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Numerical study of laminar flame speed of fuel-stratified hydrogen/air flames

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ABSTRACT

Numerical studies on hydrogen/air stratified flames in 1-D planar coordinate are performed using a time-accurate and space-adaptive numerical solver A-SURF. A step change in equivalence ratio is initialized as fuel stratification. Flame characterizations including fuel consumption speed and flame front propagation speed are compared between stratified flames and corresponding homogeneous flames. Two transport models, with equal diffusivity and mixture-average diffusivity assumptions respectively, are considered. With equal diffusivity assumption and stratification thickness larger than flame thickness, local fuel consumption speeds of stratified and homogeneous flames are identical, indicating that neither thermal effect nor chemical effect is present in stratified flames. When stratification thickness is reduced to the order of flame thickness, the difference between local fuel consumption speeds of stratified and homogeneous flames is caused by chemical effect due to different level of H radical in burnt gas. The same mechanism also leads to the difference between local fuel consumption speeds with mixture-average diffusivity assumption. In addition, preferential diffusion of H radical further increases the difference. The difference between flame front propagation speeds of stratified and homogeneous flames is mainly caused by additional heat release in the burnt gas with equal diffusivity assumption, while the difference with mixture-average diffusivity assumption is mainly caused by local chemical effect. Hydrodynamic effect due to fluid continuity on flame front propagation speeds is observed in both transport models. Additionally, with increasing stratification thickness, both local chemical and hydrodynamic effect are reduced. No significant lean flammability extension of hydrogen/air mixture is introduced by fuel stratification.

1. Introduction

Fuel-stratified, overall-lean combustion has become one of the potential internal combustion engine techniques [1,2]. While lean combustion leads to low NO_x emission without losing combustion efficiency [3,4], charge stratification improves ignitability and flame stability [5,6]. In addition, fuel stratification is also regarded as a useful technique to control combustion phasing and expand load limits in piston engines[7]. Despite its wide application in industries, fundamental understanding of stratified flames is still incomplete, which impedes the development of advanced direct fuel injection control strategies. In particular, as laminar flame speed of stratified charge is a key factor to determine the interaction between fuel auto-ignition events and flame propagation in stratified compression ignition engines, how laminar flame speed of stratified flame varies compared to the corresponding homogeneous flames is crucial but still not well understood.

There are two typical types of stratified flames: stratified flames propagating perpendicular to the mixture stratification layer, or along the layer. The first type of stratified flames is often investigated with a detailed discussion on structure of tribrachial triple flames [8–10], as a diffusion flame branch is created along the stoichiometric mixture fraction line. In comparison, the second type of stratified flames, when stratified flames propagate along the mixture stratification layer, only has the premixed flame branch. It is relatively complicated as flame characteristics are transient and alter in time due to flame passing through different local mixture compositions across the stratification layer. This study focuses on the latter stratified flames, which propagate along fuel stratification layer.

There have been extensive theoretical, experimental and numerical research on stratified flames propagating along mixture stratification layer: Effects of stratification on flammability limit [11–13], flame propagation speed [14,15], flame structure [16–18] and etc. have been investigated, with regard to different fuel components

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Nomenclature

ϕ	equivalence ratio
ϕ_u	equivalence ratio of unburnt mixture
ϕ_f	equivalence ratio at flame front based on local element composition
X_k	mole fraction of species k
δ_S	stratification thickness
S_c	fuel consumption speed
Y_k	mass fraction of species k
$\dot{\omega}_F$	fuel consumption rate
S_L	laminar flame speed relative to unburnt mixture
S_b	flame front propagation speed
ρ_u	density of unburnt mixture
ρ_b	density of burnt mixture
S_{exp}	fluid expansion speed
x_c	grid cell size
t	time
T	temperature
q	heat release
$\dot{q}$	heat release rate
c_p	specific heat
x_f	flame front location
D_T	thermal diffusivity
λ	thermal conductivity
ρ	density
D_k	mass diffusivity of species k
u	fluid velocity
HF	homogeneous flames
SF	stratified flames

including hydrogen [13], methane [14,15] and iso-octane [16]. As to the effect of stratification on laminar flame speeds, two mechanisms have been proposed to explain the behavior of stratified flames. Cruz et al. [19] conducted 1-D planar, unsteady laminar flame simulations on stratified methane/air mixture with detailed chemistry. Both rich and lean mixtures undergoing through positive or negative equivalence ratio gradients with regard to flame propagation direction were investigated. They suggested that the propagation of lean stratified flames is influenced mainly by burned gas temperature, i.e. thermal effect. When flame is burning from stoichiometry to lean, additional heat and composition fluxes from hotter products accelerate combustion at the flame front compared to the corresponding homogeneous flames at the same equivalence ratio. For rich stratified flames, the propagation is additionally influenced by production and consumption of molecular hydrogen in the flame front and the burnt gas, i.e. chemical effect. This causes the stoichiometric to rich flames to slow down and the rich to stoichiometric flames to accelerate, compared to homogeneous flames. However, only the fuel consumption over the entire domain was investigated and the impact of stratification on local flame characteristics was missing. In the content of computational fluid dynamics (CFD), local fuel consumption is especially more relevant in internal combustion engine applications and turbulent combustion. Moreover, although the differences in temperature and species distribution between stratified flames and homogeneous flames were reported, how they actually led to the difference in flame characteristics is not fully understood. In the second mechanism study, by performing numerical simulation of methane/air counterflow stagnation flames, Zhou and Hochgreb [20] confirmed that methane/air stratified flames are primarily dominated by the diffusion of heat under lean conditions, and diffusion of H_2 under rich conditions. However, these observations are only valid in the cases of certain strain rates under steady state. How stratification relates to unstretched propagating flames is still unclear. In fact,

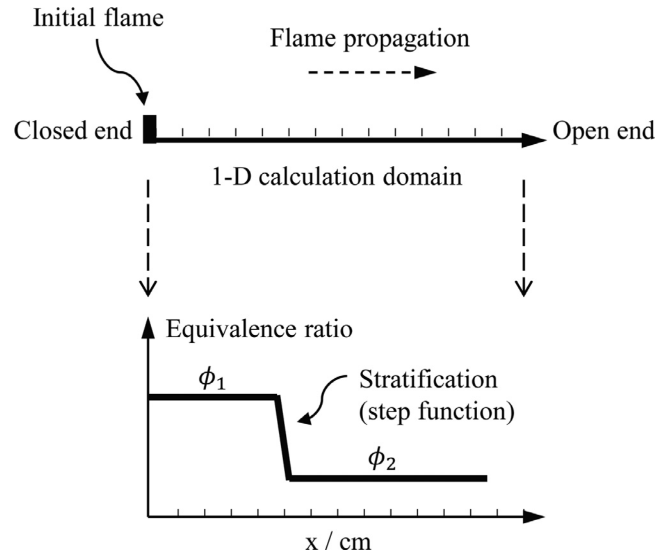

Fig. 1. Schematic of stratified flame propagating in 1-D planar coordinate.

stratified flames are difficult to characterize, e.g. location of flame front, equivalence ratio at flame front and definition of flame speeds. Especially when differential diffusion exists, gas composition at the flame front can be quite different from that of unburnt mixture, making the characterization even harder. Furthermore, observation from one particular fuel stratification might also not hold for another fuel, as different fuel species burn through different chemical pathways. As one of the fundamental combustible mixtures, hydrogen/air flame generates intermediate radicals, which appear in almost all hydrocarbon flames. Therefore a thorough understanding of hydrogen/air flames is essentially important to establish the first picture of fuel stratification concept.

The objective of this study is to understand how hydrogen/air stratified flame behaves differently in comparison to homogeneous flames. More specifically, the following questions are to be answered:

1. What is the detailed mechanism that stratification introduces thermal effect or chemical effect, if any, leading to variation of flame characteristics between stratified flames and homogeneous flames?
2. What is the role of differential diffusion of chemical species in stratified flames? Is it related to the chemical effect?
3. How do flame characteristics respond to different degrees of stratification?

To answer these questions, fuel consumption speed as well as flame front propagation speed are used to quantify the differences between stratified and homogeneous flames. Two transport models with equal diffusivity and mixture-average diffusivity assumptions respectively are considered and analyzed. The effect of stratification thickness on stratified flames as well as the potential on lean flammability extension are also investigated.

2. Numerical model and setup

The present numerical model represents hydrogen/air flame propagation in one-dimensional (1-D) planar coordinate with one end closed and the other open, as sketched in Fig. 1. The flame is initialized at the closed end and propagates toward the open end. Stratification is introduced by specifying a step change in the initial equivalence ratio profile. The simulated condition is analogous to constant-volume bomb experiments where ignition occurs in the center and flame propagates outwardly [21], or to tube experiments where flame propagates in a pipe from its closed bottom to the open end [22].