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Predicting the heat release rates of liquid pool fires in mechanically ventilated compartments

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ABSTRACT

In this paper we perform predictive simulations of liquid pool fires in mechanically ventilated compartments. We show that steady state burning rates are accurately predicted using a detailed model for the liquid phase heat transfer. The effect of lowered oxygen vitiation on the burning rate of pool fires is correctly captured. Simulations were done using the Fire Dynamics Simulator and the experiments considered were conducted in the OECD PRISME project. The main difference between the present study and previous simulation studies is the use of a detailed liquid evaporation model and the direct calculation of the vitiation and thermal environment interactions through the CFD solver.

1. Introduction

Liquid pool fires are a significant hazard to industrial facilities. The liquids could originate e.g. from leaking transformers, generators or other machinery. Knowing the fire burning rate is the starting point of any fire safety analysis. The factors affecting the burning rates of liquid pool fires in open atmosphere are well known for a wide variety of liquids. However, many fire scenarios, especially in nuclear facilities, involve fires in confined spaces.

The burning rates in confined spaces, possibly coupled with mechanical ventilation, can be significantly different from the ones measured in open atmosphere. These differences are caused by e.g. air vitiation and heat radiation from hot walls and the hot gas layer. An international research program PRISME was conducted between January 2006- June 2011 to study fires in air-tight mechanically ventilated compartments. Results from this program have been previously used in validation of CFD codes for compartment fire scenarios [1–5]. For the purposes of this paper the studies of Wahlqvist and Van Hees [1,3] are of interest. In [3] they showed that the Fire Dynamics Simulator (FDS) and especially the HVAC model in it were able to accurately predict the temperatures and pressures in a mechanically ventilated compartment. In this paper, we build upon their model of the PRISME experimental facility.

Relatively few attempts have been made of predicting rather than prescribing the burning rates in compartments. The proposed models vary in complexity. The simplest model is a correlation such as the one by Peatross and Beyler [6]. Suard et al. [4] implemented this model as a boundary condition for ISIS-CFD code. Pretrel et al. [5] used a simple heat balance at the liquid surface to predict the burning rates.

Wahlqvist and Van Hees [3] combined the empirical correlation of Peatross and Beyler and added a term to account for enhanced vaporization due to heat flux from hot walls and the gas layer. Their model takes as an input the mass loss rate of the pool fire in open atmosphere. This may come from correlations or from a experimentally determined mass loss curve. If a mass loss curve is used, it is simplified and the steady state burning rate is assumed to continue indefinitely. This predetermined mass loss rate is reduced according to the correlation or enhanced based on the radiative heat feedback from the walls. Their model was implemented as an boundary condition for FDS and the oxygen concentration near the flame base was obtained from the gas phase solution. They added an output quantity to extract the external radiation without any influence from the flame radiation.

In this study, we will not rely on such an “engineering” approach but try to model the liquid evaporation rate from the first principles. The benefit of our approach is that the burning rates can also be predicted for fuels for which the experimental data is not available. On the other hand, much more detailed information about the thermophysical properties of the fuels is needed.

In this paper we investigate the capability of the detailed liquid evaporation model in the FDS to predict the pool fire burning rates in a series of compartment fire experiments. We focus on 0.4 m^2 pool fires. First the model predictions are compared against experimental data from open air experiments. We look at both the burning rate predictions and the temperatures within the liquid. After this we turn to

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Nomenclature

c	heat capacity (kJ/kg/K)
$D_{l,q}$	binary diffusion coefficient (m/s)
g	gravitational acceleration (m/s^2)
h	heat transfer coefficient (W/m^2/K)
h_m	mass transfer coefficient (m/s)
Δh_v	latent heat of vaporization (kJ/kg)
k	thermal conductivity (W/m/K)
L	length scale (m)
$\dot{m}''$	mass flux (kg/m^2/s)
$\dot{m}$	burning rate (kg/s)
p	Pressure (Pa)
$\dot{q}''$	heat flux (kW/m^2)
$\dot{q}'''$	volumetric heat source (kW/m^3)
R	universal gas constant (J/mol/K)
T	temperature (K)
t	time (s)
u	velocity (m/s)
X	Species volume fraction (dimensionless)
x	dimension into the liquid (m)

Greek

δx	grid cell size (m)
ϵ	emissivity (dimensionless)
κ	absorption coefficient (1/m)
σ	Stefan-Boltzman constant (kg/s^3/K^4)
μ	viscosity (kg/m/s)
ρ	density (kg/m^3)

subscripts

c	convective part of heat flux
g	gas phase conditions
r	radiative part of heat flux
s	surface conditions
0	ambient conditions

under-ventilated fires. We look at predicted burning rates and extinction times as function of the ventilation rate.

2. Simulation methods

2.1. Gas-phase

The simulations considered in this paper were conducted using Fire Dynamics Simulator. The details of the physical and numerical models can be found in [7]. In this section a brief overview of the relevant models and methods is given. FDS is a Large Eddy Simulation (LES) code that solves a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow with an emphasis on smoke and heat transport from fires. The governing equations 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. 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. The RTE solution method for condensed phase will be described below.

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. All simulations in this study were performed by using dodecane as the fuel. The combustion reaction was assumed to yield 1.5% soot and 0.6% carbon monoxide [3]. The radiative fraction of the combustion reaction is assumed to be 0.35 and the heat of combustion Δh_c is set to 42 MJ/kg.

FDS contains a simple extinction model based on the concept of critical flame temperature. For each computational cell, the extinction is determined by two criteria: The first criterion suppresses the combustion if the temperature in the computational cell does not exceed a user defined auto ignition temperature. The second criterion considers a stoichiometric pocket of fuel, air and products in a computational cell. If the combustion energy of this fuel is not sufficient to raise the temperature of the gas mixture over the critical flame temperature, the combustion reaction is again suppressed. Both the critical flame temperature T_{CFT} and auto ignition temperature T_{AIT} are user defined constants. For the simulations in this paper, these temperatures are 1650 K and 373 K, respectively. The former is the default value for the FDS extinction model and is a typical value for hydrocarbon fuels. Since the temperature field of a LES is not fully resolved, the measured value of auto ignition temperature cannot be used as an input. The value of 373 K for the auto ignition temperature was chosen by experimenting.

FDS has a dedicated module for modelling Heating, Ventilation and Air-conditioning (HVAC) systems connected to the gas space of the fire simulation [8]. The ventilation network is described as a series of ducts and nodes. The nodes are placed at points where the ducts intersect each other or the CFD computational domain. The ducts are uninterrupted domains of fluid flow which can encompass elbows, expansion/contraction fittings and various other fittings. The losses due to friction and various other duct fittings are assigned as dimensionless loss numbers to the ducts. The node losses are attached to the ducts as loss terms only appear in the duct equations. The module does not presently store any mass. Therefore, mass flux into a duct is equal to the mass flux out of the duct.

2.2. Liquid evaporation

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 relation, the volume fraction of the fuel vapor above the surface in an equilibrium state is a function of the liquid surface temperature T_s and boiling temperature T_b

$$X_{F,\ell} = \exp\left[-\frac{h_v W_F}{R}\left(\frac{1}{T_s} - \frac{1}{T_b}\right)\right] \tag{1}$$

where h_v is the heat of vaporization and W_F is the molecular weight of the fuel gas (170.3 g/mol for dodecane). The local evaporation rate of the fuel at time t is governed by Stefan diffusion:

$$\dot{m}'' = h_m \frac{\overline{p}_m W_F}{R T_g} \ln\left(\frac{X_{F,g} - 1}{X_{F,\ell} - 1}\right); \quad h_m = \frac{Sh\, D_{\ell,g}}{L} \tag{2}$$

where h_m is the mass transfer coefficient and $\overline{p}_m$ is the pressure. T_g and $X_{F,g}$ are the gas temperature and the fuel vapor volume fraction. They are given the values in the first grid cell adjacent to the pool surface. The diffusivity calculated from gas viscosity: $D_{\ell,g} = \nu_g/Sc$. The molecular viscosity is obtained from the gas phase solution. The Schmidt number is given a constant value of 0.6. A model with variable and fuel dependent Schmidt number is under preparation. However for the simulations in this paper the effect is negligible.

The liquid fuel itself is treated like a thermally-thick solid for the purpose of computing the heat conduction. There is no computation of the internal liquid convection within the pool. The one-dimensional