CHEMICAL ENGINEERING TRANSACTIONS
VOL. 91, 2022

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Valerio Cozzani, Bruno Fabiano, Genserik Reniers

ISBN 978-88-95608-89-1; **ISSN** 2283-9216

DOI: 10.3303/CET2291038

Experimental and Numerical Study of Heptane Pool Fire in Airtight Enclosures

Sylvain Brohez[a]*, Dario Saladino[b], Matteo Perelli[b]

[a] University of Mons, Faculty of Engineering, Department of Chemical Engineering, 20 Place du Parc, 7000 Mons, Belgium.
[b] Università di Bologna, Dipartimento di Ingegneria Civile, Chimica, Ambientale e dei Materiali, Via Zamboni, 33 - 40126 Bologna, Italia
sylvain.brohez@umons.ac.be

The need for sustainability and a smaller ecological footprint lead to the construction of more airtight building envelopes with better thermal insulation to increase energy efficiency according to the Energy Performance of Buildings Directive (EPBD 2010/31/EU). However, specific fire risks can be encountered by the occupants since they can be blocked for a long period due to the fire-induced pressure increase and the inward door opening. In a previous experimental campaign, wood crib fire tests were carried out for measuring fire-induced pressure in a 70m^3 airtight building. High pressure inside the rooms was observed highlighting the problems for the evacuation of the occupants. Moreover, these experimental results were also used to validate the Fire Dynamics Simulator (FDS). Satisfactory predictive capability of FDS was obtained for fire-induced pressure and mechanical ventilation considering the influence of the pressure on the area of the leakages but the heat release rate (HRR) was fixed as input data for the simulations. Computational Fluid Mechanics CFD modeling is regularly used in fire safety engineering but generally, a significant limitation comes from the HRR which has to be imposed as input data.
This paper presents an evaluation of FDS v6.7.6 capability to predict fire-induced pressure without setting the HRR as input data. Fire tests were carried out with a simple fuel load such as heptane pool fire. At first, heptane pool fires were performed in an open atmosphere for preventing complex interactions between the compartment and fuel vaporization rates and evaluating the ability of FDS to predict liquid pool fire fuel mass-loss rates. Secondly, twenty-one heptane pool fires were performed in a 70 m^3 setup for evaluating the capability of FDS to predict heptane mass-loss rates, fire-induced pressure, and temperature field in the fire room in several enclosure configurations.

1. Introduction

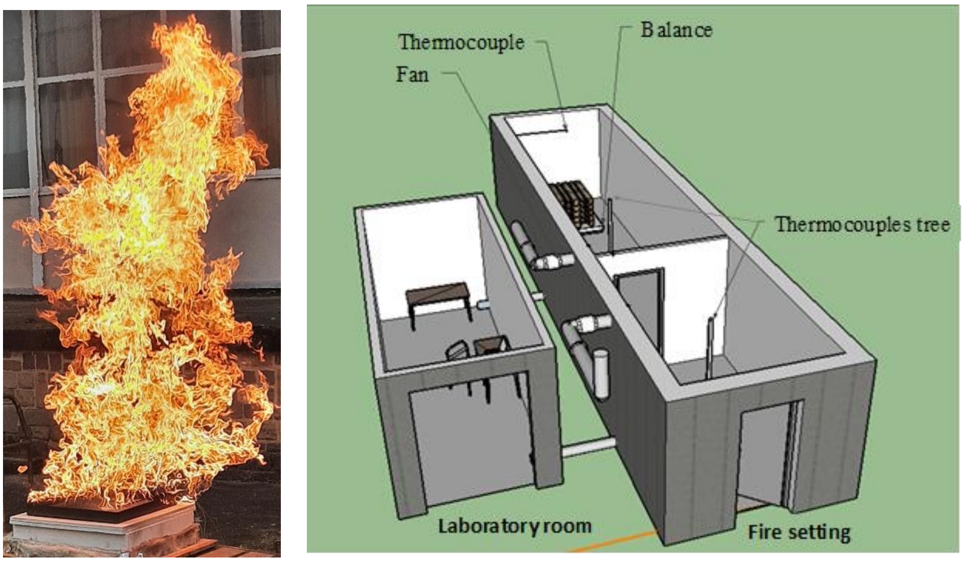
The need for sustainability and a smaller ecological footprint lead to the construction of more airtight building envelopes with better thermal insulation in order to increase the energy efficiency of houses, according to the Energy Performance of Buildings Directive (2010). However, specific risks could occur during the evacuation of the occupants in case of fire in « confined » dwellings as was observed on the night of 5 February 2013 when a fire occurred in a passive apartment in Cologne, the occupant being blocked for 2 minutes inside his apartment due to the thermal expansion of fumes and the inward door opening (Brohez et al, 2018). Learning from fire accidents is essential for preventing as far as possible accidents of the past are being repeated in the future (Hailwood, 2016), relying on research practical results and fire safety regulations.
A 70 m^3 full-scale fire-setting was built in 2015 in Bauffe by the Régie Provinciale Autonome Hainaut Sécurité RPA on its fire brigade training site for studying the effects related to the fire development in a building with high airtightness. Two different ventilation duct configurations were tested during pallets or wood cribs fires tests carried out by the University of Mons (Brohez et al, 2020): one with mechanical ventilation on, the other one with the ducts being closed with an airtight metal cap (the mechanical ventilation being off). Fire-induced peaks pressures from 870 to 2035 Pa were measured without mechanical ventilation (ducts closed), while values from 420 to 750 Pa were observed with the mechanical ventilation on. These high pressures inside the rooms highlighted the problems for the evacuation of the occupants in case of fire. These experimental results were

Paper Received: 14 January 2022; Revised: 15 March 2022; Accepted: 20 May 2022
Please cite this article as: Brohez S., Saladino D., Perelli M., 2022, Experimental and Numerical Study of Heptane Pool Fire, Chemical Engineering Transactions, 91, 223-228 DOI:10.3303/CET2291038

also used to validate the Fire Dynamics Simulator (FDS). Satisfactory predictive capability of FDS was obtained for fire-induced pressure and mechanical ventilation taking into account the influence of the pressure on the leakages area, but the HRR was fixed as input data for the simulation.
This paper presents new experimental results obtained from fire tests carried out with heptane pool fire. At first, heptane pool fires were performed in an open atmosphere for preventing complex interactions between the compartment and fuel vaporization rates and evaluating the ability of FDS to predict liquid pool fire fuel mass-loss rates. Secondly, twenty-one heptane pool fires were performed in the 70 m^3 setup for evaluating the capability of FDS to predict heptane mass-loss rates, fire-induced pressure, and temperature field in the fire room in several enclosure configurations.

2. Experimental setup

Two different sizes of square heptane pool fire were used for the open atmosphere fire tests: 0.3m x 0.3m and 0.5m x 0.5m steel pans (with a 2 mm thickness). The pan height was 3 cm and 5 cm respectively for the little and the large pan. A volume of 1.5 L and 2 L of heptane was used respectively for the small and the large pool fires. Four strain gauges were used to measure the mass of the fuel every second. To prevent unwanted temperature effects on the strain gauges, a Wheatstone measuring bridge was used for the gauges and a box made of non-combustible mineral board was placed between the pan and the strain gauges. Thermocouples were also placed in the liquid pool at different heights.
In addition to open atmosphere fire tests, tests were also performed in the 70 m^3 setup in the Régie Provinciale Autonome Hainaut Sécurité RPA. The structure is divided into two compartments: the first room is 4 m long, the second one is 8 m. They are separated by a 0.12 m thick wall composed of a steel stud frame filled with mineral wool covered with plasterboards on both sides. A partition door is in this wall, a gap of 0.9 m x 0.01 m is located at the bottom of this door for air circulation. The walls are composed of three layers of different materials: 26 mm plasterboards, 50 mm insulation layer, and 200 mm concrete blocks finished with plaster on the inside to ensure airtightness. The floor and the ceiling are made of 150 mm concrete slabs; the latter being insulated with 50 mm of mineral wool protected by 130 mm thick plasterboards to reduce the heat losses. The building has no window but only one external door. The ventilation of the building is guaranteed thanks to the mechanical ventilation network. However, for the experiments presented in this paper, the ducts were tightly closed, and the partition door was opened (the external door was closed). The fire tests were carried out with both the steel pans, the center of the pan being located about 1.4 m from the back wall and 1.2 m from the side walls.



(a) *(b)*

Figure 1: (a) Heptane pool fire in open atmosphere (50cm x 50cm pan); (b) Sketchup of the 70 m^3 airtight setup

3. Numerical modelling

3.1 CFD model and pool vaporization sub-model

The Fire Dynamics Simulator (FDS) v6.7.6 (McGrattan et al., 2012, 2021) was used to perform the simulations. FDS is a Large Eddy Simulation CFD model that solves a discretized form of the Navier-Stokes equations appropriate for low-Mach number, thermally driven fluid flows. Pool fires are modelled in two ways in FDS: the fuel mass loss rate (or HRR) is prescribed or is predicted from a pyrolysis model. In the pyrolysis model, the liquid fuel itself is treated like a thermally thick solid for simplicity. There is no computation of the convection of the liquid within the pool. A one-dimensional heat conduction equation is solved for the temperature of the liquid fuel $T_l(x,t)$:

$$\rho_l\, c_l \frac{\partial T_l}{\partial t} = \frac{\partial}{\partial x}\left(k_l \frac{\partial T_l}{\partial x}\right) + \dot{q}_l''' \quad (1)$$

where ρ_l, c_l and k_l are respectively the fuel density, specific heat and thermal conductivity. The source term $\dot{q}_l'''$ consists of the sum of heat loss rate given by the pyrolysis model and radiative absorption.
The surface temperature of the pool surface is given by the boundary condition:

$$-k_l \frac{\partial T_l(0,t)}{\partial x} = \dot{q}_c'' + \dot{q}_r'' \quad (2)$$

where $\dot{q}_c''$ and $\dot{q}_r''$ are respectively the convective and radiative fluxes at the surface of the pool.
The rate at which a liquid fuel evaporates when burning is a function of the liquid temperature and the concentration of fuel vapor above the pool surface. According to the Clausius-Clapeyron relation, the volume fraction of the fuel vapor above the surface $X_{F,l}$ is a function of the liquid boiling temperature:

$$X_{F,l} = exp\left[-\frac{h_v\, W_F}{R}\left(\frac{1}{T_l} - \frac{1}{T_b}\right)\right] \quad (3)$$

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

$$\dot{m}'' = h_m \frac{\bar{p}_m W_F}{R\, T_g} ln\left(\frac{X_{F,g}-1}{X_{F,l}-1}\right) \quad (4)$$

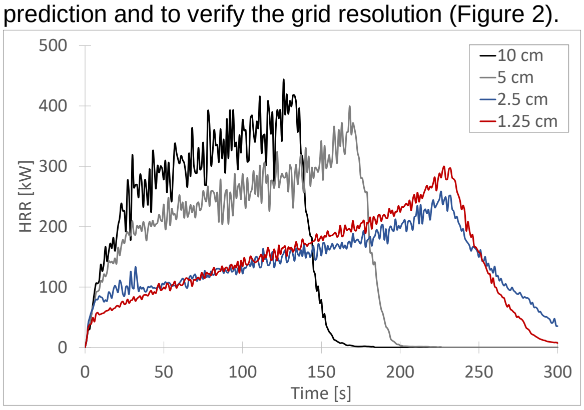
where $\bar{\boldsymbol{p}}_{\boldsymbol{m}}$ is the pressure, $\boldsymbol{T_g}$ is the temperature, and $\boldsymbol{X_{F,g}}$ is the volume fraction of fuel vapor in the grid cell adjacent to the pool surface.

3.2 Mesh resolution and computational domain

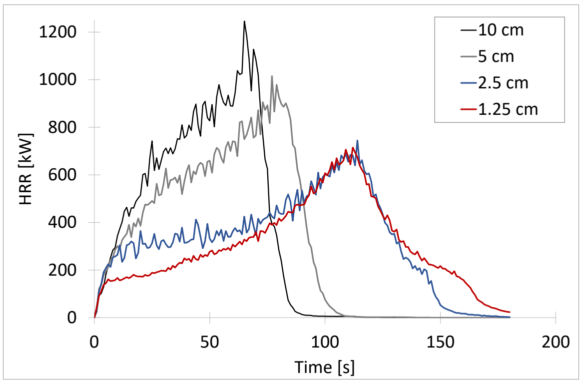
The computational domain, 3x3x6 times the fire diameter, was specified to ensure the minimal effect of the open boundary conditions on the air entrainment near the fire and fuel combustion within the simulated domain.
For buoyant plumes simulation, the non-dimensional expression $D^*/\delta x$ is used to calculate the suitable mesh size δx, where the characteristic length D^* is calculated according to:

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

$\dot{Q}$ is the HRR (kW), ρ_∞ is the ambient air density, c_p is the specific heat of the fluid, T_∞ is the ambient air temperature. A 0.63 m (0.88 m) characteristic length D^* was estimated from a measured peak HRR of 350 kW for the little pan (850kW for the large pan). The recommended ratio of $D^*/\delta x$ is between 5 and 25 leading to a mesh cell size respectively of 0.125 and 0.025 m for the small pan (0.157 and 0.035 m for the large pan). Different meshes sizes (0.1, 0.05, 0.025 and 0.0125m) were used for performing a grid sensitivity for the HRR prediction and to verify the grid resolution (Figure 2).



(a)



(b)

Figure 2: Grid sensitivity analysis for HRR prediction. Square pool fires: (a) 0.3 x 0.3m; (b) 0.5 x 0.5m

As can be seen in Figure 2, the 10 and 5 cm mesh cell sizes are too coarse for satisfactory grid resolution. While these mesh resolutions would give satisfactory results for plume temperature and pressure in airtight enclosures with fixed HRR as input data (Brohez, 2020), no satisfactory results are observed for the HRR predictions.

However, similar HRR results are obtained for the 2.5 and 1.25 cm mesh cell sizes. In the present study, a 1.25 cm mesh cell size was chosen for all the calculations. Higher burning rates are observed in Figure 2 with coarse grids. Sikanen et al (2016) showed that the predicted incident heat flux on the pool surface increases as the grid is too coarse which is linked to the inability of the coarse grid to capture the fuel rich core of the flame and a faster mixing of fuel and oxidizer. The blocking effect of the fuel vapors is weakened.

4. Experimental results – FDS validation

4.1 Open atmosphere

Heptane pool fires were carried out in open atmosphere in the absence of wind or with light wind across the pool. After ignition, a rapid increase of the HRR is observed as the flame heats the fuel surface. Heat propagates into the liquid and a thermal equilibrium seems to be reached with a quasi-steady HRR for a period of about 60 seconds for the large pan (about 110 seconds for the little pan). Then a transition to bulk boiling was observed, the pool surface appears unsteady with huge bubbling through the surface.

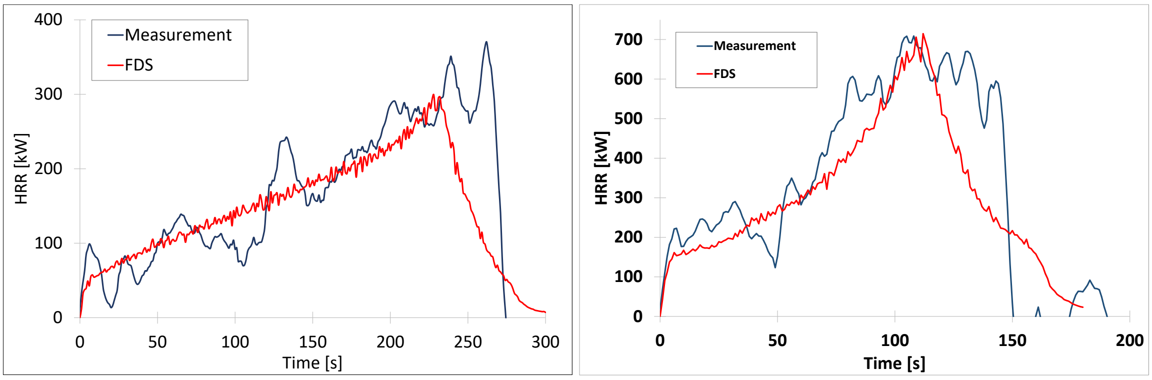


Figure 3: Comparison of measured and predicted HRR. Square pool fires: (a) 0.3 x 0.3m; (b) 0.5 x 0.5m

The combustion model used in FDS is an infinitely fast, mixing-controlled reaction scheme (McGrattan et al., 2021). The combustion occurs in the model wherever fuel vapor and oxygen co-exist. For a fuel such as heptane having a low boiling temperature, ignition of the fuel is instantaneous in FDS and the flame covers the entire fuel surface immediately (as observed during the experiments). Comparing the model predictions with the experimental measurements shows that FDS consistently predicts the heating phase involving ignition and the subsequent rapid increase of the HRR (Figure 3). Globally, FDS predicts consistently all the phases of the HRR at the exception of the extinction one which is slower. In the FDS simulation, the extinction begins at the center of the heptane pan before going outwards to complete extinction at the pan edge (the heat feedback to the fuel surface is higher in the center of the pan and decreases towards the edge of the fuel pan). With the cell-by-cell solution procedure of FDS, the fuel is consumed more quickly at the fuel pan center than around the edges of the pan due to the non-uniformity distribution of heat feedback to the fuel surface (Stewart et al, 2021). Consequently, the fuel evaporation sub-model predicts a stepwise decay of the HRR. However, the remaining fuel would be able to flow within the pan to remain at an approximately constant depth across the entire pan area until extinction (with a more abrupt extinction). Moreover, a one-dimensional heat conduction equation is used in FDS which leads certainly to an underestimation of the conduction heat transfer especially during the extinction phase.

4.2 Heptane pool fires in the 70 m^3 setup

Measurements were made for gas pressure in the fire room and between both rooms, gas temperatures in the center of each room using 1 mm in diameter K-type thermocouples trees with 0.2 m vertical separation and fuel mass from load cell. The fuel mass loss rate $\dot{m}_f$ was calculated from a smoothing technique and the heat release rate $\dot{Q}$ was then calculated with a 44.6 MJ.kg^{-1} heat of combustion ΔH_c:

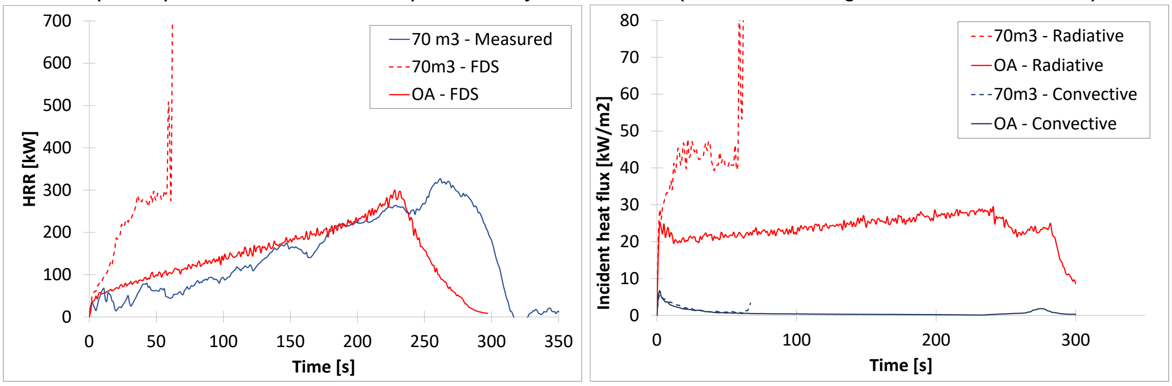
$$\dot{Q} = \Delta H_c \, \dot{m}_f \tag{6}$$

Both the HRR and the leakages area of the building envelope are key parameters for fire induced pressure prediction in an airtight building. The leakages area of the building was fixed as input data. But, in a typical building, as the pressure increases, the leakages area increases as small gaps, cracks and other leakage paths open-up. Overpressure tests were carried out in a large pressure range Δp (0–600Pa) according to the ASTM

E779 to characterize the leakages area of building. The leakages area can be expressed as function of the pressure according to the following equation:

$$A_L = A_{L,ref}\left(\frac{\Delta p}{\Delta p_{ref}}\right)^{n-0.5} \quad (7)$$

The pressure zone leakages model was used in FDS 6.7.6 with the actual 0.7 value for the leakage pressure exponent n, and a 20.7 cm^2 leakage reference area at a reference pressure of 58 Pa tanks to the overpressure tests (Brohez et al, 2020).Figure 4 compares the measured and the predicted time varying HRR obtained in the 70 m^3 setup with ducts tightly closed and partition door opened, the external door being closed. While satisfactory comparisons were obtained for heptane pool fires in open atmosphere, FDS overpredicts the HRR of the heptane pool fire inside the compartment by a factor of 3 (before obtaining numerical instabilities).



(a) (b)

Figure 4: (a) Comparison of measured and predicted HRR for the 0.3 x 0.3m pool fires in the 70 m^3 airtight setup and in open atmosphere (OA); (b) Simulated incident heat flux on the pool surface

For pool fires with diameters higher than 10 cm, the contribution of the radiative heat transfer (compared to convection) increases with pool diameter and becomes the main mode of heat transfer to the pool surface (Beyler, 2002). Unfortunately, the radiative heat flux to the pool surface was not measured during the heptane fires. However, the radiative and convective heat fluxes on the pool surface was calculated thanks to FDS and are presented in Figure 4(b) for both the open atmosphere and the compartment heptane pool fires. As expected, it can be observed that radiation is the main mode of heat transfer. Moreover, the heat feedback to the pool surface is overestimated for the pool fires in the compartment (in comparison to the open atmosphere heptane pool fire) which is linked to heat feedback from the compartment.

As can be observed in Figure 3(a) and 4(a), the HRR measured in the 70 m^3 setup is similar to the one obtained in an open atmosphere. It was then decided to fix the predicted HRR obtained with FDS for the open atmosphere fire as input data for the simulation of the pool fire in the 70m^3 setup. Figure 5 compares the measured and the predicted fire induced pressure as well as the temperature in the fire room obtained from this simulation (at 0.1 and 2.1 m high).

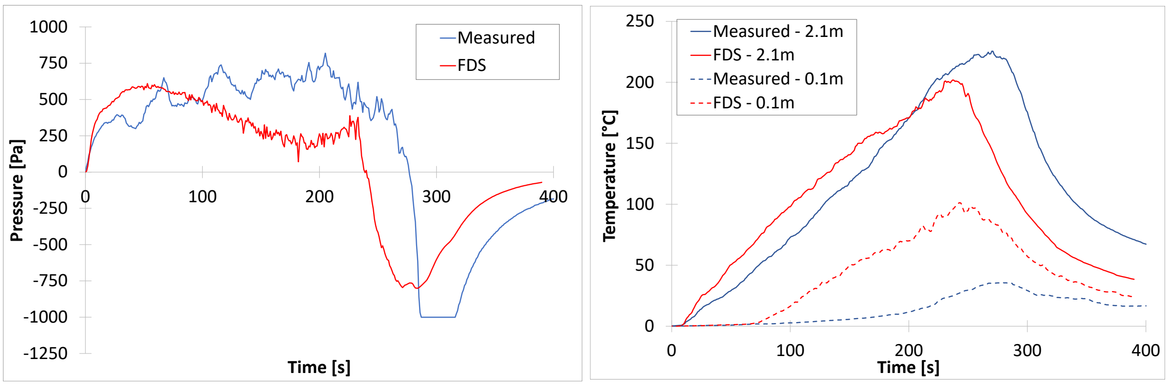


Figure 5: Comparison of measured and predicted fire induced pressure and fire room temperature for the 0.3 x 0.3m pool fire in the 70 m^3 airtight setup.

Fire-induced pressure of about 800 Pa were measured with the small heptane pool fire which could prevent the safe evacuation of the occupants in case of inward door opening, the door opening forces resulting from this range of fire-induced pressure being higher than the maximum design value given by building and life safety regulation (133N). Globally satisfactory predictions are obtained with FDS for fire-induced pressure and temperatures in the fire room at the exception of the temperature near the floor in the 70m^3 setup. Pressure peaks of about 800 and 600 Pa were respectively measured and predicted. A shift can be observed for the predicted pressure due to the HRR curve shape which is not exactly the same as the measured one (Figure 4a). While satisfactory predictions are obtained for fumes temperature at 2.1 m high (30 cm below the ceiling), the temperature near the floor (0.1 high) is overestimated by the model. Forthcoming research is needed to better understand the temperature fields discrepancies which could be linked to the air recirculation in the airtight room.

5. Conclusions

CFD modeling is regularly used in fire safety engineering but generally, a significant limitation comes from the HRR which is imposed as input data. This paper presents an evaluation of FDS v6.7.6 capability to predict fire-induced pressure in an airtight compartment without setting the HRR as input data. At first, heptane pool fires were performed in an open atmosphere for preventing complex interactions between the compartment and fuel vaporization rates. It has been shown that FDS gives consistent results for the fuel mass loss rate but only with the finest mesh to correctly simulate the heptane vapor-rich core above the fuel surface. Secondly, heptane pool fires were performed in a very airtight setup. Unfortunately, the mass-loss rate was overestimated by a factor of 3 by FDS due to the incident radiative heat flux on the pool surface (heat feedback from the compartment). As the HRR measured in the 70 m^3 setup was similar to the one obtained in an open atmosphere, it was decided to fix the predicted HRR obtained with FDS in the open atmosphere as input data for the simulation of the fire in the airtight compartment. Globally satisfactory predictions are obtained with FDS for fire-induced pressure and temperatures in the fire room at the exception of the temperature near the floor. Forthcoming research is needed to better understand the temperature field discrepancies which could be linked to the air recirculation in the airtight room. It can be pointed out that fire-induced pressure of about 800 Pa were measured with the small heptane pan which could prevent the safe evacuation of the occupants in case of inward door opening. In a forthcoming publication, experimental results obtained from the opening of a natural smoke exhaust activated with a smoke detector will be presented as a mitigation measure to avoid the blocking of the occupants within a confined dwelling subjected to a fire.

Acknowledgments

The authors thank the Régie Provinciale Autonome (RPA) Hainaut Sécurité for the construction and the access to the experimental setup for the heptane pool fire tests

References

ASTM E779-19, 2019, Standard Test Method for Determining Air Leakage Rate by Fan Pressurization, ASTM International, West Conshohocken, PA, USA.

Beyler C.L., 2002, Fire Hazard Calculations for Large, Open Hydrocarbon Fires, chapter 3, 268-314 in in P.J. DiNenno et al, SFPE Handbook of Fire Protection Engineering, third edition, National Fire Protection Association, USA.

Brohez S., Duhamel P., 2018, Inwards doors blocked by fire induced overpressure in airtight apartment: a real case in Germany. Chem Eng Trans, 67, 25-30.

Brohez S., Caravita I., 2020, Fire-induced Pressure in Passive Houses: Experiments and FDS Validation, Fire Safety Journal, 114, 15p.

Directive of the European Parliament and of the Council of 19 May 2010 on the energy performance of buildings, (Directive 2010/31/EU).

Fourneau C., Cornil N., Delvosalle C., Breulet H., Desmet S., Brohez S., 2012, Comparison of fire hazards in passive and conventional houses. Chem Eng Trans, 26, 375–380.

Hailwood M., 2016, Learning from accidents – reporting is not enough, Chem Eng Trans, 48, 709- 714.

McGrattan K., K., McDermott R., Floyd J., Hostikka S., Forney G., Baum H., 2012, Computational fluid dynamics modelling of fire, International Journal of Computational Fluid Dynamics, 26, 349-361.

McGrattan K., Hostikka S., Floyd J., McDermott R., Vanella M., 2021, Fire Dynamics Simulator, Technical Reference Guide, NIST special publication 1018-1, sixth ed.

Sikanen T., Hostikka S., 2016, Modeling and simulation of liquid pool fires with in-depth radiation absorption and heat transfer, Fire Safety Journal, 80, 95-109.

Stewart J.R., Phylaktou H.N., Andrews G.E., Burns A.D., 2021, Evaluation of CFD simulations of transient pool fire burning rates, Journalof Loss Prevention in the Process Industries, 71, 14