Combustion and Flame 173 (2016) 89–98

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Large-eddy simulation of methanol pool fires using an accelerated stochastic fields method

Mehdi Jangi*, Mohammednoor Altarawneh, Bogdan Z. Dlugogorski

School of Engineering and Information Technology, Murdoch University, WA 6150, Australia

ARTICLE INFO

Article history:
Received 2 April 2016
Revised 12 May 2016
Accepted 20 August 2016
Available online 11 September 2016

Keywords:
Pool fire
Methanol
LES
Stochastic fields method

ABSTRACT

Large-eddy simulation with transported probability density function (t-PDF) method for modelling pool fires is presented. The PDF method that is used here is based on the Eulerian stochastic fields method (SF), and is accelerated with chemistry coordinate mapping (CCM) technique. SF-CCM for large-eddy simulation is formulated and applied to simulate methanol pool fires with various pool sizes for the first time. The model includes finite rate chemistry effects with detailed chemistry of the methanol combustion. The simulation results agree well with experiments in terms of the averaged flame height and the maximum ceiling temperature. More important is the capability of the current approach in reproducing the dynamic characteristics of the fire plume. Especially, the intermittent behaviour of pool fires and its response to the effects of the pool size are predicted, accurately. The key factor to success is the capability of the method in handling multiple modes of combustion in both premixed and non-premixed mixtures. It is shown that a pool fire involves the local and global extinction which is mainly due to the large entrainment of the fresh and cold ambient air to the base of fire plume. It is shown that the quenching and re-ignition are key processes in the understanding the dynamic behaviour of pool fires.

1. Introduction

From safety perspective, prediction of compartment fires, namely the flame height, maximum ceiling temperature and the rate and type of toxic emissions are important. In this context, pool fires are of great importance, especially in oil and petroleum industries, and in the transportation sector; because of the enormous damages that could be associated with this category of fires. On the other hand, from fundamental combustion science point of view, pool fire is an interesting phenomenon because it involves several key physical processes among them: evaporation and mixing, pyrolysis and turbulent combustion.

In a pioneering empirical study by Blinov and Khudiakov [1], three regimes of pool fires were proposed: laminar flow; transient flow; and fully turbulent flow regimes. This classification is based on Froude number (dimensionless heat release), and still remains applicable. Regardless of the nature and regime of the flow, fires in general and pool fires in particular are classified as diffusion flames. Therefore, the dynamics of fires is described based on the theory of non-premixed flames [2]. The assumption behind this classification is that combustion occurs with infinite fast reaction rates in thin reaction fronts, and the "all mixed are burned" rule is valid. Most of the literature modelling studies rely on this understanding of the physics of fire. For example the combustion sub-model in the widely used Fire Dynamics Simulator (FDS) package is based on the eddy dissipation concepts (EDC) [3]. Modified version of EDC approach [4] and non-premixed flamelet approach have also been used in the past [5]. The latter can be computationally very efficient if combustion in the problem at hand belongs to the non-premixed flamelet regime of combustion.

However, the validity of the above mentioned assumptions has not been thoroughly examined, yet. Indeed, pool fires usually involve pyrolysis (fuel dissociation and low-temperature chemistry) which can be much slower process than mixing and turbulence. The rate of evaporation (the regression rate of the pool) is also much smaller than that require of matching the massive entrainment which is up to 20 times of the stoichiometric air to fuel ratio [6], and to form a stable non-premixed flame. Such entrainment can potentially give rise to the quenching and eventually local/global extinction of the fire plume. Flame height and the intermittency of the fire plume also cannot be fully understood and predicted by the theory of non-premixed flames. Although the dynamics of pool fires may be reproduced, to some extent, by using EDC model together with sub-models for the flame extinction [7]. However this type of modelling approach requires *ad hoc*sub-model and model constants tuning. It is highly possible that pool fires, at least in some flow regimes, involve premixed combustion

* Corresponding author.
E-mail address: m.jangi@murdoch.edu.au (M. Jangi).

http://dx.doi.org/10.1016/j.combustflame.2016.08.017
0010-2180/

in a form of ignition and/or premixed flame fronts propagation. Under these conditions non-premixed based modelling strategies are not physically correct modelling approaches. Perhaps, the so-called partially premixed combustion (PPC) better describes the nature of pool fires.

In this study, we revisited the problem of combustion in compartment pool fire configurations to examine the structure of combustion in more details. We are presenting a new modelling approach. The originality of our approach is in the combustion sub-model that is used. We used Eulerian stochastic fields (SF) method [8]. SF method is an Eulerian formulation of the transported probability density function (t-PDF) method. This class of combustion sub-models have been designed to handle multiple modes of combustion from ignition to premixed flames to non-premixed flames when they can potentially co-exist in a problem and interact with each other [9,10]. In this approach, the chemical source terms in the transport equations of the chemical species and the energy equation of turbulent reacting flows appear in a closed form. In this way, no further assumption on the structure of combustion and the reaction fronts is needed to obtain a closed form of the conservation equations.

The drawback with t-PDF is that, this method can become computationally very expensive, when applied to simulate realistic combustion problems in which reasonable details of the kinetic mechanism is required to correctly predict the chemistry of combustion. Modelling of pool fires is of this class of problem in which reasonably detailed chemistry has to be adopted for pyrolysis and fuel dissociation near the pool surface and the formation of emissions in the fire plume. Here, this issue is addressed by employing chemistry coordinate mapping (CCM) technique [11,12]. In the past, we developed and validated this method for both Lagrangian [13] and Eulerian based PDF [14] formulations. Those studies are based on Reynolds-averaged Navier–Stokes (RANS) approach. Here, for the first time, we formulated and applied the SF method with CCM for large-eddy simulation (LES). The SF introduced by Valino [8] and Sabelnikov [15]. SF method has been used by Jones and co-workers for modelling combustion in gas turbines related configurations [16], cf. references therein, and also by Jangi et al. [14] for modelling diesel spray combustion applications.

In this study, we use (LES) which is desirable because it allows us to capture the temporal and spatial evolution of the flow motions and combustion processes. In this work, the simulations are based on the experiments of Ji and colleagues [17,18], where they studied the maximum ceiling temperature and the flame height of methyl alcohol pool fires with various pool sizes in a compartment. The detailed kinetic mechanics of methyl alcohol involves relatively less number of chemical spices compared with that of larger hydrocarbons. This allows us to use LES with t-PDF approach and detailed chemistry, yet reasonable computational costs. The main objectives of current study are: to formulate and apply SF-CCM for modelling pool fires; to examine the structure and the modes of combustion of the modelled pool fires; to understand the role of premixed combustion in the dynamics of the modelled fire plume.

2. Mathematical model: CCM accelerated SF method

Favre-filtering LES conservation equations for gas phase can be written:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\tilde{u}_j}{\partial x_j} = 0, \tag{1}$$

$$\frac{\partial \overline{\rho}\tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}[\overline{\rho}\tilde{u}_i\tilde{u}_j - \overline{\tau}_{ij} + \tau_{ij}^{sgs}] = 0, \tag{2}$$

the overline denotes the general filtering, e.g.,

$$\overline{u(x,t)} = \int G(r,x)u(x-r,t)dr, \tag{3}$$

the integration is over the entire field and the filter function G satisfies the normalization condition

$$\int G(r,x)dr = 1. \tag{4}$$

Tilde denotes the Favre filtering

$$\overline{\rho u} = \overline{\rho}\tilde{u}. \tag{5}$$

In Eq. (2), u is velocity, and $\overline{\tau}_{ij}$ is filtered stress tensor obtained from resolved strained rate $\tilde{S}_{ij}$ using $\overline{\tau}_{ij} = -\overline{p}\delta_{ij} + 2\overline{\mu}\tilde{S}_{ij} + 1/3\tilde{S}_{kk}\delta_{ij}$. $\tau^{sgs} = \overline{\rho}(\widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j)$ is the sub-grid scale stress tensor which is modelled using the Smagorinsky model.

2.1. Combustion sub-models

We use Eulerian stochastic fields (SF) method in which the exact transport equation of the joint sub-grid scales PDF is solved with the Monte Carlo method [8]. In SF method the joint sub-grid PDF is estimated by an ensemble of N_F stochastic fields. Each stochastic fields involves $N_s + 1$ number of scalars accounting for N_s number of chemical species in addition to the enthalpy variable. The stochastic equation for the nth stochastic field is:

$$\overline{\rho}d\phi_\alpha^{(n)} = -\overline{\rho}\tilde{u}_i\frac{\partial \phi_\alpha^{(n)}}{\partial x_i}dt + \frac{\partial}{\partial x_i}(\Gamma_t\frac{\partial \phi_\alpha^{(n)}}{\partial x_i})dt + \overline{\rho}S_\alpha^r(\phi^{(n)})dt - \frac{1}{2}\overline{\rho}C_\phi(\phi_\alpha^{(n)} - \tilde{\phi}_\alpha)\omega^{sgs}dt + \overline{\rho}\sqrt{2\frac{\Gamma_t}{\overline{\rho}}}\frac{\partial \phi_\alpha^{(n)}}{\partial x_i}d\boldsymbol{W}_i^{(n)}, \tag{6}$$

with $1 \leqslant \alpha \leqslant Ns + 1$ and $1 \leq n \leq N_F$. The above equation implies invoking the gradient transport hypothesis for approximating transport by turbulent velocity fluctuations. Here $\Gamma_t = \frac{\mu}{\sigma} + \frac{\mu^{sgs}}{\sigma^{sgs}}$ is the total molecular plus sub-grid scale diffusivity, and $S_\alpha^r(\phi^{(n)})dt$ is increments in $\phi_\alpha^{(n)}$ due to chemical reactions.

The term involves C_ϕ, where $C_\phi = 2$, is the micro-mixing modelled by the Interaction with Exchange to the Mean (IEM) model. In this term, ω^{sgs} is sub-grid scale turbulent frequency obtained from $\omega^{sgs} = \frac{\mu+\mu_{sgs}}{\overline{\rho}\Delta^2}$, with Δ being the filter width.

The $d\boldsymbol{W}_i^{(n)}$ represents a vector Wiener process that is spatially uniform but different for each field. Here $d\boldsymbol{W}_i^{(n)}$ is approximated by time-step increment $\sqrt{dt}\eta^{(n)}$ and $\eta^{(n)}$ is a $\{-1, 1\}$ dichotomic random vector [8].

The mean and moments of each variable α can be approximated from the ensemble of N_F notional fields, for example the mean is:

$$\tilde{\phi}_\alpha = \frac{1}{N_F}\sum_{n=1}^{N_F}\phi_\alpha^{(n)} \tag{7}$$

An operator splitting strategy is used to isolate the chemical source terms. The calculation of those source terms involves evaluating the integral $\int_{t_0}^{t_0+dt} S_\alpha(\phi^{(n)})dt$. A potentially more efficient way to evaluate the chemical source terms would be to first identify and cluster all cells in all notional fields that have similar thermodynamic states into phase-space zones, and then perform the ODE integration once for all of the particles in the zone. This approach is known as clustering [19], or sometimes is referred to as an agglomeration [20] technique.

In principle, the phase space consists of a subset of the composition space. The mapping of the nth field with composition $\phi^{(n)}(Y_1, ..., Y_{N_S}, h)$ into the discretized phase space can be considered as a mapping between the CFD cell index (i, j, k) in nth to the zone index in discretized phase space. The (i, j, k) CFD cell at time t in nth field is mapped to the lth zone in direction α of the phase