Dynamics of Volumetric Ignitions Induced by Free Radicals Injection

S. Mori and N. Yoshikawa

Department of Aerospace Engineering, Nagoya University Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan E-mail: yoshi@nuae.nagoya-u.ac.jp

Abstract

Some of the important aspects of volumetric ignitions triggered by free radicals injection are presented. The defining conditions between volumetric and point ignition modes are obtained through a model analysis of ignitions in non-uniformly activated O_3 - O_2 mixtures. The chemical kinetic mechanisms of ignitions by free radicals injection are compared with the heated ignitions in H₂- O_2 mixtures. The laser photochemical ignition phenomena in NO₂ sensitized H₂- O_2 mixtures and a comparison with numerical predictions of induction times are also reported.

Introduction

Volumetric ignition mechanisms have a great potential for the application to stable ignitions in automobile lean-burn engines and supersonic combustion engines, in which conventional point ignition mode becomes unstable. We have elucidated that volumetric ignition occurs in the hot jet injection of burned gas into a fresh gas mixture [1]. The activated volume of the rapid turbulent mixing contains high concentration of hot free radicals, this enhances simultaneous explosions of multi-spot ignition kernels. The usual flame propagation does not occur in the volumetric mode. We report the recent progress on the volumetric ignition phenomena.

Model analysis of ignition in O₃-O₂ mixtures

The volumetric ignition mode is compared with the point ignition mode through the finite difference computations of spherically symmetric reactive flow fields of O_3 - O_2 mixtures. The initial non-uniform distributions of O radicals and temperature are assumed, and the effects of the gradient field are especially emphasized. The computer code includes elementary reactions, thermal conduction, and molecular diffusion. Because the simple reaction mechanisms of O_3 - O_2 did not increase too much the computer machine time, we could pursue the defining conditions between the volumetric and point ignition modes by means of a parametric study. The computations are divided into two parts, that is, non-reacting flow and constant volume combustion process. The first part is solved by a fourth order accurate FCT method (Boris et al. [2]), and the second part is solved by a linear implicit scheme (Lomax and Bailey [3]). The elementary reactions of Heimerl and Coffee [4] are used. The validity of the computer code was tested by the burning velocity prediction of 25% O_3 – 75% O_2 mixture at 1atm. The burning velocity is 49±1cm/sec, that is comparable with the experimental value of about 50cm/sec. The same gas mixture was used for the analysis of the reactive flow field.

Figure 1 shows a typical point ignition mode. The initial temperature distribution is uniform at 560K, and oxygen atoms are concentrated near the ignition kernel. A flame surface is established near the kernel and propagates outward. Figure 2 is a typical volumetric mode. The surrounding mixture around the kernel starts the exothermic process when the flame surface is established. The flame propagates a very short distance prior to the simultaneous explosion of the outer region. The results indicate that the initial gradients of temperature and radicals concentrations are dominant factors that distinguish the two ignition modes. We suggest a simple criterion for distinguishing the volumetric mode from the point mode by the following equation:

$$(L \Box L_{in})/f_{v\Box} \Box \Box t_A \Box t_B$$

 f_v : average flame speed, t_A : induction time in the outer region, t_B : induction time in the kernel, L_{in} : radius of the kernel, L: location for determining whether a flame sheet with a steep gradient is established or not (5mm in this case).

Ignition kinetics in H₂-O₂ mixtures including free radicals

The constant volume combustion of atmospheric, stoichiometric H_2 -O₂ mixtures including O, H, and OH radicals are computed using the reaction data of Oran et al. [5]. Figure 3 shows an ignition process triggered by OH radical injection of 10% mole fraction in the gas mixture initially at room temperature. The ignition mechanism consists of two parts. The first part is an induction process in which the added free radicals enhance the chain reactions at relatively low temperature. The concentration of the injected radical species decreases due to the consumption in the chain reactions. The subsequent stage is a typical thermal explosion process in which

heat release and chain reactions couple together to accelerate the extremely rapid rate. Figure 4 shows a heated ignition in the mixture initially at 1000K. In the induction process, the concentration of radicals increases monotonically. The thermal explosion stage is common to the two ignition modes. Figure 5 shows the change of induction times for different ignition means with different initial enthalpies of gas mixtures. The results demonstrate that the ignition by free radicals addition is more effective than the conventional heated ignition.

Volumetric laser ignitions in H₂-O₂-NO₂ mixtures

In addition to the above computations, we demonstrated that the volumetric ignition occurs in the photosensitized mixture of H₂-O₂ mixtures. We used the 355nm beam of the 3rd harmonic wave of a Nd:YAG pulse laser for the volumetric ignition of a stoichiometric H₂-O₂ mixture with NO₂ addition of 20% mole fraction at 0.1 atm and 300K. The photo-dissociation of NO₂+hv \rightarrow NO+O is the dominant elementary reaction generating the free radicals of oxygen atoms. Figure 6 shows the experimental setup of laser ignition. The FWHM of laser pulse is about 6nsec and the maximum power is 250mJ/pulse. The laser beam of 2mm diameter was directly introduced to the window. The ignition phenomena near the window of the incident laser beam was observed by a CCD camera, and the ignition delay times were obtained by ion probe measurements changing the laser power. The spontaneous emission of gas mixture in Fig.7 shows that the volumetric ignition occurs and the flame surface propagates in the radial direction of the laser beam. The ignition delay times were determined by subtracting the flame propagation time from the detection time of ion probe signal. Figure 8 shows the ignition delays of experiments and numerical analysis of constant volume reactions. In the theoretical model, the quantum yield of oxygen atom generation is 100%, that is, every photon-absorbing NO_2 molecule dissociate to NO and O without loss. We assumed that the excess internal energy, that is the energy difference between the bond energy of NO-O and the laser energy, is converted for heating up the mixture. The temperature rise due to this effect is less than 60K. This result indicates that the photochemical effect is the dominant process for generating the free radicals. The chain reaction mechanisms of H_2 - O_2 are included for calculating the change of temperature and species concentrations. The ignition delay time sharply increases in the region of laser power below 100MW/cm². The laser power at the ignition limit is about 60MW/cm² in the present experiment. The computation predicts slightly smaller laser power of 56MW/cm² at the ignition limit.

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Fig.3 Time Evolution of OH Radical (Injected Ignition)



Fig.4 Time Evolution of Heated Ignition



Fig.5 Induction Times for Different Ignition Means



Fig.6 Experimental Apparatus of Laser



4 mus

10 mus

70 mus

Fig.7 Sequential Self-luminescence of Laser Ignition



Fig.8 Ignition Delay Times of Laser Photochemical Reactions