Progress in Energy and Combustion Science 41 (2014) 1–55

Contents lists available at ScienceDirect

Progress in Energy and Combustion Science

journal homepage: www.elsevier.com/locate/pecs

Review

Recent advances in understanding of flammability characteristics of hydrogen

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ARTICLE INFO

Article history:
Received 26 August 2013
Accepted 29 October 2013
Available online 2 December 2013

Keywords:
Hydrogen combustion
Flammability limits
Reduced chemistry
Crossover temperature

ABSTRACT

The current increasing interest in hydrogen utilization and increasing understanding of hydrogen combustion motivate this review of flammability characteristics of hydrogen. The intent is to present a thorough and self-contained tutorial that covers the existing fundamental knowledge in a uniform and concise manner. The presentation begins with an up-dated exposition of the elementary chemical mechanism of hydrogen oxidation, including the latest chemical-kinetic results, with evaluated selections of reaction-rate parameters. Understanding of the mechanism is emphasized through presentation of systematically reduced overall steps and their associated rates. Useful simplifications of the chemistry are thereby exposed and appraised, identifying applicable quasi-steady-state approximations. The status of our knowledge of the fundamental transport properties for hydrogen combustion is then summarized, with indication of the relevance of thermal diffusion for hydrogen. Hydrogen–oxygen autoignition processes are next analyzed, including the important differences found under conditions above and below the crossover temperature at which the rates of the branching and recombination steps are equal, with an explanation of the classical explosion diagram that exhibits three explosion limits. Time-dependent and counter-flow mixing layers are addressed in the context of ignition processes. Knowledge of hydrogen deflagrations is reviewed, including their flame structures, burning velocities, and flammability limits, with special emphasis on peculiarities and simplification that occur in the vicinity of the lean limit. Deflagration instabilities and effects of strain and curvature on deflagrations are described, resulting under appropriate circumstances in flame balls, the structures, characteristics, and importance of which are analyzed. The structures and stabilization mechanisms of hydrogen diffusion flames are reviewed, pointing out the current state of knowledge and current uncertainties in their extinction conditions. Hydrogen detonations also are considered, with explanations given of their detonation velocities, structures, and instabilities, including cellular detonations and emphasizing the importance of future studies of vibrational relaxation effects in these detonations. Finally, some comments and observations on the applications and future prospects for hydrogen usage are offered from viewpoints of safety and energy production.

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http://dx.doi.org/10.1016/j.pecs.2013.10.002

1. Introduction

The practical motivation for investigating the combustion of hydrogen falls into two broad categories, one concerning its utilization and the other concerning its safety. From the viewpoint of utilization, there is increasing interest in hydrogen usage for power production because of its inherent cleanliness. In addition to being well adapted to fuel cells, it tends to produce fewer pollutants in direct combustion than do other fuels. Notably absent in hydrogen combustion, for example, is the greenhouse gas carbon dioxide, which is of increasing concern for energy generation from fossil fuels. One of many marks of the attractiveness of hydrogen in this respect is the existence of the International Journal of Hydrogen Energy, devoted to publication of scientific and engineering aspects related to energy production through hydrogen. In this context, it is relevant to bear in mind that, unlike fossil or nuclear fuels, combustible hydrogen is not found in deposits on Earth but instead must be generated in energy-consuming processes, so that it is best viewed as an energy carrier. Not only is hydrogen an effective energy carrier, but it also serves as one of the most powerful propellant constituents for rocket and air-breathing engines. There are thus many varied applications for extracting energy, power, or force from hydrogen.

Along with its increasing utilization come increasing safety concerns about hydrogen. It is much easier to ignite hydrogen than most other fuels, and its range of flammability is considerably broader. In addition, transition to detonation occurs more easily for hydrogen mixtures than for the vast majority of other mixtures, thereby making it potentially more dangerous. Coupled with the facts that hydrogen flames generally are more difficult to detect and that combustible hydrogen–air mixtures can be (and have been) generated from coolants in nuclear-reactor accidents, considerable efforts are warranted in evaluating and planning mitigation of potential hydrogen fire hazards. Prevention of hydrogen fires may be deemed essential. It thus becomes of paramount importance to ascertain accurately the flammability limits of hydrogen mixtures under different circumstances. Complications arise from the fact that the limits may be appreciably different in spacecraft, for example, than on Earth. Safety aspects thus warrant extensive investigation for hydrogen.

Studies of hydrogen combustion also are of interest from the viewpoint of enhancing scientific understanding. The chemistry of hydrogen oxidation is considerably simpler than that for any other fuel, and in fact it is part of the oxidation mechanisms of carbon monoxide and all hydrocarbons, alcohols, and other biofuels. It thus should be possible, in principle, to develop a better scientific