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Modeling and simulation of liquid pool fires with in-depth radiation absorption and heat transfer

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ABSTRACT

In this paper we present a computational fluid dynamics model for predicting the heat release rates of liquid pool fires. The model makes use of the one-dimensional heat transfer solver to provide the liquid surface boundary condition for the gas phase solver. The in-depth radiation transport is solved by a one-dimensional radiation transport model together with effective absorption coefficients determined from experimental data. The model accounts for the convective heat transfer in the liquid phase by modifying the thermal conductivity. The model is implemented as a boundary condition in the fire dynamics simulator (FDS). The model is validated by comparing experimental and predicted evaporation rates for water and a range of hydrocarbon fuels. The sensitivity of the results to the modelling assumptions and model input parameters is studied. The in-depth heat transfer appears to have a significant effect on the fire dynamics, except for the peak burning rates, which depend most importantly on the gas phase combustion.

1. Introduction

Pool fires are an important class of industrial fire hazards due to the large amounts of flammable liquids present in most industrial facilities, and because the rapid development of the heat release rate in such fires poses a challenge to the safety systems. Pool fires have been studied for decades and these works have been collected in several review articles [3,24,38]. The focus of the research has usually been on the steady state behavior and maximum burning rates of pools of different sizes. The results from such studies are often empirical correlations for the burning rate. A recent example is the study by Ditch et al. [13] where the authors correlated the mass burning rate with the fuel heat of gasification and smoke point.

Fire safety analyses are commonly performed using the computational fluid dynamics (CFD) type of fire simulations. The most important boundary condition for these simulations is the fire source burning rate, or liquid evaporation rate in case of the pool fires. While many of the analyses can be performed by prescribing the pool burning rate using either experimental data or empirical correlations as sources of information, there are situations where the conditions of the fire scenario are so much different from any experimental study that a reliable prediction of the pool burning rate cannot be made in advance. Examples of such conditions are the ambient temperature, radiation level, side wind and vitiation of the atmosphere. On the other hand, the heat transfer within the pool itself can be significantly different from the situation behind the empirical conditions. Furthermore, the transient nature of the analyses may require knowledge on the time-dependent burning rate, not just the peak or steady state value. It is therefore necessary to develop sub-models for the CFD fire models that can predict the pool fire dynamics and burning rate during the simulation.

Predictive CFD simulation of the pool burning rate were previously performed by Hostikka et al. [22]. In their model, the liquid evaporation rate was calculated iteratively over the course of the simulation to maintain an equilibrium fuel vapor pressure in the first gas-phase cell above the liquid boundary. The heat transfer inside the liquid layer was calculated using a one-dimensional heat conduction solver. In the results, only the steady state burning rate value was observed paying no attention to the temporal development. The main weakness of this kind of evaporation model is that the realized vapor concentration is highly sensitive to the spatial resolution. Suard et al. [40] used a more robust methodology by relating the total pool burning rate to the pool size and local oxygen concentration according to the empirical correlations. Three experiments with hydrogenated tetrapropylene fuel in a mechanically ventilated compartment were used to validate the model.

The main heat transfer mechanisms in a burning liquid pool are illustrated in Fig. 1. The heat from the flame is transported to the

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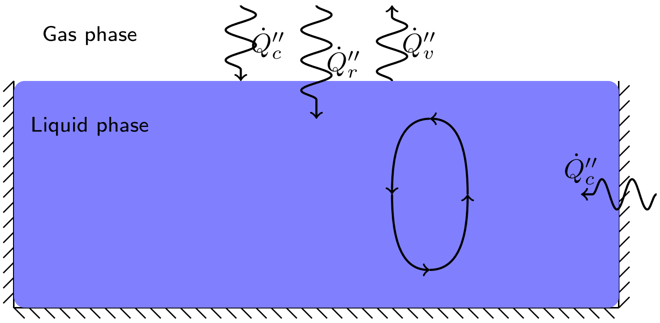

Fig. 1. Heat transfer mechanisms in pool fires.

liquid by thermal radiation and convection. Heat conduction takes place between the vessel and the liquid. The size of the pool dictates which mode of heat transfer dominates, although the type of fuel also plays a role [3,38]. For very small pool diameters, the conduction through the vessel walls dominates the heat transfer. For slightly larger pool fires, convective transport is the most important mode, and for the large pool fires, the radiative transport dominates. The exact diameters where these transitions between dominant heat transfer mechanisms occur are fuel dependent.

Studies have also been conducted to determine the spectra of emitted radiation [42] and to characterize the radiation absorption by gases within the flame [51]. The question of heat transport within the fuel has received less attention. In the liquid phase, the dominant modes of transport are convection (liquid movement) and radiation. The convection can be driven by heat transfer from the walls, unsteady burning rate, uneven surface temperature and buoyancy. Higuera [20] explored numerically the situation of a liquid layer with a cold bottom plate heated nonuniformly from above. For liquids with Prandtl numbers near unity, both thermocapillary and buoyant flows were induced.

Very little experimental data exists on the importance of liquid side convection in determining the burning rates of pool fires. In fact, steps are sometimes taken in order to minimize both convection and in-depth radiation absorption. For example, Ditch et al. [13] and Suo-anttila [41] used glass beads in the fuel bed in order to minimize in depth radiation absorption and convection. Suo-anttila and Blanchat [41] also investigated the effect of convection by removing the glass from the pools. They found that convection and in-depth radiation absorption had a small effect on the steady state burning rate. Vali et al. [50] found that there is a near constant temperature region directly below the surface of a pool fire. In this region, the heat transfer was found to be dominated by convection driven by heated pool walls. In another study, Vali et al. [49] noted that varying the temperature of the pool boundary had an effect on burning rate. The importance of the initial temperature of the liquid fuel on pool fire dynamics has been previously noted by Hayasaka et al. [18] and investigated more thoroughly by Chen et al. [11], who recorded the temperature gradient within the fuel. They found that the initial temperature did affect the temporal development of the burning rate but did not significantly affect the steady state burning rate.

To investigate the heat transfer within the liquid, we must also consider the depth over which the radiation reaching the liquid surface is absorbed. Depending on the fuel, the thickness of absorption can vary significantly, which has a great influence on how the radiation should be taken into account in numerical modelling. In fuels which are optically very thick in the infrared region, the thermal radiation is absorbed within a very thin layer on the surface, and the radiation can be taken into account as a boundary condition of the liquid's internal heat transfer problem. If the liquid is not optically thick the in-depth absorption must be taken into account as an internal source term of the heat conduction/convection problem. Additionally, the re-radiation of the fuel and vessel must be taken into account to ensure the conservation of energy in case of optically thin fuels and high temperatures. The in-depth absorption by semi-transparent fuels has been studied for PMMA [39], polymer films [48] and liquid pool fires [42]. Most of the research related to the in-depth radiation absorption in liquids considers the boil-over of liquid pool fires on water [9]. The effect of in-depth radiation absorption on evaporation of fuel droplets has also received some attention [36].

The objectives of the present study are to improve the previous model [22] by replacing the equilibrium-based vaporization model with an engineering mass transfer expression, to find an appropriate technique for the specification of the liquid phase radiation absorption coefficients, to investigate the relative importance of the internal convection to the pool burning rate dynamics, and to validate the proposed modelling approach using experimental results for different fuels.

2. Mathematical models

In this section we describe the mathematical model of liquid under consideration.

2.1. Gas phase model

The liquid model is included as a boundary condition in the CFD software Fire Dynamics Simulator [31,28,27]. FDS is a large Eddy simulation (LES) code that solves a form of the Naiver–Stokes equations appropriate for low-speed, thermally driven flow with an emphasis on smoke and heat transport from fires. The governing equations of for momentum transport are discretized by second-order central finite differences on a cartesian staggered grid. A two stage explicit Runge–Kutta method is used for time-stepping. In the present paper, gas phase combustion is treated by the single step, mixing-controlled chemical reaction scheme using three lumped species. These lumped species are air, fuel, and products. Radiative heat transfer is included in the model via the solution of the radiation transport equation (RTE) for a gray gas. In the gas phase, the RTE is solved using the finite volume method radiation. The absorption coefficients of the gas–soot mixtures are computed using the RadCal narrow-band model [17].

The gas-phase model has been validated for a wide range of fire scenarios that are relevant to the current investigation [32]. Since the evaporation in a pool fire is driven by the heat feedback from the flames, the accuracy of the heat flux predictions will propagate directly to the evaporation rate predictions. The uncertainties in the predictions can be summarized with two parameters: the bias δ and standard deviation σ. Given a model prediction M, the true value y is assumed to be normally distributed as $y \sim N(\frac{M}{\delta}, \sigma^2(\frac{M}{\delta})^2)$.

Predicted heat fluxes outside diffusion flames have bias of 0.97 and standard deviation 0.27. Heatfluxes resulting from flame impingement are predicted with standard deviation 0.37 and bias 0.93. These numbers imply that heat fluxes tend to be under predicted and that the 68% confidence interval for the predictions is $\pm$ 30%. Additionally, simulations of experiments by [43] have shown that the vertical distribution of heat release rate approaches experimentally determined values as the grid is refined. The results in this paper have been calculated with FDS version 6.2.0.

2.2. Liquid evaporation model

The rate at which liquid fuel evaporates when burning is a function of the liquid temperature and the fuel vapor pressure above the pool surface. According to the Clausius–Clapeyron