Analytical Approach for Predicting Effects of Vitiated Air on the Mass Loss Rate of Large Pool Fire in Confined Compartments

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ABSTRACT

The aim of this study is to determine the vaporization rate of an under-ventilated pool fire in a closed environment. A theoretical model that allows the burning rate of fuels to be determined for compartment fires under vitiated conditions is presented. The radiative and convective components of the heat flux from the flame to the pool surface are both evaluated and related to the ambient oxygen mass fraction. The model was first compared with the empirical correlation determined by Peatross and Beyler [1] before being applied to pool fires using heptane and PMMA as fuels in a small-scale apparatus. The global model presented here was then implemented in the CFD code ISIS and was validated against experiments involving a hydrogenated tetra-propylene pool fire test in a confined and mechanically ventilated compartment. It is shown that the model is able to correctly predict the fuel mass loss rate and provides a reasonable assessment of the heat flux from the flame to the pool surface.

KEYWORDS: CFD, compartment fires, modeling, heat transfer, heat release rate.

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NOMENCLATURE LISTING

$\begin{array}{llll} h & \mbox{convective heat transfer coefficient (W/m}^2 \cdot K) & \beta & \mbox{mean beam length corrector (-)} \\ L & \mbox{mean beam length (m)} & \varepsilon & \mbox{emissivity (-)} \\ L_v & \mbox{heat of gasification (J/kg)} & \kappa & \mbox{absorption coefficient (m}^{-1}) \\ L_m & \mbox{modified heat of gasification (J/kg)} & \sigma & \mbox{Stefan-Boltzmann constant (W/m}^2 \cdot K^4) \\ \hline \dot{m}'' & \mbox{mass loss rate of fuel per unit area (kg/m}^2 \cdot s) & \chi_r & \mbox{flame radiative fraction (-)} \\ \dot{q}''_{e,r} & \mbox{external radiative heat flux (W/m}^2) & \Delta H_c & \mbox{heat of combustion (J/kg)} \\ \dot{q}''_{f,r} & \mbox{convective heat flux from the flame (W/m}^2) & \Delta h_{vap} & \mbox{heat of vaporization (J/kg)} \\ \dot{q}''_{g,r} & \mbox{re-radiative heat flux from the flame (W/m}^2) & \mbox{subscripts} \\ \dot{q}''_{g,r} & \mbox{re-radiative loss (W/m}^2) & f & \mbox{flame} \\ r & \mbox{stoichiometric oxygen to fuel mass ratio (-)} & g & gas \\ r & \mbox{temperature (K)} & s & \mbox{pool surface} \\ Y_{O_2} & \mbox{oxygen mass fraction (-)} & w & \mbox{wall} \\ & & \mbox{ambient} \\ & & \mbox{ambient} \\ & & \mbox{ambient} \\ & \mbox{21} & \mbox{well-ventilated conditions} \\ \end{array}$	c_p	specific heat at constant pressure (J/kg·K)	Greek	
L_v heat of gasification (J/kg) κ absorption coefficient (m-1) $L_{\rm m}$ modified heat of gasification (J/kg) σ Stefan-Boltzmann constant (W/m²·K⁴) \dot{m}'' mass loss rate of fuel per unit area (kg/m²·s) χ_r flame radiative fraction (-) $\dot{q}''_{\rm f,r}$ external radiative heat flux (W/m²) ΔH_c heat of combustion (J/kg) $\dot{q}''_{\rm f,r}$ radiative heat flux from the flame (W/m²) $\Delta h_{\rm vap}$ heat of vaporization (J/kg) $\dot{q}''_{\rm s,r}$ re-radiative loss (W/m²) f flame r stoichiometric oxygen to fuel mass ratio (-) g gas T temperature (K) g gas Y_{O_2} oxygen mass fraction (-) g	h	convective heat transfer coefficient (W/m ² ·K)	β	mean beam length corrector (-)
$L_{\rm m}$ modified heat of gasification (J/kg) σ Stefan-Boltzmann constant (W/m²·K⁴) m'' mass loss rate of fuel per unit area (kg/m²·s) χ_r flame radiative fraction (-) $\dot{q}_{\rm e,r}^{\prime\prime}$ external radiative heat flux (W/m²) ΔH_c heat of combustion (J/kg) $\dot{q}_{\rm f,c}^{\prime\prime}$ convective heat flux from the flame (W/m²) $\Delta h_{\rm vap}$ heat of vaporization (J/kg) $\dot{q}_{\rm s,r}^{\prime\prime}$ radiative heat flux from the flame (W/m²) subscripts $\dot{q}_{\rm s,r}^{\prime\prime}$ re-radiative loss (W/m²) f flame f flame f stoichiometric oxygen to fuel mass ratio (-) f g gas f temperature (K) f subscripts f function f subscripts f flame f stoichiometric oxygen to fuel mass ratio (-) f g and f subscripts f function f subscripts f flame f subscripts f function f s	L	mean beam length (m)	$\mathcal E$	emissivity (-)
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$\dot{q}_{\text{f,r}}^{\prime\prime}$ radiative heat flux from the flame (W/m ²) subscripts $\dot{q}_{\text{s,r}}^{\prime\prime}$ re-radiative loss (W/m ²) $_{\text{f}}$ flame $_{\text{r}}$ stoichiometric oxygen to fuel mass ratio (-) $_{\text{g}}$ gas $_{\text{T}}$ temperature (K) $_{\text{s}}$ pool surface $_{\text{V}_{O_2}}$ oxygen mass fraction (-) $_{\text{w}}$ wall $_{\text{m}}$ ambient	$\dot{q}_{\mathrm{e,r}}''$	external radiative heat flux (W/m ²)	ΔH_c	heat of combustion (J/kg)
$\dot{q}_{\mathrm{s,r}}''$ re-radiative loss (W/m ²) $_{\mathrm{f}}$ flame $_{\mathrm{r}}$ stoichiometric oxygen to fuel mass ratio (-) $_{\mathrm{g}}$ gas $_{\mathrm{g}}$ T temperature (K) $_{\mathrm{s}}$ pool surface $_{\mathrm{g}}$ oxygen mass fraction (-) $_{\mathrm{w}}$ wall $_{\mathrm{w}}$ ambient	$\dot{q}_{ m f,c}''$	convective heat flux from the flame (W/m^2)	Δh_{vap}	heat of vaporization (J/kg)
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T temperature (K) s pool surface Y_{O_2} oxygen mass fraction (-) s wall s ambient	$\dot{q}_{ m s,r}''$	re-radiative loss (W/m ²)	f	flame
Y_{O_2} oxygen mass fraction (-) $_{ m w}$ wall $_{ m \infty}$ ambient	r	stoichiometric oxygen to fuel mass ratio (-)	g	gas
∞ ambient	T	temperature (K)	S	pool surface
	Y_{O_2}	oxygen mass fraction (-)	w	wall
well-ventilated conditions			∞	ambient
			21	well-ventilated conditions

INTRODUCTION

General Context and Motivations

During recent years, there has been a growing concern about the potential of compartment fires to cause major accidents. The pool fire scenario has been widely used by researchers to study the burning process at the vaporizing surface since it represents a simplified version of many fires that occur in practice. The present study proposes a theoretical approach to predict the rate of vaporization of a pool fire, based on the energy balance equation at the pool surface. This is considered to be an effective way to describe any fire scenario.

Most investigators have concentrated on determining important quantities, such as the heat release rate or fire power due to the combustion of the vaporizing fuel. The latter may be expressed as the product of the fuel mass loss rate, the combustion efficiency (that takes into account incomplete combustion) and the heat released by chemical reactions. Prescribed constant conditions for the burning rate or the fuel mass loss rate have been used in various numerical fire studies showing good agreement with experimental results. A practical way to determine the burning rate was also described in Ref. [1] where it was shown that the fuel mass loss rate or the burning rate in an open-atmosphere system can be estimated with a simple correlation that only requires the knowledge of fuel properties.

Previous investigations of hazardous conditions associated with compartment fires have included empirical methods such as that given by Peatross and Beyler [1] as well as theoretical methods [2–4]. The empirical correlation reported in Ref. [1], obtained under a steady-state combustion regime, gives the fuel mass loss rate as a function of oxygen concentration measured at the base of the flame for large-scale fire compartments. One of the main drawbacks of this empirical relationship lies in the fact that it was obtained in conditions for which external heat fluxes were negligible, therefore limiting its relevance to situations where low gas and wall temperatures prevail. In a more recent theoretical study [5], which made use of a well-stirred reactor approach, good agreement between the measured fuel mass loss rate with the linear correlation of Peatross and Beyler [1] was obtained. The theoretical model presented in Refs. [2–4] is also based on the burning rate approach in an open-atmosphere and includes fuel response to vitiated air along with burning enhancement due to hot gases and confinement. In this study, the predicted mass loss rate was properly validated with small-scale heptane pool fire experiments. However, because the flame radiative heat feedback to the pool fire was neglected in this theory, the formulation was found to be ineffective for large-scale fires as shown in Ref. [6].

In the scientific literature addressing the modeling of compartment fires, few studies have addressed the problem of the determination of the heat fluxes back to the fuel surface in order to determine the fuel mass loss rate. The study performed by Orloff and de Ris [7] illustrated the application of Froude modeling principles to the development of an homogeneous fire radiation model. The convective heat transfer from the flame to the fuel surface was determined according to the stagnant film theory, which gives its variation with the mass transfer rate at the pyrolyzing surface. The study performed by Tewarson et al. [8] focused on the determining the convective and radiative fluxes by using a steady-state heat balance equation at the fuel surface with a radiation correction for the Spalding number. Beaulieu and Dembsey [9] carried out an analytical study to quantify the effect of enhanced ambient oxygen concentration on flame heat flux. The flame emissivity, temperature and height were measured and used to calculate the convective and radiative heat fluxes. The flame was considered as a surface emitter so that a view factor was used to express the flame radiative heat flux. A global model was also developed by Hamins [10] to predict the mass burning flux for pool fires. Total radiation to the pool surface was given according to Ouintiere [11] and the convective heat transfer was approximated using the stagnant film model [7]. More recently, an analytical model, based on the energy balance at the fuel surface and on the stagnant film layer theory, was derived by Nasr et al. [6] and first applied in a CFD code to predict the fuel mass loss rate of a TPH pool fire in a confined and mechanically ventilated compartment. The validation of this model was performed against experimental measurements [12,13] and showed good agreement for the prediction of the time evolution of the heat release rate. The main advantage of this global approach is that no assumptions were made about the relative importance of each mode of heat transfer and therefore the convective and the radiative components of the heat flux from the flame to the fuel surface were accounted for. However, the air vitiation effect on the fuel mass loss rate was not investigated in this study.

Outline of the Paper

In the second section, we present a detailed description of the theoretical model used to predict the burning rate of the fuel. The net radiative component of the heat transfer from the flame to the fuel surface is obtained using the usual definition of radiative heat transfer while the convective part is determined using the stagnant film layer theory. We then explain in detail the developments and assumptions made to relate the convective and radiative fluxes to the air vitiation in the fire compartment. In this approach, a reference temperature is defined and depends on the ambient oxygen concentration; then an additional assumption allows us to link this to an effective flame temperature. In the third section we present the validation of this model by comparison with the results on TPH pool fires published in Refs. [12,13] and against the empirical correlation proposed by Peatross and Beyler as well [1]. Moreover, predicted variations of convective and radiative heat fluxes are compared with data from the theoretical and experimental study of Tewarson et al. [8]. Finally, the results of a predictive simulation of a pool fire in a confined and mechanically ventilated compartment, performed by the CFD code ISIS [14], are then presented and compared to experimental measurements [13].

MODEL FORMULATION

General Formulation

The burning of a liquid is often used to simply describe the pyrolysis process of a general material. In the following formulation, an ideal representation is adopted by considering that unsteady physical phenomena involved in charring pyrolysis processes are neglected. The steady burning analysis including an external radiative flux for this ideal approach reads:

$$\dot{m}'' L_{\nu} = \dot{q}_{f,c}'' + \dot{q}_{f,r}'' + \dot{q}_{e,r}'' - \dot{q}_{s,r}'', \tag{1}$$

where \dot{m}'' is the mass loss rate, L_{ν} is the heat of gasification, $\dot{q}''_{\rm f,c}$ and $\dot{q}''_{\rm f,r}$ are the convective and radiative flame heat fluxes respectively. The external radiative heat flux is defined by $\dot{q}''_{\rm e,r}$ and the re-radiative loss by $\dot{q}''_{\rm s,r}$. Heat conduction is assumed to be negligible and the heat of gasification is taken as being equal to the heat of vaporization $\Delta h_{\rm vap}$.

$$L_{v} = \Delta h_{\text{vap}} \tag{2}$$

In Eq. 1 it is implicitly assumed that conductive heat transfer through the burner walls into the liquid pool can be neglected, which amounts to assuming a relatively large pool diameter (D> 0.1 m).

Convective Feedback

According to the stagnant layer film theory [2], the average convective transfer from the flame to the fuel surface reads

$$\dot{q}_{\mathrm{f,c}}'' = \frac{h}{c_p} \left(\frac{\gamma}{\mathrm{e}^{\gamma} - 1} \right) \left[\frac{Y_{O_{2,\infty}} \Delta H_c}{r} \left(1 - \chi_r \right) - c_p \left(T_{\mathrm{s}} - T_{\infty} \right) \right]$$
(3)

where h is the convective heat transfer coefficient, c_p is the specific heat, $Y_{O_{2,\infty}}$ is the ambient oxygen mass fraction near fuel, r is the stoichiometric oxygen to fuel mass ratio, χ_r is the radiative fraction of the combustion process and ΔH_c is the heat of combustion. The variation of the radiative fraction as a function of the oxygen concentration was studied by Tewarson et al. [8]. According to experimental values usually observed near the pool surface, the radiative fraction should vary only about 10 percent. For simplicity, the

ambient value of the radiative fraction is used. In Eq. 3, the term $\gamma/e^{\gamma}-1$ with $\gamma=c_p\dot{m}''/h$ is defined as the blocking factor. Its impact on the convective flux plays a central role in this modeling as it diminishes convective transfer when the fuel mass loss rate increases. The blocking factor can also be written using the mass transfer number called the Spalding number [2].

$$\frac{\gamma}{e^{\gamma} - 1} = \frac{\ln(1+B)}{B} \tag{4}$$

where B is given by:

$$B = \frac{Y_{O_{2,\infty}} \Delta H_c (1 - \chi_r) / r - c_p (T_s - T_\infty)}{L_m}$$
 (5)

and the modified heat of gasification is defined as:

$$L_{\rm m} = L_{\rm v} - \frac{\dot{q}_{\rm f,r}'' + \dot{q}_{\rm e,r}'' - \dot{q}_{\rm s,r}''}{\dot{m}''} \tag{6}$$

Radiative Feedback

Following the definition given by Hottel [15], the net radiative flux from the flame to the pool surface is given by:

$$\dot{q}_{\rm f,r}^{"} = \sigma \left(1 - e^{-\kappa L}\right) \left(T_{\rm f}^4 - T_{\rm s}^4\right) \approx \sigma \left(1 - e^{-\kappa L}\right) T_{\rm f}^4 \tag{7}$$

where $T_{\rm s}$ corresponds to the pool surface temperature and $T_{\rm f}$ to an effective grey-gas flame temperature.

Here, the flame is considered as a homogeneous media with a cylindrical shape. σ is the Stefan-Boltzmann constant, κ is an effective soot absorption coefficient and L is the mean beam length [7] crossing the flame. The first term inside the parentheses is the flame emissivity. Its value (\approx 1 for large pool fires -D > 1 m) mainly depends on fuel properties, combustion processes and pool diameter.

Re-radiative Heat Loss

The surface re-radiation heat loss is expressed in term of ambient temperature by

$$\dot{q}_{\rm s,r}^{"} = \sigma \left(T_{\rm s}^4 - T_{\infty}^4 \right) \tag{8}$$

where the pool surface is assumed to be opaque (surface emissivity equals to 1). This term can often be neglected compared with flame radiation but it will be considered in the further development because of the use of dodecane as the fuel (high vaporization temperature).

External Heat Flux

This term can be significant in enclosure fires and takes into account the radiative flux coming from the hot gas layer and from the hot walls. According to Utiskul [4] it can be written as:

$$\dot{q}_{\rm e,r}'' = \sigma(1 - \varepsilon_{\rm f})\varepsilon_{\rm g}(T_{\rm g}^4 - T_{\rm s}^4) + \sigma(1 - \varepsilon_{\rm f})(1 - \varepsilon_{\rm g})(T_{\rm w}^4 - T_{\rm s}^4), \tag{9}$$

where $T_{\rm g}$ represents the gas compartment temperature, $T_{\rm w}$ stands for the wall temperature, and ε_f and ε_g represent the flame and smoke emissivity, respectively. The shape factors from the fuel to the walls and compartment gases are set to 1. In some cases, where soot production inside the compartment causes high opacity of the media the heat feedback from walls can be neglected and the external heat flux then reduces to:

$$\dot{q}_{\rm e,r}'' = \sigma(1 - \varepsilon_{\rm f})\varepsilon_{\rm g}(T_{\rm g}^4 - T_{\rm s}^4) \tag{10}$$

Modeling the Effect of Vitiated Air on the Fuel Mass Loss Rate

The difficulty in establishing a theoretical model under vitiated air conditions, in a compartment, mainly lies in the way the flame radiation relates to ambient conditions. More specifically, the average flame temperature used to express the radiative feedback, Eq. 7, must be related to the ambient oxygen mass fraction. Quintiere [16] suggests using the flame heat flux formulation in the case of a one-dimensional diffusion flame to express the flame temperature as a function of oxygen concentration. This definition can not be used in the case of radiating flames because flame temperature assessment leads to a strong overestimation of the radiative feedback. Another way to determine an average flame temperature is to consider Babrauskas' formulation [17] where the fuel mass loss rate in an open atmosphere is given as a function of the pool diameter D and two empirical factors \dot{m}_{∞}^{r} and $(\kappa\beta)$:

$$\dot{m}_{21}'' = \dot{m}_{\infty}'' \left(1 - e^{-\kappa \beta D} \right) \tag{11}$$

where κ is the absorption-extinction coefficient of the flame and β is a mean beam length corrector.

For a radiative burning mode and for large pool diameters (i.e., neglecting re-radiative heat loss), the fuel mass loss rate in open atmosphere is given by:

$$\dot{m}_{21}'' L_{\nu} = \dot{q}_{\rm f,r,21}'' \approx \sigma \varepsilon_{\rm f,21} T_{\rm f,21}^4$$
 (12)

In this formulation, the equivalent grey-gas flame temperature in open atmosphere $T_{\rm f,21}$ is determined by equating the two preceding relations:

$$T_{f,21} = \sqrt[4]{\frac{L_{\nu} \dot{m}_{\infty}'' \left(1 - e^{-\kappa \beta D}\right)}{\sigma \varepsilon_{f,21}}}.$$
(13)

From the convective heating formulation [16], a reference temperature can be determined and related to the ambient oxygen concentration:

$$T_{R,21} = \frac{Y_{O_2,21} \Delta H_c (1 - \chi_r)}{c_p r} + T_{\infty} . \tag{14}$$

The effective flame temperature and the reference temperature can be combined with the assumption that the ratio is independent of the oxygen concentration:

$$\frac{T_{\rm f}}{T_{\rm R}} \approx \frac{T_{\rm f,21}}{T_{\rm R,21}}.\tag{15}$$

With this approximation the equivalent flame temperature can now be written as:

$$T_{\rm f} = \alpha Y_{O_2,\infty} + \eta \,, \tag{16}$$

where
$$\alpha = (T_{f,21}/T_{R,21})\Delta H_c (1-\chi_r)/(c_p r)$$
 and $\eta = (T_{f,21}/T_{R,21})T_{\infty}$.

As a first approach, to compare with the experimental correlation given by Peatross and Beyler [1], the external heat flux from the hot gas layer and hot walls are not considered. According to this equivalent flame temperature formulation, the fuel mass loss rate becomes:

$$\dot{m}'' L_{v} = \frac{h}{c_{p}} \left(\frac{\gamma}{e^{\gamma} - 1} \right) \left[\frac{Y_{O_{2}, \infty} \Delta H_{c}}{r} (1 - \chi_{r}) - c_{p} (T_{s} - T_{\infty}) \right] + \sigma \varepsilon_{f} \left(\alpha Y_{O_{2}, \infty} + \eta \right)^{4} - \sigma \left(T_{s}^{4} - T_{\infty}^{4} \right)$$

$$= a_{4} \left(\alpha Y_{O_{2}, \infty} + \eta \right)^{4} + a_{1} Y_{O_{2}, \infty} + a_{0}$$
(17)

with
$$a_4 = \sigma \varepsilon_f$$
, $a_1 = \left| hG(\gamma)(1-\chi_r)\Delta H_c/(rc_p) \right|$, $a_0 = -\left| \sigma \left(T_s^4 - T_\infty^4\right) + hG(\gamma)(T_s - T_\infty) \right|$ and $G(\gamma) = \gamma/(e^{\gamma} - 1)$.

The fuel mass loss rate normalized by its value in open atmosphere is then defined as:

$$\frac{\dot{m}''}{\dot{m}_{21}''} = c_4 \left(\alpha Y_{O_2,\infty} + \beta \right)^4 + c_1 Y_{O_2,\infty} + c_0 , \qquad (18)$$

where
$$c_i = a_i / \delta$$
 and $\delta = a_{4,21} (\alpha Y_{O_2,21} + \eta)^4 + a_{1,21} Y_{O_2,21} + a_{0,21}$.

MODEL VALIDATION

Effect of Vitiated Air on Mass Loss Rate

In order to validate our model, the results were compared to experimental data corresponding to a large-scale compartment fire [12,13] and to the linear correlation reported in Ref. [1]. The normalized mass loss rate variations with oxygen concentration are shown in Fig. 1. This term is defined as the ratio of the mass loss rate in a confined environment with the mass loss rate that results from the burning in normal oxygen concentrations.

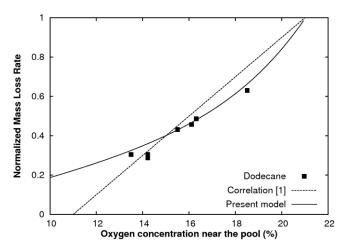


Fig. 1. Effect of oxygen concentration on normalized mass loss rate per unit area.

The present model agrees well with the linear correlation of Peatross and Beyler [1] as well as with the experimental data. Poor agreement with this correlation around an oxygen concentration of 13 % can be explained by the fact that the extinction phenomenon was not taken into account in the proposed approach. Unlike this modeling, the empirical correlation used the critical value of 11 % of oxygen concentration to simulate the flame extinction. Figure 1 indicates that when the oxygen concentration is within the range of 15–21 %, the linear correlation tends to overestimate the mass loss rate by 10 % in comparison to the value calculated by the present model. The nonlinear formulation of the radiative heat transfer indicates that the variation of the mass loss rate is larger when the oxygen concentration approaches the value in open atmosphere. In vitiated environments, the decrease is lower since the influence of radiative transfer becomes negligible compared to convective transfer, that depend linearly on the oxygen concentration. This trend is also amplified by the blocking factor which tends to increase the convective heat transfer when the mass loss rate decreases.

Flame Heat Flux Variations in a Vitiated Air Environment

To illustrate the previous observations, Fig. 2 presents a comparison between the radiative and convective fluxes predicted by the present model and those obtained by Tewarson et al. [8] for various oxygen fractions in the case of a heptane pool fire test in a small-scale apparatus. The authors have investigated the influence of oxygen concentration in pool fires for different solid and liquid fuels. In their study, the convective and radiative fluxes were determined from a steady-state heat balance equation at the pool surface and measurements of the mass loss rate, convective and radiative fraction of heat of complete combustion and mass fraction of oxygen. As for the previous comparison, the proposed modeling shows good agreement between the calculated and reference values. The same variations with oxygen concentration are observed for the convective and radiative fluxes and the present model indicates that the flame convective heat flux decreases as the oxygen fraction increases. Fuel properties are taken from [8]: $h/c_p = 13.6 \text{ g/m}^2$ -s; $\Delta H_c = 44.56 \text{ kJ/g}$; r = 3.52 kJ/g; $L_v = 0.48 \text{ kJ/g}$; $T_s = 371 \text{ K}$; $\chi_r = 0.42/0.83$.

The empirical factor $\kappa\beta$ is taken from Ref. [17], $\kappa\beta=1.4~\text{m}^{-1}$ and \dot{m}_{∞}'' used to determine the effective flame temperature (Eq. 13). This was taken as 0.15 kg/(m² s) instead of 0.11 kg/(m² s) in order to fit the data for large pool fires proposed by Babrauskas [17] to the small-scale fire apparatus of Tewarson et al. [8].

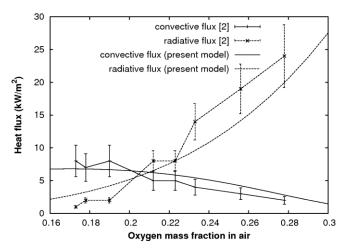


Fig. 2. Effect of oxygen concentration on convective and radiative fluxes for a heptane diffusion flame.

Application to a Large-Scale Pool Fire in a Confined Compartment

Code Description

The global model described in this work has been implemented in the CFD code ISIS [14]. This open-source software is a low Mach number computational tool dedicated to the simulation of fires in confined and ventilated compartments. Aerodynamic, turbulence, combustion and heat transfer are treated in detail using basic local conservation laws. The system of balance equations is discretized in time using fractional time-step methods, including a pressure correction technique for solving hydrodynamic equations. Discretization in space uses the finite elements method for hydrodynamic equations and the finite volumes method for scalar transport equations. In the case of confined compartments, the influence of the fire development on ventilation is taken into account through a relationship between the ventilation flow rate and the thermodynamic pressure of the fire room. The oxygen mass fraction in the convective heating term of Eq. 1 is considered at the bottom of the compartment near the pool fire. The gas temperature $T_{\rm g}$ and T_{∞}

in Eqs. 3, 8 and 10 are determined on the whole compartment. The flame emissivity is determined by the CFD model through the absorption coefficient and is taken into account to calculate the radiative heat feedback as in (Eq. 7). Flame ignition is not considered in this work and the mass loss rate in an open atmosphere is used as a boundary condition to start the simulation. The numerical simulation of the fire scenario described hereafter was performed with a structured mesh of 150,000 elements. The grid was refined near the pool, the walls and the admission and the extraction branches. An adaptive time-step and a parallel strategy were used to reduce the CPU time. The simulated physical time was 4,000 s and the time-step varied within the range [10⁻³ s, 1 s].

Experimental Setup

The experiment used to validate this global approach was performed by the IRSN Fire Test Laboratory at Cadarache (France), in the DIVA facility. This test was conducted as part of the experimental research program PRISME-SOURCE, which studied the propagation of smoke and hot gases between full-scale, well-confined and mechanically ventilated fire compartments. The infrastructure of this large scale multiroom device consists of four rooms and a corridor outfitted with an industrial ventilation network. A single room (6 m \times 5 m \times 4 m) was used for the fire test. The walls are composed of concrete material with a thickness of 0.3 m. The mechanical ventilation system consists of inlet and exhaust branches situated in the upper part of the compartment. The initial ventilation rate was set at 560 m³/h in the room. The pool fire consisted in a 0.4 m² circular steel pan of 10 cm deep hydrocarbon liquid fuel called TPH (an isomer of dodecane, $C_{12}H_{26}$, widely used as a solvent in nuclear power plants). The pan was placed on a weighing device, located at about 0.4 m above the floor and in the center of the fire room. Measurements performed include the fuel mass loss rate, the fire duration, the pressure, temperature and chemical species

concentration of gases filling the compartment, as well as the wall temperatures and the total heat flux. More details of this fire test can be found in a description of the PRISME-SOURCE program [1].

Results

In Fig. 3a comparison between the measurements and the computed values by the predictive simulation is shown. The pool fire burned for 200 s with the mass loss rate measured in the open atmosphere. After this time, the mass loss rate was established using Eq. 18. The temporal variation of this quantity is shown in Fig. 3a. The peak is well matched by the predictive model, as well as the decreasing phase. The value of the mass loss rate is over-predicted during the steady-state phase but no calibration of model constants was done.

The variation of the oxygen mass fraction versus time is shown in Fig. 3b. The measurement location corresponds to a zone at the base of the flame, outside the fire. The level of the oxygen concentration is well reproduced during the first phase until 240 s. Figure 3b indicates also good agreement of the model with experimental measurements during the decreasing phase of the oxygen concentration. The underestimated result during the steady state phase is mainly due to the overestimation of the mass loss rate which acts as the burning rate in the boundary condition for the balance energy equation.

The gas temperature variation versus time, at three heights in the room and located in the northeast quadrant of the room, are presented in Fig. 3c. Once again, there is good agreement between the fire model ISIS and experimental measurements. The peaks of temperature and the three levels calculated during the steady-state phase are approximately predicted with a difference of 10 °C with experimental data. This result is an important finding to predict the hot gas layer temperature and smoke movement in an enclosed space. These results also show that the overestimation of the mass loss rate has little influence on gas temperature prediction far enough from flames.

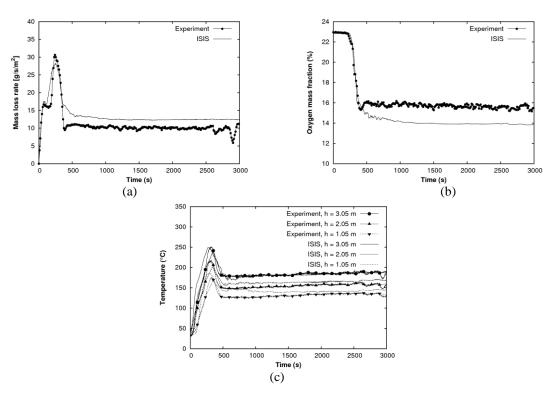


Fig. 3. Comparisons between the predicted values and experimental measurement versus time: (a) Mass loss rate; (b) oxygen mass fraction; (c) gas temperature at three heights.

Variations of the convective and radiative surface heat flux, from the flame to the pool surface, are depicted in Fig 4. At the beginning of the fire, the results indicate that the radiative flux is preponderant as a value of 7 kW/m^2 is predicted by the model whereas the convective part of the flame heat flux is about $2-3 \text{ kW/m}^2$.

This result is consistent with experimental measurements conducted in open atmospheres. Once the smoke layer develops in the fire compartment, the vitiated air affects the fuel mass loss rate and then strongly decreases the radiative heat flux from the flame. At the same time, due to the blocking factor $G(\gamma)$ in Eq. 18, the convective part of the flame heat flux increases. This behavior cannot be validated against PRISME fire test results but is in agreement with the experimental and theoretical work of Tewarson et al. [8]. The gap between the two heat fluxes predicted by the model is probably increased because the fuel mass loss rate is also overestimated. However, this outcome describing the mass loss rate behavior in enclosed environments shows that it is essential for a good prediction of this complex phenomenon to take into account, in the mass loss rate formulation, both radiative and convective heat flux, although the dominant regime in an open environment is purely radiative for large pool diameters.

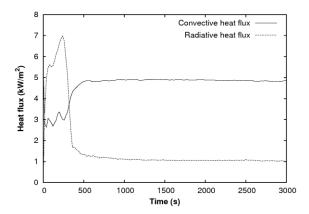


Fig. 4. Predicted Heat flux variations versus time.

CONCLUSION

The effects of vitiated air on the fuel mass loss rate behavior of TPH pool fires in confined compartments were theoretically and numerically investigated. A global formulation, based on the energy balance at the fuel surface and on the stagnant film layer theory, was initially used in the proposed modeling. Two temperatures, an effective and a reference one, which are related to the convective and radiative heat fluxes, were then introduced in the mass loss rate modeling. From that, a relation was proposed to relate the effective flame temperature to the oxygen concentration near the flame base.

The global modeling was first validated against experimental mass loss rate measurements as a function of oxygen concentration near the pool. A comparison was also performed with the linear correlation of Peatross and Beyler [1]. The results are in good agreement with data in the literature and the nonlinearity of the model highlights some behaviors of the mass loss rate, hidden in the empirical correlation. Heat flux variations were validated against results in literature data. The model predicts a decrease of the flame radiative flux as the oxygen concentration decreases. On the other hand, the flame convective heat flux increases as the oxygen concentration decreases near the flame.

Similar observations were made on a predictive simulation of a TPH pool fire in a confined compartment. Results show that the model predicts well the temporal variations of the fuel mass loss rate, oxygen concentration and local gas temperature. Variations of the convective and radiative surface heat flux as a function of oxygen concentration near the flame base are also predicted by the model. The results indicate that an accurate prediction of mass loss rate behavior should contain both the radiative and convective components in the heat flux formulation. The oxygen concentration, for a given pool fire, seems to play the same role as the pool diameter on the fuel mass loss rate in open atmosphere, in terms of heat flux variations. This scale effect is not discussed in this paper but this work is in progress and a particular effort is undertaken to properly predict the influence of the vitiated air on the decrease of the mass loss rate. In addition to this theoretical approach, an experimental study has been conducted in a reduced-scale fire compartment in order to correctly measure the variation of the radiative and convective heat flux during an under-ventilated fire.

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