This paper presents, buoyant and subsonic vertical propane jet fires, in which the non-dimensional expression D^*/δ_x (i.e., characteristic fire diameter and cell size) is recommended to measure how effectively the fluid flows in buoyant and subsonic regimes [10].

III. MATERIALS AND METHODS

A total of twenty fire vertical scenarios—jet orientation—simulations were conducted under FDS, for nozzle diameters of 12.75, 20, and 43.1, all in mm, and mean mass flows of 0.007, 0.016, 0.020, 0.066, and 0.142, all in kg/s. The flame length and flame area are parameters that can be obtained with no further analysis using FDS. However, the diameter must go through a different process due to FDS not being able to read the real diameter because it depends on a suitable cell size and the fire regime. Therefore, a sensitivity analysis was carried out following suggested values, proposed by Rengel [5], given four different D^*/δ_x for the analyses, which are: 8, 12, 16, and 32. Once the correlation of the equivalent diameter is defined, cell sizes can be calculated as well.

A treatment to the data must be carried out in which Eq. (2) shows the non-dimensional expression D^*/δ_x , is recommended to measure how well the fluid flows in buoyant and subsonic fire regimes.

$$D^* = \left(\frac{\dot{Q}}{\rho_{air} C_p T_{\infty} \sqrt{g}} \right)^{\frac{2}{5}} \quad (2)$$

where D^* is the characteristic diameter of the fire, \dot{Q} heat release rate of the fire, ρ_{∞} the ambient air density, C_p the specific heat, T_{∞} ambient temperature, and g the gravitational acceleration. The D^*/δ_x expression can be seen as the number of grid cells spanning the characteristic diameter of the fire, whose values ranged between 4 and 16.

Table 1 shows the diameters obtained for the five vertical jet fires with different nozzle sizes and mass flows. All data were prior corroborated along with Rengel [5] information.

Table 1. Equivalent diameter for vertical propane jet fires obtained from experimental data

Experiment	D^* (mm)	Mass flow (kg/s)	D^*/δ_x			
			8	12	16	32
V12.75_0.007	12.75	0.007	60	40	30	20
V12.75_0.016	12.75	0.016	90	60	40	20
V20_0.020	20	0.020	100	60	50	20
V43.1_0.066	43.1	0.066	150	100	80	40
V43.1_0.142	43.1	0.142	200	150	100	50

The bare set-up for modelling jet fires in COMSOL Multiphysics was selected as one of the simulations predefined by the software. For COMSOL to properly achieve the primary goal of developing a jet fire, a different approach was selected, in which the simulation would start with air and further in the reaction section propane would be added as the fuel to change the primary characteristics of the jet fire. Therefore, COMSOL requires the velocity and the density of the air. Table 2 registers the air density and velocity input as parameters for COMSOL.

Table 2. Air parameters used as input data for COMSOL v5.6

Name	Value	Units	Description
v_{air}	9	m/s	Air velocity
ρ_{air}	1.2	kg/m ³	Air density

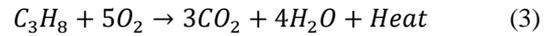
After, the geometry is specified. For this, a rectangle shape is desired with a width of 15 m and a height of 20 m. These measures were selected to have a broader range of simulation. The construction of the nozzle is fixed at a certain length from the width previously established. For making the nozzle distance (i.e., equivalent diameter) the remaining measure is added in comparison with the data obtained from FDS. The value of the nozzle changes according to the simulation running, hence simulations having a mass flow of 0.007 kg/s

will not have the same nozzle constructed as for mass flows of 0.142 kg/s. The geometry set-up that has COMSOL gives the user the availability to either insert the real nozzle size or the equivalent diameter without having errors during the simulation.

Then the turbulent flow $k-\varepsilon$ (spf) is added. The model is the most common used in CFD to simulate mean flow characteristics for turbulent flow conditions. During the selection of the model, different boundaries were applied to understand the movement of the jet fire. The inlet selected for the jet fire carrying the substance as fuel enters through the nozzle, placed at the middle of the 15 meters of width, where the propane mixed with oxygen will come out to start the combustion mechanism. In this case, the outlet boundaries are defined as the perimeters of the geometry—the right, left, and upper walls—without counting the floor. Since from the bottom will come the fuel.

Once the flow is coupled, the Heat transfer in fluids (ht) is added. This interface accounts for conduction and convection in gasses and liquids as the default heat transfer mechanism [8]. This interface requires the user to set-up the range of temperatures the jet fire will have. For example, as a first approximation, the jet fires were performed from 293 K to 500 K on the same domains for the turbulent flow, meaning that it is supposed that air is entering at 293 K and leaving the boundary at 500 K. Nevertheless, the range can change depending on the conditions.

Finally, the Chemistry (chem) is added, where the reaction is added and is the primary interface since the jet fire combustion reaction will take place. In here, an irreversible reaction is added and four different species as well. The four different species correspond to the propane combustion rate seen in Eq. (3).



The Chemistry interface also requires the constant rates defined by the Arrhenius model, observed in Eq. (4).

$$k = A \cdot e^{-\frac{E_A}{RT}} \quad (4)$$

where the frequency factor (A) and the activation energy (E) were input from the power law model for the combustion of propane [11]. As final parameters, COMSOL requires the molar mass and density of the species (i.e., propane, oxygen, carbon dioxide, and water). All prior parameters mentioned can be found on Table 3.

Table 3. Propane combustion parameters

Substance	Value	Units	Description
Propane	44.09	kg/kmol	Propane molar mass
Oxygen	31.99	kg/kmol	Oxygen molar mass
Carbon Dioxide	44.009	kg/kmol	Carbon dioxide molar mass
Water	18.01	kg/kmol	Water molar mass
T_inletP	400	K	Inlet temperature
T_inletA	303.15	K	Inlet temperature
E_A	8.43×10^4	J/mol	Activation Energy
A	$2.38 \times (10^5) \times 101325$	1/s	Frequency Factor
k_{cte}	$A \times \exp(-E/(R_{cont} \times T_{inletP}))$	1/s	-
H_I	-2220100	J/mol	Reaction enthalpy

Quantitative comparison between simulations results and experimental measurements have been carried out to assess the result's accuracy obtained with the CFD codes [5]. Statistical measurements of the flame geometry descriptors obtained in FDS for vertical subsonic propane as a function of the cell size and geometrical variables are compared with COMSOL results using the Fractional Bias Eq. (5) and Normalized Mean Square Error Eq. (6) statistical methods, where x_m are the mean experimental values and x_p the mean experimental predicted values.

$$FB = \frac{1}{n} \sum_{i=1}^n 2 \frac{x_m - x_p}{x_m + x_p} \quad (5)$$

$$NMSE = \frac{1}{n} \sum_{i=1}^n \frac{(x_m - x_p)^2}{x_m x_p} \quad (6)$$

Finally, an assessment of predictions is done by graphical methods—qualitative comparison—in the form of scatter plots, illustrating the level of agreement found in each simulation. The solid diagonal line indicates perfect agreement between simulated and experimental values, while long-dashed lines represent the $\pm 20\%$ and $\pm 40\%$ prediction error with regard to the measurements.

IV. RESULT AND DISCUSSION

As it can be seen from Table 1, a total of 20 simulations were performed using FDS. The sizes of the cells determined (δ_x) are always greater than the original nozzle diameter (D_{or}). Consequently, equivalent nozzle diameters are defined with the same size as the calculated cell. For example, the V12.75_0.007 ($D^*/\delta_x = 8$) scenario will be modelled with an equivalent nozzle diameter of 0.06 m and a cell size of $0.06 \times 0.06 \times 0.06 \text{ m}^3$.

Besides the quantitative analyses a validation analysis must be performed for both software's. The validation of numerical codes consists in a comparison process between experimental and predicted data. This step is a first necessary requirement before their use in real applications. The physical phenomena of interest can be determined and the uncertainties generated either in the conceptual modelling or during the computational design phase can be highlighted. The first comparison method used is a quantitative statistical method. These methods are used to evaluate the computational uncertainties and the agreement reached over time. Table 4 summarizes the quantitative error of the experimental and predicted data for both FDS and COMSOL.

Table 4. Quantitative error of the experimental and predicted data for FDS and COMSOL

CFD	Simulation	L_f [m]		D_{eq} [m]		A_f [m ²]	
		FB	NMSE	FB	NMSE	FB	NMSE
FDS	V12.75_0.007	-1.71	10.70	1.46	4.56	-1.71	10.90
	V12.75_0.016	-1.46	4.58	1.33	3.15	-1.40	3.85
	V20_0.020	-1.31	3.02	1.44	4.25	-1.09	1.70
	V43.1_0.066	-0.55	0.33	1.71	10.84	0.84	0.85
	V43.1_0.142	-0.45	0.22	1.66	8.81	0.95	1.15
COMSOL	V12.75_0.007	-1.71	11.01	1.46	4.58	-1.69	10.12
	V12.75_0.016	-1.47	4.74	1.33	3.18	-1.36	3.48
	V20_0.020	-1.35	3.38	1.44	4.28	-1.11	1.79
	V43.1_0.066	-0.46	0.22	1.71	10.87	0.99	1.30
	V43.1_0.142	-0.38	0.15	1.66	8.79	1.06	1.55

The use of the statistical methods FB and NMSE show a performance measurement of the evaluated codes. These methods were selected as a recommendation for the evaluation of predictions of CFD codes according to Hanna and Hansen *et al.* [11]. In the case of the FB, negative results indicate that the values have been overestimated, while positive results show that the values have been underestimated. In the case of the NMSE, is a measure of the scatter that reflects the fit of the estimation data [5]. Therefore, the simulations that best approach the experimental data from [3] are the simulations with a nozzle size of 43.1 mm and a mass flow of 0.066 and 0.142 kg/s.

Qualitative scatter plots illustrate the level of agreement reached between predictions and measurements. The assessment of predictions was studied in comparison to the validated data from Palacios and Muñoz *et al.* [7], with reference lines that work as a qualitative error, ranging from $\pm 20\%$ and $\pm 40\%$.

Closer to the solid diagonal line, the more accurate the predictions are. Fig. 2 shows the mean jet flame length obtained for vertical propane jet fires in FDS and COMSOL.

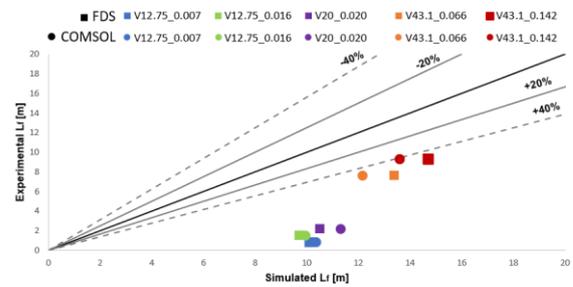


Fig. 2. Mean jet flame length comparison for FDS and COMSOL.

As seen from Fig. 2, both software's show good agreement for the highest diameter nozzle (i.e., 43.1 mm) and higher mass flow rates, jet fires having 0.066 and 0.142 kg/s, ranging in areas near the agreement line of +40%. Demonstrating that these simulations performed agree with also the statistical measurements (i.e., FB and NMSE). Although the correlation regarding the length flame shows good results, a better approximation can be performed. The length flame was calculated with stationary image frames by obtaining the average of the pictures according to each flame.

Fig. 3 indicates the mean jet flame area for FDS and COMSOL. FDS and COMSOL show a better approximation for all fire propane scenarios that were conducted for nozzle sizes of 12.75 and 20 mm—colored in blue, green and purple. The results show that a good agreement occurred near the agreement line of +40%. However, for higher mass flow rates and nozzle diameter of 43.1 mm, the programs seem to obtain discrepancies due that the area was calculated with stationary frame images enclosing the flame into an oval, having black space accounted for during the calculation that must not be considered.

Another studied variable is the mean equivalent diameter shown in Fig. 4 for both FDS and COMSOL. The CFD results estimations lead to an error of -40% for the simulations with a nozzle sizes of 12.75 and 20 mm with their corresponding mass flow rates of 0.007, 0.016, and 0.020 kg/s. As seen from Fig. 4, FDS and COMSOL have the same value, since as in FDS, the equivalent diameter is an input parameter prior

calculated to run the simulations, while for COMSOL, the user has the option to either input the real or equivalent nozzle diameter and hence the equivalent diameter was selected to be able to compare results.

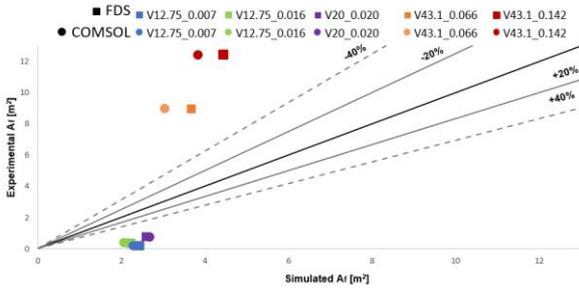


Fig. 3. Mean jet flame area comparison for FDS and COMSOL.

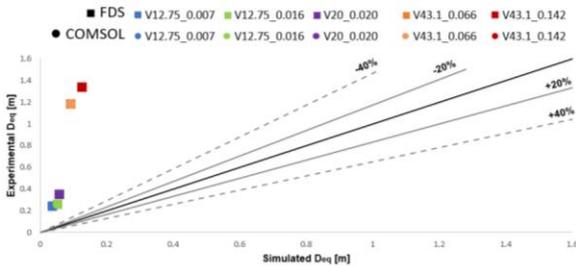


Fig. 4. Mean jet flame equivalent diameter comparison for FDS and COMSOL.

To completely evaluate the performance of the system a close relationship must exist within the mesh and the computational time. This implies the most arduous step during the simulation since it will define the results presented. All simulations and results presented were run at a time frame of 30 s. The time was selected in order to facilitate and speed up the simulations and to lower the computational time. Even though both CFD fire simulators can run up to various times, each one within their mechanisms and interfaces performed the simulations at a delimited time linking the amount of necessary data to yield a result. In this case, COMSOL proved to be faster at the time of running the codes.

V. CONCLUSION

The study of jet fires is important due to different descriptors that must be examined in order to prevent the domino effect or to predict the flame shape and form. CFD tools help the user predict a risk and are important instruments for understanding and mitigating the hazard. Either FDS or COMSOL give the same output with a different interface. On one hand, it can be seen that both programs seem to work properly and better for partial nozzle ruptures—including nozzle diameters of 12.75 and 20 mm—while for bigger ruptures (i.e., nozzle of 43.1 mm) shows less agreement. On the other hand, COMSOL Multiphysics v5.6 enriches and gives the user the knowledge behind the simulation and even shows the results with higher resolution.

All flame geometry descriptors analyzed, showed an error ranging between $\pm 40\%$, expressing good approximations. Nevertheless, FDS serves as a primary tool to develop fire hazards, COMSOL Multiphysics v5.6 has rarely been used as a study tool for jet fire scenarios. As a primary result, to study jet fires in COMSOL, a set of input data given by the

user must be defined, such as: geometry, material, borders, hydrodynamics model, substances (i.e., propane), heat transfer mechanism, and the reaction.

The experimental results obtained with vertical propane jet fires with a nozzle sizes of 12.75 and 20 mm with mass flows of 0.007, 0.016 and 0.020 kg/s have shown both good quantitative and qualitative features. Three descriptors of the jet flames were studied in this paper; (a) for the equivalent diameter both software’s demonstrated agreement near -40% ; (b) for the jet flame area FDS and COMSOL demonstrated results near the agreement line of $+40\%$; (c) for the length flame, the propane jet fire of 43.1 mm with both mass flows showed an agreement near the $+40\%$, while FDS being follow behind and also approximated to the agreement line of $+40\%$. Thus, the results offer a good comparison between a commercial and an open-source software.

As future work, a binary code in a programming language using a gray scale can be further studied to attempt to calculate the real length and area of the jet fire. Finally, the simulations performed during this analysis were at 30 s each to obtain proper results and good resolution. However, it is suggested that the simulations are runed at least 1 min to observe the flame behavior under the same circumstances and compare further results.

NOMENCLATURE

A	Frequency factor (1 s^{-1})
A_f	Flame area (m^2)
C_p	Specific heat ($\text{kJ kg}^{-1} \text{K}^{-1}$)
C_x	LES model constant
D	Diameter (m)
D_{eq}	Equivalent diameter (m)
D_{or}	Nozzle diameter (m)
D^*	Characteristic fire diameter
E_A	Activation energy (J mol^{-1})
g	Gravitational acceleration (m s^{-2})
H_f	Total flame reach (m)
H_1	Reaction enthalpy (J mol^{-1})
$k \text{ cte}$	Arrhenius rate constant
L_f	Flame length (m)
\dot{m}	Mass flow rate (kg s^{-1})
P	Inlet pressure (Pa)
\dot{Q}	Heat release rate (kW)
R	Ideal gas constant ($\text{J K}^{-1} \text{mol}^{-1}$)
S_f	Lift-off distance (m)
T	Temperature (K)
T_∞	Ambient pressure (Pa)
Greek	
δ_x	Cell size (m)
Δ_x	Lattice spacing
ε	Turbulent dissipation rate ($\text{m}^2 \text{s}^{-3}$)
v_{air}	Air velocity (m s^{-1})
ν_t	Turbulent Eddy viscosity ($\text{kg m}^{-1} \text{s}^{-1}$)
ρ_{air}	Air density (kg m^{-3})
x_m	Mean experimental value
x_p	Mean experimental predicted value
ϖ	LES model operator

Abbreviations

CFD	Computational Fluid Dynamics
FB	Fractional Bias
FDS	Fire Dynamics Simulator
NMSE	Normalized Mean Square Error

CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHOR CONTRIBUTIONS

A. Palacios; P. M. Castro-Olivera; A. Llante-Salas; V. Foroughi; J. Casal conducted the research, analyzed the data, and wrote the paper. All authors had approved the final version.

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