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Effects of Soret diffusion on the laminar flame speed and Markstein length of syngas/air mixtures

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Abstract

The effects of Soret diffusion on premixed syngas/air flames at normal and elevated temperatures and pressures are investigated numerically including detailed chemistry and transport. The emphasis is placed on assessing and interpreting the influence of Soret diffusion on the unstretched and stretched laminar flame speed and Markstein length of syngas/air mixtures. The laminar flame speed and Markstein length are obtained by simulating the unstretched planar flame and positively-stretched spherical flame, respectively. The results indicate that at atmospheric pressure the laminar flame speed of syngas/air is mainly reduced by Soret diffusion of H radical while the influence of H_2 Soret diffusion is negligible. This is due to the facts that the main reaction zone and the Soret diffusion for H radical (H_2) are strongly (weakly) coupled, and that Soret diffusion reduces the H concentration in the reaction zone. Because of the enhancement in the Soret diffusion flux of H radical, the influence of Soret diffusion on the laminar burning flux increases with the initial temperature and pressure. Unlike the results at atmospheric pressure, at elevated pressures the laminar flame speed is shown to be affected by the Soret diffusion of H_2 as well as H radical. For stretched spherical flame, it is shown that the Soret diffusion of both H and H_2 should be included so that the stretched flame speed can be accurately predicted. Similar to the laminar flame speed, the Markstein length is also reduced by Soret diffusion. However, the reduction is found to be mainly caused by Soret diffusion of H_2 rather than that of H radical. Moreover, the influence of Soret diffusion on the Markstein length is demonstrated to decrease with the initial temperature and pressure.

Keywords: Soret diffusion; Syngas/air; Laminar flame speed; Markstein length

1. Introduction

Mass diffusion is essential in laminar flames and it strongly affects, or even determines, the fundamental combustion processes such as ignition, flame propagation, and extinction [1,2]. The dominant mode of mass transport is the Fickian diffusion, which is due to the appearance of concentration gradient. In the modeling of multi-component

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reactive flow, usually only the Fickian diffusion is considered. However, in the presence of very light or heavy species and steep temperature gradient, Soret diffusion [1–3], which drives light (heavy) species toward (away from) the hot zone, is also important for the mass transport.

The effects of Soret diffusion on laminar flames have been extensively studied in the literature. Except the work on heavy species such as metal particle [4], soot [5], and *n*-heptane [6], most of the studies are focused on the Soret diffusion of light species. For examples, Ern and Giovangigli [7,8] studied the influence of Soret diffusion on the flame structure and extinction of hydrogen/air and methane/air mixtures; Bongers and De Goey [9] investigated the effects of Soret diffusion on the laminar flame speed of hydrogen/air and methane/air mixtures; Grcar et al. [10] examined the Soret effects in lean hydrogen/air premixed flames; and Yang et al. [11,12] presented a mechanistic interpretation on Soret diffusion in hydrogen/air and *n*-butane/air flames. In these studies [4–12], discernable effects of Soret diffusion were observed.

However, to our knowledge, in the literature there is no study investigating the effects of Soret diffusion on syngas/air flames. Currently, syngas (synthesis gas) is expected to play an important role in future energy production, particularly for stationary power generation using Integrated Gasification Combined Cycle (IGCC) systems [13]. However, there are gaps in the fundamental understanding of syngas combustion characteristics, especially at elevated temperatures and pressures that are relevant to practical combustors. Syngas is primarily composed of H_2 and CO, and usually it has high concentration of light species, hydrogen [13]. Therefore, it is expected that Soret diffusion will affect syngas/air flames. Previous studies [4–12] only examined the Soret diffusion at normal temperature and pressure. Therefore, the influence of Soret diffusion at high temperatures and pressures remains unknown. Since syngas combustion in gas-turbine occurs at high temperatures and pressures, it is of interests to understand the effects of Soret diffusion at elevated temperatures and pressures as well as at normal conditions.

The objective of this study is to computationally assess and interpret the effects of Soret diffusion on syngas/air flames at normal and elevated temperatures and pressures. Two most important parameters of premixed syngas/air flames are investigated: one is the laminar flame speed (or laminar burning flux) and the other is the Markstein length. The laminar flame speed is defined as the propagation speed of an adiabatic planar flame relative to the unburned gas [1,2] and it affects the fuel burning rate in combustion engines. The Markstein length characterizes the variation in the local flame speed due to the influence of external stretching [14]. It determines the flame instability related to preferential diffusion and is one of the basic input physicochemical parameters in certain turbulent combustion models [14]. In the next section, the problem specification and numerical methods are presented. Then in Section 3, the effects of Soret diffusion on the laminar flame speed and Markstein length of syngas/air mixtures are discussed. Finally, the conclusions are given in Section 4.

2. Problem specification and numerical methods

Two premixed flame configurations are considered in this study: one is the unstretched freely-propagating planar flame and the other is the positively-stretched propagating spherical flame. The laminar flame speeds of syngas/air mixtures at different conditions (equivalence ratio, temperature, and pressure) with and without Soret diffusion are obtained by simulating the one-dimensional propagating planar flame using the CHEMKIN–PREMIX code [15]. In all simulations, the detailed chemical mechanism for syngas oxidation developed by Davis et al. [16] is used and it consists of 13 species and 38 elementary reactions. The number of grid points is always kept to be above 800 so that the flame structure is well resolved and the results are grid-independent.

In order to get the Markstein length of syngas/air mixtures, the one-dimensional expanding premixed spherical flame is simulated using the in-house code A-SURF [17,18]. A-SURF solves the conservation equations of one-dimensional, compressible, multi-component, reactive flow in a spherical coordinate using the finite volume method [17,18]. The CHEMKIN packages [19] are incorporated into A-SURF to calculate the temperature- and component-dependent thermodynamic and transport properties as well as the reaction rates based on the detailed chemistry of Davis et al. [16]. A-SURF has been successfully validated and used in previous studies [17,18,20,21]. Details on the governing equations, numerical schemes, and code validation can be found in Refs. [17,18] and thus are not repeated here. The computational domain is set to be $0 \leqslant r \leqslant 50$ cm and a multi-level, dynamically adaptive mesh is used. The propagating spherical flame is initiated by a small hot pocket (1–2 mm in radius) of burned product surrounded by static fresh mixture at initially specified temperature and pressure.

3. Results and discussion

3.1. Effects of Soret diffusion on unstretched laminar flame speed

In order to assess the effects of Soret diffusion on the laminar flame speed of syngas/air mixtures,