Chapter 6

Applications of CFD for Process Safety

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Additional information is available at the end of the chapter

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Abstract

Nowadays, the statistical studies have revealed that major accidents (MA) are frequent in diverse industries, which has originated the development of strategies and normative focussed in foreseeing and preventing these. Thus, the process safety is in continuous improvement. The experimental studies in this field result in situations of high risks and are usually expensive. Therefore, the implementation of developments as the computational fluid dynamics (CFD) techniques is now applied, and has proven to be advantageous. In this work, CFD models for pool and jet fires are presented, as these kinds of fires are usually involved in major accidents. The results of the CFD models show orders of magnitude and behaviors in good agreement with experimental observations found in literature. The outputs of the simulations showed values of around 500 and 1400 K for the pool fires; while the jet fires predictions were of temperatures around 500 and 1050 K. Furthermore, the information obtained by these models can be used in order to develop safety plans to diminish risks in the facilities designs, safe zones and emergency exit routes.

Keywords: CFD multiphysics, mathematical modeling, safety, major accident, process safety

1. Introduction

The development of the chemical industries, as well as emerging fields of nanotechnology, energy generation, biotechnology and pharmaceutical, among others, as well as the storing, handling, transport and transformation of their products, has resulted in an increasing need of handling and storing flammable and explosive substances. Consequently, the risks in chemical plants have increased dramatically and major accidents (MA) have taken place more frequently [1]. It has been recorded that these kinds of accidents represent great losses in terms of lives, environmental impact and destruction of equipment and buildings. In fact, only in 2015 the National Fire Protection Association (NFPA) reported that there were 1,345,500 fires in the USA, that caused the death of 3280 civilians and injured 15,700 more, and represented $14.3 billion dollars in property damage [2].

Statistical studies of MA, such as those shown in **Table 1**, show how these events have been constantly present throughout history and throughout the civilized worldwide. And therefore, further efforts must be carried out in researching on the process safety.

This has conducted to the development of a scientific discipline: The Process Safety [7]. This concept must be now part of our daily life in order to ensure the sustainable development of the planet [4], to ensure the safety of the people and to reduce the economical impact. Furthermore, the risk analysis is yet in continuous development. Large multi-sector efforts for identifying hazards to ensure the safe design and operation of a system in process plants and other facilities [8] are being developed, with the challenge of dealing with real-time support for decision-making, in the multiple scenarios with unpredictable conditions [7].

Regarding the study of MA in the process safety, three kinds of accidents can be distinguished: breaching, explosions and fires [5]. All of which have been widely studied, mostly through experimental methods, that have led to the generation of a great number of semi-empirical correlations [9, 10]. These have been used like tools or guidelines as assistance for the Inspection Management in Chemical Plants, and for the calculation of consequences by simplified procedures [11].

Authors, year	Description
Girgin and Krausmann [3]	Incidents at US onshore hazardous liquid pipeline systems were analyzed with an emphasis on natural hazards (natechs). The analysis covered about 7000 incidents in 1986–2012. Natechs resulted in 317,700 bbl of hazardous substance release and 597 million USD economic damage.
Kannan Pranav et al. [4]	A collection of 96 incidents of process safety from across de world is categorized and analyzed to identify proximate causes and deficiencies in the safety management. Emphasis is placed in that these are not statistically representative due to the lack of a universal database of incidents.
Mannan [5]	In Chapter 2, incidents and loss statistics are discussed, with information from proper sources. The arrangements for the control of major hazards in the European Community and in the United States are briefly reviewed. Chapter 26 shows important things to be learned from the incident about case histories and information from some recognized databases in the world.
Chen Yinting et al. [1]	From 1951 to 2012, 318 domino accidents were collected and analyzed. Flammable substances are the most common material involved in Domino effects. Of all 318 samples, 237 cases associated with flammable substances. 71.1% domino accidents occurred in developed countries, while only 28.9% occurred in developing countries. It can be explained by the massive presence of large-scale chemical plants with giant facilities which contain large quantities of flammable substances and toxic materials. Besides, the accidents reporting mechanisms in developed countries allow getting information easier.
Vílchez et al. [6]	A survey of accidents involving hazardous materials has been performed. A total of 5325 accidents taken from the database MHIDAS, covering from the beginning of twentieth century up to July 1992. The data show the distribution of percentages of accidents in various areas.

Table 1. Selection of statistical and historical studies of MA.

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However, despite the extensive efforts and development in the study of fires in MA, the unpredictability of the phenomena and the difference in the length scales that these take place, as well as the influence and limitations given by the experimental conditions in the reported works, have motivated the development of mathematical models that allow the prediction of fires and their consequences. It is noteworthy that the implementation of these models implies further complications in the evaluation of parameters and variables that are frequently unknown, such as the heat transfer coefficient (*h*), emissivity, radiation models, transmissivity, reflectance, among others, leading to a great gamut of approaches. For example, the hybrid models, where the semi-empirical correlations are coupled with the mathematical models in order to find valid solutions to the transport equations; and also, in recent years, with the development of computers and numerical methods, the computational fluid dynamics (CFD) applied in these topics have shown to be advantageous. Principally, due to that these techniques and models provide not only accurate hazard assessments such as thermal energy flux level, overpressure contour and distribution of toxic cloud, but also detailed information about the spatial and temporal evolution of accidental events [7], allowing detailed three-dimensional analysis in the presence of obstacles, bunds and congested industrial layouts [12]. Thereby, several specialized CFD software in the study of fires have been developed, as well as applications for general purpose CFD software. A selection of general purpose and specialized CFD software can be seen in **Table 2.**

This approach, through CFD simulations, has been of great advantage compared with experimental methods, as experiments are usually expensive, dangerous and practically impossible

Software	Characteristics	Developer/ License	Platform
COMSOL Multiphysics	General-purpose CFD software, based on FEM, specialized in the modeling of coupled multiphysics phenomena, such as non-isothermal flows with mass transfer and chemical reactions	COMSOL/ Paid	Windows Mac OS X Linux
Ansys CFX	CFD software, part of the ANSYS family of products of Fluid Dynamics. Allows to simulate chemical reactions and combustions as well as fluid flow	ANSYS/ Paid	Windows, Linux
FLAIR	Special-purpose CFD software for HVAC systems, smoke movement and fire spreading	CHAM/ Paid	Windows, Linux
Fire dynamic simulator and smoke view (FDS – SMV)	FDS is a special-purpose CFD model for fire-driven fluid flow. SMW is the visualization software for the FDS simulations results	NIST/Free	Windows, Mac OS X, Linux
SmartFire	Special-purpose CFD software for fires simulation and analysis, as well as evacuation analysis	FSEG/Paid	Windows
Kobra-3D	Special-purpose CFD software for smokes simulation and heat transfer in buildings. Includes mass transfer with generation equations	IST GmbH/ Paid	Windows
Solvent	Special-purpose CFD software for the simulation of fluid flows, heat transfer and smoke transport in tunnels	Solvent/ Paid	Windows

Table 2. Commercial CFD software with application for process safety and fires analysis.

to perform at very low scales, such as microscales [13], or very large scales of hundreds of meters. Thus, there are still lots of unsolved issues in the process safety engineering. Many of those issues related to the domino effect usually presented in MA [3, 6, 14].

It is common to find turbulent flows when studying the MA, and thus this has been a great motivation for their study and modeling, besides the motivation due to the costs reduction, as the need to build and test prototypes is avoided [15]. The main approaches through CFD in order to model the turbulent flows in MA leading to acceptable results are the implementation of Reynolds-Averaged Navier-Stokes (RANS) models, large eddy simulations (LES), direct numerical simulation (DNS) and hybrid LES/RANS techniques. However, computational costs may exceed the computing capacities if the detailed characteristics of reactive turbulent flows are intended to be observed, such as eddies, velocity patterns, high-vorticity regions, large structures that stretch and engulf, etc. And thus, generally the standard $\kappa-\varepsilon$ turbulence models provide good results; although sometimes, certain modifications need to be taken into account.

The procedure to approach the solution of problems through CFD techniques is depicted in **Figure 1**. In general, the process consists of three important steps: preprocessing, processing and postprocessing. It is also of great importance the validation of the outputs of the CFD models results against experimental data. Special attention should be drawn to the preprocessing step, as in this step the understanding of the phenomena will be developed; and a correct understanding of the phenomena will allow to take into account the proper considerations and simplifications. As seen in the diagram, when there is a bad agreement between the models results and the experimental observations, sometimes the problem lays in the definition of the problem itself, this means, in the preprocessing steps. In this chapter, following the CFD modeling process

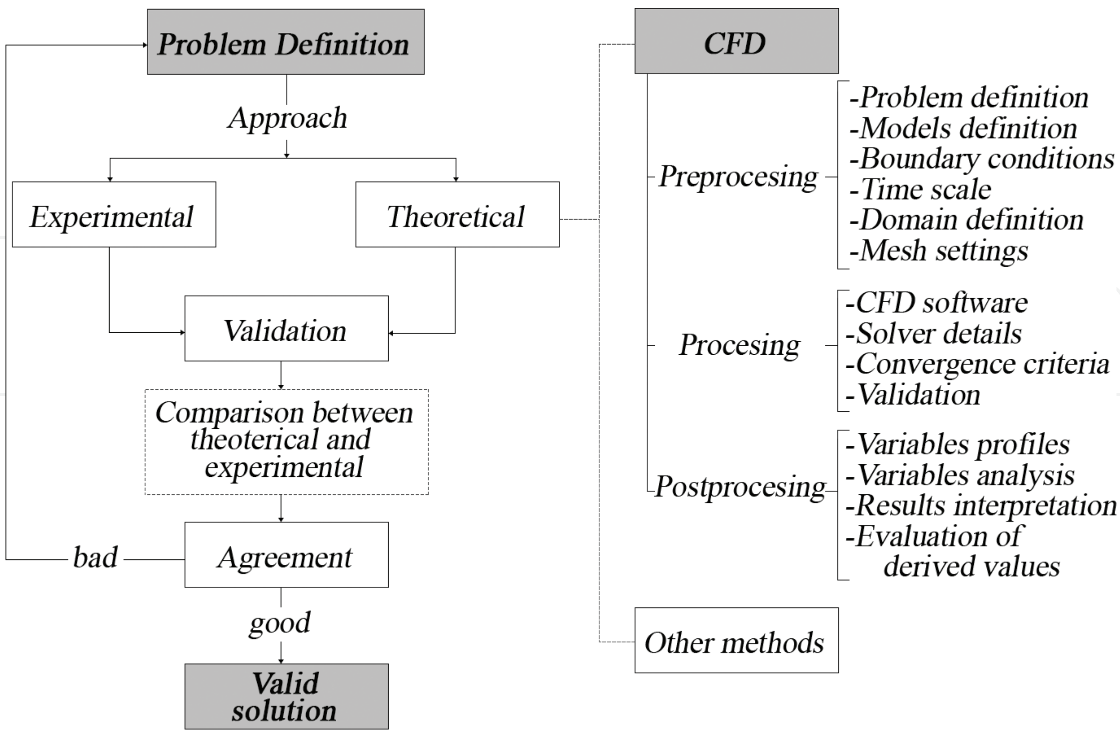

Figure 1. Proposed CFD modeling process considering comparison against experimental approaches.

aforementioned, two characteristic kinds of fires in MA are presented. Sections 2 and 3 present the preprocessing steps; the processing step is also depicted in Section 3; and lastly Section 4 presents the postprocessing steps. The models for these fires are developed though COMSOL Multiphysics CFD simulations, coupling momentum, mass and heat transfer, considering radiation, for pool and jet fires. The models also consider the turbulence flows through Reynolds-Averaged Navier-Stokes (RANS) equations, using the $\kappa - \varepsilon$ model. The predictions obtained with the models properly predict the behavior of experimental observations reported in literature.

2. Fire modeling

The fire consists of a process where complex physical and chemical phenomena occurs simultaneously producing heat. In order to study fires, there are several classifications according to the materials involved, the source or the place in which they are presented. These are of great importance in order to understand how to control the fires, which kind of fire extinguisher should be selected, the consequences of the fire and the radius of impact of these. Two of the main classifications are the following

i. By the material: Fires involving solid, liquid or gases, which gives rise to the following classification or class. For each class, there is a suggested kind of fire extinguisher.

  a. Combustible materials: wood, paper, textiles, rubber

  b. Flammable liquids and gases: gasoline, solvents, hydrocarbons

  c. Electrical fires

  d. Flammable metals: sodium, potassium, magnesium, titanium, zirconium and other metals

  e. Cooking oils and fats

ii. By the source or the place where they are presented.

  a. Wildfire or forest fires: sub classified in other three types: crown fires, surface fires and ground fires

  b. Industrial process fires: vapor clouds fires, fireballs, jet flames, pool fires, running liquid fires, fires of solid materials, dust fires, warehouse fires, sea fires, fires in oil spills in the ocean

  c. Building fires: Structures of diverse dimensions, from small houses to large buildings

Regarding MA, these take place in uncontrolled places and times, which is actually what defines, up to a great extent, the characteristics and dynamics of the fire. Thus, in order to properly model the fire, the behavior of each kind of fire must be understood, as this will allow the adequate establishment of the differential equations and their most convenient boundary conditions. Due to the aforementioned, a further discussion of the phenomena in jet and pool fires is presented in the subsequent pages.

2.1. Pool fire

Pool fires occur when a flammable liquid spills or is poured in the ground and ignites. The shape and dynamics of these fires depend on many variables, such as obstacles, barriers found, whether the leaking is continuous or of a brief duration, as well as the surroundings meteorological and environmental conditions. This prior is highly important as MA usually takes place in open areas, and thus there is a remarkable effect of the wind over the geometry of the flame, the oxygen inflow and the heat transfer mechanisms. These kinds of incidents represent a major complexity as great quantity of phenomena take place simultaneously. **Figure 2** depicts a simplified representation of the phenomena involved in pool fires.

The volatile flammable compounds feed the combustion zone in gas phase under the proper conditions. The drag of the air can be impelled by the wind force or the free convection, depending on the conditions surrounding the fire. The combustion can consist of up to thousands of elementary reactions with intermediate steps that may include hundreds of more chemical species (this great amount of species is commonly observed in MA involving hydrocarbons, as fuels and diesel). Also, generally fires produce smokes with solid particles. Depending on the nature of the combustible, the smoke may contain high concentrations of finely dispersed particles, commonly known as soot, and somniferous gases, as carbon monoxide, as well as other commonly produced products of combustions. Due to these complexities, it can be understood why this is yet an issue of research.

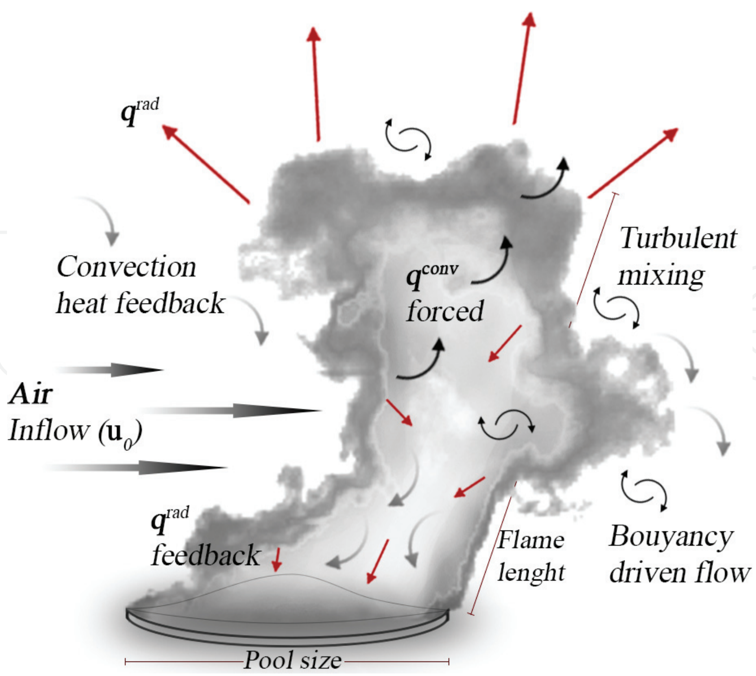

Figure 2. Typical pool fire in presence of wind.

For many years and with diverse approaches, pool fires have been widely studied. Experimental approaches that have led to correlations to predict the fire characteristics are noteworthy, such as burning rate [16], flame tilt angle [17], flame length [18], surface emissive power [19], soot production and radiation [20]. However, it is important to point out that major efforts in the amount of experiments over diverse scenarios, large scales and wind influence, are yet required [21]. The theoretical proposal, that consist in the resolution of the transport equations coupled with the kinetics for the diverse reactions taking place in the phenomena, will be discussed in the upcoming section.

Despite the great advances in the study of pool fires, there is still no model that accurately predicts the proper behavior of fires at the diverse length-scales, and describes all the relevant variables satisfactorily [22]. This is by reason of that most of these have been developed in small scales, and due to the complexity and variability of fires. Furthermore, in theoretical studies turbulence models are still being developed [15], and the multiphysic-multiscale nature is still a challenge to overcome [23]. Moreover, there are also restrictions in theoretical approaches due to the high computational costs.

2.2. Jet fire

Jet fires are characterized by the presence of stationary turbulent diffusion of flames that can reach great lengths and short amplitudes. This kind of fires can be present in closed or open areas. This can be whether generated or accidental, without having notable differences. The source of generated jet fires are usually valves, and can reach supersonic velocities; while accidental jet fires are usually due to holes caused by breakings in pipelines or flanges, and thus the outlet velocities are usually lower, reaching at most (most cases) sonic velocities. Jet fires can arise from gases, liquids or biphasic mixtures. **Figure 3** depicts a simplified diagram of some of the phenomena present in jet fires.

The properties of jet fires depend on the composition of the fuel, the release conditions, the amount of released mass, geometry of the outlet hole, wind direction and the surrounding conditions. These have been widely studied, and thus several models have been developed, mostly through experimental observations [24–28]. Nowadays, aside from the experimental studies [29, 30], computational methods have been implemented into the study of jet fires, allowing the inclusion and development of more complex numerical methods, in order to solve hundreds of equations simultaneously [31–33].

Jet fires are, in a great extent, of paramount importance due to their frequent presence in industrial applications. For example, in hydrocarbon process plants to eliminate undesired gases in the production of crude oil; in oil refineries and industrial processes to evacuate undesired sub-products, or released gases through security valves; or in controlled areas such as furnaces, gas turbines or industrial burners.

Regarding MA, it has been observed through historical analysis of accident, that when accidental jet fires are present, one of each two causes another greater accident. [34]; 90% of them leading to an explosion [35].

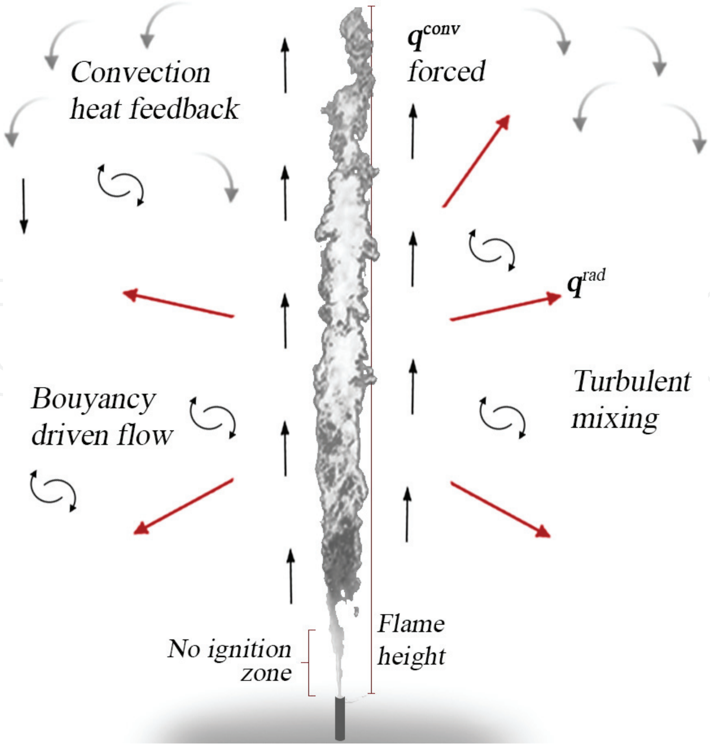

Figure 3. Typical jet fire.

3. CFD modeling

3.1. Geometry

Defining the geometrical representation of the model and the domains is part of the preprocessing. This will set the regions where the mathematical models (the partial differential equations) are valid; and defines the region where the phenomena will be studied. **Figure 4** depicts the geometrical representations of the models and the implemented mesh.

The size of the mesh in these representations is determined by the detail of the required information. It is clear that a 3D representation will require greater computational resources, and it may not provide further information than the 2D representation, depending on the required information from the model.

3.2. Mathematical models: partial differential equations and kinetics expressions

The phenomena described in the foregoing section are simulated by coupling and simultaneously solving the models described in **Table 3** [36]. Momentum balance, heat transfer and mass with combustion reaction are solved, using the hydrodynamics solution in the energy and mass balances, as well as the solution of the energy balance in the two other constitutive equations. It is important to note that the energy balance considers the generation due to the reaction, thus the energy balance is coupled with mass balance. It is important to consider that corrections to the mass and energy balance equations due to the turbulence should be added.

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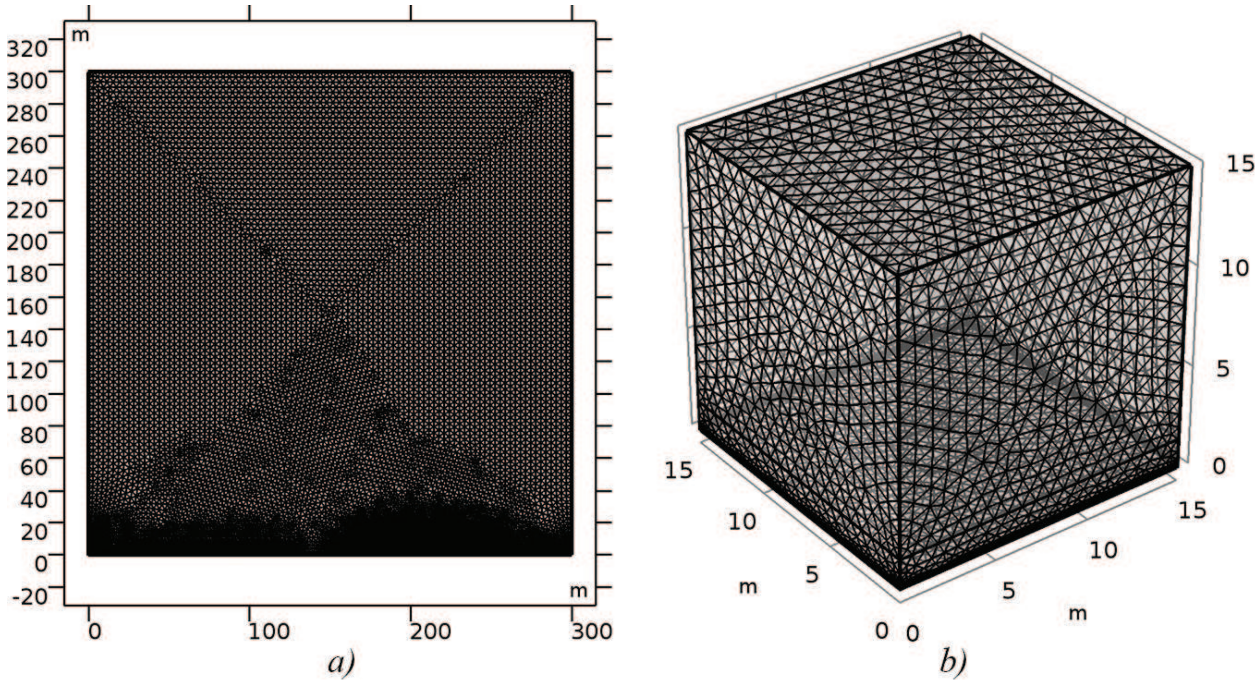

Figure 4. Geometry, domain and mesh considered for the simulations, (a) 2D domain of 300 m^2, (b) 3D domain with 15 m per side.

Momentum	$\rho\frac{\partial \mathbf{u}}{\partial t}+\rho(\mathbf{u}\cdot\ \nabla)=\ \nabla\cdot\left[-p\mathbf{I}+(\mu+\mu_T)\left(\ \nabla\mathbf{u}+(\ \nabla\mathbf{u})^T-\frac{2}{3}(\mu+\mu_T)(\ \nabla\mathbf{u})\mathbf{I}\right)\right]+\mathbf{F}$ $\rho\frac{\partial \mathbf{u}}{\partial t}+\ \nabla\cdot(\rho\mathbf{u})=0$
Turbulence	$\rho\frac{\partial \kappa}{\partial t}+\rho(\mathbf{u}\cdot\ \nabla)\kappa=\ \nabla\cdot\left[\left(\mu+\frac{\mu_T}{\sigma_\kappa}\right)\ \nabla\kappa\right]+P_\kappa-\rho\varepsilon$ $\rho\frac{\partial \varepsilon}{\partial t}+\rho(u\cdot\ \nabla)\varepsilon=\ \nabla\cdot\left[\left(\mu+\frac{\mu_T}{\sigma_\varepsilon}\right)\ \nabla\varepsilon\right]+C_{\varepsilon 1}\frac{\varepsilon}{\kappa}P_\kappa-C_{\varepsilon 2}\rho\frac{\varepsilon^2}{\kappa};\quad \varepsilon=ep$ $\mu_T=\rho C_\mu\frac{\kappa^2}{\varepsilon};\quad P_\kappa=\mu_T\left[\ \nabla\mathbf{u}\mathbf{:}\left(\ \nabla\mathbf{u}+(\ \nabla\mathbf{u})^T\right)-\frac{2}{3}(\ \nabla\cdot\mathbf{u})^2\right]-\frac{2}{3}\rho\kappa\ \nabla\cdot\mathbf{u}$
Energy	$\rho C_P\frac{\partial T}{\partial t}+\rho C_P\mathbf{u}\cdot\ \nabla T+\ \nabla\mathbf{q}=Q_{gen}$ $\mathbf{q}=-k\ \nabla T;\qquad Q_{gen}=-\Delta H_{rxn}R_i$
Mass	$\frac{\partial c_i}{\partial t}+\ \nabla\cdot(-D_i\ \nabla c_i)+\mathbf{u}\cdot\ \nabla c_i=R_i$ $\mathbf{N}_i=-D_i\ \nabla c_i+\mathbf{u}c_i$

Table 3. Models solved in CFD software.

However, this prior would add further non-linearities and would require greater computational resources.

The solution of these models require the proper evaluation of the thermophysics variables and parameters. Also, a fundamental task is determining the combustion reaction, which is included in the mass balances. Due to the nature of the studied fires, the inclusion of all chemical species involved is practically impossible, not only due to the great computational resources that the kinetics models would consume, but the determination of all chemical species reaction rates expressions, which are often unknown, mostly for the emerging alternative fuels that are still being developed. Despite the implementation of new methodologies to characterize and design new fuels, where molecular structures of the mixtures are studied in order to obtain a deeper and better understanding of the kinetic, physical and chemical properties that conduct the combustion in the energy conversion processes [37], it is still necessary to approach the combustion processes by simplified steps and considering only a representative mixture or selection of components (more common when fuel surrogates are involved). Regarding this last point, when studying the gasoline surrogates, several authors have proposed different representative mixtures, for example, Battin-Leclerc [38] considers a ternary mixture of iso-octane, 1-hexane and toluene; while Zhang [39] considers a mixture of 22 components.

The simplest combustion reaction for a hydrocarbon is:

$$Fuel + n_1 O_2 \rightarrow n_2 CO_2 + n_3 H_2 O \tag{1}$$

where the stoichiometric coefficients ni are determined by the selected fuel. And the global reaction rate must be represented by a suitable average of all reaction rates for the involved components. The simplest expression for the reaction rate can be expressed as

$$R_i = A_i T^n e^{\left(\frac{-Ea_i}{RT}\right)} [fuel]^a [O_2]^b \tag{2}$$

The general reaction rate constant depends on the temperature and is given by a modified form of the Arrhenius equation: $K_i = A_i T^n e^{\left(\frac{-Ea_i}{RT}\right)}$, where A is a collision pre-exponential factor and Ea is the activation energy. Also, the exponents a and b are experimentally determined empirical constants. Most of the cases, it is assumed that the global reaction is of first order for the fuel and the oxidant, and thus $a = b = 1$. However, it has been seen that this assumption may lead to great errors. **Table 4** shows some examples of common fuels with their kinetic parameters for the combustion kinetics expressions, which have been published in specialized literature.

3.3. Boundary conditions

In recent years, the boundary conditions have been widely investigated, as these are essential to find a valid solution, and often a misled selection of these conduces to significant errors in

Fuel	a	b	A	Ea (kcal)
Metano	−0.3	1.3	1.3×10^9	48.4
Propano	0.1	1.65	8.6×10^{11}	30
n-Heptane	0.25	1.5	4.3×10^{11}	30
n-Undecae	1	0.8	5×10^{15}	45
Kerosene	1	0.8	2.8×10^{15}	45

Table 4. Kinetic parameters for common fuels.

the results [40]. In the study of fires, as well as for other engineering fields, involving closed domains, three kinds of boundary conditions can be usually found:

1. The dependent variable derivate is specified (Neumann condition): $\mathbf{n} \cdot \nabla\varphi = f(r)$ in the surface.

2. The value for the dependent variable is specified (Dirichlet condition): $\varphi = f(r)$ in the surface.

3. A function of the normal component of the gradient and the dependent function is specified. Hence, a combination of the other two boundary conditions (Cauchy condition): $\alpha\mathbf{n} \cdot \nabla\varphi + \beta\varphi = f(r)$ in the surface.

Also, the values for the boundary values can fluctuate according to a determined behavior, as the ones shown in **Figure 5**. For example, the fuel inflow may vary following a Gaussian distribution due to the increase in the vaporization of the fuel that feeds the combustion zone. Another fluctuation commonly seen are the differences in the air inflow velocities, which have important consequences not only in the turbulences and the geometry of the flame, as seen in **Figure 2**, but also in the inflow of oxygen, which determines the reaction rate. The fluctuation of air should be taken into account properly as it will vary depending on the height that it is observed and also depending on the time. Furthermore, this air inflow is usually not symmetrical, and depending on the studied region, the surroundings conditions and the atmospheric conditions, at different times the air may be going as an inlet to the control volume through a boundary, and sometimes it may go as an outlet from the same boundary.

The proper understanding of the phenomena is of great importance in order to stablish adequate boundary conditions that may even reduce computational times and save computational resources, as symmetry conditions in the applicable cases. However, these same simplifications must be supported by scientific background. Sometimes, the lack of a scientific background for these lead to oversimplified models that do not properly describe the phenomena. **Table 5** shows the boundary conditions used in both of the models.

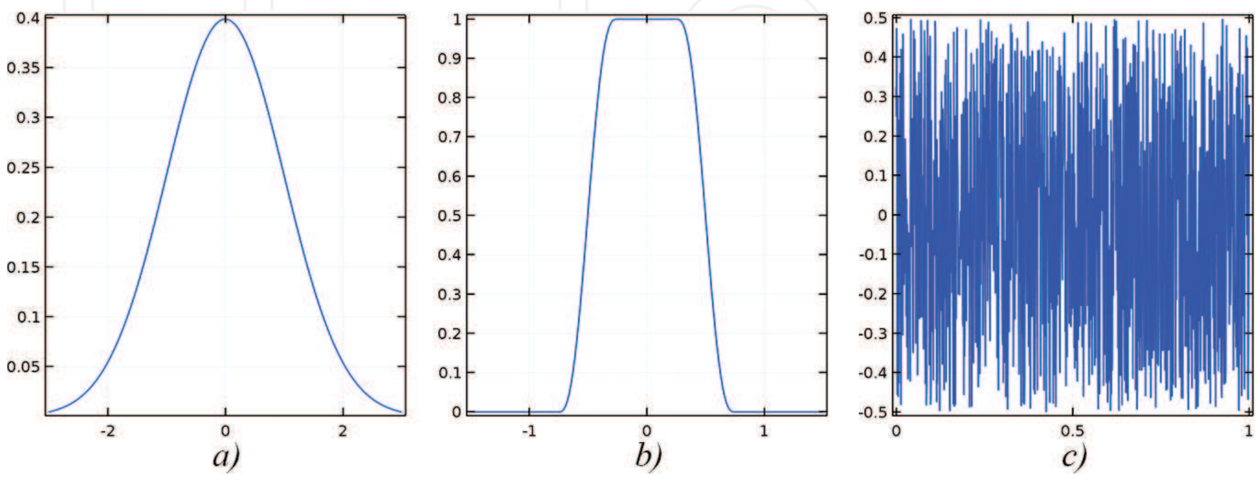

Figure 5. Variables distributions examples (a) Gaussian, (b) smooth rectangle step and (c) random.

	Pool fire		Jet fire	
Momentum	**Value**	**Boundary (m)**	**Value**	**Boundary (m)**
$\mathbf{u} = -u_{fuel}\mathbf{n}$ (*Fuel inlet*)	$u_{fuel} = 0.316[m/s]$	$\begin{pmatrix} 125 \le x \le 175 \\ y = 0 \end{pmatrix}$	$u_{fuel} = 50[m/s]$	$\begin{pmatrix} 4.98 \le x \le 5.01 \\ y = 0 \end{pmatrix}$
$\mathbf{u} = -u_{air}\mathbf{n}$ (*Air inlet*)	$u_{air} = 7.2[m/s]$	$\begin{pmatrix} x = \{0, 300\} \\ 1.5 \le y \le 300 \end{pmatrix}$	$u_{air} = 7.2[m/s]$	$\begin{pmatrix} x = \{0, 10\} \\ 1.5 \le y \le 10 \end{pmatrix}$
$\mathbf{u} = -u_{air}\mathbf{n}$ (*Air inlet*)	$u_{air} = 2.88[m/s]$	$\begin{pmatrix} x = \{0, 300\} \\ 0 \le y \le 1.5 \end{pmatrix}$	$u_{air} = 2.88[m/s]$	$\begin{pmatrix} x = \{0, 10\} \\ 0 \le y \le 1.5 \end{pmatrix}$
$[-p\mathbf{I} + a]\mathbf{n} = -p_0\mathbf{n}$ $a = (\mu + \mu_T)(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$ (*Outlet pressure*)	$p_0 = 1[atm]$	$\begin{pmatrix} 0 \le x \le 300 \\ y = 300 \end{pmatrix}$	$p_0 = 1[atm]$	$\begin{pmatrix} 0 \le x \le 10 \\ y = 10 \end{pmatrix}$
$\mathbf{u} \cdot \mathbf{n} = 0$ (*Wall*)		$\begin{pmatrix} 125 \ge x \ge 175 \\ y = 0 \end{pmatrix}$		$\begin{pmatrix} 4.98 \ge x \ge 5.01 \\ y = 0 \end{pmatrix}$
Mass transport	**Value**	**Boundary (m)**	**Value**	**Boundary (m)**
$c_i = c_j^0$ (*Specie inflow*)	$c^0_{C_7H_{16}} = 12[mol/m^3]$	$\begin{pmatrix} 125 \le x \le 175 \\ y = 0 \end{pmatrix}$	$c^0_{C_7H_{16}} = 12[mol/m^3]$	$\begin{pmatrix} 4.98 \le x \le 5.01 \\ y = 0 \end{pmatrix}$
$c_i = c_j^0$ (*Specie inflow*)	$c^0_{O_2} = 8.6[mol/m^3]$	$\begin{pmatrix} x = \{0, 300\} \\ 0 \le y \le 300 \end{pmatrix}$	$c^0_{O_2} = 8.6[mol/m^3]$	$\begin{pmatrix} x = \{0, 10\} \\ 0 \le y \le 10 \end{pmatrix}$
$-\mathbf{n} \cdot D_i \nabla c_i = 0$ *if* $\mathbf{n} \cdot \mathbf{u} \ge 0$ $c_i = c_j^0$ *if* $\mathbf{n} \cdot \mathbf{u} < 0$ (*Open boundary*)	$c^0_{O_2} = 8.6[mol/m^3]$	$\begin{pmatrix} 0 \le x \le 300 \\ y = 300 \end{pmatrix}$	$c^0_{O_2} = 8.6[mol/m^3]$	$\begin{pmatrix} 0 \le x \le 10 \\ y = 10 \end{pmatrix}$
$-\mathbf{n} \cdot \mathbf{N}_i = \mathbf{0}$ (*Wall*)		$\begin{pmatrix} 125 \ge x \ge 175 \\ y = 0 \end{pmatrix}$		$\begin{pmatrix} 4.98 \ge x \ge 5.01 \\ y = 0 \end{pmatrix}$
Energy transport	**Value**	**Boundary (m)**	**Value**	**Boundary (m)**
$T = T_0$ (*Ignition temperature*)	$T_0 = 488.15[K]$	$\begin{pmatrix} 125 \le x \le 175 \\ y = 0 \end{pmatrix}$	$T_0 = 488.15[K]$	$\begin{pmatrix} 4.98 \le x \le 5.01 \\ y = 0 \end{pmatrix}$
$T = T_0$ (*Air temperature*)	$T_0 = 300[K]$	$\begin{pmatrix} x = \{0, 300\} \\ 0 \le y \le 300 \end{pmatrix}$	$T_0 = 300[K]$	$\begin{pmatrix} x = \{0, 10\} \\ 0 \le y \le 10 \end{pmatrix}$
$T = T_0$ *if* $\mathbf{n} \cdot \mathbf{u} < 0$ $-\mathbf{n} \cdot \mathbf{q} = 0$ *if* $\mathbf{n} \cdot \mathbf{u} \ge 0$ (*Open boundary*)	$T_0 = 300[K]$	$\begin{pmatrix} 0 \le x \le 300 \\ y = 300 \end{pmatrix}$	$T_0 = 300[K]$	$\begin{pmatrix} 0 \le x \le 10 \\ y = 10 \end{pmatrix}$

Table 5. Boundary conditions set to the CFD models.

4. Results

4.1. Computation

The described models were implemented in COMSOL Multiphysics 5.2a models. The simulations were carried out in the described 2D models, due to the computational resources that the 3D models required, as well as the great computing times. Then, two different domains were stablished, a 300 m^2 domain for the pool fires and a 15 m^2 for the jet fires. These were selected according to the common lengths of these kinds of fires. The mesh for the pool fire model consisted of 71,665 triangular elements; while the mesh for the jet fire model consisted of 63,821 triangular elements.

The pool fire simulation was a time dependent simulation. 20 s in steps of 0.02 s were simulated (a total of 1001 frames). It consumed 3.72 GB of RAM and 3.96 GB of virtual memory, and required a computing time of 6.72 hours.

The jet fire simulation was also a time dependent simulation. 10 s in steps of 0.02 s were simulated (a total of 501 frames). It consumed 3.4 GB of RAM and 3.95 GB of virtual memory, and required a computing time of 9.73 hours.

The simulations were carried out in a HP z600 Workstation with an Intel® Xeon® E5620 CPU (quad-core, 2.4 GHz, 12 Mb of Cache), with 24 GB of RAM.

4.2. Pool and jet fire CFD model results

Figure 6 shows a sequence of the results from the pool fire CFD model previously described at different times. This pool fire model considers the combustion of heptane (C_7H_{16}) as the main

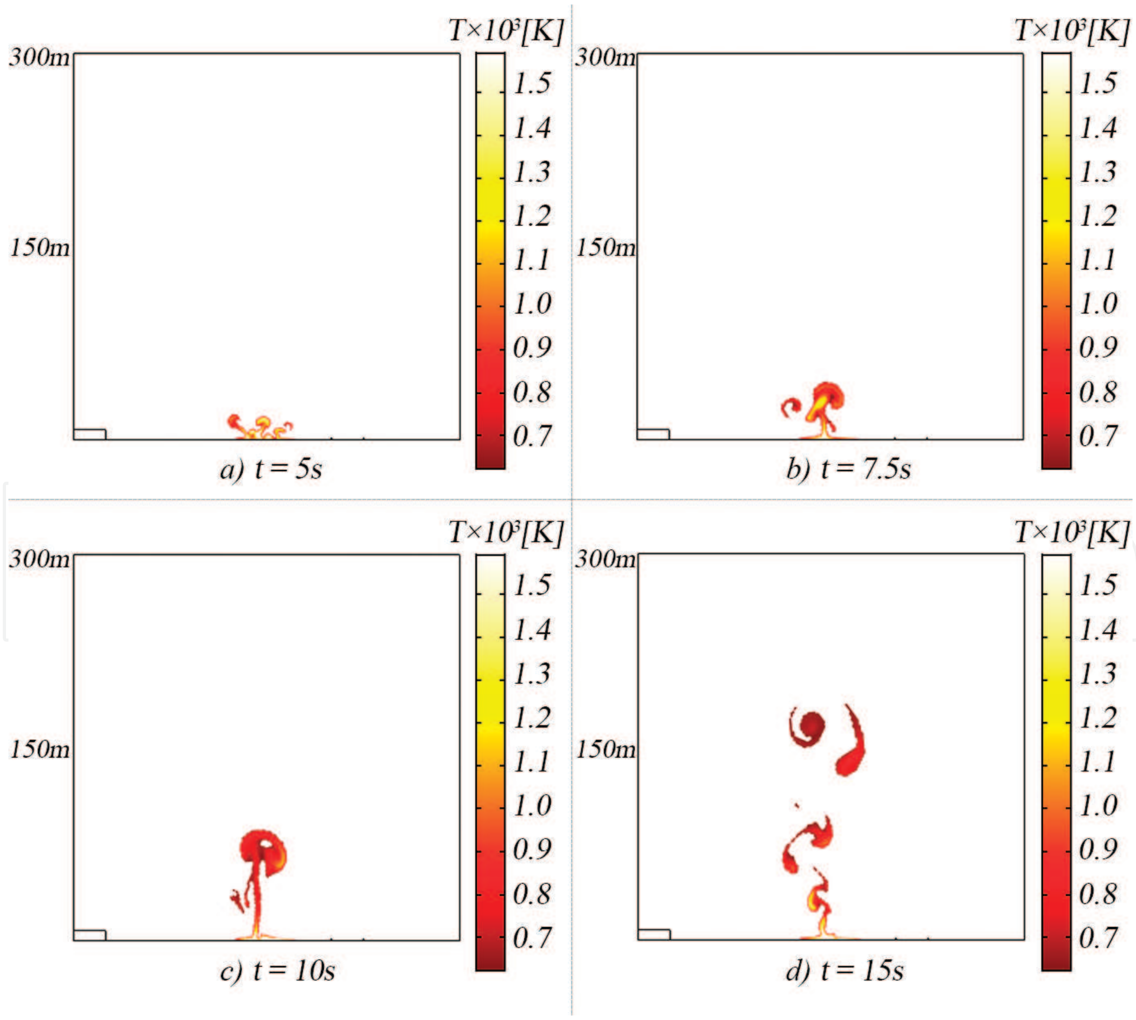

Figure 6. Results sequence from the pool fire CFD model temperature field (a) t = 5 s, (b) t = 7.5 s, (c) t = 10s, (d) t = 15 s.

combustion, a pool diameter of 50 m, a total time of 20 s, and a 300 m^2 domain. It is important to note that in these images, highly turbulent flames can be seen which tend to develop in large-size eddies, and that from the beginning moments of the pool fire, very high temperatures and flame heights can be reached.

Figure 7 shows a similar sequence of results for the jet fire CFD model. In this model, the fuel inflow was modified in order to follow a smooth rectangle distribution over the time, and thus it can be appreciated in the figures that in the beginning times the flame develops, then it reaches an almost steady behavior and afterwards it starts to diminish until it is consumed. Again, in this simulation, the main considered reaction was the combustion of heptane (C_7H_{16}). The shown images also consider a hole of 3 cm from where the jet fire arises, a total time of 10 s and a 15 m^2 domain.

The results of these models allow the analysis and evaluation of important variables in the process safety, such as the maximum and average temperatures and flame lengths. **Table 6** shows the resume of the average flame lengths in pool fires, taking as criteria the reaction rate; as well as the maximum temperature, which is evaluated in the whole domain, and thus this value might not necessary be found in a flame zone, it can be a hot zone where no

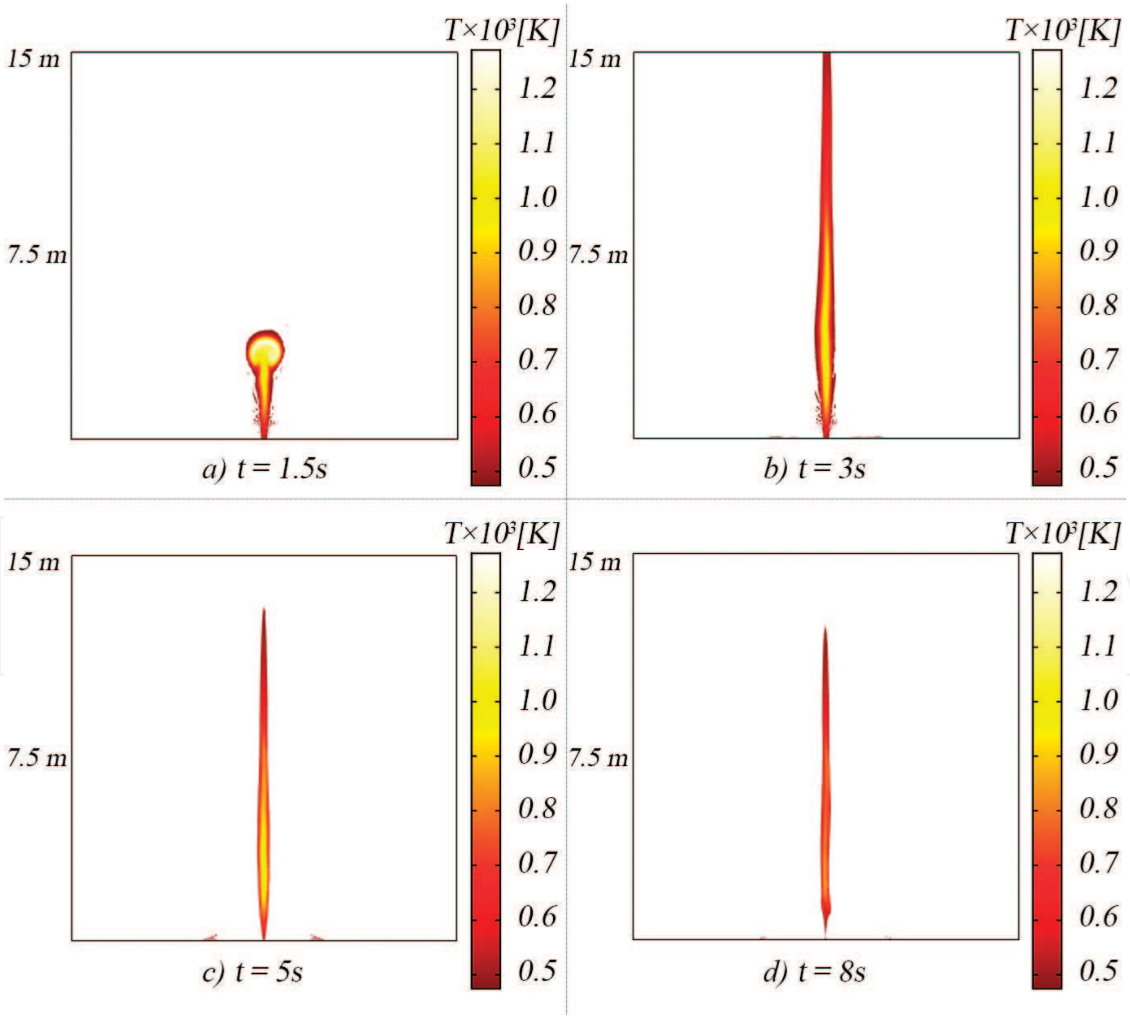

Figure 7. Results sequence from the jet fire CFD model temperature field (a) t = 1.5 s, (b) t = 3 s, (c) t = 5 s, (d) t = 8 s.

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combustion reaction is taking place. Note that there is no proportional correlation between the flame height and the flame diameter, nor between the flame diameter and the temperature. Furthermore, it was observed that the highest reaction rate values did not always correspond to the highest temperatures. It can also be seen that the fire exhibits lower temperature values when starting, and these values tend to increase with time, presenting great fluctuations not only in the temperature but other parameters as the flame geometry. These observations are an expected behavior for turbulent flames. Also, several pool diameters were tested, from 3 to 60 m.

Table 7 show a similar analysis to the one in **Table 6**, but for the jet fire CFD model. Different diameters for the hole of the jet fire were tested, from 3 to 19 cm. It is noteworthy that, despite that the jet fires arise from a breach of a few centimeters, these fires can reach great magnitudes,

Diameter (m)	Time (s)	Height (m)	$T_{average}$ (K)	T_{max} (K)
3	0.2	0.5	480	362
	3.0	11.6	697	1572
	9.5	11.6	620	1371
15	0.2	1.1	540	613
	3.0	8.2	1185	1411
	9.5	40.3	538	1363
30	0.2	2.3	541	614
	3.0	4.5	1470	1973
	9.5	96.4	669	1959
60	0.2	4.6	541	616
	3.0	21	1276	>2000
	9.5	31.1	1006	>2000

Table 6. Observed flame height and temperatures average values for different pool fires diameters models.

Diameter (cm)	Time (s)	Height (m)	$T_{average}$ (K)	T_{max} (K)
3	0.2	0.7	569	755
	3.0	7.1	754	938
	4.5	15.0	657	944
9	0.2	1.6	612	770
	3.0	11.5	722	1029
	4.5	15.0	831	996.49
19	0.2	1.42	657	863.9
	3.0	15.0	1054	1352
	4.5	>15.0	1039	1309

Table 7. Observed flame height and temperatures average values for different hole diameters for jet fire models.

with average temperatures around 550 and 1100 K, and punctual maximum values that can reach over 1300 K.

For both kinds of fires models, the results were compared against experimental data, and similar behaviors were found [29, 41].

Even though the detailed study of fires is not the objective of this chapter, it is important to point out that when the CFD heat, momentum and mass transport models are solved, the information of a great number of variables are obtained as an output. A way to use this information is through the dimensionless numbers analyses [42], as the evaluation of these will allow the comparison of different phenomena presented, neglecting the length-scales. For example, by evaluating the Reynolds numbers, it can be seen when will a flame be highly distorted; and the Froude number will show small values in the region near to surface area ($Fr \leq 1$) and increases with the flame height, where the forces of momentum are dominant.

As a resume, the results of the CFD fires simulations presented here show that for pool fires can reach over 90 m in height, average temperatures fluctuating between 500 and 1400 K, and punctual temperatures between 1500 and 1900 K; while the jet fire CFD simulation results predicted flame heights of over 15 m, with average temperatures fluctuating 550 and 1050 K. These results are in good agreement with the observations in experimental studies. Due to the aforementioned, it is important to point out that, even though that as aforementioned the pool fires and jet fires are usually present in other MA, they are by their own considered as MA.

Other applications of CFD models of MA, which are recently developed and widely applied, are the prediction of consequences in a combination of possible scenarios [43]. This is done by combining the CFD models' predictions with vulnerability values, proposing intervention zones, safe distances, equipment distribution in a plant, etc. For example, in the scenario depicted in **Figure 6**, it can be seen that only a few seconds after the pool fire started, temperatures of up to 1500 K can be found, with average temperatures of around 1000 K, and heights over 200 m. With this information, as shown in **Figure 8**, it can then be proceeded to

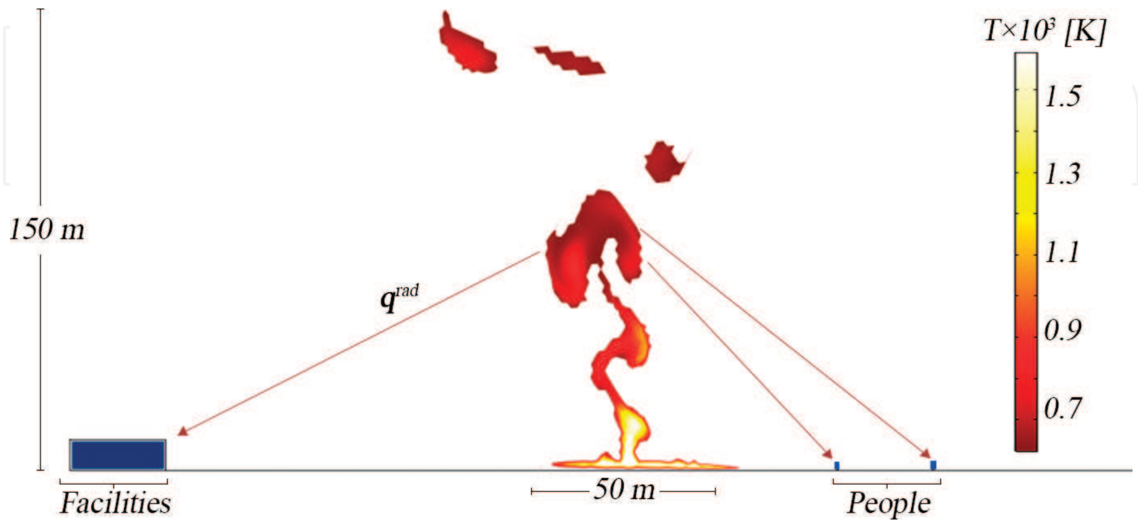

Figure 8. Possible scenario of MA considering the effect in the surroundings.

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evaluate the thermal radiation that an industrial facility 150 m away from the fire and persons 50 and 75 m away would receive, considering the view factors. This can be done by applying the Stefan-Boltzmann equation:

$$q_{rad} = \varepsilon\sigma F_{1-2}\left(T_1^4 - T_2^4\right) \tag{3}$$

where σ is the Stefan-Boltzmann constant, ε is the emissivity and $F_{1\text{-}2}$ is the view factor, defined as

$$F_{ij} = \frac{1}{A_i}\sum_{i=1}^{n}\sum_{j=1}^{m}\frac{\cos\theta_i \cdot \cos\theta_j}{\pi \cdot r^2}dA_i dA_j \tag{4}$$

Also, the determination of the thermal radiation can be coupled with the analytical equations developed for several geometries [44]. The maximum thermal radiation fluxes defined by the vulnerability factors have been widely studied, and are reported in the specialized literature. For example, Jagger [45] studied the consequences of the exposition of personal to different levels of thermal radiation, and proposes recommendations for the gas and petrol offshore industries, suggesting a review of the structural damage that may represent obstacles in emergency exit routes criteria. Raj [46] makes a review of the criteria of diverse normative regarding the exposition of people to fires. Further studies in specific cases can be found in the works of Casal [47].

When vulnerability factors are evaluated, it is important to take into account the maximum observed values, as these will represent the worst-case scenario, with the highest risks for the people and the structures. In this sense, as observed by the simulation results, taking as an example the 50 m pool fire results, the maximum temperature produces a thermal radiation of over 200 kW/m^2, which if far above the safe criteria. Taking in consideration the consequences in the reported vulnerability criteria for people and objects found in literature, it can be concluded that no one would survive that amount of thermal radiation flux; and that the steel structures would lose all their mechanical integrity. This scenario would definitely cause domino effects with greater consequences.

If the 3 m pool fire is considered, the consequences would be lower. However, due to the produced thermal radiation, the safe zone for a person would be no closer than 25 m, as a person can receive a maximum amount of thermal radiation between 4.7 and 5 kW/m^2 [46]; and for the metal structures, the safe zone would be found in a distance of 7.5 m, in order to avoid the collapse of the structure, that can receive a maximum thermal radiation of 37.5 kW/m^2. Although, exposition to this value of 37.5 kW/m^2 would lead to the death of a person, even in a short exposition period of time [46].

5. Conclusions

Process safety is of major importance due to the consequences in matter of lives, economy and wide regions affections. Thus, the prediction of the behavior of major accidents is of key importance in the better development of process safety engineering. In this context, CFD tool represent an opportunity to provide more accurate solutions in the prediction of the complex multiscale and multiphysic phenomena that MA involve (some problems that have been experimentally impossible to solve). These tools are of special necessity in the quantitative analysis of results, as the previously developed methods still have great restrictions and failures in predictions, for example, of highly turbulent flows, rapid compressions or expansions, low Reynolds number effects and chemical reactions.

Despite the development of diverse strategies for the CFD simulations that allow taking into account the turbulence present in MA (LES, DNS, RANS), the RANS equations have been widely used, as the results predicted by those have shown a good agreement compared with experimental methodologies. Also, applying other methodologies require greater computational resources, and are in many cases unpractical. On the other hand, the CFD simulations provide a great advantage to study large-scale MA, as these would be practically impossible to control and study in experimental studies (due to the high costs and the scientific and technical challenges).

Finally, it is noteworthy that the results of the CFD simulations of MA have several practical applications in diverse Process Safety fields and issues. For example, the study of safe distances, emergency exit routes and facilities design. Even though, the aforementioned manifests that there is still a strong need of developing research in these underexplored fields, which have special application in the process safety engineering.

Nomenclatures

Abbreviations

MA	Major accidents
NFPA	National Fire Protection Association
CFD	Computational fluid dynamics
RANS	Reynolds-Average Navier-Stokes
LES	Large eddy simulations
DNS	Direct numerical simulations

Symbols

h	Convective coefficient
$\mathbf{u}$ (m/s)	Velocity vector
$\mathbf{N}$ (mol/m^{2}s)	Total mass flux
D_i	Specie i diffusivity
C_P (J/mol K)	Heat capacity

ΔH_{rxn} (J/mol)	Heat of reaction
R_i (mol/m^{3}s)	Reaction rate
A_i	Pre-exponential collision factor
Ea	Activation energy
a	Kinetics empirical constant 1
B	Kinetics empirical constant 2
n_i	Stoichiometric coefficient for specie i
K_i	Reaction rate constant
$\mathbf{n}$	Unitary vector
p (Pa)	Pressure
c_i (mol/m^3)	Specie i concentration
k (W/mK)	Thermal conductivity
$F_{1\text{-}2}$	View factor
Sub-superscripts	
0	At reference conditions
Greek letters	
μ (Pa s)	Dynamic viscosity
ε	Emissivity factor
σ (W/m^{2}K^4)	Stefan-Boltzmann constant

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