

INDUSTRIAL RISK ASSESSMENT THROUGH THE NUMERICAL ANALYSIS OF THE THERMAL EFFECTS PRODUCED BY A HYDROCARBON FIRE IN A MILD HYDROCRACKING UNIT

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ABSTRACT

The paper presents a preliminary numerical assessment of the thermal effects produced by a high-intensity hydrocarbon fire developing within a three-dimensional configuration representative of a mild hydrocracking unit. The analysis was based on an existing model developed in PyroSim and computed using the Fire Dynamics Simulator software, in which n-heptane was used as a surrogate fuel and the prescribed nominal heat release rate was approximately 73.5 MW. The available set of results was analysed through the evolution of the heat release rate, fuel mass flow rate, the main terms of the global energy balance, and the visualizations obtained in Smokeview for flame, smoke, temperature, and gas movement. The final available interval, from 45 to 59.4 s, was used to characterize the period during which the source operated at the prescribed maximum intensity. During this stage, the mean heat release rate was 72.855 MW, while the maximum value recorded over the available simulation duration was 84.020 MW. The mean global radiative term was approximately 15.769 MW, representing 21.64% of the mean heat release rate. Depending on the heat release rate and radiative fraction used, the calculated radiant heat flux ranged between 34.86 and 68.72 kW/m² at a distance of 6 m and between 8.71 and 17.18 kW/m² at 12 m. The results highlight the possibility of severe thermal exposure near the source and the influence of the facility configuration on the movement of smoke and hot gases. The proposed method clearly distinguishes the results obtained directly through CFD simulation from analytical estimates and can be used for the preliminary identification of vulnerable areas, the establishment of protection priorities, the placement of monitoring systems, and the substantiation of emergency response measures.

Keywords: industrial risk, mild hydrocracking, hydrocarbon fire, CFD simulation, thermal radiation.

INTRODUCTION

Mild hydrocracking is used in petroleum refining for the partial conversion of vacuum gas oil into products with lower boiling points and for the simultaneous improvement of feedstock quality through hydrogenation, hydrosulfurization, and hydrodenitrogenation reactions. Compared with conventional hydrotreating, the process operates at a higher severity and

combines catalytic cracking with hydrogen addition, facilitating the production of middle distillates and improved feedstocks for downstream conversion units. These technological advantages are achieved under conditions characterized by high hydrogen concentrations, elevated temperatures, and high pressures, which require maintaining the mechanical integrity of the facility and preventing loss of containment of process fluids [1].

The containment of hazardous substances within process systems represents a fundamental objective of process safety, because an uncontrolled release may develop into a fire, an explosion, or a toxic dispersion. In hydrocarbon processing facilities, the consequences of an initial loss of containment depend on both the properties and quantity of the released substance and the operating conditions, time to ignition, geometric configuration of the site, and distance from adjacent equipment. The prevention and control of such events are part of the general framework of process safety and are regulated at European Union level by Directive 2012/18/EU on the control of major-accident hazards involving dangerous substances [2],[3].

The ignition of liquid hydrocarbons spread over a large area may produce an intense flame, extremely hot gases, and strong thermal radiation. The severity of thermal exposure depends on the burning area, heat release rate, flame shape, amount of soot, atmospheric conditions, and distance from the source. Thermal radiation may affect personnel, structures, and process equipment even without direct contact with the flame [4-7].

Thermal radiation produced by hydrocarbon fires is frequently assessed using simplified models, such as the point-source model and the solid-flame model. These methods are useful in preliminary analyses because they can be applied rapidly and require limited data. In congested industrial facilities, these simplifications may limit the accuracy of the estimates because the surrounding platforms, piping, and equipment influence flame development, the movement of hot gases, and thermal radiation transfer [4-7].

If a vessel or pipeline is exposed to intense thermal radiation for a sufficient period, the temperature of the material may increase, while its strength may decrease. Under these conditions, a new loss of containment may occur, extending the initial accident and generating a domino effect. Its assessment must take into account the type of exposed equipment, the duration of heating, the radiation intensity, and the existing protective measures [8-11].

Computational fluid dynamics enables a more detailed analysis of fires in industrial facilities, particularly when equipment geometry influences flame development and smoke movement. Fire Dynamics Simulator, developed by the National Institute of Standards and Technology, is used to simulate the propagation of heat and smoke produced by fires. The software can represent three-dimensional structures and calculate time-dependent quantities such as gas temperature, gas velocity, smoke concentration, and heat release rate [12].

Fire Dynamics Simulator has been used in numerous studies to analyse industrial fires and has been compared with experimental results. The research has examined fires of various sizes and configurations, including scenarios occurring in petroleum product storage areas. The results have shown that CFD simulation can provide useful information on flame development, temperature distribution, smoke movement, and the level of thermal exposure. At the same time, the accuracy of the results depends on how the fire source, fuel, and simulation conditions are defined [13-16].

Existing studies provide important information on the behaviour of hydrocarbon fires; however, most analyse fires occurring in open spaces, medium-scale experiments, or scenarios associated

with storage tanks. These configurations differ from a mild hydrocracking unit, where equipment, piping, and platforms are located in close proximity and may influence flame development, smoke movement, and heat distribution. Furthermore, simplified radiation models estimate exposure primarily as a function of fire power and distance from the source, without fully capturing the effects of facility geometry [4-7],[14-17]. Therefore, the problem addressed in this paper consists of assessing the thermal effects within a complex industrial configuration by combining the spatial information provided by CFD simulation with the analytical estimation of radiative exposure.

The aim of the paper is to assess the initial phase of a hydrocarbon fire occurring within a configuration representative of a mild hydrocracking unit. The analysis examines the evolution of the heat release rate, the movement of smoke and hot gases, temperature distribution, and the radiative component of the released energy. The results are used for the preliminary assessment of thermal exposure at representative distances and to highlight the influence of facility geometry on fire development. The contribution of the study is primarily application-oriented and consists in the complementary use of CFD simulation and the point-source model to evaluate fire behaviour and radiative exposure within a complex industrial configuration. Rather than proposing a new numerical or radiation model, the study applies established methods in an integrated manner to support the preliminary identification of areas potentially exposed to significant thermal effects and to provide a basis for subsequent risk-reduction and protection assessments.

MATERIALS AND METHODS

Materials and input data

The analysis was conducted based on the results of a simulation representative of a fire occurring in the area of a mild hydrocracking unit. The scenario configuration file, data on the evolution of the heat release rate and energy balance, as well as the resulting images for flame, smoke, and temperature, were used. This information formed the basis for the numerical assessment and the subsequent estimation of thermal exposure. [12],[18-20].

N-heptane was used as a surrogate fuel because a detailed multicomponent representation of vacuum gas oil (VGO) was not available in the numerical model. The simulation therefore focuses on the thermal effects of a prescribed high-heat-release hydrocarbon fire rather than on reproducing the evaporation and combustion chemistry of VGO; the use of n-heptane does not imply physicochemical equivalence between the two fuels. The fire source was defined by a prescribed thermal power. The main data used in the analysis and for the model configuration are summarized in Table 1.

Table 1. Data used for the analysis of thermal effects.

<i>Parameter</i>	<i>Value</i>
Modelling software	PyroSim
Computational software	Fire Dynamics Simulator
Surrogate fuel	n-heptane
Maximum nominal power	approximately 73.5 MW
Prescribed radiative fraction	0.37
Distances analysed from the source	6 m and 12 m
Atmospheric conditions	no imposed wind

The computational domain covered approximately $33.6 \times 21.6 \times 48.2$ m and was divided into 16 computational meshes, using cubic cells with a side length of 0.2 m. The resulting model contained approximately 4.37 million computational cells. This spatial resolution was used throughout the simulation to represent the development of the fire and the interaction of hot gases and smoke with the surrounding equipment and structures.

The selected cell size influences the spatial resolution of the calculated temperature, velocity and flame fields. A finer mesh could provide a more detailed representation of local gradients, but would also substantially increase the computational cost. Since simulations with alternative cell sizes were not performed, mesh independence was not assessed in the present study, and this aspect is considered when interpreting the results.

The three-dimensional geometry was used to capture the influence of platforms, pipelines, and equipment on the movement of the flame, smoke, and hot gases.

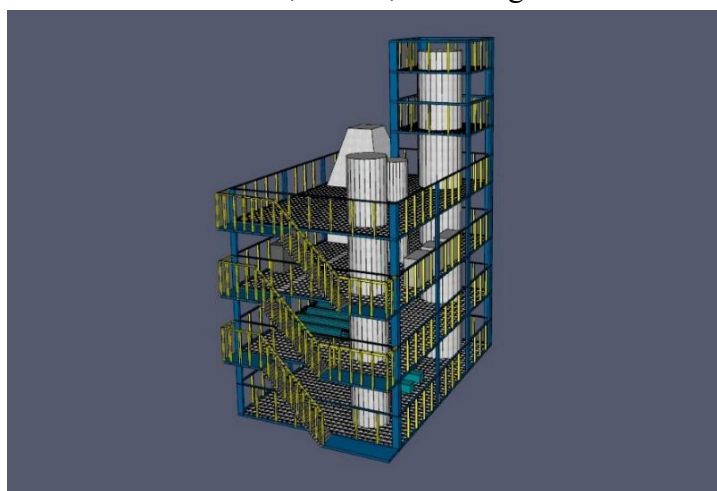


Figure 1. Three-dimensional model of the representative configuration of the mild hydrocracking unit used in the simulation.

Method for analysing the CFD results

The simulation results were analysed both qualitatively, based on the images generated in Smokeview, and quantitatively, by processing the numerical data provided by the simulation. The visual analysis examined:

- flame development at 5 s and 50 s;
- smoke propagation at 15 s, 35 s, and 55 s;
- temperature distribution in the available vertical section;
- movement of the hot gases in relation to the installation structures.

The images were used to identify the direction of smoke propagation, the extent of the thermal plume, and the interaction between the fire and the installation geometry.

The quantitative analysis considered the heat release rate, the fuel mass flow rate, and the main terms of the overall energy balance. To characterize the operating phase at maximum intensity, the data recorded between 45 and 59.40 s were analysed, and the mean value, minimum value, maximum value, and standard deviation were determined for each parameter.

The mean of a variable X was calculated using the following relationship:

$$\bar{X} = \frac{1}{n} \sum X_i \quad (1)$$

where n represents the number of values analysed, and X_i represents the value of the variable at time i .

The selected interval corresponds to a period of constant source feeding. Because the heat release rate continues to exhibit variations caused by the combustion process, this stage was considered a quasi-steady-state regime.

Determination of the radiative component

The overall radiative component of the fire was evaluated based on the Q_{RADI} term provided by FDS. The net radiative fraction was calculated as the ratio of the mean absolute value of the radiative term to the mean heat release rate:

$$\chi_{r,net} = \frac{|\bar{Q}_{RADI}|}{\bar{Q}} \quad (2)$$

where:

$\chi_{r,net}$ = net radiative fraction;

Q_{RADI} = mean absolute value of the global radiative term;

$\bar{Q}$ = mean heat release rate.

The net radiative fraction resulting from the energy balance was analysed separately from the radiative fraction of 0.37 entered into the model. The former expresses the net radiative component calculated for the entire domain, whereas the latter represents the value prescribed for the combustion reaction. The global Q_{CONV} term was used only to describe the overall energy balance.

Method for Assessing Thermal Exposure

To assess radiative exposure at equipment level, the global energy results of the simulation were supplemented by applying the point-source model. This method, frequently used in preliminary assessments of hydrocarbon fires, enables the estimation of heat flux at representative distances from the source [4],[5],[21-24].

The incident radiant heat flux was calculated using the following relationship:

$$q''_{rad} = \frac{\chi_r \dot{Q} \tau}{4\pi R^2} \quad (3)$$

where:

q''_{rad} – incident radiant heat flux, expressed in kW/m²;

χ_r – radiative fraction;

$\dot{Q}$ – heat release rate, expressed in kW;

$\tau = 1$, atmospheric transmissivity;

R – distance between the source and the analysed point, expressed in meters.

The assessment was carried out for distances of 6 m and 12 m, considered representative of the positions of equipment located in the vicinity of the source.

To highlight the possible variation in exposure, the following were used:

- the mean heat release rate;
- the maximum heat release rate;

- the net radiative fraction determined from the FDS energy balance;
- the radiative fraction of 0.37 prescribed in the model.

Combining these values made it possible to obtain a radiative exposure range for each distance. The method provides a preliminary estimate of the severity of the thermal effects, without providing the exact distribution of the heat flux over the surface of a piece of equipment.

RESULTS AND DISCUSSIONS

Evolution of the Heat Release Rate

The main set of results, shown in Figure 2, includes the evolution of the heat release rate, together with the absolute values of the radiative and convective terms in the global energy balance. In the simulation results, the Q_{RADI} and Q_{CONV} terms are reported with a negative sign, in accordance with the energy balance convention used by the software.

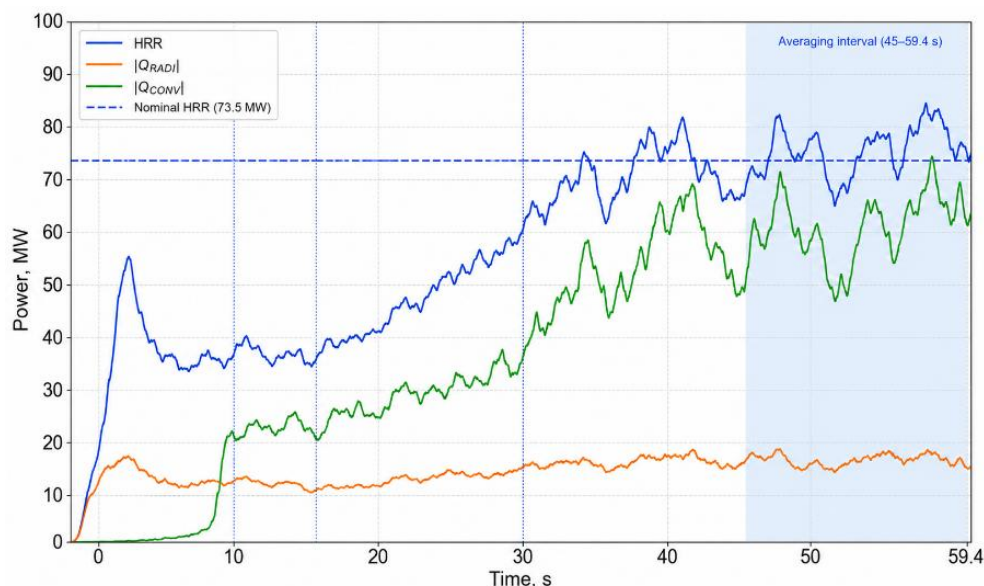


Figure 2. Evolution of the heat release rate and the main terms of the global energy balance over the highlighted interval.

After reaching the prescribed maximum intensity, the HRR oscillates around the nominal power of 73.5 MW. The observed fluctuations are characteristic of the turbulent combustion process and reflect the temporal variation in the fuel mixing and consumption rates. The statistical parameters obtained are presented in Table 2.

Table 2. Statistical parameters of the heat release rate.

Parameter	Value
Nominal source power	73.5 MW
Number of values analyzed	73
Mean HRR	72.855 MW
Minimum HRR	58.261 MW
Maximum HRR within the averaging interval	82.534 MW
Standard deviation	5.28 MW

Coefficient of variation	7.25%
Maximum HRR over the entire simulation	84.020 MW
Time of maximum HRR	44.601 s

The relative difference between the prescribed nominal power and calculated mean value is:

$$\varepsilon_Q = \frac{73.5 - 72.855}{73.5} \times 100 \approx 0.88\% \quad (4)$$

The low value of this difference confirms the consistency between the source intensity defined in the input file and the resulting mean HRR. The maximum value of 84.020 MW represents a transient peak in the combustion process and not a change in the nominal power of the source. The analysed interval can be characterized as a quasi-steady-state regime with constant feeding, because the HRR continues to exhibit turbulent fluctuations around the mean value.

Flame development

The visual development of the flame is presented in Figure 3 at 5 s and 50 s. At 5 s, the flame reaches a height of approximately 13 m, is concentrated near the source, and appears vertically fragmented by the intersected platforms and structural elements. At 50 s, after the maximum fuel flow rate is reached, the combustion region extends across several levels and forms an almost continuous column, reaching a height of approximately 23 m.

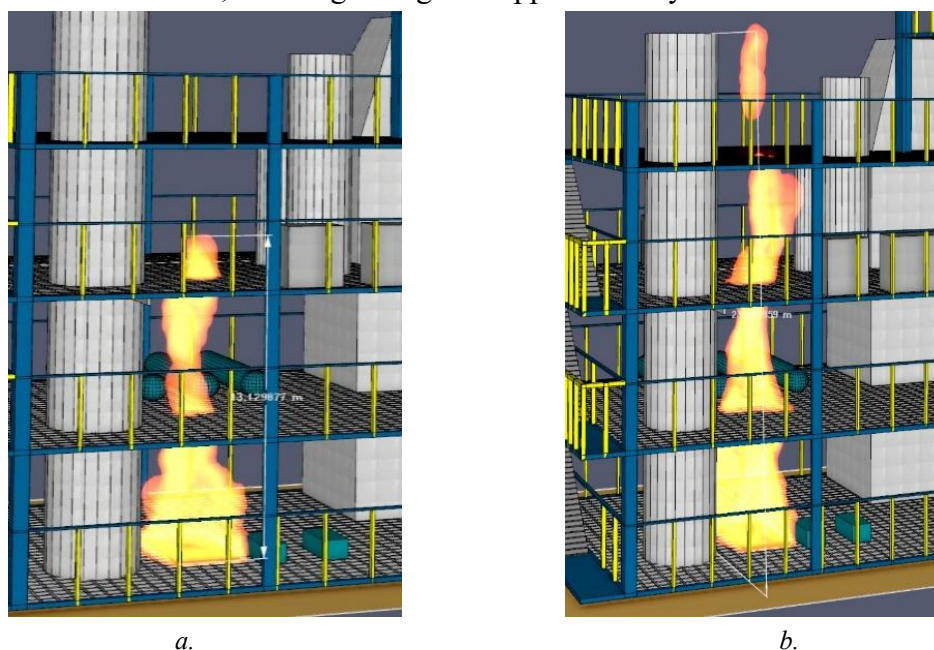


Figure 3. Visual development of the flame: (a) 5 s; (b) 50 s.

Smoke Propagation and Temperature Field

The evolution of smoke and temperature was analysed at 15 s, 35 s, and 55 s. At all three time points, the hot gases and smoke move primarily vertically, in the absence of an imposed wind field. The observed evolution highlights the influence of the facility configuration on the movement of hot gases and smoke in the vicinity of the fire source. These results are relevant for the preliminary identification of areas where thermal exposure may become significant and for guiding further assessment of nearby equipment.

At 15 s (Figure 4), a compact smoke column has already formed above the source. Its dark appearance is influenced by the prescribed soot yield of 0.10 kg/kg. The thermal field reveals a high-temperature core in the source region and an ascending plume that passes through the lower levels of the structure.

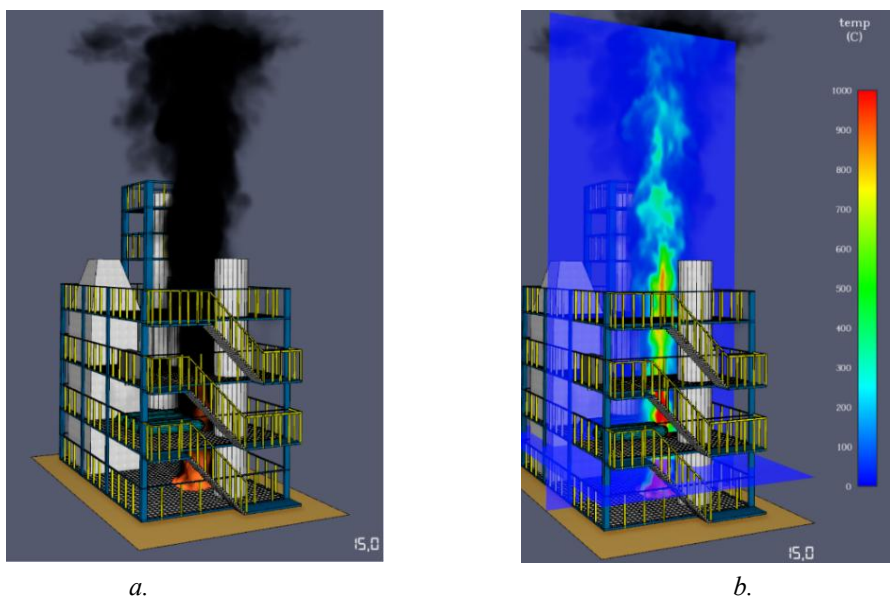


Figure 4. Smoke propagation and temperature distribution at 15 s:
 (a) smoke visualization; (b) vertical temperature section

At 35 s (Figure 5), the source operates at the prescribed maximum intensity. The hot-gas region extends to the upper levels, and the smoke becomes denser. The lateral displacement observed near the platforms highlights the influence of obstacles on gas circulation. The upper limit of the temperature scale is 1,000 °C.

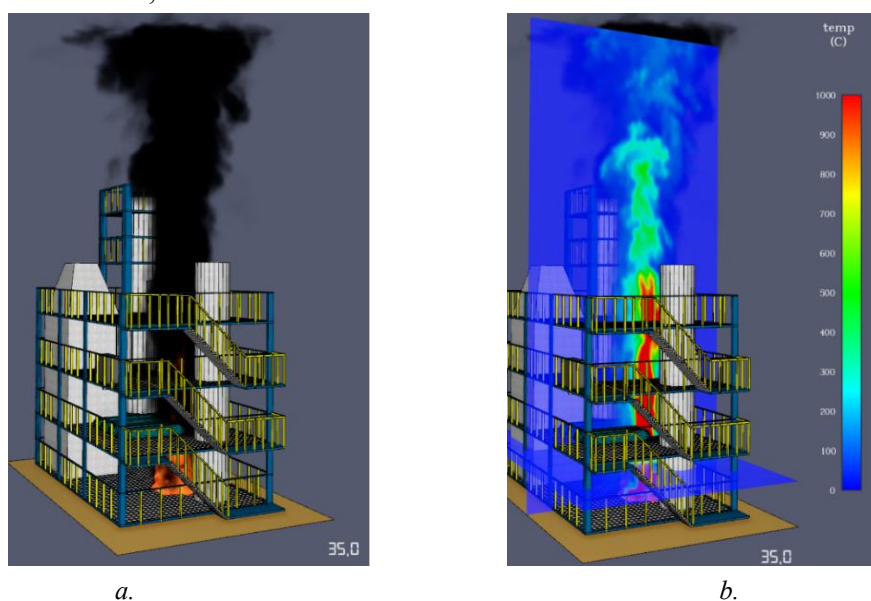


Figure 5. Smoke propagation and temperature distribution at 35 s:
 (a) smoke visualization; (b) vertical temperature section.

At 55 s (Figure 6), the smoke column extends above the upper level of the structure, while the temperature section indicates the extension of the hot-gas region across several levels. The result highlights the influence of the geometry on the movement of smoke and heat, without allowing the direct determination of wall temperatures or local heat flux.

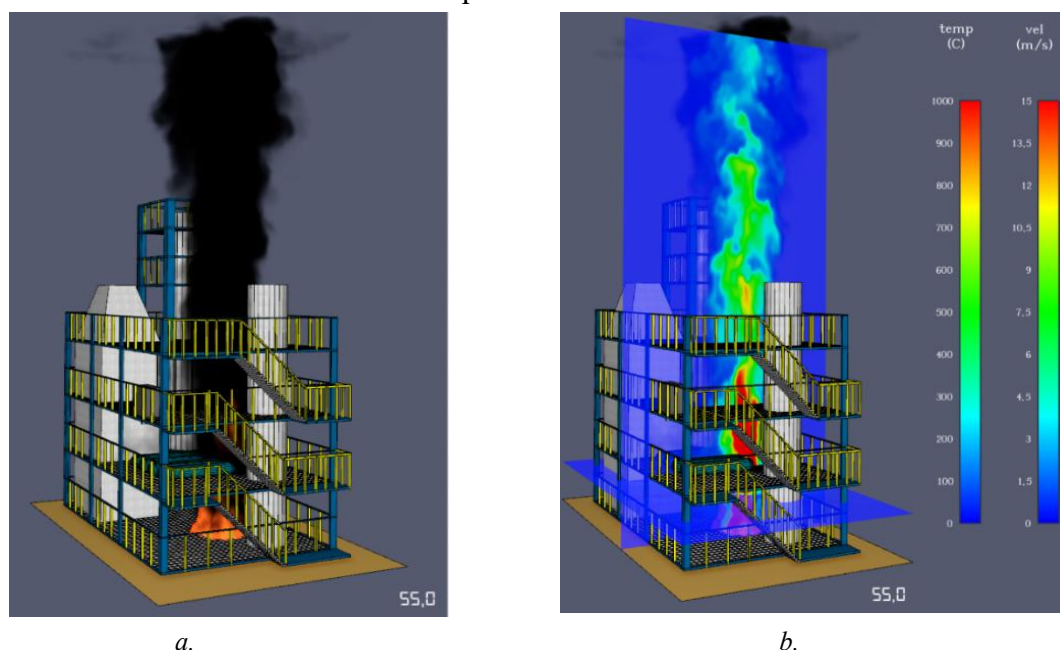


Figure 6. Smoke propagation and temperature distribution at 55 s:
(a) smoke visualization; (b) vertical temperature section.

Global Energy Balance

The mean values of the main energy terms, calculated for the representative interval, are summarized in Table 3.

Table 3. Mean values of the global energy balance terms.

Term	Mean value	Ratio to HRR
HRR	72.855 MW	100%
Q _{RADI}	-15.769 MW	21.64%
Q _{CONV}	-54.485 MW	74.79%
Q _{COND}	-1.169 MW	1.60%
Q _{DIFF}	+0.250 MW	0.34%
Q _{TOTAL}	+1.682 MW	2.31%

The net radiative fraction resulting from the energy balance is:

$$\chi_{r,net} = \frac{|\bar{Q}_{RADI}|}{\bar{Q}} = \frac{15.769}{72.855} = 0.2164 \quad (5)$$

The value of 21.64% differs from the radiative fraction of 0.37 prescribed in the combustion reaction. The prescribed fraction controls the distribution of energy in the reaction zone, whereas Q_{RADI} represents the net radiative exchange at the domain level. The difference is associated with the absorption and redistribution of radiation by gases, smoke, and surfaces

[12],[18],[24]. The radiative fraction also depends on the fuel and the flow regime; therefore, the prescribed value should not be interpreted as a universal constant [24],[25].

The Q_{CONV} term, representing 74.79% of the mean HRR in absolute value, characterizes the global convective transport of energy.

Analytical estimation of radiative exposure

In the absence of local heat flux measurement devices, radiative exposure was estimated using the point-source model [24],[26]:

$$q''_{rad} = \frac{\chi_r Q \tau}{4\pi R^2} \quad (6)$$

In the calculations, a unit atmospheric transmissivity, $\tau=1$, corresponding to the neglect of atmospheric attenuation, was adopted. Two HRR levels and two radiative fraction values were analysed: the net fraction of 0.2164, obtained from the FDS balance, and the fraction of 0.37 prescribed in the reaction.

Table 4. Analytical estimation of radiant heat flux at representative distances.

Distance	HRR used	Radiative fraction	Estimated radiant heat flux
6 m	72.855 MW	0.2164	34.86 kW/m ²
	84.020 MW	0.2164	40.20 kW/m ²
	72.855 MW	0.37	59.59 kW/m ²
	84.020 MW	0.37	68.72 kW/m ²
12 m	72.855 MW	0.2164	8.71 kW/m ²
	84.020 MW	0.2164	10.05 kW/m ²
	72.855 MW	0.37	14.90 kW/m ²
	84.020 MW	0.37	17.18 kW/m ²

The values in Table 4 represent screening estimates rather than heat fluxes calculated directly on equipment surfaces. The point-source model does not account for the actual flame shape, receptor orientation, view factor, smoke absorption, or shielding by surrounding structures [24]. At 6 m, the estimated radiant heat flux ranges from approximately 35 to 69 kW/m², depending on the HRR and radiative fraction considered, while at 12 m the values range from approximately 9 to 17 kW/m². These results highlight the sensitivity of the analytical estimate to the selected radiative parameters.

For comparison, API Standard 521 specifies thermal radiation levels of 9.46 kW/m² for areas where personnel may be required to perform urgent actions and 6.31 kW/m² for exposure periods of up to 30 s, under the conditions specified by the standard. All estimated values at 6 m exceed these levels, while the values at 12 m are close to or above 9.46 kW/m² [26]. These values are used only to contextualize the severity of thermal exposure and should not be interpreted as equipment failure thresholds.

A detailed assessment of equipment integrity under such thermal exposure would require a separate thermal-mechanical analysis, including information on material grade, wall thickness, operating conditions and service environment. For hydroprocessing equipment operating in hydrogen service, material-specific considerations addressed for Cr-Mo-V reactors and in API RP 941 may provide additional guidance for such an assessment [27],[28].

Visual comparison with a real fire

Figure 7 presents a visual comparison between the simulation and the real fire, captured 6 seconds after initiation. In both images, the vertical development of the flame and the formation of a dense smoke column can be observed. The real incident involved the release of naphtha from a pressurized vessel, the formation of a vapor cloud, and its ignition [29],[30].

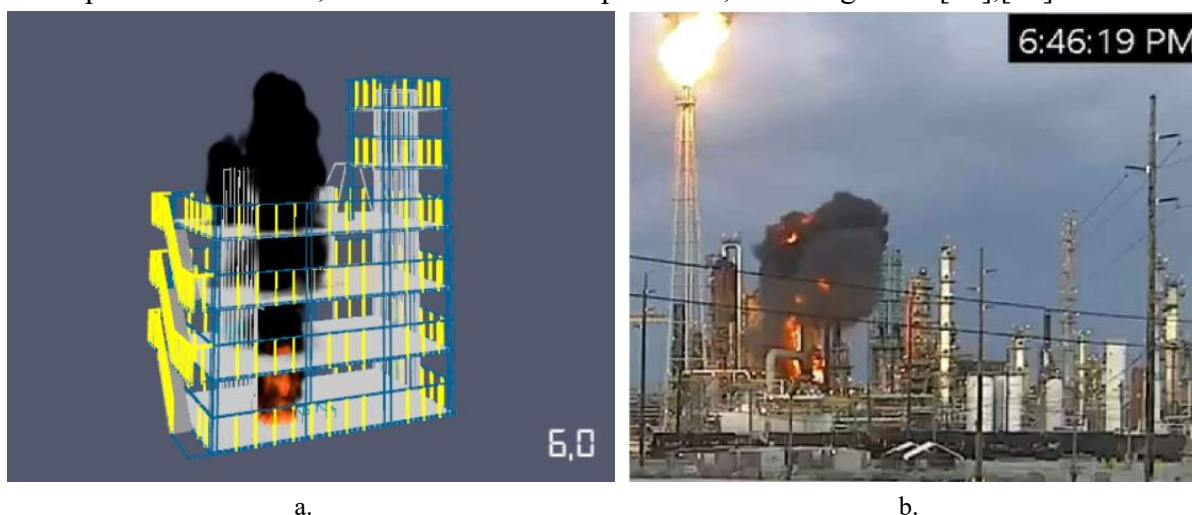


Figure 7. Qualitative visual comparison between: (a) the simulation result at 6 s; (b) the fire of 20 September 2022 at the BP-Husky Toledo refinery, Oregon, Ohio. Source of image (b): BP, with CSB annotations, reproduced by Hale [29] and in the CSB report [30].

CONCLUSIONS

The study analysed the initial development phase of a high-thermal-power hydrocarbon fire in a configuration representative of a mild hydrocracking unit. The CFD simulation was used to examine the evolution of the heat release rate, the movement of smoke and hot gases, the temperature distribution, and the main terms of the energy balance. The results highlighted the predominantly vertical propagation of smoke under conditions without an imposed wind field and the influence of structures and equipment on the local circulation of hot gases.

During the interval corresponding to operation at maximum intensity, the mean heat release rate was 72.855 MW, a value close to the nominal power of 73.5 MW. The difference of approximately 0.88% indicates good agreement between the source defined in the model and the resulting energy response. The maximum value of 84.020 MW represented a short-term variation in the combustion process, without altering the nominal level imposed on the source. The energy analysis showed that the mean global radiative term was approximately 15.769 MW, representing 21.64% of the mean heat release rate. To supplement the CFD results, radiative exposure was estimated using the point-source model. At a distance of 6 m, the resulting heat fluxes ranged between 34.86 and 68.72 kW/m², while at 12 m they ranged between 8.71 and 17.18 kW/m². These values confirm the decrease in radiation with increasing distance, but also indicate the possibility of significant thermal exposure for equipment located near the source.

The main contribution of the research consists in combining two levels of analysis. The CFD simulation was used to describe the evolution of the fire in relation to the geometry of the installation, while the analytical model was applied to estimate radiative exposure at

representative distances. This approach enables the use of the spatial information provided by the simulation without confusing the global numerical results with heat fluxes measured directly on equipment surfaces.

The practical usefulness of the study lies in the possibility of preliminarily identifying areas and equipment with high thermal exposure. The results can support the preliminary identification of equipment that may require further assessment regarding separation distances, passive fire protection, water cooling or additional monitoring measures. The methodology can also guide the placement of detectors, sensors, and observation points in areas considered vulnerable.

Overall, the research demonstrates that combining CFD simulation with an analytical estimate of thermal radiation represents a useful method for the preliminary assessment of industrial risk generated by fires in refining installations. The study provides a clear basis for further analyses of local heat fluxes, equipment response, and the effectiveness of protective measures, contributing to the prevention of fire propagation and the reduction of consequences for the installation.

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