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Large Eddy Simulation of Ethanol-gasoline Fire

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Abstract

The multi-component fuel based eddy dissipation concept(EDC) model, PaSR based soot model and grey gas based FvDOM radiation model etc in ExfireFoam is further extended to simulate a 30cm × 30cm ethanol-gasoline square pool fire. The predictions achieved good agreement with the measurements for flame height and the radial temperature profiles at different heights, demonstrating the good potential of the ExfireFoam for predicting the combustion process of pool fires from multi-component fuels.

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Keywords: fire safety, large eddy simulation, multi-component fuels, pool fire

1. Introduction

In practical energy systems, every energetic material is basically made of multi-component fuels, e.g. liquid fuels (gasoline, diesel, kerosene etc), solid fuels (wood, plastic etc) and gas fuels (natural gas, petroleum gas etc). If these fuels accidently catch fires, the characteristics of the formed solid fire, liquid pool fire or gas jet fire etc will be different from pure-fuel fires. So from the standpoint of fire safety, there is hence the need to understand the fire behavior involving multi-component fuels and develop predictive capability to assist related consequence analysis.

As for liquid fuels, in past decades, the pure-fuel fire has been extensively studied, focusing on its every fields such as the burning rate, fire height, fire pulsation, its radiation and soot etc. However, multi-component fires have not been touched extensively. Only Chatris et al. [1] focused on the burning rate, fire height etc. of two typical car fuels such as gasoline and diesel. Additionally, recently in State Key Laboratory of Fire Science, Ding and Wang et al.[2] performed a series of experimental investigations on ethanol-heptane, ethanol-gasoline and heptanes-gasoline fires.

Following our experimental study [2], we developed ExfireFoam for numerical simulation and comparison. It should be noted that ExfireFoam extended from fireFoam in OpenFOAM platform and mainly focused on combustion models, soot models, radiation models and pyrolysis models etc. Here, by comparison in fire height and fire plume temperature at given locations, current ExfireFoam was validated for blended fuel fire simulations.

2. Mathematical modeling

2.1. Governing equations

The flow is governed by spatially filtered and Favre averaged reactive Navier-Stokes equations in the LES framework.

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

$$\frac{\partial \overline{\rho}\widetilde{u}_j}{\partial t}+\frac{\partial \overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\overline{\rho}\left(v+v_t\right)\left(\frac{\partial \widetilde{u}_i}{\partial x_j}+\frac{\partial \widetilde{u}_j}{\partial x_i}-\frac{2}{3}\frac{\partial \widetilde{u}_k}{\partial x_k}\delta_{ij}\right)\right)-\frac{\partial \overline{p}_d}{\partial x_i}-g_i x_i\frac{\partial \overline{\rho}}{\partial x_i} \tag{2}$$

$$\frac{\partial \overline{\rho}\widetilde{h}_s}{\partial t}+\frac{\partial \overline{\rho}\widetilde{u}_j\widetilde{h}_s}{\partial x_j}=\frac{D\overline{p}}{Dt}+\frac{\partial}{\partial x_j}\left[\overline{\rho}\left(D+\frac{v_t}{\mathrm{Pr}_t}\right)\frac{\partial \widetilde{h}_s}{\partial x_j}\right]+\dot{q}'''-\nabla\cdot\dot{q}_r'' \tag{3}$$

$$\frac{\partial \overline{\rho}\widetilde{Y}_m}{\partial t}+\frac{\partial \overline{\rho}\widetilde{u}_j\widetilde{Y}_m}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\overline{\rho}\left(D+\frac{v_t}{\mathrm{Pr}_t}\right)\frac{\partial \widetilde{Y}_m}{\partial x_j}\right]+\overline{\omega}_{m,gas}+\overline{\omega}_{m,soot} \tag{4}$$

$$\frac{\partial \overline{\rho}\widetilde{Y}_s}{\partial t}+\frac{\partial \overline{\rho}\widetilde{u}_j\widetilde{Y}_s}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\overline{\rho}\left(D+\frac{v_t}{\mathrm{Pr}_t}\right)\frac{\partial \widetilde{Y}_s}{\partial x_j}\right]+\overline{\omega}_s \tag{5}$$

$$\overline{p}=\overline{p}_d+\overline{\rho}g_j x_j \tag{6}$$

where ρ , u , p , h_s and Y are the density, velocity, pressure, sensible enthalpy and mass fraction of gas mixture, respectively. v , v_t , D , Pr_t denote laminar dynamic viscosity, turbulent dynamic viscosity, laminar diffusion coefficient and turbulent Prantl number. The source term, $\overline{\omega}_s$, is computed as a sum of soot formation and oxidation rates, $\overline{\omega}_s = \overline{\omega}_{sf} + \overline{\omega}_{so}$. $\overline{\omega}_{m,gas}$ is the production/sink rate due to gas reaction whileas $\overline{\omega}_{m,soot}$ is the one due to soot formation and oxidation. $\dot{q}$ is the heat release rate per unit volume from a chemical reaction. The thermal radiation $\dot{q}_r$ is the sum of gas and soot radiative fluxes.

2.2. Combustion model

In current study, we employed multi-component fuel based eddy dissipation model(EDC) for fuel combustion. The EDC, originally proposed by Magnussen et al. [3,4] , has been extensively used to simulate the combustion of fires and other energy generating systems and it were successful in the Reynolds Averaged Navier Stokes (RANS) context. But in LES framework, the EDC model requires formulation of the total kinetic energy and its dissipation rate with the SGS kinetic energy and eddy viscosity. Fureby et al. [5, 6] directly replaced them using SGS kinetic energy k_{SGS} and other SGS parameters. Chen et al. [7] followed the energy cascade concept but derived the total kinetic energy and its dissipation rate using the SGS quantities. Following Chen's work [7], Wang et al. [8] have extended the modified EDC to account for the combustion of multi-component fuels using infinitely fast chemistry and applied it to hydrogen/methane jet fire simulations. Here, this combustion model is applied to multi-component fuel pool fire simulations for further validation.

2.3. Soot model

Chen [7] extended the laminar smoke point based soot model to turbulent combustion using the Partially-Stirred-Reactor (PASR) concept. However, the original extension was limited by the over simplified assumptions for soot oxidation assuming infinitely fast soot oxidation chemistry and constant soot formation characteristic time. Further development by Wang et al. [9] has overcome these limitations through the use of a finite rate soot oxidation model and especially a newly proposed time-and-space dependent soot formation and oxidation characteristic time.

2.4. Radiation model

For optially-thick fires such as heptane, heptane-ethanol fires, etc, the grey mean absorption emission-based finite volume discrete ordinate method(fvDOM) in OpenFOAM is used to account for both gas and soot radiation. The total absorption coefficient is calculated as the sum of the component gas and soot absorption coefficients with the former evaluated by the RADCAL program [10] and the later computed following Chatterjee et al. [11], $\kappa_s = 1226 f_v T$,where f_v , where T are soot volume fraction and gas temperature, respectively.

3. Numerical setup

Although numerous large scale gasoline and crude oil pool fires have previously been conducted by industry and these were all essentially multi-component fuels, there were no detailed measurements available from these tests for model validation. Otherwise, there is no other detailed experimental data available in the literature for pool fires involving well defined multi-component fuels. In the light of this knowledge gap, new tests have been designed and conducted for heptane-ethanol pool fires using the extensive facility in State Key Laboratory of Fire Science at University of Science and Technology of China.

Free burning heptane-ethanol pool fire tests are performed in a large quiescent test hall. The square steel tray is 30cm × 30cm and 0.5 cm thick and 4 cm high. The fuel is a uniform blend of n-heptane and ethanol with their properties listed in Table 1. A top-loading balance is positioned below the tray to measure the mass loss of this two-component fuel. The temperature profiles along the centerline are measured with 1mm diameter K-type thermocouples which are arranged at 0.2m, 0.6m, 1.0m and 1.6m above the pool surface. A camera with the frame rate of 25 fps is set facing the fire to record fire images which are later used to derive the transient flame height.

Table 1. Fuel parameters

Fuel	density(kg/m^3)	boiling point (K)	Laminar smoke point height (m)
Ethanol	695	371.59	0.225
Gasoline	～725	308～478	0.08

The computational domain is also set to be a cylinder with the diameter of 2m and the height of 4m. It has been tested that 32 grids across the square tray width are sufficient to obtain the converged heptane-ethanol pool fire in the range of current mass flow rate. As shown in Fig. 1, non-uniform meshes are used with grid points clustered around the tray and their sizes gradually increased in the radial and vertical directions. The inlet boundary representing the evaporating pool surface is set according to the time-varying mass burning rate of the mixed heptane-ethanol fuel with the mass ratio of 0.4649:0.5351 as shown in Fig. 2. In order to keep the stability of the computation, the smoother fitted red curve is used. The wall boundary is set around the tray on the cylinder bottom while typical outflow and inlet open boundaries are used for the side and top.

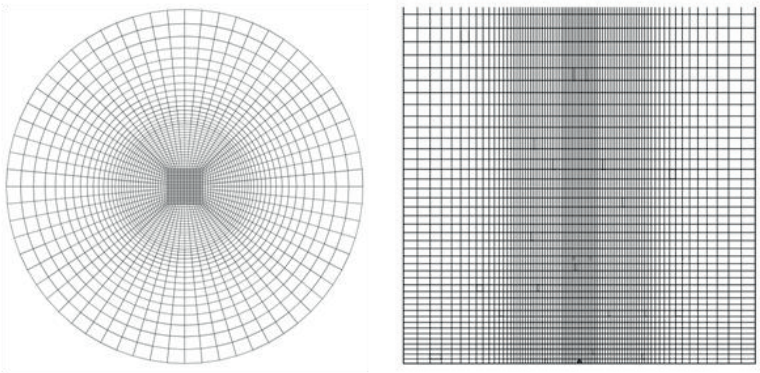

Fig. 1. The computational grid at the base of the ethanol-gasoline fire case

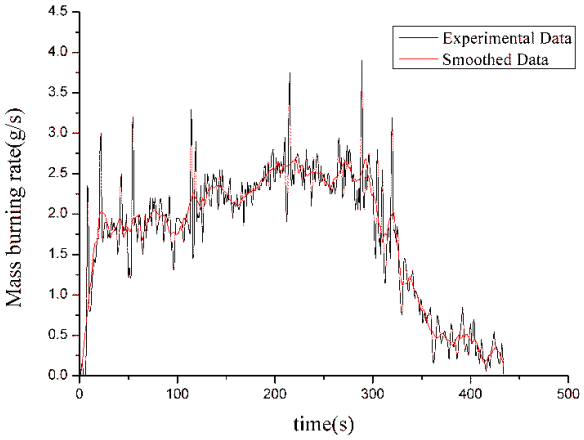

Fig. 2. The measured mass burning rate *vs* time.

4. Results and discussions

The predicted flame height is compared with the measurements in Fig. 3. The transient flame height in the experiment is characterized as the luminous visible flame height. The predicted flame height is defined as the highest location where the fuel and oxygen coexist since infinitely fast chemistry is involved. Figure 3 demonstrates that the predicted flame height agrees very well with the measurements during the fire growth. During quasi steady stages of ethanol-gasoline fire, the deficit between the predicted and experimental values is about 10%. Main reasons can be summarized as: (1) Actual ethanol in experiments included 5% water, but it is regarded as pure one in simulation; (2) No.90 gasoline is employed in experiments and resultantly the content of iso-octane is 90%. The remaining components of 10% are not clear, so iso-octane was used to replace the gasoline in simulation, which is one reason of the resulted deviation; (3) the different boiling points of ethanol and gasoline leads to the different mass burning rates. Moreover, the vapour ratio of ethanol and gasoline is varied with time. Such changes have the effect on gas reaction, soot generation and radiation etc. So the constant proportion of ethanol and gasoline used in simulation should result in computational deviations at different degree; (4) Certainly, mathematical model is also another reason for this. However, basically, the predicted fire height is well consistent with the experimental data.

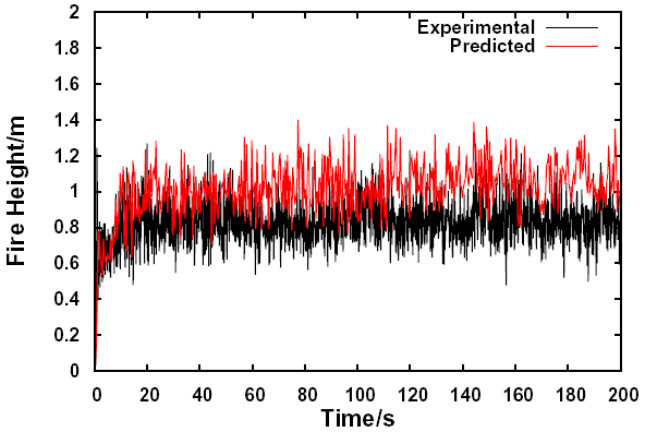

Fig. 3. The predicted and measured flame height *vs* time.

Fig. 4 plots the predicted and measured temperature profiles at different centerline heights. The temperature measurements have been corrected for thermocouple radiative exchange with the surrounding gas. It shows that very good agreement has been achieved between the predictions and the measurements, especially for the continuous flame zone (H=0.2m) and fire plume zone (H=2.0m). At H=0.6m and H=1.0m, the temperatures are over-predicted by about 200K. This over-prediction can be possibly attributed to the assumption of the infinitely fast chemistry. It might have also been caused by the differential burning rates of the two fuel components due to the different boiling points of heptane and ethanol,

and the resulting heptane-ethanol mass fraction ratios is time-varying in the experiment, different from the initial value which is set as fixed in the numerical simulation. Furthermore, such discrepancy could also influence the change of soot formation and oxidation rates in this region, as well as soot endothermicity/exothermicity, etc. Nevertheless, the predictions should be considered as very satisfactory while the aforementioned points are useful to guide further improvement of the model in the future.

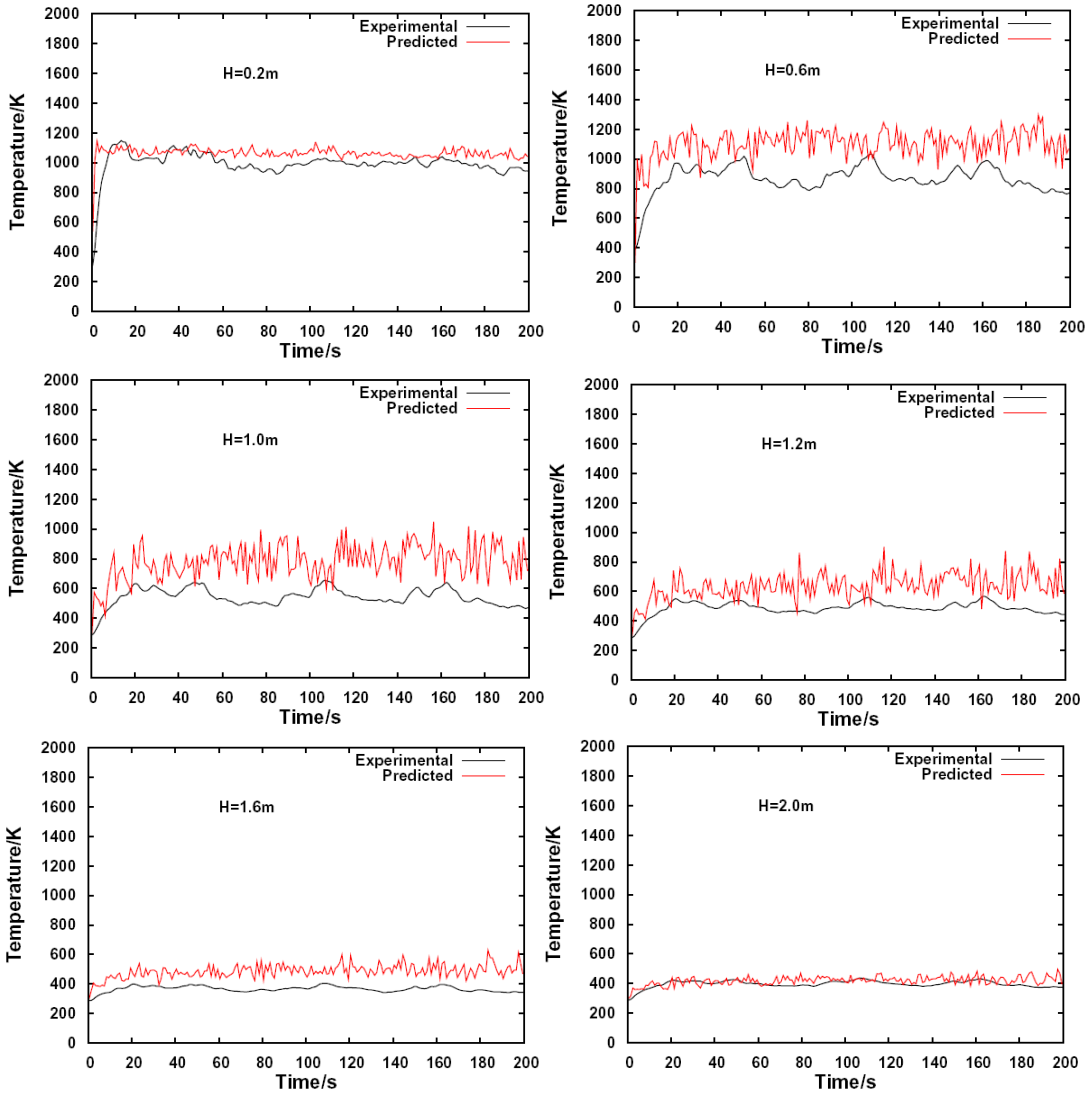

Fig. 4. The predicted and measured centerline temperature profiles *vs* time at different heights.

5. Concluding remarks

In this paper, ExfireFoam, which covers multi-component fuel based EDC combustion model, PaSR based soot model and grey gas based FvDOM radiation model etc, was employed to simulate a 30cm × 30cm ethanol-kerosene square pool fire. The predictions achieved good agreement with the measurements for flame height and the radial temperature profiles at different heights, demonstrating the good potential of the ExfireFoam for predicting the combustion process of pool fires from multi-component fuels.

Detailed analysis of the results, especially the discrepancies, indicates possible directions to improve the model. These include modifications to allow for consideration of the different boiling points of the fuel components and their mass burning rates, which would result in the mass fraction of the different fuel component to change with the progress of the fire.

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