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Numerical analysis and model development for laminar flame speed of stratified methane/air mixtures

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ABSTRACT

Numerical simulations of stratified methane/air flames with various stratification configurations are conducted using an 1-D unsteady reacting flow solver. Among all the stratified flame cases investigated, rich-to-lean stratified flames show significant departures from homogeneous flames, i.e., up to 50% increase in fuel consumption speeds, primarily due to preferential diffusion of lighter species and radicals from rich burnt products. A sensitivity study of transport properties further reveals that preferential diffusion of molecular hydrogen H_2 along with radicals H, OH is the dominant factor in increasing stratified flame speeds, compared to the influence of heat diffusion and diffusion of H_2O. Larger departure of stratified flames from homogeneous flames is observed in those cases with higher degree of stratification. In order to model transient behaviors of stratified flames with arbitrary stratification configurations, a local stratification level (LSL) model is proposed. LSL incorporates the effect of preferential diffusion by introducing a transfer function from molecular hydrogen concentration gradients to equivalence ratio gradients, and the memory effect by solving the transient model equation of LSL. The model results match well with directly simulated results quantitatively with error less than ∼10% for both lean and rich conditions.

1. Introduction

Stratified combustion exists in a wide range of practical combustion phenomena and industrial applications, from forest wildfires [1], mine gas and vessel ruptures [2,3], to gas turbines and internal combustion (IC) engines [4–6]. Fuel stratification affects a wide range of combustion characteristics from flame speed, autoignition, to even instability. For gas turbines, oscillations in equivalence ratio may trigger thermo-acoustic instabilities in the combustion chamber, which can deteriorate the turbine performance or even cause severe physical damages [7]. In contrast, stratified combustion in direct-injected spark-ignited internal combustion engines has been an effective technique to improve fuel efficiency and reduce emissions [8,9]. Flame propagation speeds of in-cylinder stratified fuel/air mixtures can differ from those of homogeneous mixtures based on local and instantaneous equivalence ratio [10]. Therefore, it is of practical significance as well as fundamental interest to understand the effect of stratification on flame speed. Moreover, an accurate prediction of stratified flame speeds can benefit experiment interpretation and turbulent combustion modeling by developing more comprehensive flame speed look-up tables with consideration of fuel stratification.

There have been several analytical and experimental studies, aiming at understanding the departure of stratified flames from homogeneous flames in terms of flame speed. Karim and Tsang [11] first used a circular pipe filled with two mixtures separated by a plate, where a stratified mixture was formed after removing the separation plate. They found that the flame speeds of a rich-to-stoichiometric methane/air stratified flames were close to the corresponding quasi-homogeneous flame speeds, while the stoichiometric-to-lean stratified flame were ∼ 30% faster than the corresponding homogeneous flames. Badr and Karim [12] performed a similar experimental investigation and extended Karim and Tsang's conclusion: stratified flames propagating from mixtures with higher flame speeds to those with lower speeds, e.g., stoichiometric to either lean or rich, were faster than the corresponding homogeneous flames, while stratified flames with opposite directions were close to homogeneous flames. Moreover, the observed stratified flame speeds can be correlated to the homogeneous flame speeds corresponding to fuel concentrations at the ignition point and concentration gradients. However, the correlation was case-specific and valid only under simple stratification cases, where stratification does not change its direction. Around the same time, Mikolaitis [13] performed an asymptotic analysis using exponential scaling of premixed flame propagation with thermal and

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Nomenclature

Greek symbols

δ	Local Stratification Level (LSL)
δ_f	Local Stratification Level (LSL) at flame front
$\dot{\omega}_F$	fuel consumption rate
ϕ	equivalence ratio
ϕ_b	equivalence ratio of burnt mixture
ϕ_f	equivalence ratio at flame front
ϕ_f^b	equivalence ratio at flame front on burnt side
ϕ_f^u	equivalence ratio at flame front on unburnt side
ϕ_u	equivalence ratio of unburnt mixture
T_u	temperature of unburnt mixture

Roman symbols

U	vector of independent variables (governing equation)
$\mathcal{C}$	convection term (LSL model)
$\mathcal{D}$	diffusion term (LSL model)
$\mathcal{R}$	reaction term (LSL model)
C_F	scale constant (LSL model)
$C_{\mathcal{R}}$	reaction constant (LSL model)
C_{grad}	gradient constant (LSL model)
C_{rlx}	relaxation constant (LSL model)
d_f	flame thickness
D_k	diffusivity of species k
d_s	stratification thickness
F	convection term (governing equation)
F_v	diffusion term (governing equation)
Le	Lewis Number
P	pressure
S_c	fuel consumption speed
S_R	chemical source term (governing equation)
T	temperature
t	time
T_b	temperature of burnt mixture
T_u	temperature of unburnt mixture
U	velocity

concentration gradients. The results were restricted to the scenario where the flame preheat zone thickness is very thin and smaller than the length scale of initial temperature or concentration variations. Under this restriction, the author concluded that the flame propagation can be simply determined by the local values of temperature and mixture composition from the initial conditions. As the author pointed out in the paper, such an exponentially thin flame is not of practical significance for most applications. For this reason, Bissett and Reuss [14] adopted a similar approach and obtained a slowly-varying flame with the usual algebraic distance scaling for the flame. They demonstrated that the burning rate of the slowly-varying flame propagating through a region of varying temperature or mixture composition is different from that of corresponding homogeneous flames. In recent years, Kang and Kyritsis [15–17] conducted extensive research on stratified flames, both experimentally and theoretically. They established stratified mixtures through convective-diffusive balance of two methane/air streams in a tube-like burner. Their conclusions were very similar to that of [14] and they pioneered the development of stratified flame speed model. Two different models were proposed: (1) A integrated measure Q model was proposed in [15], where Q is the product of the average equivalence ratio gradient times the ratio of the average over the local value of equivalence ratio. A critical value $Q_0 = 0.018\ \text{mm}^{-1}$ is used to determine whether a stratified flame starts to deviate from its corresponding homogeneous flames. (2) A theoretical model was further proposed [17] on the basis of the hypothesis that stratified flames differ from homogeneous flames due to the effect of cumulative heat support from burnt gas. The model predicted quantitatively well with their experimental results of stoichiometric-to-lean or lean-to-leaner stratified flames but not rich flames. Balusamy et al. [18] performed stratified flame experiments of propane/air in a constant volume chamber, where a rich mixture was ignited and the corresponding flame propagated into lean mixtures. The flame propagation in the lean mixtures was found back-supported by the ignition in richer conditions, as the flame benefited from the rich composition of the burnt gas compared to that of lean homogeneous flames.

In spite of many interesting experimental observations and insights, all the above studies did not study the effect of preferential diffusion, which has been shown to play an important role in hydrocarbon stratified flames by many numerical studies [19–21]. For example, in a rich-to-lean stratified methane/air flames, rich flames can generate a significant amount of molecular hydrogen which diffuses faster than the flame front so that the excess hydrogen can penetrate into unburnt mixtures. A corresponding enhancement in flame speeds is thereby observed. As Kang and Kyritsis [17] pointed out in their latter model, the reason why the model did not work in rich flames was probably due to the single-step-chemistry approximation which did not include hydrogen as an intermediate species.

This paper examines the effect of preferential diffusion on the enhancement of flame speed with a detailed quantitative analysis, including a sensitivity study of transport properties. Furthermore, to the best of the authors' knowledge, there does not exist a stratified flame speed model that takes into account of differential diffusion and covers a wide range of conditions, both rich and lean. In order to improve current understanding of stratified flames and to facilitate development of stratified flame speed models, this paper

1. presents detailed one-dimensional stratified flame numerical results of methane/air flames with mixture-average diffusivity model and validated reduced chemical kinetic model;
2. discusses various stratification configurations of stratified methane/air flames;
3. conducts a sensitivity study of diffusivities to identify the root cause for the difference between laminar flame speeds of stratified and homogeneous mixtures;
4. proposes a transient local stratification level (LSL) model incorporating both the effect of preferential diffusion and the memory effect.

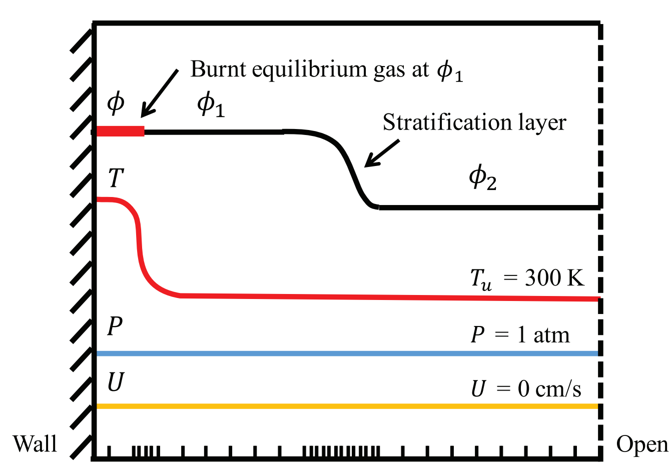

Fig. 1. Schematic of stratified flame propagating from unburnt mixture of ϕ_1 to that of ϕ_2 in 1-D planar coordinate.