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Ignition of hydrogen/air mixtures by a heated kernel: Role of Soret diffusion

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ABSTRACT

Effects of Soret diffusion on the ignition of hydrogen/air mixtures by a heated kernel, and the structure and dynamics of the embryonic flame that is subsequently formed, were investigated numerically with detailed chemistry and transport. Results show that Soret diffusion leads to larger (smaller) *minimum ignition energy* (MIE) for relatively rich (lean) mixtures, that this effect is mainly engendered by the Soret diffusion of H_2 while that of the H radical is almost negligible, and that Soret diffusion also leads to an increase (decrease) of the Markstein length for rich (lean) mixtures. Satisfactory agreement with literature experimental data on the MIE is shown, especially for the critical states near lean and rich flammability limits. Evolvement of the flame structure shows that before the self-sustained flame is formed, the high temperature gradient associated with the ignition kernel has driven the H_2 in the mixture towards the ignition kernel and formed a locally high H_2 concentration region, which consequently renders lean (rich) mixtures easier (harder) to ignite. It is further shown that Soret diffusion of both H and H_2 affect the *propagation dynamics* of the stretched spherical flame that is subsequently formed, from its embryonic state until that of free propagation, in that Soret diffusion of H_2 is the dominant mode at small flame radius with the large strain rate, while that of H is the dominant mode at large flame radius with the small strain rate similar to that of the unstretched adiabatic planar flame.

1. Introduction

Ignition of a flammable mixture by a localized thermal deposition is of extensive practical interest, ranging from spark ignition within internal combustion engines to the accidental initiation of fires and explosions. Mechanistically, a successful ignition event would require both the formation of an embryonic flame before the ignition kernel is diffusively dissipated, and the attainment of this embryonic flame to achieve free propagation independent of the imposed state of the ignition kernel. Since steep temperature gradients result from the application of the localized high-temperature ignition kernel, Soret diffusion [1,2], which drives light species towards the high temperature region and heavy species away from it, could exert notable influence on the failure or success of ignition. Furthermore, it is also well established that successful ignition depends on the amount of energy deposited, which is characterized by the minimum ignition energy (MIE) [2,3] and has been extensively studied numerically [4,5] and experimentally [3,6]. It is clear that Soret diffusion, whose influence depends on the steepness of the temperature gradient, could substantially affect the MIE.

In terms of prior contributions on Soret diffusion in combustion problems, we note the studies on metal particles [7], soot [8–10], and *n*-heptane [11] for the heavy fuel species, and those on the light fuel species of hydrogen, methane, and syngas by Ern and Giovangigli [12,13], Bongers and De Goey [14], Grcar et al. [15], Yang et al. [16,17], Liang et al. [18] and Faghih et al. [19] with specific interests on the flame propagation velocities and stretch-induced extinction limits. The problem has also been theoretically analyzed by Han and Chen [20]. Mechanistically, in these studies the temperature gradients driving Soret diffusion arise from existing flames, while large concentration gradients are also already present such that Fickian diffusion is expected to be dominant, with Soret diffusion having only secondary effects. For the present ignition problem, however, the initial species concentrations are uniform and the imposed heat deposition generates a local high-temperature region before chemical reactions can substantially alter the concentration profiles. Consequently, Soret diffusion could impose substantial and mechanistically quite different influences.

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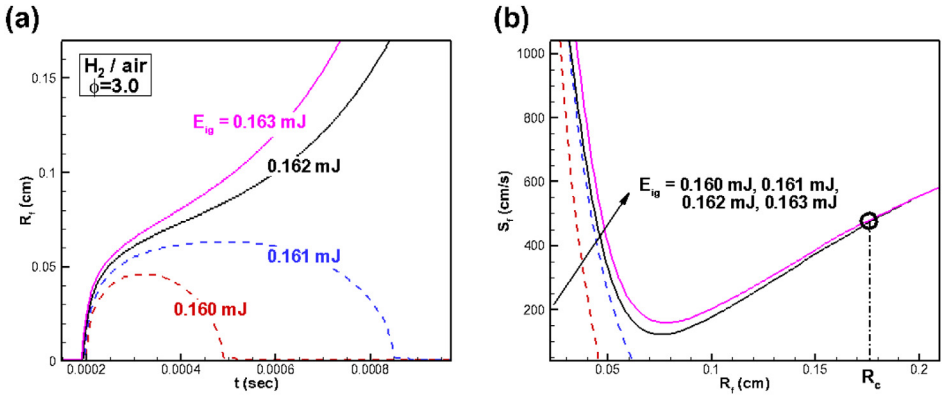

Fig. 1. Spherical flame initiation for hydrogen/air mixtures ($\phi = 3.0$) at different ignition energies: (a) temporal variation of flame radius; (b) flame propagation speed as a function of flame radius.

The objective of the present study is to study the effects of Soret diffusion on ignition of hydrogen/air mixtures by a heated kernel, and quantitatively assess and explain its influence on the MIE. Specifically, the unsteady, spherically symmetric flame is first simulated to calculate the MIE of hydrogen/air mixtures to demonstrate the flame initiation and propagation processes. Next, the physical model and computational method used in this study are briefly described. Then, results on MIE and the related length scale – namely the Markstein length, are discussed and the flame front evolution with detailed flame structure is presented. Finally concluding remarks are given.

2. Numerical method and problem specification

The problem of interest was studied computationally, using the A-SURF code [21] which solves the conservation equations of 1-D, compressible, reactive flow in a spherical coordinate, and has been successfully used and validated in previous studies [21–23]. A multi-level, dynamically adaptive mesh is used and the moving reaction zone is always fully covered by the fine meshes. The thermodynamic and transport properties as well as the reaction rates were calculated using the CHEMKIN packages [24], using the detailed hydrogen/air reaction mechanism of Li et al. [25]. The mixture-averaged formulation [1] has been adopted to calculate both the Fickian and Soret diffusion fluxes, and the results compared with those using more detailed multicomponent formulation were found to be close.

The mixture is initially homogeneous, at 298 K and atmospheric pressure. Imposition of the ignition kernel is given by:

$$q_{iq} = \begin{cases} \dfrac{E_{ig}}{\pi^{3/2} r_{ig}^3 t_{ig}} \exp\left[-\left(\dfrac{r}{r_{ig}}\right)^2\right] & \text{if } t < t_{ig} \\ 0 & \text{if } t \geq t_{ig} \end{cases} \quad (1)$$

where E_{ig} is the total ignition energy, t_{ig} the duration of the energy source, and r_{ig} the ignition kernel radius. The ignition kernel size and duration for most cases are fixed as $t_{ig} = 200$ μs and $r_{ig} = 200$ μm, respectively. Figure 1(a) shows the time evolution of the flame radius for different ignition energies with $\varphi = 3.0$. It is seen that a self-sustained propagating flame can only be successfully initiated when the ignition energy is above the MIE. The MIE can be determined by the average of the ignition energies for the closest success and failure cases of ignition, which gives $E_{min} = 0.1615$ mJ for this mixture. The MIE for all other mixtures were determined similarly, with an uncertainty below 5%. In addition to the MIE, studies [26,27] have shown that there also exists a critical flame radius, R_c, beyond which flame propagates as a self-sustained quasi-steady flame independent of the ignition energy. This gives a characteristic dimension of the ignition and flame propagation process. Based on this criterion, the critical radius was defined as the point where the ignition energy does not affect the subsequent flame propagation; specifically $R_c = 0.176$ cm, as indicated by the circle symbol in Fig. 1(b).

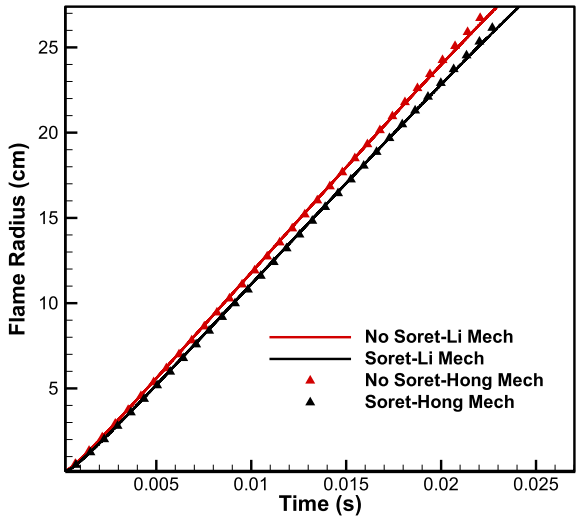

Fig. 2. Spherical flame initiation for hydrogen/air mixtures ($\phi = 3.0$) with different kinetic mechanisms (E_{ig}=0.5 mJ).

Furthermore, to validate the chosen kinetic mechanism, the flame trajectories using an updated hydrogen mechanism by Hong et al. [28] are compared in Fig. 2. It is found that given the same ignition energy, differences due to the kinetic mechanism are quantitatively small and qualitatively do not lead to any change in the understanding of the effect of Soret diffusion.

3. Results and discussion

3.1. MIE and related length scales

Figure 3(a) shows the calculated MIE for mixtures with equivalence ratio ϕ ranging up to 5.2. Since the possible candidate species for substantial Soret diffusion in hydrogen flames are H_2, the fuel, and H, the intermediate radical, we focus on their separate roles on the MIE. In Fig. 3(a), it is seen that Soret diffusion significantly affects MIE for extremely lean and rich cases, at which the MIE increases rapidly as the mixture is close to the flammability limits. Furthermore, the effect of Soret diffusion has opposite