Numerical simulations of oscillatory combustion and extinction of a liquid pool fire in a reduced-scale and mechanically-ventilated enclosure

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Highlights:

- Fire burning regimes are well predicted in a wide range of ventilation conditions
- Oscillatory combustion is captured by natural convection for evaporation modeling
- Prescribing Auto-Ignition Temperature is important in capturing fire oscillations
- Prescribing AIT prevents spurious fuel re-ignition in under-ventilated conditions

Abstract:

The paper presents a numerical study on an 18 cm-diameter liquid pool fire in a reduced-scale and mechanically-ventilated enclosure. The enclosure walls are made of a calcium silicate layer and a steel layer on five sides, the remaining sidewall is made of heat-tempered glass. The ventilation system consists of an extraction fan positioned in one duct. A second duct for air inlet is left 'open'. Three air renewal rates (ARR) and open atmosphere conditions are considered in the numerical study. Computational Fluid Dynamics (CFD) simulations are carried out with the Fire Dynamics Simulator (FDS 6.7.5). The default evaporation model in FDS, based on a forced convection approach, is compared to a natural convection approach implemented in the source code. The results show that the oscillatory combustion, occurring at ARR = 15 h^{-1}, is best captured by the natural convection approach. It is also found that prescribing the actual Auto-Ignition Temperature (AIT) of the fuel is important to capture the fire oscillations and (local) flame quenching. At ARR = 8 h^{-1}, extinction occurs. In this case, it is found that prescribing the actual fuel AIT allows to prevent spurious oscillatory combustion. At ARR = 22.5 h^{-1}, there is a stable steady-state burning regime for which (as well as for open atmosphere conditions) prescribing the actual fuel AIT is not crucial.

Keywords: compartment fires; modeling; CFD; liquid pool fires

1. Introduction

When a fire occurs in confined and mechanically-ventilated compartments, such as in nuclear facilities, there is a potential loss of confinement due to pressure changes. An associated subsequent risk is the release of harmful products. A specific fire scenario in this configuration is the oscillatory combustion phenomenon that has been observed in a large-scale mechanically-ventilated compartment called DIVA [1]. The compartment dimensions were 5 m × 6 m × 4 m (height). The walls were made of re-enforced concrete partially covered with rock-wool panels. The ceiling was covered with a double layer of a 30 mm – thick panel. The mechanical ventilation consisted of a fresh air inlet duct and an exhaust duct with a 0.3 m × 0.6 m-ventilation area, each positioned at 0.8 m below the ceiling. The inlet and exhaust ducts were connected to a complex mechanical ventilation network with fans delivering in the room (prior to ignition) flow rates corresponding to Air Renewal Rates (ARRs) between 8 and 17 h^{-1}. The fire source consisted of a 0.4 m^2 circular heptane pool fire positioned in the center of the room. During the

fire growth period, the room pressure increased substantially because of the release of hot combustion products in an air-tight compartment. Consequently, the inflow of fresh air reduced, causing a 'weakening' of the flame to the point of near-extinction. Therefore, the pressure has decreased allowing for an increase in the inflow of fresh air and a subsequently 'revitalized' flame, which caused (again) and increase in pressure, leading to a cyclic behavior. This phenomenon, as described above, results from a coupling between the liquid (evaporation) burning rate and the ventilation through the room pressure. It is described as a low-frequency oscillatory behavior because the calculated frequency of the transient burning rate profile (which is similar to the dominant frequency in the pressure and ventilation profiles) is significantly lower than the puffing frequency of a pool fire in open atmosphere conditions due to hydrodynamic instabilities. The onset of oscillatory combustion (with frequencies between 5 and 7 mHz) has been observed at ARRs of 12 and 15 h^{-1}; a lower ARR of 8 h^{-1} caused a sudden extinction due to lack of oxygen and a higher ARR of 17 h^{-1} yielded sustained stable burning without low-frequency oscillations. Furthermore, a mapping of the burning modes has been proposed in [1] based on a Global Equivalence Ratio (GER) that has been defined using the steady burning rate in open atmosphere conditions and the ventilation flow rate at the inlet. At GER < 0.3, there is sustained stable burning. At GER > 0.8, sudden extinction occurs due to lack of oxygen. Oscillations occur at intermediate values of the GER. In addition to the effect of the ventilation it has been shown in [1] that, under similar ventilation conditions, oscillations occur for liquid fuels (heptane and dodecane) and not for a gaseous fuel, namely propane. This suggests that the response of the liquid surface in terms of evaporation rate under the radiative heat feedback effect plays a major role in triggering and sustaining oscillatory combustion. That is why, as will be further discussed in this paper, evaporation modelling is considered as a key modelling aspect in capturing oscillatory combustion for the fire scenarios of interest here. Therefore, the focus in this study is on liquid pool fires in mechanically-ventilated compartments because it is carried out in the context of fire safety in nuclear installations (with mechanically-ventilated rooms and liquids such as Hydrogenated TetraPropylene (HTP) stored therein for reprocessing). Nevertheless, it is important to mention that oscillatory combustion has also been observed in naturally-ventilated compartment fires [2], as well as in a mechanically ventilated compartment with a gaseous fuel (propane) [3].

In order to further characterize the oscillatory combustion, a 1:4 scale reproduction of the room in the DIVA facility, called NYX, has been used in [4]. The ARR varied between 4 and 22.5 h^{-1}. Heptane and dodecane were used as fuels with burner diameters varying from 12 to 24 cm. Unstable oscillatory combustion (with frequencies of about 12 to 33 mHz) has been mainly observed at ARRs between 10 and 16.5 h^{-1}, with variations depending on the fuel (heptane or dodecane) and the burner diameter.

Several numerical studies have been carried out in order to assess the current Computational Fluid Dynamics (CFD) capabilities in the prediction of the oscillatory combustion phenomenon at either large-scale (DIVA) or reduced-scale (NYX). In [1], the CFD code ISIS has been used to simulate the large-scale experiments. The Mass Loss Rate (MLR) prediction is based on a heat balance (i.e., net heat flux divided by the heat of gasification of the liquid). Extinction is modeled using the Eddy Dissipation Concept (EDC) in conjunction with a Flame Extinction Factor (FEF) defined as a function of a lower oxygen index, $Y_{O2,c}$ = 0.15, and a critical flame temperature, T_c = 1500 K, that were determined experimentally. The oscillatory behavior was qualitatively well captured. Nevertheless, the frequency was overestimated by 112% (14 mHz instead of 7 mHz)

and the amplitude was underestimated by 64%. In [5], the Fire Dynamics Simulator (FDS 6) has been used for a similar scenario with a similar approach for turbulent combustion [6], but with a fuel evaporation modelling based on the mass transfer number approach. An improvement has been observed in the predicted frequency (about 10 mHz). However, the amplitude remained significantly underestimated. Further simulations carried out in [7] with FDS have shown that oscillations were observed in the simulations whereas they were not observed in the experiments. In order to suppress the spurious oscillations, the authors hinted in [7] at the importance of the fuel Auto-Ignition Temperature (AIT) that was calibrated numerically at AIT = 373 K = 100°C. Finally, numerical simulations of the small-scale experiments, carried out in [4] using the CFD code SAFIR and in [8] using the CFD code ISIS, confirmed the difficulty of current state-of-the-art modelling in capturing correctly the oscillatory phenomenon.

As mentioned above, liquid evaporation is very important for the fire scenarios of interest, given the importance of the liquid response to the radiative heat feedback at the surface. Regarding this aspect, it has been shown in [9] that using a natural convection approach, as opposed to the forced convection approach used in [6], is fundamentally more appropriate and yields improved predictions for the liquid surface temperature in open atmosphere conditions. The objective of the paper is to explore the potential improvement (by using a natural convection approach) in capturing the oscillatory behavior observed in the NYX compartment. Regarding extinction (in the gas phase), the importance of the fuel Auto-Ignition Temperature (AIT) is analyzed. FDS 6.7.5 is used in this study.

2. Experimental configuration and settings

As mentioned in the introduction, the enclosure fire tests considered in this numerical work, have been conducted in a 1.50 × 1.25 × 1.00 m^3 mechanically-ventilated compartment called NYX [4] (which is a 1:4 scale reproduction of the room of DIVA facility of IRSN [1]). Schematic drawings are shown in Fig. 1.

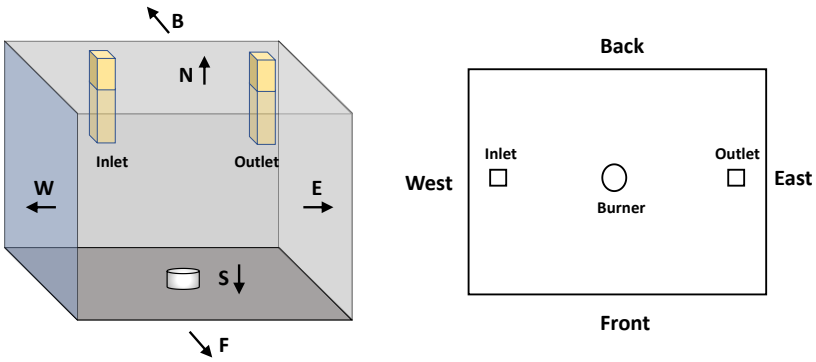

Fig. 1. The schematic drawings of the NYX compartment, reproduced from [4]. (left) view from the FW side; (right) top view.

On the west (W) side of the compartment, heat-tempered glass allows video recording by a CCD camera outside the compartment. On the E, S, N, B and F sides of the compartment, the walls are made of a 45 mm-thick calcium silicate layer and a 2 mm-thick steel layer facing outward. The air flow is mechanically extracted and the inlet flow is free. The rectangular-shaped ventilation pipes are located in the upper part of the compartment at 0.8 m from the floor. The ventilation rate is represented as an Air Renewal Rate (ARR), which is defined as the ratio of inlet volume

flow rate of air before ignition to the volume of the enclosure. The fire source is an 18 cm-diameter burner made of steel and filled with heptane up to 4.3 cm height. Ignition is carried out by a propane burner. In this study, three ventilation flow rates are considered, namely 22.5, 15 and 8 h^{-1} in order to study the three different modes of under-ventilated burning: (*i*) stable steady burning, (*ii*) unstable oscillatory burning, and (*iii*) sudden extinction due to lack of oxygen.

Gas temperatures are measured in each corner of the compartment and in the ventilation ducts. Oxygen, CO_2, and CO are measured in the exhaust duct and inside the enclosure. Gas velocities are measured in the inlet and the outlet pipes. The pressure difference is measured by a pressure transducer between the inside and outside of the compartment. The fuel MLR is recorded by a load cell. The time delay of the measurement is corrected and all measurements are recorded with the same frequency of 1 Hz. More details can be found in [4].

3. Numerical modelling

As mentioned above, FDS 6.7.5 is used this work. The main modelling aspects will be described in this section, with a particular focus on liquid heat-up and evaporation. More details can be found in [6].

3.1 Liquid evaporation

The liquid evaporation rate, calculated on a cell basis, is governed by Stefan diffusion:

$$\dot{m}'' = \left(\frac{\mathrm{Sh}\,D}{L}\right)\left(\frac{p\,MW_F}{RT_g}\right)\ln\left(\frac{X_{F,g}-1}{X_{F,l}-1}\right) \qquad (1)$$

where Sh is the Sherwood number, D is the binary diffusion coefficient, L is a length scale, p is the pressure, MW_F is the molecular weight of the fuel, R is the universal gas constant, T_g and $X_{F,g}$ are, respectively, the gas temperature and the volume fraction of fuel vapor in the first cell above the liquid, and $X_{F,l}$ is the volume fraction of fuel vapor at the surface (calculated using the integrated Clausius–Clapeyron equation). The latter is a function of the liquid surface temperature, which is calculated using the liquid heat-up model described in the next sub-section.

3.2 Liquid heat-up

In FDS, the liquid fuel is viewed as a 1-D thermally thick solid. Therefore, Fourier's equation reads:

$$\rho_\ell c_\ell \frac{\partial T_\ell(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(k_\ell \frac{\partial T_\ell(x,t)}{\partial x}\right) + \dot{q}_r''' \qquad (2)$$

where x is the distance from the liquid surface, t is the time, ρ_l, c_l, and k_l are the density, specific heat, and thermal conductivity of the liquid fuel and $\dot{q}_r'''$ is the radiative exchange term. A mean absorption coefficient is applied for calculating the radiation absorption within the liquid phase, where a gray medium is assumed. In this study, the mean absorption coefficient is chosen to be 43 based on the 'M1' method discussed in [10].

The thermal boundary condition at the top of the liquid surface is:

$$-k_\ell \frac{\partial T_\ell}{\partial x}(0,t) = \dot{q}_c'' + \dot{q}_r'' - L_v \dot{m}'' \quad (3)$$

where $\dot{q}_c''$ is the convective heat flux and $\dot{q}_r''$ is the radiative heat flux. The radiative fraction is discussed in section 3.4. The convective heat flux at the liquid surface is calculated as:

$$-\dot{q}_c'' = h\left(T_g - T_s\right) \quad (4)$$

The heat transfer coefficient, *h*, is defined as:

$$h = \max\left[C\left|T_g - T_s\right|^{1/3}, \frac{\mathrm{Nu}\ k_g}{L} \right] \quad (5)$$

where *C* is a coefficient of empirical natural convection models (taken $C = 1.52$ for a horizontal plate), and k_g is the thermal conductivity of the surrounding gas.

3.3 Convective heat and mass transfer

An important modelling question at this point is the estimation of the Sherwood number (Sh) and the length scale (*L*) in Eq. (1). Two approaches are discussed in this study: a natural convection approach and a forced convection approach.

3.3.1 Forced convection

The forced convection approach (default approach in FDS) is based on empirical correlations for the Nusselt number (Nu). These correlations, derived from experiments of a parallel flow to a flat plate, read [11]:

$$\mathrm{Nu} = 0.664\,\mathrm{Re}^{1/2}\,\mathrm{Pr}^{1/3} \quad \text{if} \quad \mathrm{Re} < 3\times10^5 \quad (6)$$

$$\mathrm{Nu} = 0.037\,\mathrm{Re}^{4/5}\,\mathrm{Pr}^{1/3} \quad \text{if} \quad 3\times10^5 < \mathrm{Re} < 10^8 \quad (7)$$

where Re is the Reynolds number and Pr is the Prandtl number (Pr = 0.7). Equation (6) is applied for the laminar regime and Eq. (7) is applied for the turbulent regime.

The Reynolds number is calculated as:

$$\mathrm{Re} = \frac{\rho_g u L}{\mu_g} \quad (8)$$

where ρ_g and μ_g are the density and the dynamic viscosity of gas at the thermal boundary layer, computed according to the gas temperature, *u* is the velocity of the cross flow and *L* is the characteristic length crossing the fuel surface.

The Sherwood number is obtained using the Chilton-Colburn analogy, i.e., Sh = Nu.

3.3.2 Natural convection

It has been shown in [9] that a natural convection correlation is more appropriate for a liquid pool fire burning under quiescent conditions. More particularly, a correlation from ‘cold plate’

experiments is used in [11] to account for the ineffective heat transfer due to flow movement. This correlation reads [11]:

$$\mathrm{Nu} = 0.52\,\mathrm{Ra}^{1/5} \quad \text{if} \quad 10^4 \le \mathrm{Ra} \le 10^9 \tag{9}$$

The Rayleigh number, Ra, is defined as:

$$\mathrm{Ra} = \mathrm{Gr}.\mathrm{Pr} = \frac{g\,\beta\left|T_s - T_g\right|L^3}{\nu\,\alpha} = \frac{g\,\left|T_s - T_g\right|L^3}{\left(T_s + T_g\right)/2}\left(\frac{\rho_g^2\,c_p}{\mu\,k}\right) \tag{10}$$

where Gr is the Grashof number, g is the gravitational acceleration, β is the expansion coefficient (inverse of the film temperature, i.e., average of T_g and T_s), ν is the kinematic viscosity, α is the thermal diffusivity, ρ_g is the gas density, c_p, μ, and k are the heat capacity, dynamic viscosity and thermal conductivity calculated at T_g for Sh, and at the film temperature for Nu.

The characteristic length scale L for the natural convection approach is [11]:

$$L = A / P \tag{11}$$

where A and P are the area and the perimeter of the horizontal plate respectively.

The Sherwood number is obtained using the Chilton-Colburn analogy, i.e., Sh = Nu.

3.4 Gas phase

The treatment of turbulence is carried out by Large Eddy Simulation (LES) method, where the Wall-Adapting Local Eddy-viscosity model for the sub-grid scale viscosity applies. The Eddy Dissipation Model (EDM) is applied for turbulent combustion, assuming an infinitely fast chemistry. The Finite Volume Method (FVM) is used to solve the Radiative Transport Equation (RTE). The radiative fraction, χ_r, is predicted instead of using a prescribed default value in FDS. In fact, the default radiative fraction of χ_r = 0.40 [6] is believed to be too high for the burner diameter of 18 cm considered in this study.

The extinction model in FDS is based on local oxygen and fuel concentration, as well as the mean temperature resolved in the grid. The cell temperature must be higher than the critical flame temperature (CFT) for the combustion to occur. The flame extinguishes when the reactants fail to raise the cell temperature above the critical flame temperature. The default assumption in FDS is that the fuel and oxygen react immediately after mixing, as long as there is sufficient fuel and oxygen concentration, unless flame extinguishment occurs. This is designed to avoid the need to model the ignition process. In practice, this is done by assuming a very low auto-ignition temperature (AIT) of -273 °C. This assumption is adequate for well-ventilated and large-scale fire simulations. However, as shown in [7], this assumption can cause spurious re-ignition under low gas temperature. Specifying a higher AIT allows to prevent the spurious re-ignition because combustion will not occur when the cell temperature is lower than the specified AIT. For heptane, AIT = 215 °C [12]. The AIT has been considered in [7] as a model parameter by taking the intermediate value of AIT = 100 °C. However, we have chosen here to consider either the default value (AIT = -273 °C) in FDS, or the actual value (AIT = 215 °C). In the latter case, ignition modelling is required, which is carried out here by setting first AIT = -273 °C, stopping the simulation at t = 80 s, changing AIT to 215 °C, and restarting the simulation from t = 80 s onwards. The choice of t = 80 s is motivated by the fact that the burning in the compartment is

found to be similar to the burning in open atmosphere conditions during this period [4]. This is a simpler 'numerical ignition protocol' than, e.g., the hot surface method used in [7].

3.5 Numerical settings and test cases

Prior to the enclosure fire simulations, open atmosphere simulations are carried out. A 0.16 × 0.16 m^2 square burner is used to represent the 0.18 m-diameter burner in the simulations, as the Cartesian coordinates system is applied in FDS. The results of a simulation (not shown here) with a circular burner using the 'stair stepping method' show that the deviations with a square burner for the quantities of interest are marginal (below 1%). The lip height in the simulations is 1 cm and the fuel depth is 4.3 cm. The computational domain is 0.72 × 0.72 × 1.60 m^3; simulations with a larger domain do not yield different results (results not shown here). The top boundary and the four sides of the computational domain are set to be 'OPEN' (total pressure boundary condition allowing free flow across the domain boundary). The bottom of the domain is set as 'INERT'; the surface remains at the initial (ambient) temperature. A uniform structured mesh is used in the simulations. A sensitivity analysis on the cell size is carried out using cell sizes of 4, 2 and 1 cm without changing the default models for evaporation (forced convection approach) and fuel Auto-Ignition Temperature (AIT = -273 °C). An additional simulation is carried out with a cell size of 1 cm and using the natural convection approach. The fuel properties used are listed in Table 1.

Table 1. Fuel properties [10].

Fuel	ρ kg/m^3	C_p kJ/(kg K)	k W/(m K)	L_v kJ/kg	ΔH_c kJ/kg	T_b °C	Y_{CO} g/g	Y_s g/g
Heptane	675	2.24	0.14	317	43580	98.5	0.010	0.037

Table 2. The main simulations conducted in this study.

Sim. ID	Vent.	Forced/ Natural	Re_{min}/ Ra_{min}[1]	L	AIT (°C)	Cell size (cm)
FO-4	OPEN	Forced	5×10^5	L_b	-273	4
FO-2	OPEN	Forced	5×10^5	L_b	-273	2
FO-1	OPEN	Forced	5×10^5	L_b	-273	1
NO	OPEN	Natural	10^4	A_b / P_b	-273	1
F22.5_AIT	22.5h^{-1}	Forced	5×10^5	L_b	215	1
N22.5_AIT	22.5h^{-1}	Natural	10^4	A_b / P_b	215	1
N22.5	22.5h^{-1}	Natural	10^4	A_b / P_b	-273	1
F15_AIT	15 h^{-1}	Forced	5×10^5	L_b	215	1
N15_AIT	15 h^{-1}	Natural	10^4	A_b / P_b	215	1
N15	15 h^{-1}	Natural	10^4	A_b / P_b	-273	1
F8_AIT	8 h^{-1}	Forced	5×10^5	L_b	215	1
N8_AIT	8 h^{-1}	Natural	10^4	A_b / P_b	215	1
N8	8 h^{-1}	Natural	10^4	A_b / P_b	-273	1

[1] Re_{min} and Ra_{min} are for the forced and natural convection approach, respectively.

In the enclosure fire simulations, a 1 cm cell size is used. A 1.50 × 1.26 × 1.00 m^3 compartment is prescribed to represent the NYX compartment in the simulations. The six sides of the compartment are prescribed as insulated walls with two layers of calcium silicate and steel. The

heat-tempered glass on the West side of the compartment is not prescribed due to unavailability of the information on material properties and thickness. One simulation was carried out with glass (properties taken from [13] with the thickness of 7 mm) installed on the west side with oscillatory regime (ARR = 15 h^{-1}), where no significant difference is found in the results (not shown here). The ventilation is activated for 30 seconds before placing the fuel in the enclosure, to ensure a stable ventilation rate. As mentioned above, three ventilation flow rates are considered (ARR = 22.5, 15 and 8 h^{-1}) in order to study the three different modes of under-ventilated burning conditions: (*i*) stable steady burning, (*ii*) unstable oscillatory burning, and (*iii*) sudden extinction due to lack of oxygen. For each of the three ventilation flow rates, the following combinations are used: (1) natural convection and AIT = 215 °C, (2) natural convection and AIT = -273 °C, and (3) forced convection and AIT = 215 °C. These combinations allow to examine separately the influence of two modelling aspects of interest here: convective mass transfer and AIT. The main numerical tests and details of the numerical settings can be found in Table 2. The nomenclature is as follows: the first letter is F or N ('F' means Forced convection approach; 'N' means Natural convection approach), the following letter is the ventilation condition ('O' means open atmosphere condition; '8', '15', and '22.5' are the ARRs). After the underscore, 'AIT' means AIT = 215 °C, otherwise the default AIT = -273 °C is used. The number (4 ,2, or 1) after 'FO-' is the cell size. A 1 cm cell size is used for the remainder of the simulations. The numerical results presented in this study are time-averaged over a period of 12 s, similarly to the experimental data.

4. Results and discussions

4.1 Open atmosphere conditions

Most of the test cases shown in this sub-section have been analyzed in [9]. They are briefly recalled here for the sake of completeness.

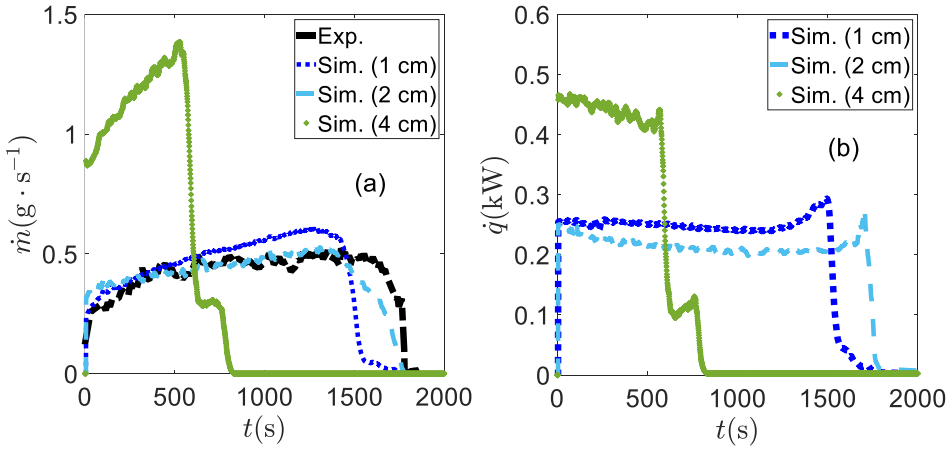

Fig. 2. The cell sensitivity analysis by the forced convection approach in open atmosphere conditions. (a) burning history; (b) integrated total heat flux on the fuel surface.

The results for the cell sensitivity analysis are reported in Fig. 2. It is shown that the transient MLR predictions correspond to the total heat flux received on the fuel surface. The predicted burning rate and heat flux on the fuel surface are significantly overestimated with a cell size of 4 cm, whereas good predictions are obtained with cell sizes of 2 cm and 1 cm. The structure of the flame is relatively well predicted, regardless of the cell size, when comparing the quasi-steady

state vertical velocity and temperature to McCaffrey's correlations (see Fig. 3). The most significant difference is found to lie in the first gas cell near the fuel surface. The gas temperature (T_g) in the first cell adjacent to the liquid fuel is much higher in the 4 cm mesh, whereas similar gas temperatures are predicted by 1 cm and 2 cm meshes (see Table 3). Strictly speaking, convergence is not yet obtained. However, the deviations for the burning rate and heat fluxes on the fuel surface are small enough (see Table 3) to carry out the remaining tests with a cell size of 1 cm.

Table 3. Results of the cell sensitivity analysis (1, 2, and 4 cm cell) by the forced convection approach.

Sim. ID	$\dot{m}$ (g/s)	$\dot{q}_{total}$ (kW)	$\dot{q}_r$ (kW)	$\dot{q}_c$ (kW)	T_g (°C)	T_s (°C)	$(T_g - T_s)$ (°C)
FO-1	0.56	0.24	0.21	0.03	171	50	121
FO-2	0.48	0.21	0.17	0.04	167	42	125
FO-4	1.26	0.43	0.27	0.16	525	24	501

* The averaging time is 800-1200 s for 'FO-1' and 'FO-2', and 300-500 s for 'FO-4' due to earlier full consumption of the fuel.

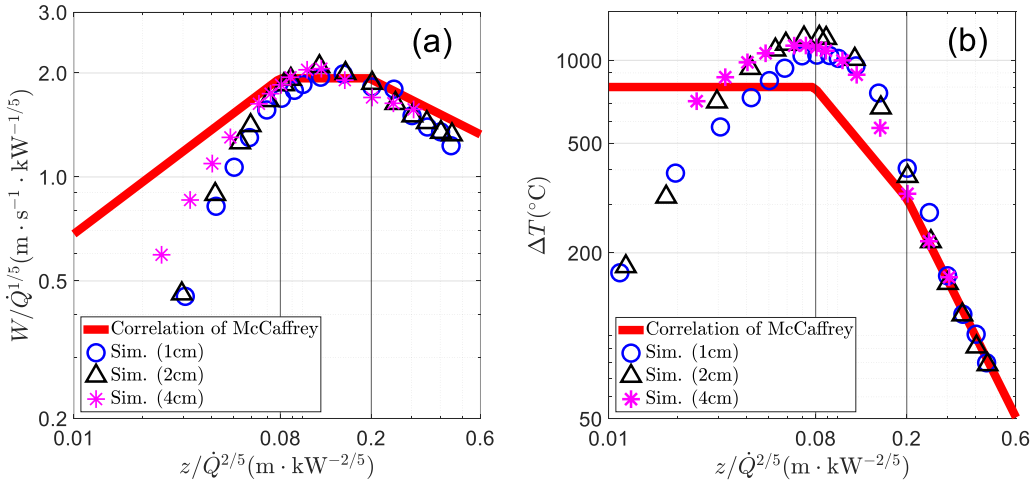

Fig. 3. The quasi-steady (a) vertical velocity and (b) temperature difference of the cell sensitivity analysis by the forced convection approach, comparing to McCaffrey's correlations.

Fig. 4 shows the transient profiles of the burning rate and surface temperature predictions by the forced and natural convection approaches. A slight improvement is observed for the burning rate when using the natural convection approach, where a peak value in closer agreement with the experimental data is observed. Additionally, the surface temperature with the natural convection approach is much closer to the boiling point, which is believed to be more representative of reality. The higher surface temperature prediction is also believed to have a significant influence on the fuel response to heat feedback at the surface in the enclosure fire configuration. One drawback of the forced convection approach is the inconsistency of the flow regime on the fuel surface and the correlation assumption [9]. The Reynolds number on the center of fuel surface is found to lie in the laminar regime (250 - 500) instead of the turbulent assumption by the forced convection approach ($\mathrm{Re_{min}} \geq 5 \times 10^5$). On the other hand, the natural convection approach is

found to have a flow regime that is consistent with the correlations, where the Rayleigh number (7×10^4) complies with the flow regime ($10^4 \leq \mathrm{Ra} \leq 10^9$) of Eq. (9).

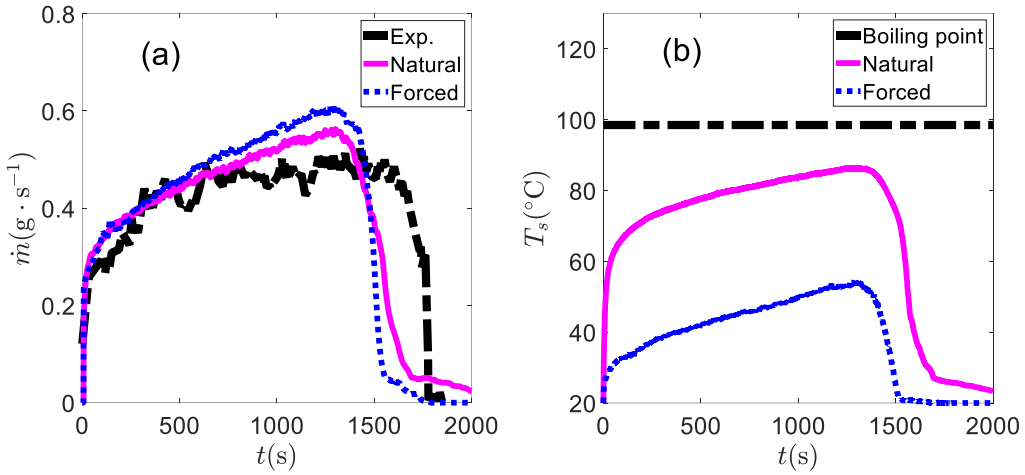

Fig. 4. Transient profiles of the (a) burning rate and (b) fuel surface temperature, by the forced and natural convection approaches in open conditions.

4.2 Stable steady-state burning

Fig. 5 shows that in the experiments with ARR = 22.5 h-1, after an initial fire growth stage, the burning rate stabilizes at 0.22 - 0.25 g/s at t = 200 to 1200 s. After 1250 s, the burning rate increases rapidly and a MLR runaway occurs around t = 1400 s before fire extinction. The rapid increase of fuel evaporation is believed to be due to the remaining small fuel quantity (around 450 g) in the burner and the conductive heat flux from the burner walls [4].

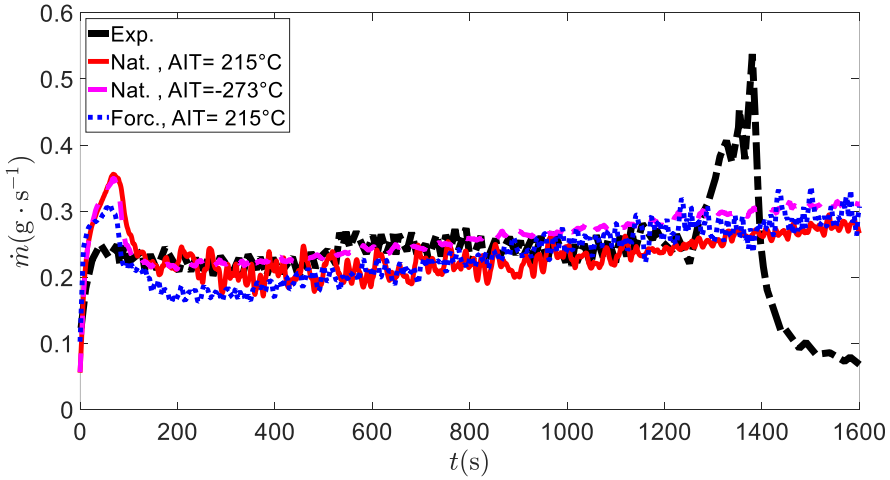

Fig. 5. The transient fire history at ARR = 22.5 $\mathrm{h^{-1}}$.

The initial fire growth is not well captured in the simulations which is believed to be due to the challenges of modeling the ignition process and heat transfer through the burner walls, which is further discussed in section 4.3. At t = 200-500 s, the natural convection approach predicts a close time-averaged MLR (0.21 g/s) to the experiment (~ 0.22 g/s), whereas the forced convection approach predicts a lower value (0.18 g/s). After t = 550 s, both approaches predict

similar (0.22 and 0.23 g/s, respectively by the natural and forced approach), but slightly lower time-averaged MLR, compared to the experiment (~ 0.25 g/s). The results show that the assumption of low AIT (= -273°C) seems to be appropriate for the stable steady-state burning scenario, where the averaged MLR predictions are close to the experiment.

The evaporation runaway and fire extinction are not predicted by the simulations, which has also been the case in a previous numerical study conducted by SAFIR [4]. The simulations predicted a stable increasing MLR until the fuel is consumed (not shown here). In [4], it is mentioned that the simplified assumptions of 1-D conductive heat transfer and not accounting for the regression of the liquid surface results in the failure to predict the MLR runaway. Similar predictions are observed here as neither of the assumptions are challenged in this study.

4.3 Unstable oscillatory combustion

For ARR = 15 h^{-1}, it is observed experimentally that the burning rate escalates at t = 0-80 s as in the open conditions [4]. After the initial fire growth stage, the burning rate stabilizes at around 0.23 g/s before undergoing an under-ventilated stage with an oscillatory combustion mode. During the latter stage, the average burning rate is about 0.16 g/s, the amplitude of the oscillations is about 0.045 g/s and their frequency is about 20 mHz. After five periods of fire oscillation, extinction occurs at 496 s and the MLR is below 0.03 g/s beyond t = 600 s.

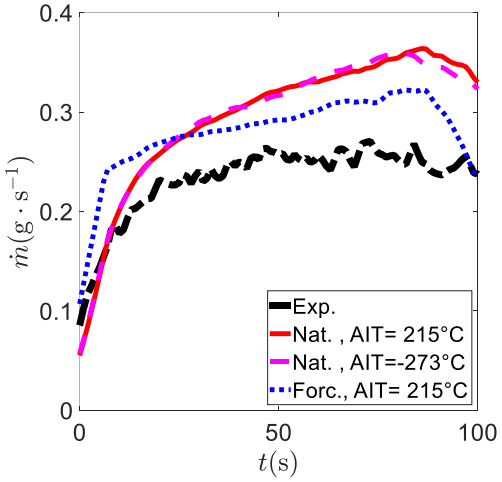

Fig. 6. The burning history of the initial fire growth at ARR = 15 h^{-1}.

The results displayed in Fig. 6 show that the initial fire growth is over-predicted by the simulations. The over-predicted initial fire growth was also found in the enclosure fire simulations of PRISME [7] and in the numerical study conducted by ISIS code [8]. In [7], the challenges to model the ignition process and flame radiation are inferred to be the reasons of the exaggerated initial spikes. Additionally, it is mentioned that the heat loss to the fuel pan was not fully captured by the simplified assumption of 1-D Fourier transfer and results in over-prediction of the initial burning rate [8].

Fig. 7 shows that the oscillatory combustion is relatively well captured by the natural convection approach along with a specified AIT = 215°C. The average burning rate during this phase is relatively well predicted with an average value of 0.13 g/s (vs. 0.16 g/s in the experiments). The periodicity and frequency (14 mHz) of the oscillations are not the same as in the experiments (20

mHz). Nevertheless, the predicted average amplitude (0.05 g/s) is close (0.04 g/s in the experiments).

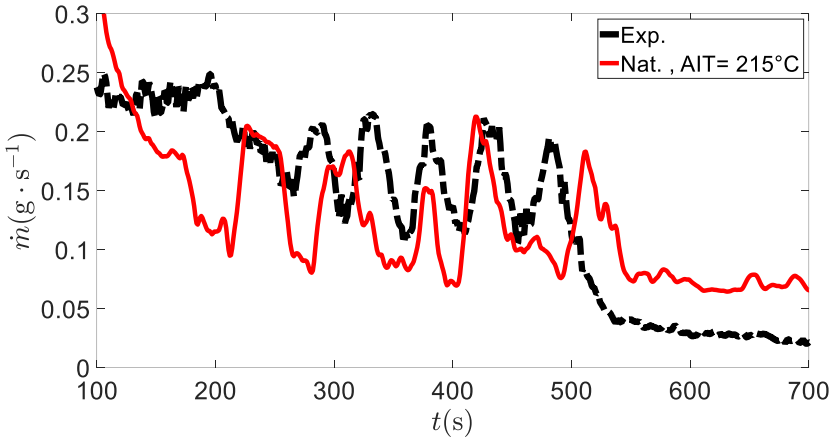

Fig. 7. The fire oscillations and near-extinction predicted by the natural convection approach with AIT = 215 °C, comparing to the experiment (ARR = 15 h^{-1}).

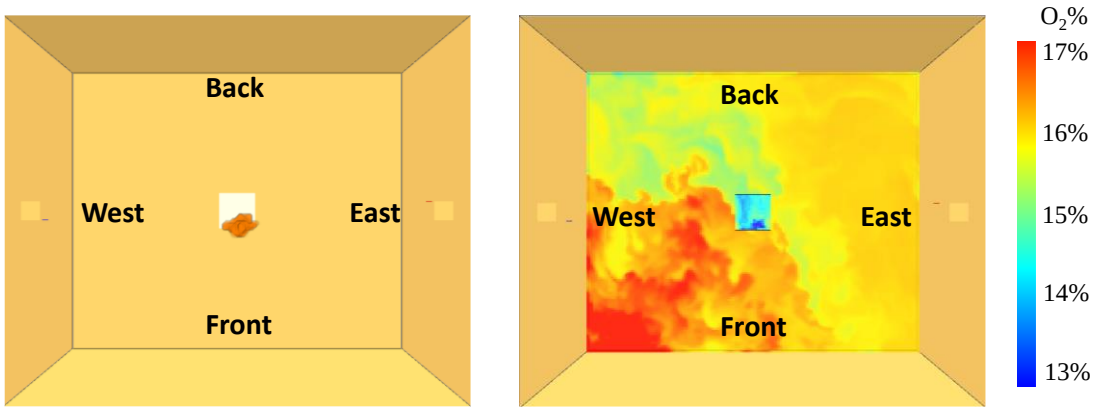

Fig. 8. Top view snapshots (at t = 276 s) by the natural convection approach with AIT = 215 °C; (left) the leaning of flame; (right) the oxygen concentration at 0.5 cm above the fuel surface.

The oscillations correspond to a periodic flame displacement, where the fire is leaning toward the 'Front' side to seek for oxygen. This has been clearly captured in the simulations (see Fig. 8), unlike in the numerical study carried out in [4]. The burning area and flame height correspond to the burning history, where a higher flame height or larger burning area is observed for the burning rate peaks, and vice versa for the valleys. Furthermore, it is quite remarkable that the near-extinction is observed after 5 cycles, as in the experiments. However, the MLR at this stage is overestimated (0.07 vs 0.03 g/s in the experiments), which perhaps caused the spurious re-ignition in the simulations that was observed at around t = 740 s (not shown here).

Fig. 9 confirms that the overall fire dynamics during the oscillatory combustion stage is relatively well predicted with respect to the room pressure, the inlet ventilation flow rate and the gas temperature at the FE corner located 0.85m from the floor. The results shows that the predicted pressure (resp. the inlet volume flow rate) oscillates between about -200 and 25 Pa (resp. -10 m^3/h and 37 m^3/h) whereas the measured values are between -300 and 0 Pa (resp. 10

m^3/h and 60 m^3/h). A reversed inlet flow is observed at $t \sim 420$ s when the burning rate revitalizes, which remains to be explained. Regarding the gas temperatures at the FE corner, the average value of 140 °C is overestimated by about 20 °C in the simulations. Furthermore, the amplitude of the oscillations is also overpredicted: 20°C in the simulations against 10°C in the experiments.

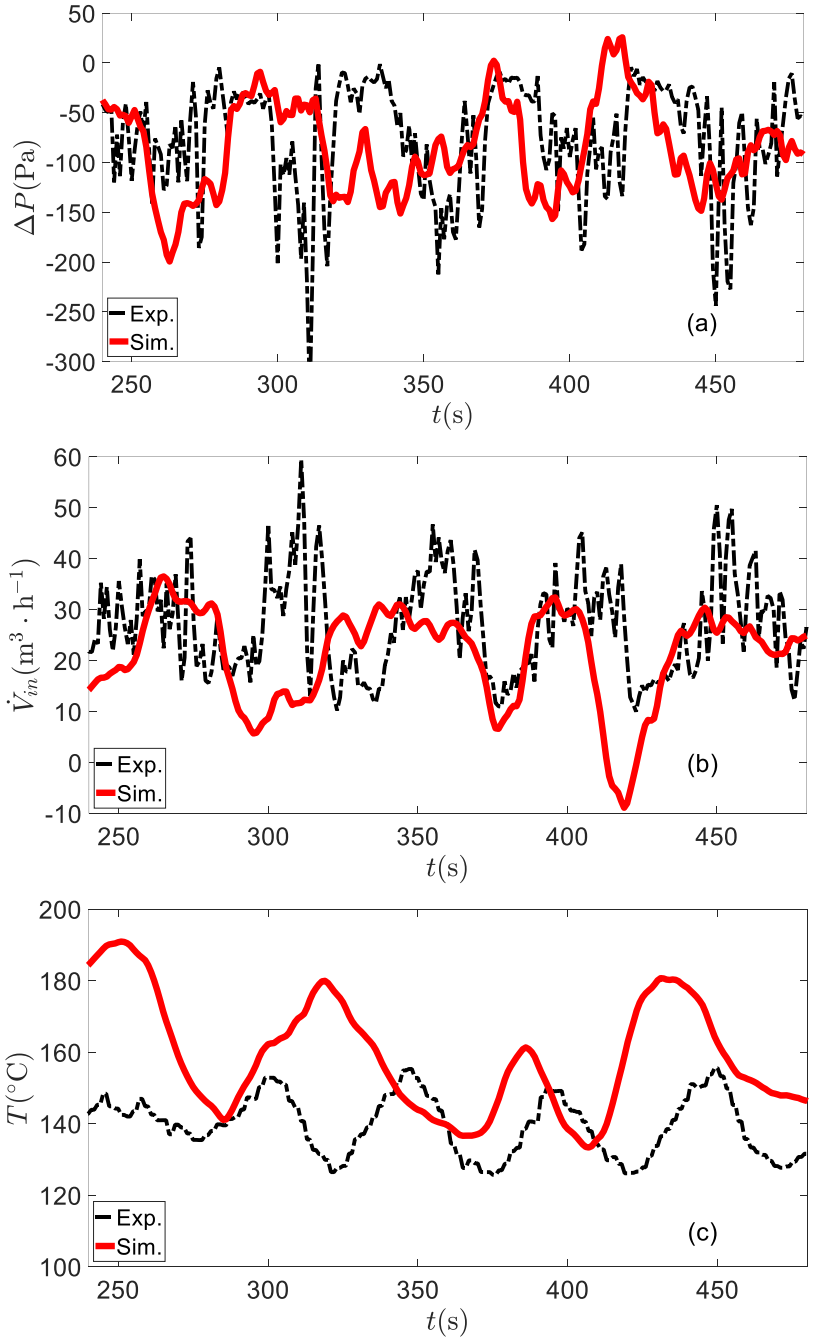

Fig. 9. The experimental and numerical results during the oscillatory period. (a) pressure difference; (b) inlet flow rate; (c) gas temperature 0.85m from the floor on the FE corner.

It appears that both the natural convection approach and a specified AIT = 215°C are important in predicting oscillatory combustion. As shown in Fig. 10(a), the forced convection approach predicts very low amplitudes. Furthermore, flame extinction is not captured. Fig. 10(b) shows that the natural convection approach with AIT = -273°C leads to a good prediction of the average burning rate, but the transient profile is 'flat' and no extinction is observed. When a very low AIT is prescribed, as the default setting in FDS, the fire will (re-)ignite when sufficient air meets the fuel gas, even if this does not happen in reality due to low gas temperature. In this case, (local) flame quenching is not observed when AIT = -273°C. On the contrary, the flame occupies the entire fuel surface and results in low but steady burning in under-ventilated conditions.

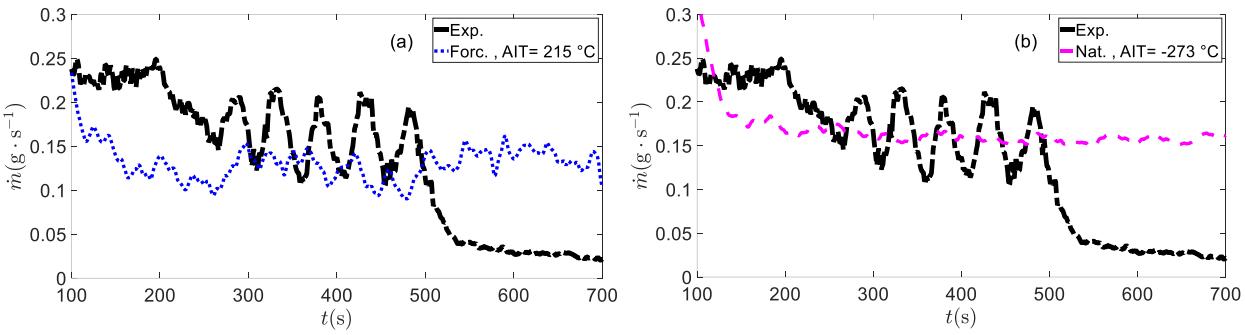

Fig. 10. The temporal profiles of burning rate during the oscillatory period at ARR = 15 h^{-1}, by (a) the forced convection approach with AIT = 215 °C and (b) the natural convection approach with AIT = -273 °C.

4.4 Sudden extinction

For an ARR = 8 h^{-1}, it is observed experimentally that, after an initial fire growth stage, the burning rate stabilizes at a value of around 0.23 g/s, before undergoing decay and extinction at about t = 200 s.

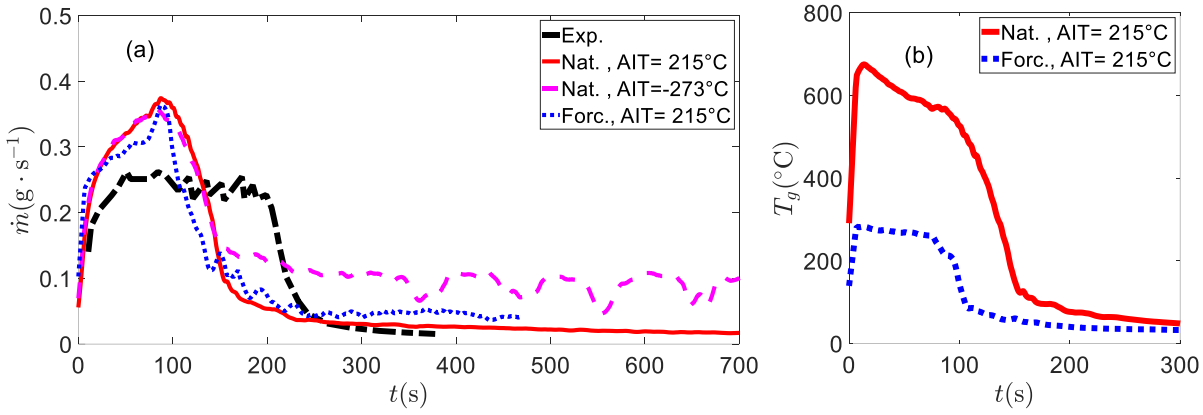

Fig. 11. The temporal profiles at ARR = 8 h^{-1}. (a) the burning history; (b) the mean temperature in the first gas cell adjacent to the fuel surface.

Fire extinction can be predicted by both forced and natural convection approaches, as shown in Fig. 11(a). The natural convection approach predicts a later extinction time (234 s) than the forced approach (165 s). A significant difference is found for the mean gas temperature prediction one cell above the fuel surface, where a much higher temperature is predicted by the natural convection

approach, as shown in Fig. 11(b). The high gas temperature near the fuel surface is believed to be the reason why the natural convection approach predicts a later fire extinction, as the AIT is prescribed as 215 °C. However, the reason for the different gas temperature prediction in the first gas cell near the fuel remains to be explained. Both approaches predict an earlier time for onset of fire decay than observed in the experiments, in line with the higher MLR values during fire growth (as for the other ARR values), which is immediately followed by extinction here.

Again, prescribing the AIT is crucial for predicting fire extinction. When the default AIT= -273 °C is applied, unburned fuel gas re-ignites, leading to a spurious oscillatory behavior as shown in Fig. 11(a). The AIT is also critical for predicting the flame displacement, as local extinction can only occur when the AIT is high enough. The flame displacement is believed to be due to a non-uniform distribution of the oxygen in the enclosure; the oxygen level is found to be higher in the FW side, due to the direction of the ventilation. This is also observed in the simulations of ARR = 15 h^{-1} (see Fig. 8). Moreover, 'ghost flames' (flames detaching from the burner) are also observed before fire extinction.

5. Conclusions

The numerical simulations carried out in this work confirm that the prediction of the low-frequency oscillatory combustion of a liquid pool fire in a reduced-scale mechanically-ventilated enclosure is sensitive to the liquid evaporation model. A natural convection correlation for the Sherwood number for estimating the evaporation rate and the Nusselt number for the heat transfer calculations has been implemented in FDS 6.7.5. The impact of the Auto-Ignition Temperature (AIT) of the fuel has also been investigated. In case of stable steady-state burning (ARR=22.5 h^{-1}), the predicted MLR is in closer agreement with experimental data when the natural convection approach is used, while a lower MLR is predicted with the forced convection approach at initial fire growth. The results are insensitive to AIT: even the default value (-273°C) provides good agreement with the experiments. For ARR = 15 h^{-1} the natural convection approach allowed to better capture the frequency and amplitude of the oscillations observed. Additionally, at the level of the gas phase, prescribing the actual AIT of the fuel is important to capture the increase in burning rate that follows near-extinction. The flame displacement is also successfully captured in the simulations. Oscillatory behavior is also found with the forced convection approach, but the amplitude is significantly under-predicted. No oscillations are found with the default AIT value, highlighting the importance of using the fuel's AIT. With the lowest ARR, equal to 8 h^{-1}, it was confirmed that the use of the actual AIT of the fuel is necessary to avoid spurious ignition to occur in a cyclic manner. The findings obtained in this work will be applied in the future for the numerical study of a large-scale mechanically-ventilated compartment fire.

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Figure captions

Fig. 1. The schematic drawings of the NYX compartment, reproduced from [4]. (left) view from the FW side; (right) top view.

Fig. 2. The cell sensitivity analysis by the forced convection approach in open atmosphere conditions. (a) burning history; (b) integrated total heat flux on the fuel surface.

Fig. 3. The quasi-steady (a) vertical velocity and (b) temperature difference of the cell sensitivity analysis by the forced convection approach, comparing to McCaffrey's correlations.

Fig. 4. Transient profiles of the (a) burning rate and (b) fuel surface temperature, by the forced and natural convection approaches in open conditions.

Fig. 5. The transient fire history at ARR = 22.5 h^{-1}.

Fig. 6. The burning history of the initial fire growth at ARR = 15 h^{-1}.

Fig. 7. The fire oscillations and near-extinction predicted by the natural convection approach with AIT = 215 °C, comparing to the experiment (ARR = 15 h^{-1}).

Fig. 8. Top view snapshots (at t = 276 s) by the natural convection approach with AIT = 215 °C; (left) the leaning of flame; (right) the oxygen concentration at 0.5 cm above the fuel surface.

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Fig. 11. The temporal profiles at ARR = 8 h^{-1}. (a) the burning history; (b) the mean temperature in the first gas cell adjacent to the fuel surface.