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Numerical simulation of a turbulent partially premixed flame with inhomogeneous equivalence ratio

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HIGHLIGHTS

- The model uses a two-scalar four delta presumed Pdf to describe mixing and reactions.
- The LW–P model is validated against the ICARE lean premixed flame.
- The model successfully predicts flow dynamics and turbulent flame characteristics.

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ABSTRACT

Reynolds averaged numerical simulation (RANS) of a turbulent partially premixed flame is performed using a presumed probability density function (Pdf) approach. The mixture fraction and the fuel mass fraction are respectively chosen to describe the local composition and the chemical reaction progress. The so called LW–P model was employed for the calculation of a lean methane–air flame stabilized by a stoichiometric pilot-flame. Numerical predictions of the jet-core as well as the mean quantities of the flame, namely the modified progress variable and the static temperature are compared successfully with the experiments.

1. Introduction

For the purpose of theoretical and numerical analysis, combustion systems are often divided into two groups: premixed systems where the fuel and oxidizer are perfectly mixed at the molecular level before being consumed by the flame and non-premixed or diffusion systems where the fuel and oxidiser enter the flame separately, mixing within the reaction zone. However, in practical situations relevant to working conditions in energy conversion devices, turbulent mixing of fuel and oxidizer prior to combustion leads to a reactive mixture that is not homogeneous.

The development of systems operating in this mixed combustion mode has been driven by the need to reduce pollutant emissions, especially nitric oxides (NOx). By operating systems under fuel lean conditions, the reduction in temperature has a beneficial effect on the NOx level. However, as a system is run increasingly lean it becomes susceptible to several problems, including extinction, ignitability and flame stability [1]. By carefully designing and controlling spatial variation of mixture strength or areas of rich mixture, it becomes possible to achieve a stable lean combustion. Accordingly the equivalence ratio of the mixture varies in space and time, and combustion occurs in the form of partially premixed flames.

Various experimental and numerical studies have been carried out to evaluate the influence of spatial equivalence ratio variations for different geometrical and initial conditions. The most noticeable effects that have been evidenced can be summarized as follows; (i) extension of the flammability limits [2,3], (ii) modification of the inner structure of the flame [4], and (iii) strong dependence of the combustion efficiency on both turbulence and scalar length scales [5,6].

Most of the models devoted to turbulent partially premixed combustion are based on approaches such as presumed Pdfs [7,8], flame surface density [9] and coherent flame modelling [10]. The most attractive among the proposed models is the presumed Pdf variety (using the joint Pdf of the mixture fraction

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Nomenclature

B	pre-exponential factor
c	progress variable
C_μ	turbulence model constant
D	burner diameter
D_T	turbulent diffusion coefficient
I	turbulence intensity (%)
k	turbulent kinetic energy
L_T	turbulent length scale
p	static pressure
$P(Y, \xi)$	probability density function
r	radial coordinate
R	turbulent mixing model constant
S	segregation factor
Sc_T	turbulent schmidt number
T	static temperature
u_k, U	velocity component, mean axial velocity
X	axial coordinate
Y	fuel mass fraction

Greek symbols

δ_F	flame brush thickness
ε	turbulent kinetic energy dissipation
ϵ_Y, ϵ_ξ, $\epsilon_{\xi Y}$	scalar dissipation rates
ξ	mixture fraction
μ_T	turbulent viscosity
ω	instantaneous fuel consumption rate
ρ	density
τ_{ij}	viscous stress tensor element

Subscripts

b	burner
0	centreline value
st	stoichiometric value

Superscripts

$\bar{g}$	Reynolds average of g
g''	Favre fluctuations of g
$\tilde{g}$	Favre average of g

Acronyms

CFD	Computational Fluid Dynamics
ICARE	Institut Combustion Aerothermique, Reactivite Environnement (Research Institute)
LDA	Laser Doppler Anemometry
ORACLES	A Combustion Test-Bench (ENSMA)
NOx	Nitrogen Oxides
Pdf	Probability Density Function
RANS	Reynolds Averaged Numerical Simulation

and a reactive scalar) which offers a combination of simplicity, reduced computational cost and reasonable accuracy [8]. There are, however, several issues that arise including the shape of the Pdf, the statistical dependence of the variables and the closure of the scalar terms which appear in the transport equations of second moment quantities [11].

The Libby–Williams (LW) approach has already demonstrated its ability to recover not only the flamelet regime of turbulent combustion but also the thickened flame regime, at least for fully premixed situation [7]. The generalized form of the LW model introduced by Robin et al. [8] for partially premixed conditions is used in the present numerical study and will be denoted LW–P (Libby–Williams–Poitiers) in the following. In the latter model, the closure relies on a presumed joint scalar Pdf performed with a four Dirac delta functions.

The application of the LW–P model to various situations involving either partially premixed or non premixed combustion has been successfully carried out by Ribert et al. [12] for the description of a reactive shear layer stabilized by a parallel incoming stream of hot products. Robin et al. [8] used the generalized form of the model to perform a RANS simulation on the ORACLES rig made of a combustion chamber fed with two parallel streams of premixed reactants, having different equivalence ratios. Recently, these authors validated the LW-P model on a stratified V-shaped flame of methane and air [13]. As stated above, the LW–P model has been validated on various partially premixed configurations witnessing slight gradients of equivalence ratio. In the present investigation turbulent partially premixed combustion is studied in the special case where a strong mean gradient of equivalence ratio exists. In this respect, a new closure expression for the scalar variances is used to interpolate between thin flamelets and thickened flame regimes.

The flow configuration consists of a turbulent lean premixed burner-flame stabilized by an annular pilot-flame at stoichiometric conditions, as already investigated experimentally by Pavé [14] and Lachaux [15].

2. Mathematical modelling

Favre averaging form for each extensive quantity (except pressure and density) is considered leading to the following mean equations of continuity, momentum and energy:

$$\begin{aligned}
&\frac{\partial\bar{\rho}}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_k}{\partial x_k}=0\\
&\frac{\partial\bar{\rho}\tilde{u}_k}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_k\tilde{u}_j}{\partial x_j}+\frac{\partial\bar{p}}{\partial x_k}=-\frac{\partial}{\partial x_j}\left(\overline{\rho u_k''u_j''}-\overline{\tau_{kj}}\right)\\
&\frac{\partial\bar{\rho}\tilde{h}}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_k\tilde{h})}{\partial x_k}=\frac{\partial}{\partial x_k}\left(\overline{\rho D\frac{\partial h}{\partial x_k}}-\overline{\rho u_k''h''}\right)+\frac{\partial\bar{p}}{\partial t}
\end{aligned} \tag{1}$$

h denotes the sensible enthalpy of the mixture, given by:

$$h=\sum\nolimits_\alpha Y_\alpha\left(\Delta h^0_{F,\alpha}+\int_{T^0}^{T}cp_\alpha(T)dT\right) \tag{2}$$

where Y_α, $\Delta h^0_{F,\alpha}$ are respectively the mass fraction and heat of formation of the species α. In the previous set of equations, body forces and radiation fluxes have been neglected.

Turbulent fluxes of velocity and enthalpy are closed using viscosity and diffusivity hypothesis, respectively as:

$$\overline{\rho u_k''u_j''}=-\mu_T\left(\frac{\partial\tilde{u}_k}{\partial x_j}+\frac{\partial\tilde{u}_j}{\partial x_k}-\frac{2}{3}\delta_{kj}\frac{\partial\tilde{u}_i}{\partial x_i}\right)-\overline{\rho u_k''h''}=\frac{\mu_T}{\mathrm{Pr}_T}\frac{\partial\tilde{h}}{\partial x_k} \tag{3}$$

where $Pr_T = 0.7$ is the turbulent Prandtl number, and μ_T is the turbulent viscosity:

$$\mu_T=C_\mu\bar{\rho}\tilde{k}^2/\tilde{\varepsilon} \tag{4}$$

The previous system is completed by the transport equations of the turbulent kinetic energy $\tilde{k}$ and its dissipation rate $\tilde{\varepsilon}$ [1].

In the LW–P model, all species mass fractions are related to the fuel mass fraction Y and the mixture fraction ξ defined as:

$$\xi=(Y^{max}_{N2}-Y_{N2})/(Y^{max}_{N2}-Y^{min}_{N2}) \tag{5}$$