Analytical Modelling of the Effect of In-Depth Radiation within a Liquid Layer in the Case of a Pool Fire

Beji T.*, Merci B.

Ghent University, Department of Flow, Heat and Combustion Mechanics, Ghent, Belgium *Corresponding author's email: <u>Tarek.Beji@UGent.be</u>

ABSTRACT

In this paper, we present a 'simplified' approach for the numerical modelling of the convective currents that occur within a liquid fuel in the case of a pool fire and which are induced by in-depth thermal radiation. This approach is based on the concept of 'effective' thermal conductivity, which is calculated herein based on the analytical solution of a steady-state one-dimensional heat conduction equation including a source term for in-depth radiation. This solution leads to a temperature profile which displays a horizontal liquid layer (of a given depth) that is bounded by a temperature that is higher at its bottom than its top. This thermal structure generates Rayleigh-Bénard instabilities which enhance heat transfer within the liquid. This effect is modeled via an increase of the 'actual' thermal conductivity of the liquid by a dimensionless heat transfer number, namely the Nusselt number. The Nusselt number is calculated based on the 'classical expression' of the Rayleigh number for the case of a 'horizontal cavity heated from below'. The paper provides the details of the derived solution for the 'effective' thermal conductivity along with examples of application to several fuels.

KEYWORDS: Pool fire, heat transfer, in-depth radiation, analytical modelling.

NOMENCLATURE

- c constant pressure specific heat $(J/(kg \cdot K))$
- D pool diameter (m)
- d_{hot} depth of the vaporizing layer (m)
- g gravitational acceleration (9.81 m/s²)
- *h* heat transfer coefficient (W/($m^2 \cdot K$))
- k thermal conductivity (W/(m.K))
- L fuel depth (m)
- L_v latent heat of vaporization (kJ/kg)
- \dot{m}'' fuel evaporation rate (kg/(m².s))
- Nu Nusselt number (-)
- Pr Prandtl number (-)
- \dot{q}''_{loss} heat loss to preheating layer (kW/m²)
- \dot{q}_{c}'' convective heat flux (kW/m²)
- \dot{q}_{r}'' radiative heat flux (kW/m²)
- $\dot{q}_{r}^{\prime\prime\prime}$ radiative source term (kW/m³)
- Q normalization constant (-)
- Ra Rayleigh number (-)

- t time (s)
- *T* temperature (K)
- *x* distance from the top fuel surface (m)
- Y_s soot yield (-)

Greek

- α thermal diffusivity (m²/s)
- β coefficient of thermal expansion (K⁻¹)
- Δh_g heat of gasification (kJ/kg)
- η normalized length scale (-)
- κ effective absorption coefficient (m⁻¹)
- *v* kinematic viscosity (m^2/s)
- ρ density (kg/m³)

Subscripts

- b bottom
- conv length scale for convection
- *eff* effective
- s top liquid surface

Proceedings of the Ninth International Seminar on Fire and Explosion Hazards (ISFEH9), pp. 693-703 Edited by Snegirev A., Liu N.A., Tamanini F., Bradley D., Molkov V., and Chaumeix N. Published by St. Petersburg Polytechnic University Press ISBN: 978-5-7422-6496-5 DOI: 10.18720/spbpu/2/k19-95

INTRODUCTION

The numerical simulation of pool fires has received a lot of interest in the fire safety community, given the potential hazard induced by these types of fires in quite a number of industrial applications such as the nuclear or the oil industry. Substantial advances have been achieved at the level of the gas phase in the prediction of the flame structure and, to some extent, the subsequent thermal radiation (although aspects related for instance to soot modelling remain a great challenge). In gas phase simulations of pool fires, the fuel mass loss rate (MLR) is generally prescribed based on direct experimental measurements or empirical correlations. The main limitation of such approach (i.e., prescribing the MLR) lies in the fact that the fuel surface response to changes in the environment (e.g., heat feedback from the flame) is not taken into account. As a consequence, some specific fire dynamics behaviours such as the combustion instabilities observed in mechanically ventilated and well confined rooms [1] might not be possible to predict. The more advanced approach consists of predicting the fuel MLR (i.e., the evaporation rate) by coupling it to the heat flux exerted by the flame at the fuel surface (and which depends on the combustion and the flame structure). In this case, it becomes important to also model heat transfer within the liquid.

As stated in [2], solving the full set of Navier-Stokes equations for the liquid phase requires prohibitive amounts of computational resources for fire dynamics simulations, considering the resources that would have been already allocated for the gas phase. Therefore, a simplified approach is required. In order to do so, it is important to understand first the thermal structure that is established within the liquid in the case of a pool fire.

As described in [3-7], at the top of the fuel layer (directly below the pool surface) (see Fig. 1), there is a very thin layer where the fuel temperature at steady-state is equal to the boiling point. This nearly uniform temperature layer is called 'vaporizing layer' [3] or 'boiling layer' [4]. Below this layer, there is a 'preheating layer' [3] or 'temperature gradient layer' [4] where the fuel temperature decays exponentially. Finally, for sufficiently 'deep pools', there is a 'bottom fuel layer' [3] where the fuel temperature does not vary substantially (see Fig. 1).



Fig. 1. Thermal structure within the liquid in the case of a pool fire. Left figure: temperature profile across the liquid height; the dashed blue line represents an increase in temperature observed numerically due to in-depth radiation. Right figure: layered structure as described in [3]; the red arrows represent the convective motion due to in-depth radiation (addressed in this work) and the white arrows represent heat transfer from the pool wall to the liquid.

The most comprehensive experimental work describing heat transfer within the liquid in a pool fire has been conducted by Vali et al. [5-8] for a 90 mm-diameter methanol pool fire. More specifically, the velocity field within the liquid fuel was determined by Particle Image Velocimetry (PIV) and the temperature was measured by type K thermocouple probes. A distinct two-layer thermal structure

was depicted and the uniform temperature within the vaporizing layer was attributed to two-counter rotating vortices. The first vortex, close to the pool wall, is explained by the 'buoyancy force near the pool wall and shear stress forces at the liquid-gas interface'. Several potential reasons are provided for the development of the second vortex, e.g., 'the liquid-gas interface shear force' or the 'non-uniformity of local evaporation rate at the pool surface'. In [9], it is stated that in-depth (radiation) absorption leads to 'in-depth temperatures' higher than the surface temperature, generating thus a convective current (due to Rayleigh convection) that drives the mixing within the boiling layer. This phenomenon causes the temperature profile across the vaporizing fuel layer to be uniform. Rayleigh convection has been confirmed experimentally in [9] using holographic interferometry for a toluene pool fire.

The numerical simulation of in-depth radiation has been undertaken in [9, 10] by considering a source term in the governing energy equation (for the liquid) where the radiative flux at a given depth within the liquid is derived by applying the 'classical attenuation law' (i.e., Beer's law) to the radiative heat flux at the fuel surface using a mean average absorption coefficient. As explained in [10], this approach generally leads to a 'temperature inversion layer' (see the broken blue line in the left figure of Fig. 1) that is not observed experimentally. This is explained in [10] by the fact that 'the onset of convective currents (Rayleigh effect) generated by the radiation absorption near the surface [is] not considered in the theoretical model'. This has been one of the main modelling aspects addressed in [2]. The approach proposed in [2] to model the effect of convective currents that are generated by in-depth radiation is based on the concept of 'effective thermal conductivity'. In [2], the 'effective' thermal conductivity coefficient is calculated as:

$$k_{eff} = \mathrm{Nu} \times k , \qquad (1)$$

where k is the thermal conductivity of the liquid and Nu is the Nusselt number. The latter is calculated in [2] for the case of an internally heated horizontal plane layer with isothermal top boundary and thermally insulated bottom boundary. In this paper, we will highlight the uncertainties related to such approach and propose a new methodology for the calculation of Nu.

MODEL DEVELOPMENT

Problem description

In order to derive an analytical solution for heat conduction within the liquid, including in-depth radiation [10], steady-state is considered as follows:

$$k\frac{\partial^2 T(x)}{\partial x^2} = \frac{\partial \dot{q}_r''}{\partial x} , \qquad (2)$$

where T and x are respectively the temperature and depth of the liquid and \dot{q}''_r is the radiative flux at a given depth x.

Based on the classical attenuation law, i.e., Beer's law, the radiative flux is expressed as [10]:

$$\dot{q}_{r}'' = \dot{q}_{r,s}''' e^{-\kappa x}$$
, (3)

where $\dot{q}''_{r,s}$ is the radiative flux at the surface and κ is the mean absorption coefficient of the liquid.

The assumption that the heat flow is unidirectional, in the direction normal to the fuel surface, is mainly based on experimental observations showing that heat loss to the walls is moderate, even for pool diameters as small as 7.4 cm (e.g., [4, 9]). The 1D assumption is most likely to be valid for pool diameters larger than 10 cm.

Inserting Eq. (3) into Eq. (2) gives:

$$k\frac{\partial^2 T(x)}{\partial x^2} = -\kappa \dot{q}_{r,s}'' e^{-\kappa x} .$$
⁽⁴⁾

When using the boundary conditions $T(x=0) = T_s$ and $T(x=L) = T_b$, where L is the liquid depth and T_s and T_b are respectively the top and bottom surface temperatures of the liquid, the analytical solution of Eq. (4) reads:

$$T(x) = T_s + \frac{\dot{q}''_{r,s}}{k\kappa} \left(1 - e^{-\kappa x}\right) - \frac{x}{L} \left(\left(T_s - T_b\right) + \left(1 - e^{-\kappa L}\right) \frac{\dot{q}''_{r,s}}{k\kappa} \right).$$
(5)

An illustration of the obtained liquid temperature profile for a hypothetical case is displayed in Fig. 2. As expected, the peak temperature does not occur at the surface but at $x = d_{hot}$, yielding a so-called 'inverse temperature profile' under the effect of in-depth radiation.



Fig. 2. Liquid temperature profile for a hypothetical case with the following parameters: $T_s = 50^{\circ}$ C, $T_b = 20^{\circ}$ C, $\kappa = 1000 \text{ m}^{-1}$, $\dot{q}''_{r,s} = 20 \text{ kW/m}^2$, k = 0.2 W/(m.K) and L = 0.1 m. A zoom is applied to the top 10 mm

of the liquid layer.

Depth of the well-mixed layer

Assuming that the well-mixed layer spans across the liquid layer from the surface up to the location of the peak temperature within the liquid, the analytical expression of d_{hot} is calculated as follows:

$$\left(\frac{\partial T}{\partial x}\right)_{x=d_{hot}} = 0 \quad . \tag{6}$$

Applying Eq. (6) for the temperature profile obtained in Eq. (5) gives:

$$d_{hot} = -\frac{1}{\kappa} \ln \left(\frac{k}{\dot{q}_{r,s}'L} \left(T_s - T_b \right) + \frac{\left(1 - e^{-\kappa L} \right)}{\kappa L} \right).$$
⁽⁷⁾

Note that at depths below d_{hot} (i.e., $x > d_{hot}$) the temperature may remain higher than the surface temperature, as illustrated for example in Fig. 2. Nevertheless, it is monotonically decreasing. Therefore, according to the analytical solution displayed in Eq. (6), at $x > d_{hot}$, there are no instabilities that would generate convective currents which occur when a portion of a cold fluid is sitting on top of a hot fluid.

It is also important to note that if Eq. (7) gives $d_{hot} > L$, this means that the estimated depth, d_{hot} , of the well-mixed layer exceeds the actual depth, L, of the liquid. In that case the model considers the entire liquid layer to be well-mixed, i.e., $d_{hot} = L$.

Before continuing the model development, Eq. (7) is assessed based on the experimental data in [7]. Fluid motion and energy transfer within a 90 mm-diameter burning methanol pool have been examined experimentally in [7] for pool depths, L, of 18, 12 and 6 mm and a wide range of bottom temperatures, i.e., between -4 and 50°C. More specifically, temperature measurements within the liquid pool using type-K thermocouple probes allowed to depict a two-layer thermal structure ('most easily recognized in deep pools' [7]) with estimates of the thickness of the lower layer. Given the fact that in [7] a steady fuel level (i.e., the top edge of the wall) was maintained in the pool, the thickness of the top layer can be easily retrieved from the data displayed therein.

The liquid depth, *L*, and the bottom temperature, T_b , are provided in [7]. The top surface temperature is assumed to be the boiling temperature of methanol, i.e., $T_s = 64.8 \text{ °C}$ [2]. The thermal conductivity of methanol is taken as $k = 0.2 \text{ W/(m \cdot K)}$ [2]. The steady-state radiative heat flux incident on the pool surface, is based on the empirical correlation derived by [11]:

$$\dot{q}_{r,s}^{"} = 68.3 Y_{s}^{1/4} \left\{ 1 - \exp\left(-\left[\left(4/3\right)\Delta h_{g} D\right]^{3/2}\right) \right\},$$
(8)

where Y_s is the soot yield (taken as $Y_s = 0.001$ [2]), Δh_g is the heat of gasification (taken here as the latent heat of vaporization, $\Delta h_g = L_v = 1099$ kJ/kg [2], because the liquid temperature is assumed to have reached the boiling point) and D is the pool diameter, i.e., D = 0.09 m. Thus, applying Eq. (8) for the methanol pool fire considered herein gives: $\dot{q}''_{r,s} = 12.1$ kW/m².

The remaining unknown in Eq. (7) is the effective absorption coefficient, κ . Unfortunately, to the authors' best knowledge, there are no direct measurements of κ for methanol in the literature. Only measurements for toluene, crude oil, hexane and benzene are reported in [9]. According to [2], although the absorption coefficient spectrum was available for methanol, the assumption of blackbody radiation is not applicable. Therefore, the absorption coefficient of ethanol has been used instead. According to [2], the latter varies between 35 and 1236 m⁻¹, depending on the calculation method (two methods were proposed in [2]) and the path length (which was taken to vary between 1 mm and 50 mm). Given this wide range of values, we have chosen a value of 320 m⁻¹ that would provide a good agreement for the data with L = 18 mm, and checked the outcome of the results for the other two liquid depths. A sensitivity study on κ is discussed hereafter.

The results displayed in Fig. 3 show that several features observed experimentally in [7] are qualitatively well predicted by Eq. (7). For instance, the depth of the top layer clearly decreases as the initial fuel thickness, L, is reduced. At $T_b = 20^{\circ}$ C and for L = 12 mm, the maximum thickness of the boiling layer was around 3.4 mm, whereas for L = 6 mm it was less than 1.8 mm. Note that the decrease of the top layer depth with reduced initial fuel depth has also been depicted experimentally in [4] for gasoline pool fires with tray sizes of side lengths between 30 and 60 cm and initial liquid thicknesses of 6 mm to 15 mm.

A second feature that is qualitatively well reproduced in Fig. 3 is the increase of the top layer depth when the bottom temperature is increased. This effect is clear from Eq. (7) where a reduction in the temperature difference, $T_s - T_b$, leads to an increase (in absolute value) of the logarithmic term. The decrease in the thickness of the well-mixed layer (i.e., vaporizing layer) with decreasing pool depth and bottom boundary temperature has been explained in [7] by a 'stronger stabilizing buoyancy effect' that prevents vortical structures from 'further penetration through the thermally stabilized liquid layer'. Equation (7) provides a mathematical formulation of this effect.



Fig. 3. A comparison between the experimental measurements [7] and numerical predictions (with Eq. (7)) of the thickness of the top layer with respect to the bottom layer temperature for a 90 mm-diameter methanol pool fire.

The quantitative discrepancies shown in Fig. 3 between the predictions and the experimental measurements can be attributed to uncertainties in the radiative heat flux (calculated using Eq. (8)) but even more so in the effective absorption coefficient, which remains to be measured for a wide variety of liquids following, for instance, the experimental procedure described in [9]. In the meantime, a sensitivity analysis on the radiative heat flux and the absorption coefficient is provided in Fig. 4.



Fig. 4. Sensitivity of the depth of the top layer to the effective absorption coefficient and radiative heat flux at the surface. The base case parameters are $T_s = 64.8$ °C, $T_b = 20$ °C, $\kappa = 100 \text{ m}^{-1}$, $\dot{q}''_{r,s} = 12.1 \text{ kW/m}^2$, $k = 0.2 \text{ W/(m} \cdot \text{K})$ and L = 0.018 m.

Figure 4a shows that the onset of a temperature inversion layer, i.e., $d_{hot} > 0$, occurs for $\kappa > 5 \text{ m}^{-1}$. Then, the depth of the vaporizing layer increases with increased absorption coefficient, reaching a peak of around 7 mm at $\kappa = 50 \text{ m}^{-1}$. Increasing κ further leads to a decrease in the predicted d_{hot} . This sensitivity analysis shows that the logarithmic term in Eq. (7) dominates for low values of κ whereas for high values the term $1/\kappa$ dominates. Figure 4b shows a monotonic dependence of the predicted d_{hot} on the radiative heat flux at the fuel surface. More specifically, d_{hot} is particularly sensitive to radiative heat flux values lower than 10 kW/m². For higher values (up to 100 kW/m²), the increase in depth becomes negligible. This sensitivity analysis remains qualitative because it depends on the size of the pool (i.e., depth and diameter) and the nature of the fuel. Nevertheless, it provides a good methodology to estimate the order of magnitude of the vaporizing layer depth. By varying the absorption coefficient, an estimate of the peak value can be obtained, see Fig. 4a. By varying the radiative heat flux over a 'realistic range of values', an 'asymptotic' value of d_{hot} can be obtained, see Fig. 4b.

'Effective' thermal conductivity coefficient

The Nusselt number in Eq. (1) (used for the estimation of k_{eff}) is calculated in [2] for the case of an internally heated horizontal plane layer with isothermal top boundary and thermally insulated bottom boundary :

$$Nu = 0.338 Ra_i^{0.227} . (9)$$

The variable Ra_i denotes the internal Rayleigh number calculated as [2]:

$$\operatorname{Ra}_{i} = \frac{g \beta \dot{q}_{r}^{m} L_{conv}^{5}}{k \, \nu \, \alpha} \frac{\eta^{2}}{Q(\eta)} \left(1 - \left(1 + \frac{1}{\eta} \right) \exp \left(-\frac{1}{\eta} \right) \right) \,, \tag{10}$$

where g is the gravitational acceleration, β , v and α are respectively the coefficient of thermal expansion, the kinematic viscosity and the thermal diffusivity of the liquid, \dot{q}''_r is a volumetric heat source and L_{conv} is a characteristic length scale for in-depth radiation. The variable η is a normalized length scale associated with the source distribution and calculated as:

$$\eta = \frac{1}{\kappa L_{conv}} , \qquad (11)$$

where κ is the effective absorption coefficient of the liquid.

The variable $Q(\eta)$ is a normalization constant calculated as:

$$Q(\eta) = \eta \left(1 - \exp\left(-\frac{1}{\eta}\right) \right).$$
(12)

A significant source of uncertainty (of the above methodology) pointed out in [2] is the definition of the characteristic length scale L_{conv} taken in [2] as the depth of the liquid layer, i.e., $L_{conv} = L$. Whilst this approach may be suitable for a 'relatively thin layer of fuel', it might not be appropriate for deep pools where the convective currents would be localized in the thin top layer of the liquid. In other words, the length scale L_{conv} rather corresponds to the depth of the vaporizing layer depicted in Fig. 1 and denoted therein as d_{hot} .

Another source of uncertainty in Eq. (10) is related to the calculation of the volumetric heat source, which has been assumed to be evenly distributed over the liquid layer thickness [2]:

$$\dot{q}_{r}^{\prime\prime\prime} = \frac{\dot{q}_{r,s}^{\prime\prime}}{L} , \qquad (13)$$

where $\dot{q}_{r,s}''$ is the radiative heat flux at the fuel surface.

The work described in this paper aims at proposing an alternative methodology to the mathematical development described in [2], yet using the same concept of 'effective' thermal conductivity. The objective is to derive explicit expressions for: (1) the characteristic length scale where convection currents are generated by in-depth radiation, and (2) the temperature difference that occurs across this length scale. This will allow using the 'classical' definition of the Rayleigh number [12]:

Proceedings of the Ninth International Seminar on Fire and Explosion Hazards (ISFEH9)

$$Ra = \frac{g\beta(T_1 - T_2)L_{conv}^3}{v\alpha}$$
(14)

where T_1 and T_2 are the temperatures at the two sides of the fluid layer.

As mentioned above, the fact that the temperature at $x = d_{hot}$ is higher than the surface temperature creates a Rayleigh-Bénard instability. Expression (14) for the Rayleigh number, Ra, in the case of a 'horizontal cavity heated from below' [12] is recalled here with $L_{conv} = d_{hot}$, $T_1 = T$ ($x = d_{hot}$) and $T_2 = T_s$:

$$Ra = \frac{g\beta(T(x=d_{hot})-T_s)d_{hot}^3}{\alpha\nu}$$
(15)

The effective thermal conductivity can thus be calculated using Eq. (1) with [12]:

$$Nu = 0.069 Ra^{1/3} Pr^{0.074}$$
(16)

where Pr is the liquid Prandtl number.

Properties	Heptane	Ethanol	Methanol	Benzene	
<i>k</i> , W/(m.K)	0.14	0.17	0.20	0.14	
ρ , kg/m ³	675	794	796	874	
<i>c</i> , kJ/(kg.K)	2.24	2.44	2.48	1.74	
$\alpha . 10^{-8}, m^2/s$	9.3	7.2	10.0	9.2	
$\beta . 10^{-3}, \mathrm{K}^{-1}$	1.24	1.09	1.18	1.25	
v.10 ⁻⁷ , m ² /s	5.5	5.5	13.9	6.9	
κ , m ^{-1 a}	335	1140	1000	162	
T_b , °C	98.5	78.5	64.8	80.3	
					_

Table 1. Fuel properties

^aValues used in [2, 13].

In order to compare the approach proposed here with the approach proposed in [2], we considered the case of a liquid fuel subjected to a radiative heat flux of 20 kW/m² (at its upper surface) with depths of 0.01 m (addressed in [2]) and 0.1 m. Four liquid fuels have been tested: heptane, ethanol, methanol and benzene. Their properties are displayed in Table 1. Note that the boiling temperature is not needed for the calculation procedure of [2]. It is used in Eq. (15) where the top surface temperature is assumed to have reached the boiling point, i.e., $T_s = T_b$. The temperature at the bottom boundary (needed for the calculation of d_{hot} , see Eq. (7)) is assumed to take the value of $T_b = 20^{\circ}$ C. Furthermore, the values for the effective absorption coefficients of the liquids considered herein are those used in [2].

The Nusselt numbers displayed in Table 2 for the case L = 0.01 m have a comparable order of magnitude (between the two methods). Nevertheless, the calculation procedure described herein yields values that are 35 to 80 % lower. For the case L = 0.1 m, a similar trend is observed with relative differences between 40 and 88 %. For the latter case, note that the Nusselt numbers calculated according to the method in [13] are most likely 'too high' because taking the total liquid depth (i.e., L = 100 mm) as a length scale in Eqs. (10) and (11) does not really correspond to the physics at hand. In fact, the length scales, d_{hot} , calculated with the method proposed in this paper are

significantly lower (between 4 and 17 mm), which yields significantly lower Rayleigh numbers given the cubic dependence of the latter on the length scale.

<i>L</i> (m)	Method	Heptane	Ethanol	Methanol	Benzene	
0.01	[2, 13]	21.5 ^a	13.1 ^a	14.6 ^a	21.0 ^a	
0.01	This work	10.0	4.3	3.0	13.6	
0.10	[2, 13]	106.6	82.9	60.2	119.8	
0.10	This work	36.0	9.8	7.1	72.5	

Table 2. Calculated Nusselt numbers for $\dot{q}''_{r,s} = 20 \text{ kW/m}^2$

^a Value similar to the value reported in [13]. The calculation of the value reported in [2] is not based on the normalized length scale.

At this stage, it is difficult to be assertive with respect to the 'validity' of the calculated Nusselt numbers or the 'performance' of one calculation procedure over the other. More detailed experimental measurements are needed for this matter. The same comment holds for an important fuel property used herein, namely the effective absorption coefficient, κ . Nevertheless, in the meantime, one could implement the theoretical approach described herein in the simulation of pool fires and assess its influence on global quantities such as the peak (and steady) heat release rate and the time to reach the peak (or the steady-state). The next section is devoted to some details related to the implementation of the proposed model.

IMPLEMENTATION PROCEDURE OF THE PROPOSED MODEL

Computational Fluid Dynamics (CFD) approach

An important assumption in the mathematical development that led to Eq. (7) is the presumed steady state of the heat transfer problem (see Eq. (4)) whereas, for many applications, time-dependent calculations/simulations are required. We advocate here that the relatively low values of d_{hot} (i.e., thin vaporizing layer) allows to make the hypothesis that changes in the temporal profiles of the radiative heat flux or the temperature at the top of the liquid fuel surface will have a 'quasi-instantaneous' effect on the depth of the vaporizing layer, the temperature profile within and, subsequently, the effective thermal conductivity.

In a CFD approach, the transient one-dimensional heat conduction equation to be solved reads:

$$\rho c \frac{\partial T(x,t)}{\partial t} = k_{eff}(t) \frac{\partial^2 T(x,t)}{\partial x^2}$$
(17)

Note that, as opposed to Eq. (4), there is no source term for in-depth radiation because the effect of the latter is implicitly incorporated in the time-dependent calculation of k_{eff} (that takes the value of k as an initial condition). However, the radiative heat flux at the fuel surface is considered in the calculation at the level of the thermal boundary condition (BC) on the top surface of the liquid. The BC reads:

$$-k_{eff} \left(\frac{\partial T}{\partial x}\right)_{x=0} = \dot{q}_c'' + \dot{q}_{r,s}'' - L_v \dot{m}'$$
(18)

where \dot{q}_c'' is the convective heat flux at the liquid surface, L_v is the latent heat of vaporization of the liquid and \dot{m}'' is the evaporation rate of the fuel (which can be modeled using the 'film' theory as in [2]).

The application of the concept of 'effective' thermal conductivity has not been applied in the series of CFD simulations of liquid pool fires performed in [2] (instead, the actual conductivity has been used) because 'the layer thickness needed for absorption coefficient and thermal conductivity is not known'. Equation (7) derived herein for d_{hot} overcomes this problem.

Zone modelling approach

The concept of zone modelling is most often used in fire dynamics in the case of smoke stratification in a compartment fire. It can also be applied to the case at hand, i.e., heat transfer within the liquid in a pool fire, bearing in mind the thermal structure described in Fig. 1. In [7], a steady-state energy balance is applied to a control volume that delimits the uniform-temperature layer (i.e., boiling or vaporizing layer). This approach allowed to calculate (and 'match') the experimentally measured temperatures within the liquid for several test cases. However, in addition to the fact that the method is based on steady state, it is not fully predictive in that 'the thickness of the lower layer [which is related to the thickness of the uniform-temperature layer] is required for the solution to be complete'.

A transient solution using the zone modelling approach could be obtained by solving the following energy equation for the vaporizing layer:

$$\rho c d_{hot} \frac{\partial T(x,t)}{\partial t} = \dot{q}_c'' + \dot{q}_{r,s}'' - L_v \dot{m}'' - \dot{q}_{loss}''$$
(19)

where \dot{q}''_{loss} is a heat loss term to the preheating layer that needs to be modelled.

Note that, in this approach, the 'effective' thermal conductivity is assumed to be 'large enough' to yield a uniform-temperature within the vaporizing layer of depth d_{hot} .

CONCLUSION

Fully predictive simulations of liquid pool fires require a comprehensive modelling of heat transfer within the liquid. Solving the full set of Navier-Stokes equations for the liquid phase requires prohibitive amounts of computational resources for fire dynamics simulations, considering the resources that would have been already allocated for the gas phase. Therefore, a simplified approach is required.

Convective currents induced by in-depth radiation have been identified in [9, 10] as a significant source of heat transfer within the liquid (in a pool fire). In order to account for this phenomenon, the concept of 'effective' thermal conductivity has been employed in [2]. The ratio of the 'effective' to the 'actual' thermal conductivity of the liquid is equal to the Nusselt number, which is a function of the Rayleigh number. The latter is defined in [2] based on a volumetric source term for in-depth radiation. One of the main elements of uncertainty in such formulation is the depth of the liquid layer, d_{hot} , within which convection is assumed to occur. It is taken in [2] as the total depth of the liquid. In the methodology presented in this paper we have derived an explicit expression for d_{hot} by solving a steady-state one dimensional heat conduction equation including a source term for indepth radiation. The obtained dependence of d_{hot} with the full liquid depth and the temperature difference between the top and bottom surfaces of the liquid is in qualitative agreement with the experimental findings reported in [7]. In addition to the expression for d_{hot} , an estimate of the theoretical peak temperature that occurs beneath the liquid surface (at $x = d_{hot}$) due to in-depth

radiation is provided. This allows using the 'classical' definition of the Rayleigh number (which is based on a temperature difference between the bottom and the top surface of a liquid) and makes the concept valid not only for thin fuels, as in [2], but also for 'deep pools'.

We are planning in the future to implement the proposed approach in a Computational Fluid Dynamics (CFD) code (as described in the paper) by calculating 'dynamically' the value of the 'effective' thermal conductivity of the liquid based on the computed profiles of top and bottom temperatures as well as the radiative heat flux at the surface. In the assessment of this methodology (for a variety of several liquid fuels) we will particularly look (in addition to the temperature profiles in the liquid phase) at the transient profiles of the fuel mass loss rate. The implementation in a zone modelling approach is also envisaged.

REFERENCES

- H. Prétrel, S. Suard, L. Audouin, Experimental and numerical study of low frequency oscillatory behaviour of a large-scale hydrocarbon pool fire in a mechanically ventilated compartment, Fire Saf. J. 83 (2016) 38–53.
- [2] T. Sikanen, S. Hostikka, Modelling and simulation of liquid pool fires with in-depth radiation and heat transfer, Fire Saf. J. 80 (2016) 95–109.
- [3] H. Hayasaka, Unsteady Burning Rates of Small Pool Fires, In: Hasemi, Y. (Ed.), Fire Safety Science– Proceedings of the Fifth International Symposium, pp, 499–510, 1997.
- [4] J. Zaho, H. Huang, G. Jomaas, M. Zhong, R. Yang, Experimental study of the burning behaviors of thinlayer pool fires, Combust. Flame 193 (2018) 327–334.
- [5] A. Vali, D.S. Nobes, L.W. Kostiuk, Effects of altering the liquid phase boundary conditions of methanol pool fires, Exp. Therm. Fluid Sci. 44 (2013) 786–791.
- [6] A. Vali, D.S. Nobes, L.W. Kostiuk, Transport phenomena within the liquid phase of a laboratory-scale circular methanol pool fire, Combust. Flame 161 (2014) 1076–1084.
- [7] A. Vali, D.S. Nobes, L.W. Kostiuk, Fluid motion and energy transfer within burning liquid fuel pools of various thicknesses, Combust. Flame 162 (2015) 1477–1488.
- [8] A. Vali, D.S. Nobes, L.W. Kostiuk, Characterization of flow field within the liquid phase of a small pool fire using particle image velocimetry technique, Exp. Therm. Fluid Sci. 75 (2016) 228–234.
- [9] T. Inamura, K. Saito, K.A. Tagavi, A Study of Boilover in Liquid Pool Fires Supported on Water. Part II: Effects of In-depth Radiation Absorption, Combust. Sci. Technol. 86 (1992) 105–119.
- [10] J.P. Garo, P. Gillard, J.P. Vantelon, On the Thin Layer Boilover, In: Curtat, M. (Ed.), Fire Safety Science–Proceedings of the Sixth International Symposium, pp, 579–590, 2000.
- [11] B.D. Ditch, J.L. de Ris, T.K. Blanchat, M. Chaos, R.G. Bill Jr., S.B. Dorofeev, Pool fires an empirical correlation, Combust. Flame 160 (12) (2013) 2964–2974.
- [12] F.P. Incropera, D.P. DeWitt, Fundamentals of Heat and Mass Transfer, Fourth ed., John Wiley & Sons, New York, 1996.
- [13] T. Sikanen, Simulation of transport, evaporation and combustion of liquids in large-scale fire incidents, PhD thesis, Aalto University, Aalto, Finland, 2017.