



Effects of Soret diffusion on premixed flame propagation under engine-relevant conditions

Mahdi Faghih^a, Wang Han^b, Zheng Chen^{a,*}

^aSKLTCS, Department of Mechanics and Engineering Science, College of Engineering, Peking University, Beijing 100871, China

^bInstitute for Simulation of reactive Thermo-Fluid Systems, TU Darmstadt, Darmstadt 64287, Germany



ARTICLE INFO

Article history:

Received 15 November 2017

Revised 27 April 2018

Accepted 28 April 2018

Keywords:

Soret diffusion

Laminar flame speed

Hydrogen/air

Engine-relevant conditions

ABSTRACT

Recent studies have shown that Soret diffusion has strong impact on the laminar flame speed of hydrogen/air mixture while it has little influence for hydrocarbon fuels at normal temperature and pressure. However, it is not clear whether the same conclusions hold under engine-relevant conditions. This is investigated in the present study. A series of premixed spherical flames propagating at high temperatures and pressures are simulated for different fuels, and the corresponding laminar flame speeds with and without considering Soret diffusion are obtained. It is found that for hydrogen/air mixture, Soret diffusion has much stronger influence on burning rate at engine-relevant conditions than at normal temperature and pressure. However, for hydrocarbon fuels like methane and iso-octane, Soret diffusion still has negligible effects on the burning rate even under engine-relevant conditions.

© 2018 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

1. Introduction

It is well known that laminar premixed flame propagation is controlled by heat conduction and mass diffusion [1]. Mass diffusion mainly includes (1) Fickian diffusion due to concentration gradient and (2) Soret diffusion driven by temperature gradient [1,2]. Usually only the Fickian diffusion is considered in combustion modeling since it is the dominant mode of mass diffusion. However, under certain conditions (e.g., in the presence of very light species and very large temperature gradient), Soret diffusion cannot be neglected [3,4].

As reviewed in [3–5], there are many studies assessing Soret diffusion effects on laminar premixed flames. For examples, numerical simulation was conducted to assess Soret diffusion effects on the laminar flame speeds (LFSs) of different fuels (e.g., [6–12]). For hydrogen and syngas, LFS was shown to be reduced after considering Soret diffusion. This was found to be mainly due to the coupling between Soret diffusion of H radical and the chain branching reaction $H + O_2 = O + OH$ [9,12]. For hydrocarbon fuels such as methane, n-butane and n-heptane, the influence of Soret diffusion on LFS was shown to be negligible [8,10,11]. Theoretical analysis considering Soret diffusion [13–15] was also conducted for laminar premixed flames. It was found that Soret diffusion modifies the local equivalence ratio and thereby affects the flame propagation speed. Besides premixed flames, Soret diffusion effects on

diffusion flames were also investigated. Detailed description can be found in the recent reviews [3,4].

In previous studies, Soret diffusion effects were usually investigated under normal temperature and pressure (i.e., 298 K and 1 atm). Recently, Liang et al. [12] and Zhou et al. [16] have studied Soret diffusion effects at elevated temperatures and pressures examined. However, the elevated temperature and pressure, 500 K and 5 atm, considered in these studies are still far from engine-relevant conditions. It is still not clear whether Soret diffusion still has strong (negligible) impact on hydrogen (hydrocarbon) flames under engine-relevant conditions. The objective of this study is to answer this question. To this end, a series of premixed spherical flames propagating at high temperatures and pressures are simulated for different fuels. The corresponding LFSs with and without considering Soret diffusion are obtained, and then Soret diffusion effects on premixed flame propagation under engine-relevant conditions are assessed.

2. Numerical methods

Laminar flame speeds (LFSs) at elevated temperatures and pressures close to engine-relevant conditions are calculated through the constant-volume propagating spherical flame method (see [17] and references therein). In this method, a propagating spherical flame is initiated by spark ignition at the center of a closed spherical vessel. The evolution of chamber pressure rather than the flame radius is recorded. The pressure history, $P = P(t)$, is then used

* Corresponding author.

E-mail addresses: cz@pku.edu.cn, chenzheng@coe.pku.edu.cn (Z. Chen).

to determine LFS through the following expression [17]:

$$S_u = \frac{R_W}{3} \left(1 - (1-x) \left(\frac{P_0}{P} \right)^{1/\gamma_u} \right)^{-2/3} \left(\frac{P_0}{P} \right)^{1/\gamma_u} \frac{dx}{dt}, \quad (1)$$

where R_W is the radius of the spherical vessel, P_0 the initial pressure, and γ_u the heat capacity ratio of unburned gas. The burned mass fraction, x , is determined from pressure history through two-zone or multi-zone models in experiments (e.g., [18–20]) and it can be calculated directly in simulation. Readers who are interested in this method are referred to the Supplementary Document, which provides the detailed description of this method and detailed derivation of Eq. (1).

Compared to the other spherical flame method imaging flame front propagation (see [21] and references therein), the constant-volume propagating spherical flame method has the advantages that LFS for a given mixture over a broad range of temperatures and pressures can be simultaneously obtained from a single test and that it can be used to get LFS at engine-relevant temperatures and pressures [18]. Therefore, the constant-volume propagating spherical flame method is used here to calculate LFSs for different fuels with and without considering Soret diffusion. CHEMKIN-PREMIX code [22] is not used to calculate LFSs since it is difficult to get converged solutions at high temperatures and pressures.

One-dimensional premixed spherical flame propagating in a closed spherical vessel is simulated using the in-house code A-SURF (Adaptive Simulation of Unsteady Reactive Flow) [23–25]. Finite volume method is used to solve the conservation equations for compressible reactive flow. The CHEMKIN package [26] is incorporated into A-SURF to calculate thermal and transport properties and reaction rates. Three fuels, hydrogen, methane and iso-octane, are considered here. The detailed chemical mechanism developed by Li et al. [27] and GRI-Mech 3.0 [28] are used for hydrogen and methane, respectively. For iso-octane, the reduced mechanism in [29] is used. A-SURF has been used in previous studies on flame and detonation propagation (e.g., [30–34]). The detailed description of governing equations, numerical algorithms and code validation can be found in [23–25]. Here only the description of mass diffusion is presented.

The diffusion velocity of species k is composed of three parts:

$$V'_k = V'_{k,Y} + V'_{k,T} + V'_{k,C} \quad (2)$$

$V'_{k,Y}$ is the ordinary diffusion velocity given by the mixture-averaged formula [26]:

$$Y_k V'_{k,Y} = -D_{km} \frac{1}{\bar{M}} \frac{\partial(Y_k \bar{M})}{\partial r} \quad (3)$$

where Y_k is the mass fraction of species k ; D_{km} is the mixture-averaged diffusion coefficient of species k ; \bar{M} is the mean molecular weight of the mixture; and r is the spherical coordinate. The coefficient D_{km} is explicitly determined from the binary diffusion coefficients D_{kj} [26]:

$$D_{km} = \frac{1 - Y_k}{\sum_{j \neq k} X_j / D_{kj}} \quad (4)$$

where X_k is the molar fraction of species k . The binary diffusion coefficients D_{kj} are evaluated in CHEMKIN package based on classical kinetic theory [1].

$V'_{k,T}$ is the Soret/thermal diffusion velocity, which is proportional to the temperature gradient normalized by temperature itself:

$$Y_k V'_{k,T} = -D_{km} \Theta_k \frac{M_k}{\bar{M} T} \frac{\partial T}{\partial r} \quad (5)$$

where Θ_k and M_k are, respectively, the thermal diffusion ratio and molecular weight of species k . The correction velocity $V'_{k,C}$ is

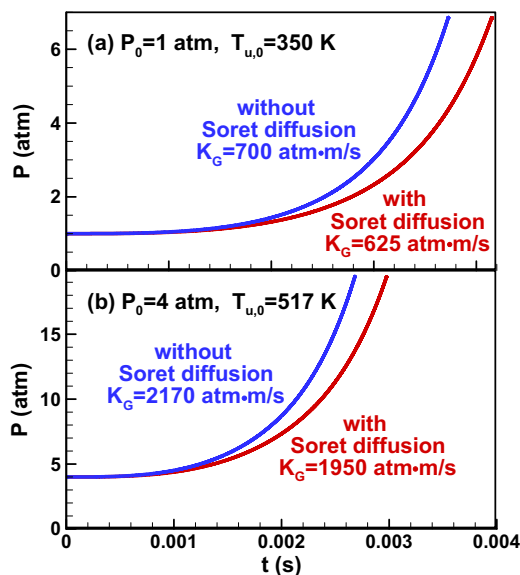


Fig. 1. Pressure rise history during spherical stoichiometric H_2 /air flame propagating in a closed spherical vessel with $R_W = 5$ cm.

included to ensure the compatibility of species and mass conservation equations [26] and it is determined by the requirement of $\sum_{k=1}^N (Y_k V'_k) = 0$ (where N is the total number of species). In the CHEMKIN package [26], the Wilke formula is used to determine the mixture viscosity and the mixture thermal conductivity is given in terms of the mass fractions and the thermal conductivity of each species. It is noted that the mixture-averaged model instead of the multi-component formulation is used here. Nevertheless, Bongers and De Goeij [8] showed that for hydrogen/air and methane/air mixtures, there is negligible difference in the LFSs predicted by the mixture-averaged and multi-component models.

In simulation, the propagating spherical flame is initiated by a small hot pocket (around 1 mm in radius). The radius of the spherical vessel is $R_W = 5$ cm. Adaptive mesh refinement is used to accurately and efficiently resolve the propagating flame front. At high pressures, the smallest mesh size is $8 \mu\text{m}$ and grid convergence is achieved. The initial temperature of $T_0 = 350$ K, pressure of $P_0 = 1$ atm, and flow velocity of $u_0 = 0$ cm/s are uniformly distributed in the whole computational domain. To reach higher temperature and pressure in unburned gas during spherical flame propagation, the initial temperature and pressure are increased to the corresponding values after isentropic compression (e.g., 517 K and 4 atm for stoichiometric H_2 /air as shown in Fig. 1b).

3. Results and discussion

We first consider spherical flame propagation in stoichiometric H_2 /air mixture. Figure 1 shows the pressure rise history. The pressure rise becomes faster once Soret diffusion is neglected, indicating higher flame propagation speed for the case without Soret diffusion. Figure 1 also shows the values of the deflagration index, K_G , which is defined as maximum pressure rise rate multiplied by the cube root of volume, i.e., $K_G = (dP/dt)_{\max} V^{1/3}$ [35,36]. The maximum pressure rise rate during gas explosions in enclosures, $(dP/dt)_{\max}$, is an important parameter in explosion. However, $(dP/dt)_{\max}$ depends not only on the mixture properties (such as mixture composition, initial temperature and initial pressure) but also on the volume of the vessel in which gas explosion takes place. Unlike $(dP/dt)_{\max}$, the deflagration index K_G is an intrinsic property of the premixture and it is independent of the volume of the vessel used in experimental measurements. Therefore, it is popularly used to quantify the

Download English Version:

<https://daneshyari.com/en/article/6593468>

Download Persian Version:

<https://daneshyari.com/article/6593468>

[Daneshyari.com](https://daneshyari.com)