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Numerical Study on Spark Ignition Characteristics of Methane-air Mixture Using Detailed Chemical Kinetics (Effect of Electrode Temperature and Energy Channel Length on Flame Propagation and Relationship between Minimum Ignition Energy and Equivalence Ratio)*

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Abstract

Involving complicated physical and chemical processes, spark ignition is considered one of the most difficult and complex problems, and it has not yet been explained sufficiently. Minimum Ignition Energy (MIE) is an important parameter to judge the ignition ability of an ignition system. In the present study, the spark ignition characteristics of methane-air mixture were investigated by numerical analysis using detailed chemical kinetics which consists of 53 species and 325 elementary reactions. Two different analytical models with and without electrode were applied to research the effect of electrode temperature and energy channel length on flame propagation and relationship between MIE and equivalence ratio. The electrode temperature is set at 300 K, 1000 K and 2000 K for analytical model with electrode, and the energy channel length is set at 1 mm, 2 mm and 3 mm for analytical model without electrode. The obtained computational results showed good agreement with experimental results. We elucidated that with the increase in the temperature of electrodes, the minima of the curve indicating the relationship between MIE and equivalence ratio move toward to leaner side, that leaner mixture is more sensitive to the heat loss to the cold surrounding gas, and that the heat loss to the electrode is an unignorable factor for the initial formation of flame kernel.

Key words: Spark Ignition, Methane-air Mixture, Minimum Ignition Energy, Equivalence Ratio, Numerical Analysis, Detailed Chemical Kinetics

1. Introduction

Spark ignition is an important way to initiate combustion, and it is widely used in SI engines. In spite of the fact that spark ignition has been studied for many years, the elucidation of ignition mechanism has remained unsatisfactory. One of the reasons is that spark ignition involves chemical kinetics, molecular transport processes and fluid dynamics, etc. It is very difficult to obtain the desired data, such as instantaneous high temperature, heat release rate and so on, during extremely short periods of time by the experiment.

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On the contrary, the numerical simulation offers attractive feather to investigate the formation process of the flame kernel and role of radicals in detailed chemical reactions as shown in the previous study[1]. Moreover, it is easy to study the specific effect of various parameters on the ignition process, and all important physical and chemical data can be obtained, which are impossible to get by the experiment.

Several studies investigated the effect of spark energy on the flame structure[2]-[5]. In some literatures[6]-[9] the early stage of flame development has been analyzed. But, a few numerical simulations[10] have studied the effect of the equivalence ratio on MIE, which is an extremely important property for safety standards as well as for the good understanding of the ignition process of combustible mixtures. After spark duration whether the flame propagates or not depends on heat release by chemical reactions and heat loss to outer atmosphere. If heat release exceeds the heat loss to the unburned cold surrounding gas and the electrode, in other words, reactions can sustain themselves, the combustion of the explosive gas starts. In the present study, we investigate the spark ignition characteristics of methane-air mixture by numerical analysis using detailed chemical kinetics. Then, we gain further understanding of how the factors such as electrode temperature and the energy channel length affect the flame propagation and the relationship between MIE and equivalence ratio.

Nomenclature

A : contact area with cold gas, m^2
L : energy channel length (electrode gap distance), mm
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 : radius of energy channel, mm
T_s : surface temperature of electrodes, K
t : time, μs
t_i : spark duration, μs
V : volume of energy channel, m^3
$ø$: equivalence ratio

2. Analytical Models and Numerical Methods

2.1 Governing Differential Equations

The early shape of the flame kernel produced by sparks in quiescent combustible gases is considered to have an axial symmetry, and we use a two-dimensional cylindrical coordinate system and a series of equations of multicomponent reactive fluid dynamics to calculate the combustion process. These equations are as follows:

(1) Equation of state
(2) Continuity equation
(3) Conservation equation of momentum
(4) Species mass conservation equations
(5) Energy conservation equation

2.2 Assumptions for Simplicity of Computations

In order to simplify the mathematical treatment, some assumptions must be made:

(1) Mixture gases are considered to be ideal gases.

(2) Soret effect, Dufour effect, and pressure effect are neglected, because diffusions by these effects are much smaller than those by temperature gradient and concentration gradient.
(3) The influence of the magnetic and electrical fields is negligible.
(4) Viscous dissipation and *Dp/Dt* are neglected in the energy conservation equation.
(5) Natural convection, heat transfer by radiation, and ionic species are ignored.
(6) The radius of the energy channel is assumed to be constant and equal to that of electrode.

The GRI-mech 3.0 consisting of 53 species and 325 elementary reactions was applied to the chemical kinetics model[11]. The specific heats at constant pressure were given by a fourth-order polynominal approximation of temperature, whose values refer to the JANAF table[12]. The simplified transport model proposed by Smooke et al[13] was used for transport properties.

2.3 Initial and Boundary Conditions

We use two different analytical models A with electrode and B without electrode shown in Figs. 1 and 2, respectively, in order to investigate the effect of heat loss. Both models have the same sizes of computational region: 5 mm and 5 mm for *r* and *z* axes, respectively. The radius of electrode *R* in Fig. 1 is 0.3 mm, and the energy channel length (electrode gap distance) is 1 mm. On the other hand, in Fig. 2 without electrode the channel length ranges from 1 mm to 3 mm, and the channel radius is 0.3 mm.

The mixture of methane and air at the computational region has an initial temperature of 300 K, and is at atmospheric pressure. During the spark duration t_i = 80 μs, the energy is given at a certain ignition energy density q in the energy channel. Total ignition energy is calculated by $Q_{total} = q \times t_i \times V$, where V is the volume of the energy channel. In order to research the effects of the energy channel length L and electrode surface temperature T_s on the flame propagation and the relationship between MIE and equivalence ratio, T_s in analytical model A is set at 300, 1000 and 2000 K, and L in analytical models B is set at 1, 2 and 3 mm, respectively. The mixture is quiescent initially. The z axis as well as the r axis is the lines of symmetry for all variables. The other two boundaries are treated as outer side boundaries, where the gradients of all variables are zero.

2.4 Numerical Method

The numerical method is almost the same used in the previous study[1]. The governing differential equations presented above are discretized using the finite volume method[14]. The SIMPLE method proposed by Patankar is employed on the coupling of velocity and

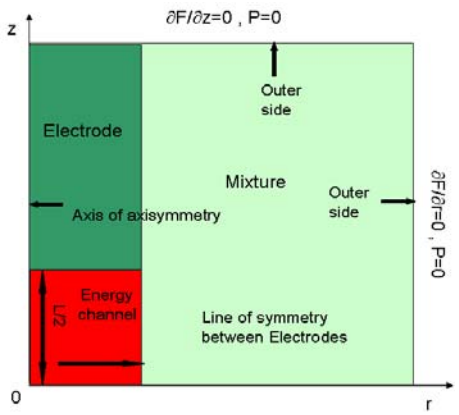


Fig. 1 Analytical model A with electrode and boundary conditions

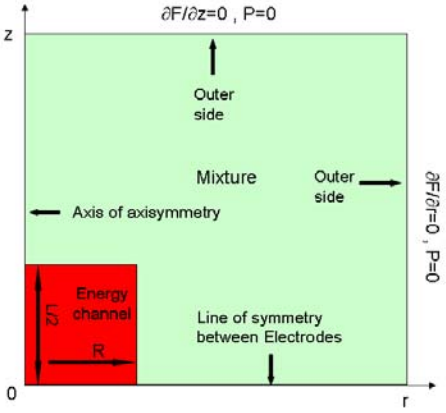


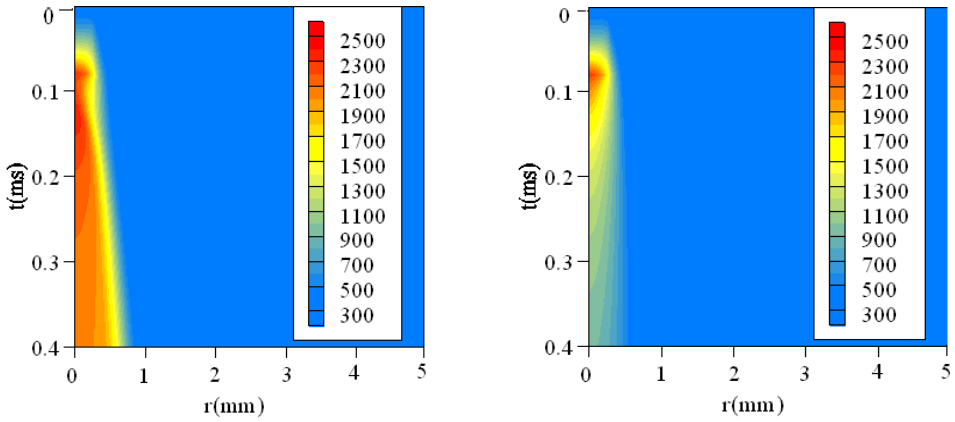
Fig. 2 Analytical model B without electrode and boundary conditions

pressure field[15]. The first-order up-wind scheme is adopted for convective terms, and the full implicit Euler method is used for the time advance. The SOR method is adopted for the iteration in the each time step. The grid size and the time step are chosen to be 0.05 mm and 1 μs, respectively.

3. Results and Discussion

3.1 Ignition Behavior

The minimum ignition energy (MIE) is an important parameter to judge the ignition ability of an ignition system, which is a function of variables such as the parameters of the gas and the electrode, etc. In this study we judge if the flame propagates by using the time history of temperature in the section of z = 0 mm. The flame spreads to the ambient cold mixture in Fig. 3(a) with larger ignition density q = 12.25 GW/m^3 (Q_{total} = 0.554 mJ), but it weakens in Fig. 3(b) with slightly smaller one q = 12.0 GW/m^3 (Q_{total} = 0.543 mJ). Thus, we can estimate the MIE in comparison between the success and the failure of flame propagation.



(a) ø = 1, L = 2 mm, q = 12.25 GW/m^3 (b) ø = 1, L = 2 mm, q = 12.0 GW/m^3

Fig. 3 Time history of temperature in section z = 0 mm of analytical model B

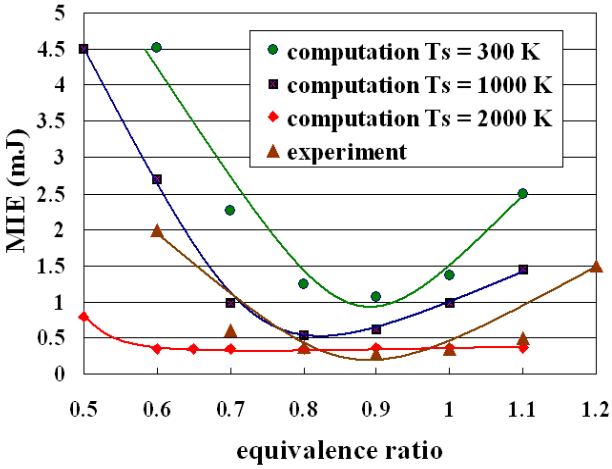


Fig. 4 Relationship between MIE and equivalence ratio (T_s = 300, 1000 and 2000 K; L = 1 mm) together with experiment result

3.2 Relationship between MIE and Equivalence Ratio and Flame Propagation for Analytical Model A

To validate our numerical simulation code, we compared our computational results with experimental data[16] [17] obtained by Lewis, B., von Elbe, et al. Figure 4 provides the computational results for atmospheric methane-air mixtures with T_s = 300 K, 1000 K and 2000 K and small electrode gap distance (L = 1 mm) by comparison with the experimental data. It can be seen that as the electrode temperature T_s is 300 K, the computational results agree well with the experimental results: MIE have minimum values for both computation and experiment, when equivalence ratio is 0.9.

Theoretically speaking, the MIE should have the minimum value for stoichiometric mixture of methane and air. But, methane is lighter and has better diffusivity than oxygen, so methane molecules get close to the initial flame kernel easier than oxygen molecules. Then, the ratio of methane molecules to oxygen molecules around flame kernel is larger than that of ambient mixture. Thus, the minimum values appear on the lean side for lighter fuels[18]. On the contrary, the minimum values appear on the rich side for heavier fuel, such as ethane, propane, butane etc. This knowledge was demonstrated by a lot of experiments[16].

In computational results of Fig. 4, an interesting observation shows that with the increase in the temperature of electrodes, the energy curves move downward, and the minima of the energy curves move toward fuel-leaner side: MIE have the minimum values at equivalence ratio $ø$ = 0.9 for electrodes temperature T_s = 300 K, at $ø$ = 0.8 for T_s = 1000 K, and at $ø$ = 0.6 for T_s = 2000 K. As we know, the temperature of the mixture of methane and air around energy channel suddenly increases because of energy input in energy channel, and high-concentration free radicals that can cause chemical reactions are generated. However, cold electrodes have quenching effect to capture the energy of radicals when the electrode gap distance is small. Then these radicals become deactivated, and the numbers of the free radicals become less. If the energy input is not strong enough, the flame

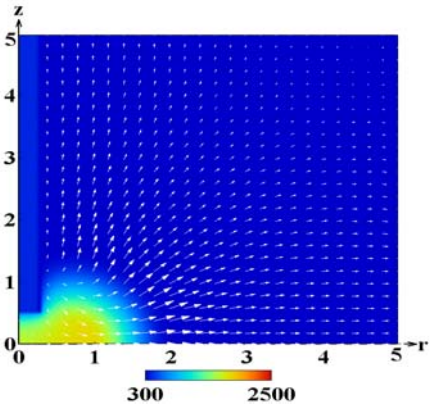


Fig. 5 Temperature and velocity vector distribution at t = 1.6 ms ($ø$ = 1, T_s = 300 K, L = 1 mm, q = 60 GW/m^3: Q_{total}= 1.36 mJ)

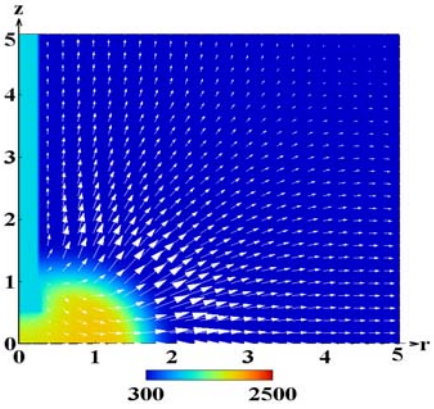


Fig. 6 Temperature and velocity vector distribution at t = 1.6 ms ($ø$ = 1, T_s = 1000 K, L = 1 mm, q = 60 GW/m^3: Q_{total} = 1.36 mJ)

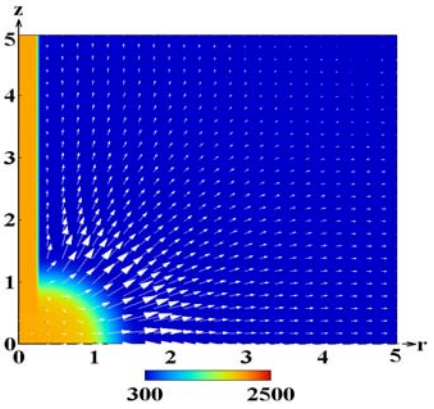


Fig. 7 Temperature and velocity vector distribution at t = 1.6 ms ($ø$ = 1, T_s = 2000 K, L = 1 mm, q = 16.25GW/m^3: Q_{total} = 0.367 mJ)

cannot propagate. As the electrodes temperature T_s is 2000 K, electrodes not only do not seize the energy of radicals, but also heat the cold mixture around electrodes. Even if the equivalence ratio is very small, for example ø = 0.6, more and more free radicals are generated, and finally the flame can propagate at these conditions. Figures 5, 6 and 7 show the distributions of temperature and velocity vector in the case of successful ignition at elapsed time t = 1.6 ms, for electrode temperatures of 300, 1000 and 2000 K, respectively. From these temperature distributions, we can find that the heat loss to electrodes effects flame propagation dramatically: the higher the temperature of electrodes is, the easier mixture of methane and air tends to get ignited.

3.3 Relationship between MIE and Equivalence Ratio and Flame Propagation for Analytical Model B

The heat release by chemical reactions is lost to not only the electrode but also the unburned cold surrounding gas. In analytical model B, the heat loss to electrode is not considered, therefore the heat loss to the cold surrounding gas is the most fundamental factor in the ignition process. The computational results for analytical model B are illustrated in Fig. 8, which describes how the energy channel length influences relationship between MIE and equivalence ratio.

When the ignition energy is put into the energy channel, the ratio of the contact area with the cold surrounding gas A to the ignition channel volume V is $A/V = 2(R+L)/RL$. It was indicated by the previous study[1] that the smaller the value of A/V is, the less the heat loss to the cold gas is, and the easier the gas tends to be ignited. In this study, we set the energy channel radius R at 0.3 mm, which is much smaller than energy channel length L, so it may be expected that the heat loss to cold surrounding gas is almost proportionate to L. As shown in Fig. 8, it is meaningful that MIE is almost proportionate to L, and with the increase in the energy channel length, the minima of the curve move toward to the leaner side which is much smaller than ø =1: MIE has a minimum value at equivalence ratio ø =0.8 for the energy channel length L = 1 mm, at ø = 0.65 for L = 2 mm, and at ø = 0.6 for L = 3 mm. This trend can be seen more clearly in Fig. 9, which provides data in terms of minimum ignition energy density (MIED). Within a range between ø = 0.7 and ø = 1, MIED of L = 1 mm is almost the same with two other cases, but much larger at lean side. To put it differently, leaner case is more sensitive to the heat loss to the cold ambient gas without considering the heat loss to the electrode.

The instantaneous temperature distribution of successful ignitions at elapsed time t = 0.4 ms for ø = 1 are shown in Figs. 10, 11 and 12, in which the energy channel length L is 1, 2

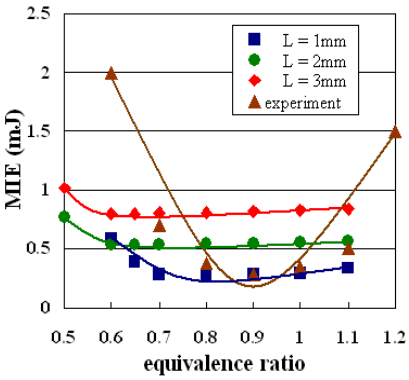


Fig. 8 Relationship between MIE and equivalence ratio (L=1, 2, 3 mm) together with experiment result

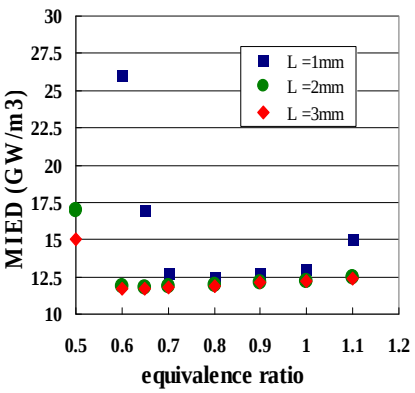


Fig. 9 Relationship between MIED and equivalence ratio (L=1, 2, 3 mm)

and 3 mm, respectively. From the figures we can find that central part of whichever has the highest temperature thanks to the least effect of the cold surrounding gas, and it is similar to Fig. 7 where the temperature of the electrode is 2000 K. In stark contrast to it, the flames depart from the electrode and temperatures between electrodes are pretty low when the temperatures of the electrode are 300 and 1000 K, as shown in Figs. 5 and 6. The figures help us to further understand that the heat loss to electrode is an unignorable factor for the initial formation of flame kernel.

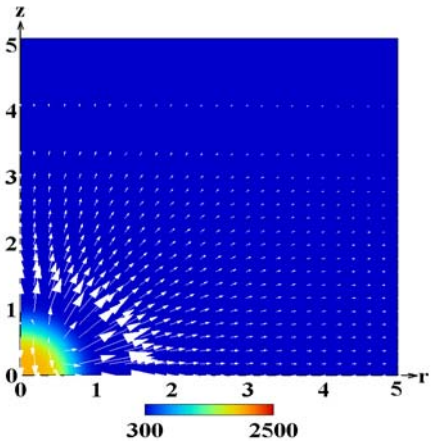


Fig. 10 Temperature and velocity vector distribution at t = 0.4 ms ($ø$ = 1, L = 1 mm, q = 13.0 GW/m^3 Q_{total} = 0.294 mJ)

4. Conclusions

The relationship between MIE and equivalence ratio in quiescent methane-air mixtures is numerically investigated by using computational results, so we reached conclusions as follows:

1. With the increase in the temperature of electrodes, the minima of the curve indicating the relationship between MIE and equivalence ratio move toward to leaner side; MIE reaches a minimum value at equivalence ratio $ø$ = 0.9 for electrodes temperature of T_s = 300 K, at $ø$ = 0.8 for T_s = 1000 K, and at $ø$ = 0.6 for T_s = 2000 K.

2. Without considering the heat loss to electrode the minima of the curves shift to much leaner side than experimental result. MIE reaches a minimum value at equivalence ratio $ø$ = 0.8 for length of L = 1 mm, at $ø$ = 0.65 for L = 2 mm, and at $ø$ = 0.6 for L = 3 mm, the leaner the mixture is, the more sensitive it is to the heat loss to the cold surrounding gas.

3. The heat loss to the electrode is an unignorable factor for the initial formation of flame kernel.

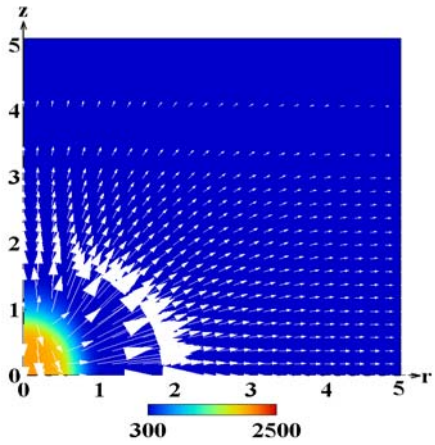


Fig. 11 Temperature and velocity vector distribution at t = 0.4 ms ($ø$ = 1, L = 2 mm, q = 12.25 GW/m^3 Q_{total} = 0.554 mJ)

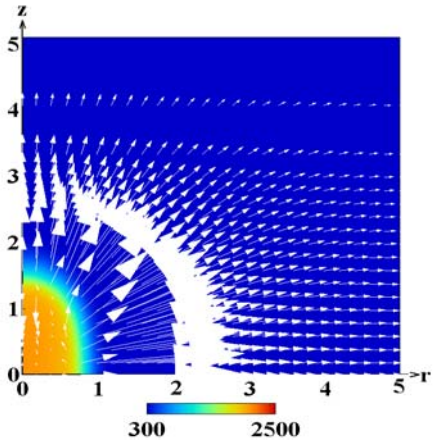


Fig. 12 Temperature and velocity vector distribution at t = 0.4 ms ($ø$ =1, L =3mm, q =12.25GW/m^3 Q_{total} = 0.831 mJ)

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