Effects of low-temperature chemistry on hot-particle ignition in a premixed fuel/air mixture

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1 Introduction

The hot particle, such as mechanical sparks in manufacturing and mining operations, is one of the typical thermal ignition sources [1]. Scientific understanding and characterizing of hot-particle ignition plays an important role on accessing and reducing the risk of accidental ignition of flammable mixture in industry and aviation [2]. Experimental work on this topic goes back to 1920s when Coward and Guest [3] studied the effect of material on the ignition of natural gas-air mixture by heated metal bars. Thereafter, extensive experiments on hot-particle ignition were performed by different groups, e.g., [4-8]. In theoretical analysis, Semenov [9] proposed an analytical expression for ignition temperature as a function of particle surface area. Law [10] solved the steady boundary equation for ignition problem and derived an explicit ignition criterion using the matched asymptotic analysis with large activation energy assumption. Kumar [11] determined the hot-surface ignition temperatures for hydrogen-oxygen-diluent mixtures through 1-D simulations and experiments. Early numerical studies have been limited to 1-D simulations of stationary particles assuming spherical symmetry. More recently, Melguizo-Gavilanes et al. [12] conducted 2-D simulations of a falling particle and studied the formation of ignition kernel influenced by the particle temperature and differential diffusion. Coronel et al. [13] developed an experimental technique for creating a moving hot particle with a well characterized and controlled temperature. Zirwes et al. [14] performed 2-D axisymmetric and 3-D direct numerical simulations to study the effect of relative flow velocity on the ignition of hydrogen/air and methane/air mixtures.

Most previous works have been focused on the effect of material, size, geometry and temperature of particles, as well as the flow field in the vicinity of hot particles. However, few studies considered the role of low-temperature chemistry (LTC) in particle induced ignition. In their 2-D simulations, Coronel et al. [13] found that inclusion of species and reactions important for LTC results in an increase in ignition temperature when the Mével mechanism is used. Mével et al. [15] proposed a simplified model to analyze the chemical kinetics of n-hexane-air along streamlines in the thermal boundary layer of a moving hot particle. They found that LTC does not play a significant role in the ignition process since the residence time of most fluid elements within the boundary layer (around 5~10 ms) is short compared to the characteristic low-temperature delay times (around 100 ms). The particle diameter considered in their work is 4 mm. However, the size of

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mechanical sparks is typically in the range of a few hundred microns up to about 2 mm [16]. Besides, Häber et al. [17] found that one-dimensional simulations have good performance on predicting surface ignition temperature for particles whose radii smaller than 2 mm, which means the density-gradient induced natural convection is not an important factor in small hot-particle ignition process. Thus, the present study uses one-dimensional simulations to investigate the effect of LTC on small hot-particle ignition in a premixed stoichiometric DME/air mixture whose characteristic low-temperature delay time is in the order of 5 ms.

2 Numerical model and methods

We consider the transient ignition process initiated by a hot spherical particle and subsequent spherical flame propagation. The hot particle is fixed in space and it is characterized by its radius R and surface temperature T_P. The mixture is initially static at specified pressure P and temperature T_u. Due to spherical symmetry, 1-D simulation in a spherical coordinate is conducted. On the surface of the hot particle, the temperature is fixed, and the flow speed and mass diffusion speed are both zero. A large computation domain of $R \leq r \leq 50$ cm is used so that the pressure is nearly constant for flame radius below 5 cm.

The 1-D transient ignition and flame propagation process is simulated using the in-house code A-SURF (Adaptive Simulation of Unsteady Reactive Flow) [18]. The conservation equations for compressible, multi-component, reactive flow are solved using the finite volume method. The time evolution of the stiff reaction terms is separated from that of the convection and diffusion terms using the Strang splitting fractional-step procedure. A-SURF has been successfully used in previous studies on ignition and premixed flame propagation. The details on governing equations and numerical methods for A-SURF are presented in [18] and thereby are not repeated here.

In this study, H_2/air and CH_4/air mixtures are considered for the validation of ignition identification while DME/air for the study of the LTC effect. The CHEMKIN packages [19] are incorporated into A-SURF to calculate chemical reaction rates and temperature-dependent thermal and transport properties. Detailed chemical mechanisms are considered: the mechanisms of Li et al. [20] for H_2, GRI-Mech 3.0 [21] for CH_4, and the mechanism of Zhao et al. for DME oxidation [22]. To accurately and efficiently resolve the reaction zone, adaptive mesh refinement algorithm is implemented. The finest mesh sizes are 4 μm, 8 μm and 16 μm for H2, CH4 and DME mixtures respectively, which ensures that there are at least 15 meshes within the hot flame front. Grid convergence is ensured.

3 Results and discussion

3.1 The transient ignition process and ignition temperature

We first study the transient particle ignition process of stoichiometric H_2/air mixture initially at T_u=300 K and P=1 atm. Figure 1 shows the temporal evolution of temperature and OH mass fraction distributions during the hot-particle induced ignition process. At the beginning, the temperature of the mixture surrounding the hot particle increases due to the heat conduction from the hot particle (lines #1~4 in Fig. 1a). Meanwhile, OH radical is produced around the hot-particle. Then around t=3.74 ms (line #5), thermal runaway occurs, which makes the temperature of surrounding mixture higher than T_P. This ignition process is triggered by high-temperature chemistry (HTC) and it occurs very close to the particle surface. A spherical flame is shown to fully develop and propagate outwardly (lines #6~10). During the transient ignition process, the heat flux on the particle surface, Q, changes its sign from positive to negative. The ignition delay time, τ_{ig}, is the time when Q=0 (i.e., the temperature gradient at $r=R$ is zero) [11].

Figure 2 shows the change of τ_{ig} with T_P for particles with different radius R. At the same T_P, τ_{ig} increases as R decreases since heat conduction and mass diffusion are stronger in the mixtures surrounding a smaller particle. Besides, at the same particle size, τ_{ig} increases exponentially as T_P approaches to a critical particle temperature, which is defined as ignition temperature, T_{ig}. As expected, T_{ig} decreases with R. Figure 3 shows the ignition temperature for H_2/air and CH_4/air mixtures. The present results are in good agreement with those from simulations [23,24] and experiments [8] reported in the literatures. Therefore, the hot-particle induced ignition process can be accurately simulated in our study.

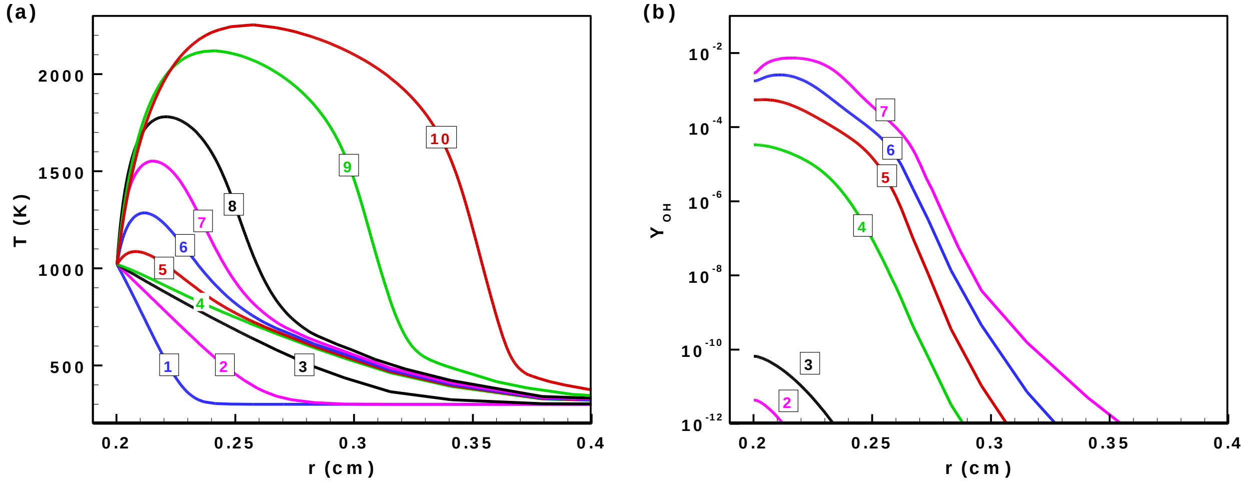

Figure 1. Temporal evolution of (a) temperature and (b) OH mass fraction distributions during the particle (R=2 mm and T_P=1020) ignition in H_2/air (ϕ=1, T_u=300 K, P=1 atm). The time sequence for lines #1-10 is respectively 0.1, 0.5, 2.0, 3.7, 3.74, 3.75, 3.755, 3.76, 3.78, 3.8 ms.

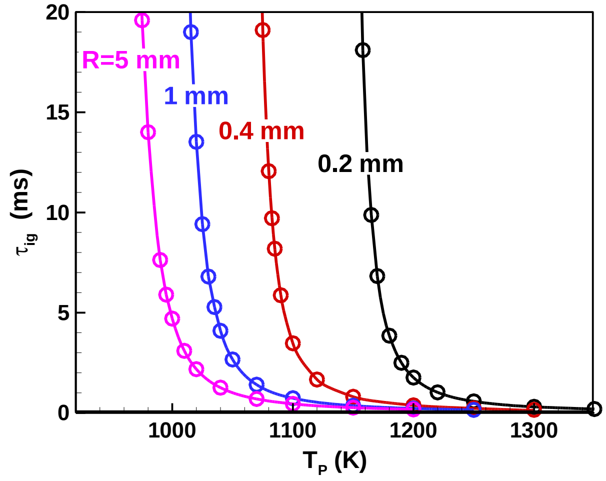

Figure 2. Change of the ignition delay time with particle temperature for particles with different radii. The mixture is H_2/air with ϕ=1, T_u=300 K, P=1 atm.

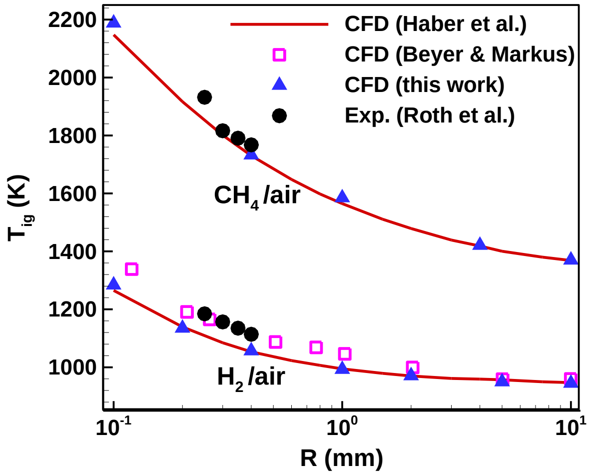

Figure 3. Change of ignition temperature with particle radius. The mixture is H_2/air or CH_4/air with ϕ=1, T_u=300 K, P=1 atm.

3.2 Ignition due to low-temperature chemistry and cool flame

Unlike H_2/air mixture for which ignition occus first near the praticle surface, DME/air mixture may ignite first at some distance away from the hot praticle due to LTC. It is known that fuels with LTC has two-stage ignition process when the initial temperature is within the NTC region. For stoichiometric DME/air mixture in a constant-pressure homogeneous ignition system, when the initial temperature is in the NTC region around 600~800 K, two-stage ignition exists. Since the temperature in the thermal boundary layer around the hot particle might be within the NTC region, LTC might happen first there and a cool flame can be first initiated before the hot flame appears. Moreover, Considering the NTC behavior, it is expected that the LTC plays an important role in hot-particle induced ignition.

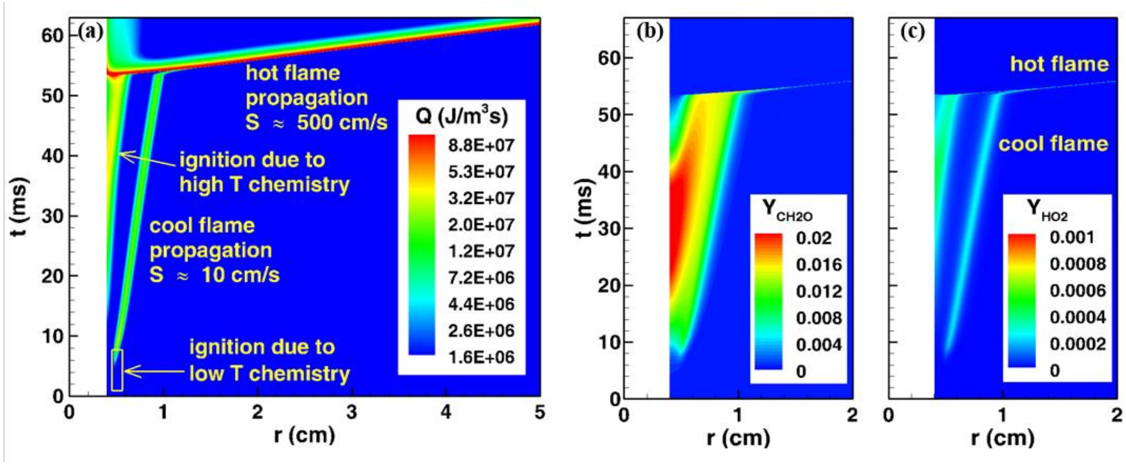

Figure 4. Temporal evolution of total heat release rate (a), CH_2O (b) and HO_2 (c) mass fractions during the particle (R=4 mm and T_P=1100 K) ignition in DME/air (ϕ=1, T_u=500 K, P=1 atm).

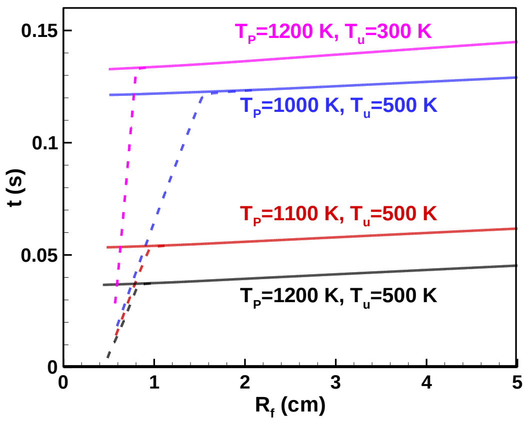

Figure 5. Trajectories of the cool flame (dashed lines) and hot flames (solid lines) induced by the particle (R=4 mm and different T_P) ignition in DME/air (ϕ=1, P=1 atm, and different T_u).

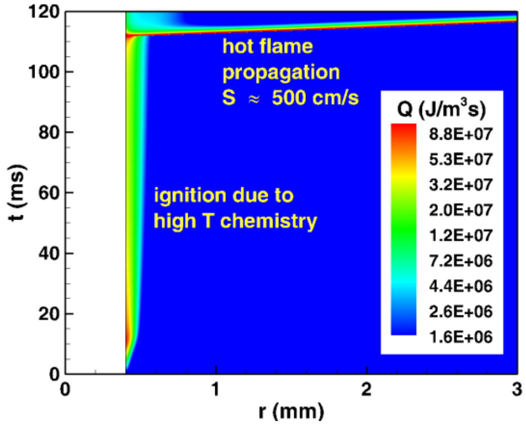

Figure 6. Temporal evolution of total heat release rate during the particle (R=4 mm and T_P=1250 K) ignition in DME/air (ϕ=1, T_u=500 K, P=1 atm). The low-temperature chemistry is not included.

The 1-D transient ignition and development of cool flame is simulated for DME/air mixture at T_P=1100 K and T_u=500 K. This initial condition is choosed deliberately so that it covers the range where two-stage ignition process exists. Figure 4 shows the temporal evolution of total heat release rate, CH_2O and HO_2 mass fractions. As expected, temperature rise pool and intermidiate species pool represented by CH_2O and HO_2 are built up first at some distance away from the particel surface due to LTC. A premixed cool flame is first initiated and it propagates outwardly at the speed around 10 cm/s. The fuel passing through the cool flame is only partially oxidized by reactions involved in LTC. At around *t*=54 ms, autoignition due to HTC occurs at the particle surface and a hot flame is initiated. The hot flame propagates behind the leading cool flame, and thereby double-flame structure for the coexistence of premixed cool and hot flames is observed. The heat release rate of hot flame is much larger than that of cool flame. The propagation speed of the hot flame is around 500 cm/s, and it is much faster than cool flame. Therefore, the hot flame finally catches up and merges with the cool flame. Similar observation was reported by Zhang et al.[25].

Figure 5 plots the trajectories of the cool and hot flames induced by the particles with *R*=4 mm and different T_P. The slope of each curve characterizes the flame propagation speed: the steeper the curve is, the slower the flame propagates. When T_P is fixed at 1200 K, increasing T_u from 300 K to 500 K makes both the LTC and HTC induced ignitions occur earlier. The corresponding cool flame and hot flame both propagate faster. On the other hand, when T_u is fixed at 500 K, increasing T_P from 1000 K to 1200 K makes both the LTC and HTC induced ignitions occur earlier while the propagation speed does not change. Therefore, the particle temperature only affects the ignition delay and does not affect the flame propagation speed.

Furthemore, we also simulate ignition process without LTC for T_p=1250 K. Figure 6 shows that ignition first occurs on the particle surface. The hot flame starts to propagate outwardly at around *t*=110 ms, which is much larger than 54 ms for the case with LTC and T_P=1100 K (see Fig. 4a). It is also noticed that the hot flame speed remains around 500 cm/s even when the LTC is terminated. Therefore, the LTC can greatly accelerate the hot-particle induced ignition but it has little effect on hot flame propagation speed.

It is should be noted that the results shown above for DME/air mixture are based on a large particle radius of 4 mm. Since the buoyancy effect is not considered, the conclusions drawn from large particles still hold for small particles qualitatively.

4 Conclusions

1-D transient ignition by a hot particle is simulated for H_2, CH_4 and DME. It is found that the particle temperature to ignite the flammable mixture increases greatly with the decrease of particle size. For DME/air mixture, the LTC is demonstrated to play an important role in hot-particle induced ignition. Since the temperature in the thermal boundary layer around the hot particle is within the NTC region, LTC ignition happens first at some distance away from the particle surface and it initiates a cool flame propagating outwardly. A hot flame is eventually initiated by HTC ignition and it catches up and merges with the leading cool flame. The LTC can greatly accelerate the hot-particle induced ignition. Therefore, LTC should be considered for hot particle ignition of DME/air mixture under the conditions considered in present study.

Acknowledgements

This work was supported by National Natural Science Foundation of China (Nos. 91741126, 51861135309).

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