Validation of Fire Dynamic Simulator (FDS) for Pool Fire in Large Enclosures

M. Pachera[*,1], P. Brunello[1], M. Raciti Castelli[2]

[1]Department of Industrial Engineering
University of Padua
Via Venezia 1, 35131 Padua (Italy)
[2]Department of Management and Engineering
University of Padua
Stradella S. Nicola 3, 36100 Vicenza (Italy)

Abstract

In this paper, computational fluid dynamics has been used for simulating an experimental pool fire within a natural ventilated room. In the experiment, carried out by the Technical Research Institute of Finland, 4.9 kilograms of heptane have been burned in a room 10 m wide, 10 m long and 5 m high with natural ventilation through an open window. This scenario has been simulated by resorting to Fire Dynamic Simulator (Version 6) with different meshes to assess the influence of the grid size on the numerical results. In order to assess the flow field inside the room, the pool fire has been initially modeled by imposing the mass loss from the pool obtained from the experiment. Then, the evaporation process from the liquid pool has also been modeled in order to evaluate the mass loss also. In both cases, the temperatures, chemical species concentrations and smoke layer height in the surrounding of the fire, obtained from the simulation have been compared with the results of the experiments using functional analysis.

Introduction

With the ongoing development of Fire Safety Engineering, several experimental studies have been performed with the aim of investigating smoke movement and fire development inside rooms or enclosures [1]: thanks to such experiments, a better understanding of the processes controlling smoke exhaust and ventilation was achieved. Several investigations were performed using liquid fuel pool fire. In fact, the adoption of such fire source allows an easy measurement of the heat release rate, determining a highly reproducible fire behavior.

Even though several experiments were performed also to understand the evaporation process due to heat transfer feedback from the fire source [2], a simplified model of the phase change still represents a challenging issue. If, generally speaking, the validation process represents one of the basis of computational fluid dynamics [3], such issue is even more pressing in the case of fire simulations, since also chemical reactions and species transport phenomena are concerned [4].

Simulation Set-up

Starting from the experimental measurements reported in [5], the hereby proposed numerical simulations were performed by resorting to Fire Dynamics Simulator (FDS) – Version 6. Accordingly, as shown in Fig. 1, simulations were performed in a naturally ventilated room (10 m wide, 10 m long and 5 m high) with a square opening on one wall, reproducing the test case.

The room was modeled without extending the simulation domain out of the window, where a constant pressure condition was simply assigned. The walls were modeled as conductive surfaces with a constant temperature equal to 15 °C on the back side. The same constant temperature of 15 °C is assumed for the external air introduced through the window, as well as for the initial temperature of the whole system.

The walls and the ceiling of the test compartment were made of a 2 mm steel plate and the floor was made of 100 mm concrete. The adopted thermal properties are summarized in Table 1.

Table 1: Material thermal properties

Material	Density [kg/m^3]	Conductivity [W/m/K]	Specific heat [kJ/kg/K]
Steel	7850	35	0.52
Concrete	2307	1.4	0.658

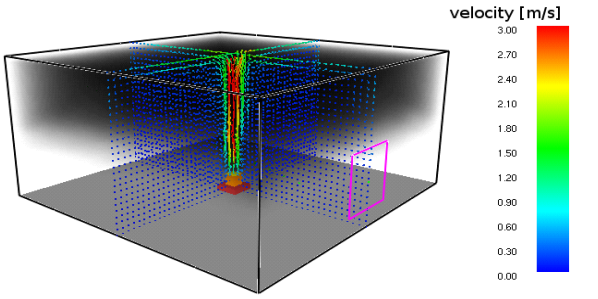

Fig. 1: Geometry of the test room, showing the smoke stratification and the velocity pattern

[*] Corresponding author: matteo.pachera@dii.unipd.it

The simulations were transient reproducing the whole experiment, during 1800 s. The radiation modeling was used with the default set-up proposed in FDS.

As required by FDS [6], a cubic uniform grid is adopted, where the grid size was chosen referring to the characteristic fire diameter D_f proposed by [7]:

$$D_f = \left(\frac{\dot{Q}}{\rho_\infty c_p T_\infty \sqrt{g}} \right)^{\frac{2}{5}} \qquad \text{Eq. 1}$$

where: Q is the HRR peak c_p is the specific heat of the air T ∞ is the temperature of the ambient and g is the gravitational acceleration.

In principle, according to [6][7], the ration between such quantity and the grid size should be between 4 and 16, to ensure adequate resolution. However, in many cases also coarser grids may guarantee acceptable resolution of the flow field. Thus, the meshes summarized in Table 2 were adopted in this study.

Table 2: Adopted meshes

Mesh	Grid size [mm]	Number of elements	$D^*/\Delta x$ [-]
Coarse	20.0	62500	2.198
Medium	13.9	202500	3.166
Fine	10.0	500000	4.397

One of the key points of the simulation set-up is obviously the fire modeling, involving chemical reactions as well as heat and mass transfer. The adopted approach will be discussed in detail in the following paragraph.

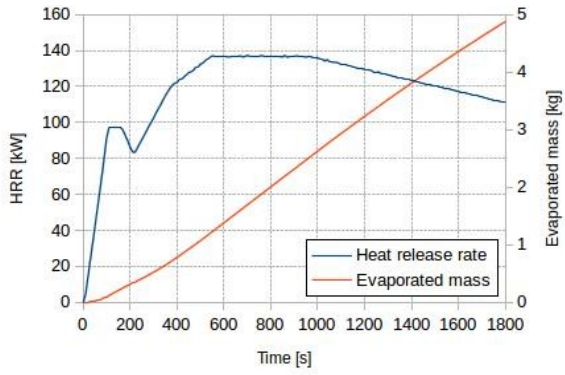

Fig. 2: Heat release rate and evaporated mass of heptane

Pool Fire Modeling

The standard combustion model used in FDS is the Eddy Dissipation Concept [8], which is infinitely fast and controlled only by the mixing of the species. The oxidation processes follow these relations:

$1\ C_7H_{16} + 7.34565\ O_2 \rightarrow 6.6913\ CO + 8\ H_2O + 0.3087\ C_{soot}$

$1\ CO + 0.5\ O_2 \rightarrow 1\ CO_2$

where the coefficients are derived from the measured CO-yield and soot-yield [5]. The experimental evaluation of heat release rate (HRR) from fire was based on heptane mass loss, which was multiplied for the heat of combustion of the heptane itself [5].

Initially, in the simulations the fire place was modeled as a burner which supplies the mass flow of heptane following the above mentioned curve.

In a second stage, an evaporation model was also introduced. The evaporation model employed in FDS [9] is based on Clausius-Clapeyron approach, where the volume fraction $X_{F,l}$ of the fuel vapor above the surface is given by:

$$X_{F,l} = \exp\left[\frac{-h_v W_F}{R} \left(\frac{1}{T_s} - \frac{1}{T_b} \right) \right] \qquad \text{Eq. 2}$$

where h_v is the heat of vaporization, W_F is the molecular weight of the fuel gas, T_s is the surface temperature and T_b is the boiling temperature of the fuel. The evaporation rate of the fuel is governed by the implementation of Stefan diffusion:

$$\dot{m} = h_m \frac{p_m W_F}{R T_g} \ln\left(\frac{X_{F,g} - 1}{X_{F,l} - 1} \right) \qquad \text{Eq. 3}$$

where pm is the pressure, T_g is the temperature, and $X_{F,g}$ is the volume fraction of fuel vapor in the grid cell adjacent to the pool surface while h_m is define in [6].

Clearly, the evaporation depends on the radiation back flux on the pool and on the species concentration above the pool fire [10]. The heat release rate is a result of the evaporation rate which, in turn, is affected by the flame [11] [12]. A steady state condition can be reached when the mass flow leaving the pool is burned and the flame re-radiates the pool without increasing or decreasing the mass flow.

Results with the Imposed Mass Flow Rate

The comparison was carried out referring to the 18 thermocouples placed inside the experimental facility: each position can be identified by three coordinates, selected according to [5]. For each position, the experimental temperature profile was compared with the numerical one, obtained using the different meshes. As usual, the agreement is assessed by means of diagrams representing the temperature evolution with time, such as Fig. 3.

However, instead of diagrams, the agreement between experimental and numerical temperatures can be assessed resorting to the functional analysis proposed by Peacock et al. [13]. According to this analysis, a couple of time-dependent numerical data can be compared using the following parameters:

$$E = \sqrt{\frac{\Sigma(E_t - N_t)}{\Sigma(E_t)}} \qquad \text{Eq. 4}$$

$$C = \frac{\langle E_t, N_t \rangle}{\|E_t\| \|N_t\|} \qquad \text{Eq. 5}$$

where: E_t and N_t represent respectively the time history of the experimental and numerical data.

The first parameter provides the magnitude of the normalized difference between the two sets of experimental vs. numerical data, while the second one provides the difference in shape between the curves.

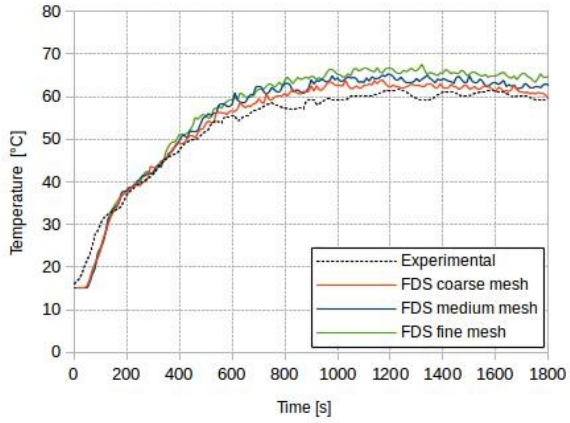

Fig 3: Experimental and numerical temperatures for the three grids at position (7.5; 5.0; 4.5)

The parameter E, evaluated for the 18 thermocouples (2 vertical arrays with 9 thermocouples each) and for the three adopted meshes, is presented in Fig. 4. It can be seen that the maximum error is present at medium height. This can be related with the temperature profile inside the smoke: in fact, the position of the interface between the smoke and the fresh air can strongly influence the temperature.

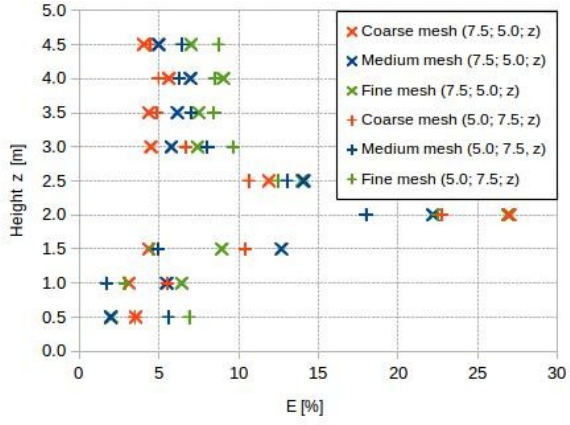

Fig. 4: Parameter E, evaluated for the 18 thermocouples

For every position also the parameter C was calculated, but it was always close to unity.

Since the amount of the smoke present in the room is obviously important, this was monitored by resorting to the so called “smoke layer height”, defined as in [6] and shown in Fig. 5.

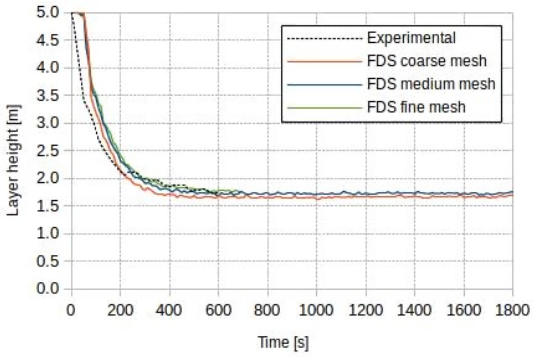

Fig 5: Smoke layer height calculated using Eq. 5 for the different grids

The smoke layer height for all the three meshes is correctly predicted both in the initial stages when the smoke begins to fulfill the room and also in the steady condition after 600 s when the smoke layer height is almost constant.

The chemical volume fraction of oxygen and carbon dioxide where also calculated near the wall, at 3.5 m height, as shown in Figs. 6 and 7.

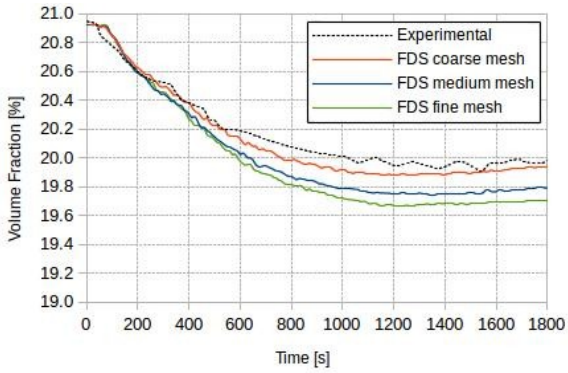

Fig. 6: Oxygen volume fraction at position (9.0; 7.5; 3.5)

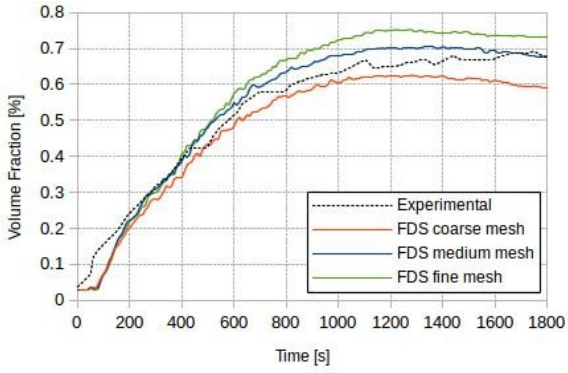

Fig. 7: Carbon dioxide volume fraction at position (9.0; 7.5; 3.5)

Instead, the double step chemistry doesn't allow to correctly predicting the partial oxidation of the carbon monoxide, which is approaching the value of 35 ppm in

the experiment while is negligible in the simulation. As also stated in [14], the oxidation of carbon monoxide is much slower than the hydrocarbon oxidation, thus the reaction modeling is not matching the second oxidation process of CO, which is immediately burned by FDS.

Results with the Evaporation Model

After an initial case where the heat release rate was imposed, the pool fire was modeled as an evaporating liquid. Confirming the results of [15], this simulation approach requires calibrating the speed of combustion, since the turbulent mixing model could be too fast, neglecting the physical time for the reaction to occur. To control the velocity of the flame, FDS allows modifying the maximum heat release rate per unit of volume (mentioned as HRRPUV in FDS) in each time-step, thus controlling the amount of fuel burned.

By using the coarse mesh, which was able also in the previous case to simulate correctly the fire inside the room, different values of HRRPUV were tested in order to match the HRR and the fuel consumption as shown in Fig. 8.

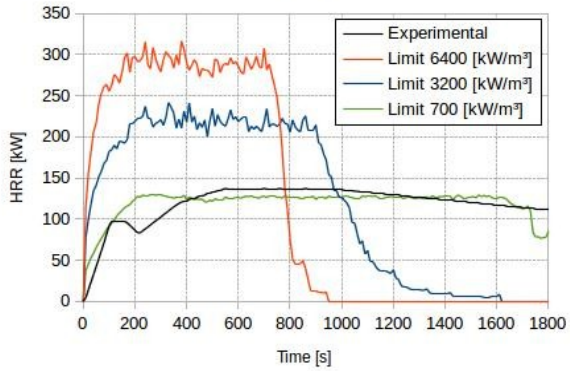

Fig 8: Heat release rate comparison for different limits of heat release rate per unit of volume

The heat release rate curve with 700 kW/m^3 used as limit, clearly fits the experimental curve unless for the peak found in the initial phase at time 300 s. The outcoming temperatures and the species concentrations are compared with the experiments in Figs 9 and 10.

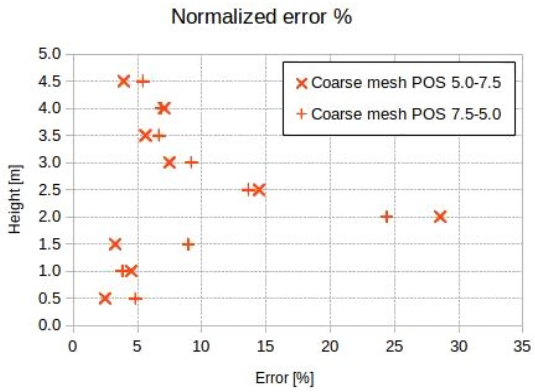

Fig. 9: Parameter E, evaluated for the 18 thermocouples

As for carbon monoxide, the same consideration reported in the previous paragraph remains valid.

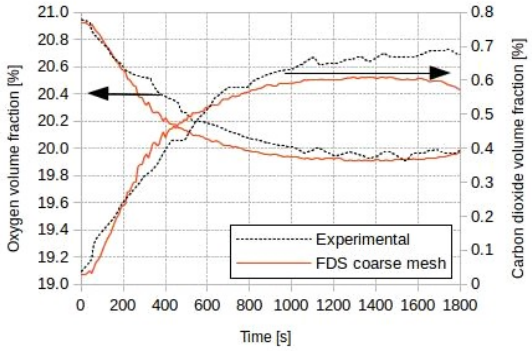

Fig. 10: Volume fractions of oxygen and carbon dioxide at position (9.0; 7.5; 3.5)

As for the smoke layer height, the comparison is presented in Fig. 11.

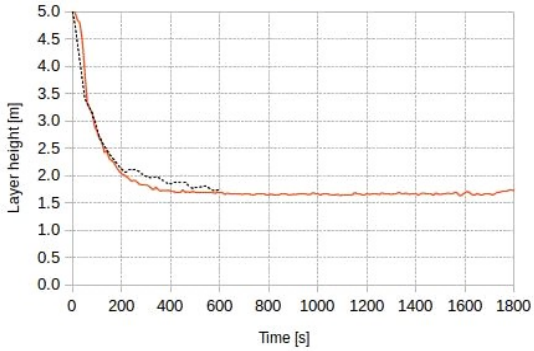

Fig 11: Smoke layer height comparison among experiment and simulation

By considering the whole set of comparisons with the evaporation model, the agreement between simulations and measurements is comparable with the simulations obtained by imposing the mass flow rate, thus confirming the reliability of the adopted evaporation and combustion model.

Conclusions

The correct simulation of a pool fire inside a room is a crucial issue in fire safety assessment. In this paper, the possibilities offered by a well established CFD computer code (FDS) were evaluated against an experimental benchmark. In doing this, two different approaches have been used for predicting the amount of fuel involved in the reaction: in the first one, the mass flow rate was imposed according to the experiments, in the second one a suitable evaporation model was used. In both cases, the results proved to be quite satisfactory, not only for the temperature distribution, but also as far as the species concentration is concerned.

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