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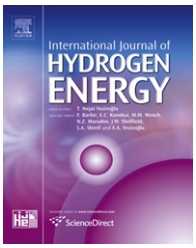

Numerical study on the spark ignition characteristics of hydrogen–air mixture using detailed chemical kinetics

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ABSTRACT

Hydrogen is a promising fuel and is expected to replace hydrocarbon fuels for its significant potentials to reduce the pollutants and greenhouse gases. It is very important to investigate Minimum ignition energy (MIE) on safety standards and ignition process of hydrogen–air mixtures. Even though the formation of flame kernels in quiescent hydrogen–air mixtures has been researched numerically and experimentally, the details of ignition mechanism have never been satisfactorily explained. In this study, the spark ignition of hydrogen–air mixture is investigated by using detailed chemical kinetics and considering the heat loss to the electrode. The purpose of this study is emphasized in the effects of the energy supply procedure, the radius of the spark channel, electrode size and electrode gap distance on the MIE. In addition, the effects of mixture temperature, electrode gap distance and electrode size on relationship between the equivalence ratio and the MIE are examined.

1. Introduction

Hydrogen is a promising fuel that could replace hydrocarbon fuels due to its potential to reduce pollutants and greenhouse gases. In particular, easily applicable utilization of hydrogen is in the SI engine as a pure fuel [1,2] and fuel blends [3,4] to start the flame propagation for its near-zero engine-out emission and high flame speed. The latter is unique to hydrogen and able to ignite premixed mixture at low equivalence ratios to achieve high thermal efficiency [5,6].

Many complex chemical and physical processes occur simultaneously during spark ignition, and these processes interact with each other. The spark ignition mechanism has never been satisfactorily explained, despite many years of research. Experimental results change if one factor is altered, but in many cases, there are insufficient experimental data on the subject to predict exactly what will happen. Numerical simulation is a convenient method for studying the specific effects of any factor on the spark ignition characteristics and for calculating important physical and chemical properties such as the instantaneous high temperature and the heat release rate, which are difficult to obtain experimentally.

The minimum ignition energy (MIE) is the minimum amount of energy required to ignite a combustible vapor, gas, or dust cloud due to an electrostatic discharge. MIE is an important parameter for judging the ignition ability of combustion systems, and is considered to be an important safety criterion for combustible gases. Factors affecting the MIE play an important role in determining the subsequent behavior of the flame. These factors include the type and composition of the

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Nomenclature

c_p	specific heat at constant pressure, J/(kg K)
D	effective diffusivity, m^2/s
h	specific enthalpy, J/kg
L	electrode gap distance, mm
Le	Lewis number
m	molar mass, kg/mol
P	pressure, Pa
q	ignition energy density, GW/m^3
q_{min}	minimum ignition energy density (MIED), GW/m^3
Q_{total}	total ignition energy, mJ
$Q_{total,min}$	minimum total ignition energy (MIE), mJ
R	electrode radius, mm
r	radial coordinate, mm
R_c	radius of the spark channel, mm
$\overline{R}$	universal gas constant, J/(mol K)
t	time, μs
t_i	spark duration, μs
V	volume of the spark channel, m^3
w	mass production rate, $kg/(m^3\ s)$
Y	mass fraction
z	axial coordinate, mm

Greek Symbols

θ	angular coordinate
λ	effective thermal conductivity, W/(m K)
μ	effective viscosity, Pa s
ρ	density, kg/m^3
τ	stress tensor, Pa
Φ	equivalence ratio

Subscript

i	species

mixture, spark duration, initial temperature, pressure, and velocity of the mixture, electrode size, electrode gap distance, and heat loss to the electrodes.

Several numerical studies have examined the details of spark ignition. Yuasa *et al.* [7] performed a two-dimensional numerical analysis with elementary reactions, including ion–molecule reactions, to investigate the effect of the energy deposition schedule on the MIE during the composite spark ignition of methane–air mixtures. Kravchik and Sher [8] simulated spark ignition and flame initiation in a quiescent methane–air mixture numerically. Kono *et al.* [9] investigated the mechanism of flame kernel formation produced by short-duration sparks using a set of partial differential equations with unsteady and two-dimensional cylindrical coordinates. Thiele *et al.* [10] investigated the early development of a stable flame kernel during spark ignition based on a detailed model for coupling two-dimensional cylindrical reactive flows with electrodynamics.

A previous study investigated the effect of the energy channel length on the relationship between the MIE and the equivalence ratio for methane–air mixture without considering heat loss to the electrodes [11]. The effects of the electrode temperature on the relationship between the MIE and the equivalence ratio, and the effects of the electrode size, electrode gap distance, equivalence ratio, and spark duration on the MIE for a methane–air mixture have also been examined [12].

From the point of view of safety, the hydrogen explosion prevention must be taken into consideration, because the MIE of hydrogen–air mixture is very small and it is easy to accidently to give rise to a disaster by spark ignition. Even though some experimental and computational research has been performed on hydrogen–air mixtures to determine the MIE for the spark ignition, the flame kernel development process, and the mass fractions of major radicals [13–17], the details of the ignition mechanism have not been satisfactorily explained.

In this study, the spark ignition of a hydrogen–air mixture was investigated using detailed chemical kinetics and considering heat loss to the electrode. The purpose of this study was to analyze the effects of the energy supply procedure, spark channel radius, electrode size, and electrode gap distance on the MIE. Additionally, the electrode gap distance, and electrode size on the relationship between the equivalence ratio and the MIE were examined.

2. Computational domain and numerical methods

2.1. Simplifying assumptions

The following assumptions were made to simplify the mathematical treatment and accelerate the calculations.

(1) The mixture gases are ideal gases.
(2) The Soret, Dufour, and Pressure effects can be neglected because diffusion due to these effects is much smaller than that due to the temperature and concentration gradients.
(3) The influence of the magnetic and electrical fields is negligible.
(4) Viscous dissipation and DP/Dt can be neglected in the energy conservation equation.
(5) Natural convection, heat transfer by radiation, and ionic species can be ignored.

2.2. Governing differential equations

Spark ignition involves many simultaneous complex chemical and physical processes. The following series of equations was used to characterize the combustion process.

(1) Equation of state,

$$P = \rho \overline{R} T \sum_i \frac{Y_i}{m_i}$$

(2) Continuity equation,

$$\frac{\partial \rho}{\partial t} + \frac{1}{r}\frac{\partial \rho u_r r}{\partial r} + \frac{\partial \rho u_z}{\partial z} = 0$$