

Numerical Calculation of Minimum Ignition Energy for Hydrogen and Methane Fuels

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Minimum ignition energies of hydrogen/air and methane/air mixtures have been investigated numerically by solving unsteady one-dimensional conservation equations with detailed chemical kinetic mechanisms. Initial kernel size needed for numerical calculation is a sensitive function of initial pressure of a mixture and should be estimated properly to obtain quantitative agreement with experimental results. A simple macroscopic model to determine minimum ignition energy has been proposed, where the initial kernel size is correlated with the quenching distance of a mixture and evaluated from the quenching distance determined from experiment. The simulation predicts minimum ignition energies of two sample mixtures successfully which are in a good agreement with the experimental data for the ranges of pressure and equivalence ratio.

Key Words : Minimum Ignition Energy, Initial Kernel Size, Quenching Distance

Nomenclature

A_i : Pre-exponential factor in i -th reaction step	\bar{M} : Mean molecular weight
a : Constant	M_j : Molecular weight of species j
b_i : Temperature exponent in i -th reaction step	n_s : Number of species
C_p : Constant-pressure specific heat	p : Pressure
D_j : Diffusion coefficient of species j	\dot{q} : Energy source
D_s : Energy source density	\bar{R} : Universal gas constant
d_q : Quenching distance	R_o : Domain size
E_{ig} : Ignition energy	r : Spatial coordinate
E_i : Activation energy in i -th reaction step	r_s : Radius of energy source (=initial kernel size)
h : Specific enthalpy of mixture	S_L : Burning velocity
h_j : Specific enthalpy of species j	T : Temperature
k_i : Reaction rate constant in i -th reaction step	t : Time
n : Exponent in Eq. (9)	u : Velocity
	V_c : Correction factor for diffusion velocity
	V_o : Mixture volume to be heated by supplied ignition energy
	V_j : Diffusion velocity of species j
	X : Mole fraction
	Y : Mass fraction

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Greek letters

α	: Geometric factor
δ	: Flame thickness
Θ_j	: Thermal diffusion ratio of species j
μ	: Viscosity of mixture
λ	: Conductivity of mixture
ϕ	: Equivalence ratio
ρ	: Density
$\tau_{rr}, \tau_{\theta\theta}$: Stresses defined in Eq. (6)
τ_s	: Duration of supplied energy
w_j	: Net production rate of species j

Subscripts

o	: Initial state
min	: Minimum

1. Introduction

Minimum ignition energy is one of the key factors in designing igniters and for the prevention of explosion hazards. There are numerous experimental data on minimum ignition energies (Rose and Priede, 1958; Moorhouse et al., 1974; Lewis and von Elbe, 1987; Au et al., 1992), frequently determined from electrical spark experiments. The measurement, however, is a difficult task, especially at high pressure, since the values of minimum ignition energy become very small. In addition, the data of minimum ignition energy scatter much depending on materials, shape of electrodes, and the characteristics of electrical discharge (Rose and Priede, 1958; Moorhouse et al., 1974; Lewis and von Elbe, 1987). Moreover, there could be an ambiguity between the energy supplied and the energy utilized for ignition. Consequently, quantitative data are sometimes partially inconsistent with each other, for example, the pressure dependence of minimum ignition energy (Lewis and von Elbe, 1987; Maas and Warnatz, 1988).

Even with numerous studies, data on minimum ignition energy are only available in the limited range of pressure, equivalence ratio, initial temperature, and degree of dilution. In this regards, it may be desirable over experiment if minimum ignition energy can be determined numerically. Since kinetic mechanisms and computa-

tional methods have been well established recently, numerical investigations have been attempted (Maas and Warnatz, 1988; Kailasanath et al., 1982; Thiele et al., 2002). In these studies, certain amount of ignition energy has been supplied locally to a premixed system and subsequent flame development has been examined. It has been demonstrated that ignition energy is quite sensitive to initial kernel size assigned in numerical calculations (Maas and Warnatz, 1988). Ignition models such as shell model for high pressure (Kim et al., 2002a; Kim et al., 2002b) have been widely used to elucidate autoignition phenomenon, but these models are case by case.

Compared to minimum ignition energy, quenching distances are relatively easier to determine experimentally, since it is associated with spark gap instead of energy measurement. As a result, the data of quenching distances are relatively consistent with each other (Lewis and von Elbe, 1987; Friedman, 1949; Calcote et al., 1952). Based on the relation between quenching distance and minimum ignition energy (Lewis and von Elbe, 1987), the present study is to test a simple method of determining minimum ignition energy numerically by utilizing quenching distance as initial kernel size for energy input. Although the complex modeling of ignition processes can be found in some literature (Sher et al, 1992; Akram, 1996), this study adopts simple models and one-dimensional approach, focusing on the macroscopic prediction of minimum ignition energy. This approach is still alive since it has many advantages (Akram and Lundgren, 1996). Hydrogen/air and methane/air are selected as sample mixtures and especially the effects of pressure and equivalence ratio on minimum ignition energy are emphasized in the present study.

2. Formulation

Model geometry is locally approximated as a spherical closed vessel. Conservation equations for mass, momentum, energy, and species are to be solved simultaneously together with the equation of state. The corresponding unsteady, one-dimensional governing equations are as follows

(Maas and Warnatz, 1988; Sohn and Chung, 1995):

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial (r^2 \rho u)}{\partial r} = 0 \quad (1)$$

$$\begin{aligned} \frac{\partial (\rho u)}{\partial t} + \frac{1}{r^2} \frac{\partial (r^2 \rho u^2)}{\partial r} + \frac{1}{r^2} \frac{\partial (r^2 \tau_{rr})}{\partial r} \\ - \frac{2}{r} \tau_{\theta\theta} + \frac{\partial p}{\partial r} = 0 \end{aligned} \quad (2)$$

$$\begin{aligned} \frac{\partial (\rho Y_j)}{\partial t} + \frac{1}{r^2} \frac{\partial (r^2 \rho u Y_j)}{\partial r} \\ + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho Y_j V_j) = w_j M_j \end{aligned} \quad (3)$$

$$\begin{aligned} \frac{\partial (\rho h)}{\partial t} + \frac{1}{r^2} \frac{\partial (r^2 \rho u h)}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \lambda \frac{\partial T}{\partial r} \right) \\ + \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho \sum_{j=1}^{n_s} h_j Y_j V_j \right) \\ - \frac{\partial p}{\partial t} - u \frac{\partial p}{\partial r} + \tau_{rr} \frac{\partial u}{\partial r} + 2 \frac{u}{r} \tau_{\theta\theta} = \dot{q} \end{aligned} \quad (4)$$

$$p = \frac{\rho \bar{R} T}{\bar{M}} \quad (5)$$

with

$$\tau_{rr} = -\mu \left[2 \frac{\partial u}{\partial r} - \frac{2}{3} \left\{ \frac{1}{r^2} \frac{\partial (r^2 u)}{\partial r} \right\} \right] \quad (6)$$

$$\tau_{\theta\theta} = -\mu \left[2 \frac{u}{r} - \frac{2}{3} \left\{ \frac{1}{r^2} \frac{\partial (r^2 u)}{\partial r} \right\} \right]$$

$$V_j = \frac{D_j}{X_j} \frac{\partial X_j}{\partial r} + \frac{D_j \Theta_j}{X_j} \frac{\partial (\ln T)}{\partial r} + V_c \quad (7)$$

where r is the spatial coordinate, ρ is the density, u is the velocity, T is the temperature, p is the pressure, μ and λ are the viscosity and conductivity of mixture, respectively, h is the mixture enthalpy defined as $h = \sum h_j Y_j$, n_s is the number of species considered, V_j is the diffusion velocity of species j , V_c is the correction factor for diffusion velocity (Kee et al., 1983), \dot{q} is the source term for energy deposition, \bar{R} is the universal gas constant, \bar{M} is the mean molecular weight defined as $\bar{M} = (\sum Y_j / M_j)^{-1}$, and w_j , M_j , D_j , Θ_j , X_j , and

Y_j are the net production rate, molecular weight, mass diffusion coefficient, thermal diffusion ratio, mole fraction, and mass fraction of species j , respectively.

Symmetric conditions at the center ($r=0$) and non-reactive, adiabatic and impermeable conditions at the wall ($r=R_o$) are represented as

$$\begin{aligned} r=0; \quad \frac{\partial \rho}{\partial r} = \frac{\partial T}{\partial r} = \frac{\partial Y_j}{\partial r} = 0, \quad u=0 \\ r=R_o; \quad \frac{\partial \rho}{\partial r} = \frac{\partial T}{\partial r} = \frac{\partial Y_j}{\partial r} = 0, \quad u=0 \end{aligned} \quad (8)$$

At the initial state, pre-mixture is assumed quiescent and homogeneous in concentration and temperature. The size of spherical volume, R_o , is taken as 2.5 cm, which is found to be sufficient to determine successful or unsuccessful ignition without appreciable pressure rise.

The energy source term for the simulation of spark ignition has been modeled as a Gaussian-like shape (Maas and Warnatz, 1988)

$$\begin{aligned} 0 \leq t \leq \tau_s; \quad \dot{q} = (D_s / \tau_s) \exp\{-(r/r_s)^n\} \\ t > \tau_s; \quad \dot{q} = 0 \end{aligned} \quad (9)$$

where D_s is the energy source density, τ_s is the duration of energy supply, r_s is the radius of energy source corresponding to the half of initial kernel size, and n is the coefficient characterizing energy-source profile, which is frequently taken as $n=2$ for the Gaussian.

Detailed reaction mechanism including 24 reaction steps for hydrogen oxidation (Maas and Warnatz, 1988), and GRI-Mech 3.0 for methane oxidation (Smith et al., 2000) are employed. Peters mechanism (Peters, 1991) and GRI-Mech 2.11 (Smith et al., 2000) are also tested for methane oxidation, however the differences among these mechanisms were found to be negligible. The specific reaction rate constant k_i of i -th reaction step is in the Arrhenius form of

$$k_i = A_i T^{b_i} \exp(E_i / RT) \quad (10)$$

where E_i is the activation energy and A_i and b_i are the kinetic constants. Thermodynamic and chemical reaction rates are evaluated from CHEMKIN-II (Kee et al., 1989), and transport

properties from TRANSPORT PACKAGE (Kee et al., 1983).

The partial differential equations are discretized based on finite volume method, through which the conservation of each variable is satisfied strictly in each control volume. For time integration, fully implicit method and Crank-Nicolson method are adopted. Thus, the accuracies are $O(\Delta r^2)$ and $O(\Delta t \sim \Delta t^2)$ for space and time, respectively.

The coupled system of equations is solved simultaneously by using Newton iteration. Adaptive gridding is employed which generates grid systems with different spacing depending on the stiffness of solution variables. Details are described elsewhere (Smooke et al., 1983; Sohn and Chung, 1995).

3. Results and Discussions

3.1 Ignition success/failure

Figure 1 shows the temperature history for the cases of successful ignition and ignition failure for stoichiometric H_2 /air mixture with $r_s=0.01$ cm, $\tau_s=1 \mu s$, $T_o=298.15$ K, and $p_o=1$ atm. For the successful ignition (a) with the ignition energy $E_{ig}=0.011$ mJ, the maximum temperature at the center ($r=0$) initially decreases due to heat conduction during ignition delay period. Subsequently, temperature increases and well-developed flame front propagates outward. Here, the ignition energy was calculated from Eq. (9). For the case of ignition failure (b) with $E_{ig}=0.010$ mJ, the initially supplied energy diffuses continuously to the surrounding, demonstrating that this ignition energy is not sufficient to initiate a flame.

These characteristics can be further substantiated from the heat release histories shown in Fig. 2. After the initial decay of heat release during ignition delay period up to, say about 0.06 ms, a well-defined reaction front starts to propagate for the successful ignition case (a), while the heat release rate keeps on decaying for the ignition failure case (b).

Minimum ignition energy is a function of initial temperature, pressure, degree of dilution, and equivalence ratio, ϕ . Numerically, it also depends

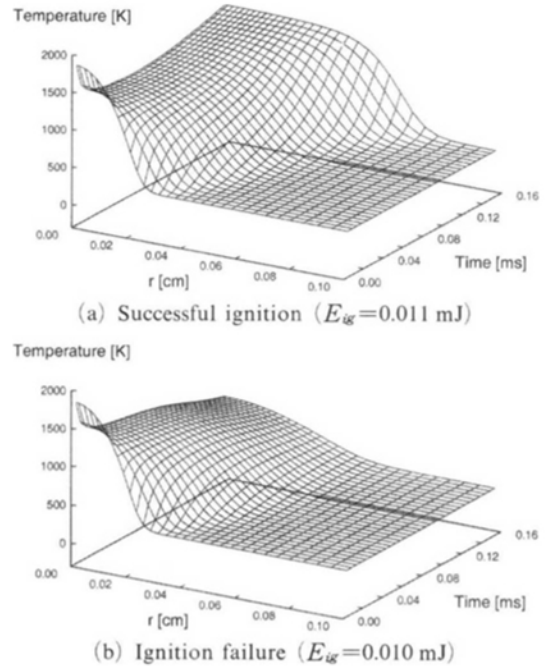


Fig. 1 Evolution of temperature profiles for stoichiometric H_2 /air mixture ($T_o=298.15$ K, $p_o=1$ atm, $r_s=0.01$ cm, $\tau_s=1 \mu s$)

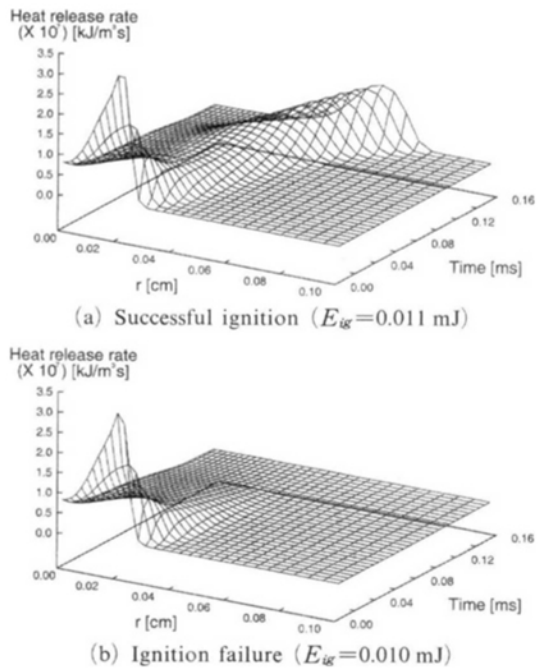


Fig. 2 Evolution of heat release rate for stoichiometric H_2 /air mixture ($T_o=298.15$ K, $p_o=1$ atm, $r_s=0.01$ cm, $\tau_s=1 \mu s$)

on both the radius of energy source, r_s , and the duration of supplied energy, τ_s . Figure 3 shows the minimum ignition energies required for successful ignition for stoichiometric H_2/O_2 and H_2/air mixtures for $T_o=298.15$ K, $\tau_s=1$ μs and $p_o=1$ atm as a function of the radius of energy source, r_s . The result demonstrates that the minimum ignition energy determined numerically varies significantly with the pre-assigned radius of energy source.

In addition to the radius of energy source, τ_s could also affect the calculation for minimum ignition energy. The effect of τ_s on minimum ignition energy is reported to be insensitive compared to the variation in r_s (Maas and Warnatz, 1988). For example, $O(10)$ change in r_s incurs $O(10^3)$ change in minimum ignition energy as demonstrated in Fig. 3, while $O(10^2)$ change in τ_s incurs $O(10)$ change. The present study also confirms this behavior for τ_s in the range of $O(10^{-6}\sim 10^{-4}$ s). Since the values of τ_s from experimental data are device-sensitive and difficult to deduce, and are rather insensitive in the numerical calculations, τ_s is set to be order of 1 μs in the present study. On the other hand, the above result demonstrates that the radius of energy source needs to be modeled properly for the prediction of minimum ignition energy numerically.

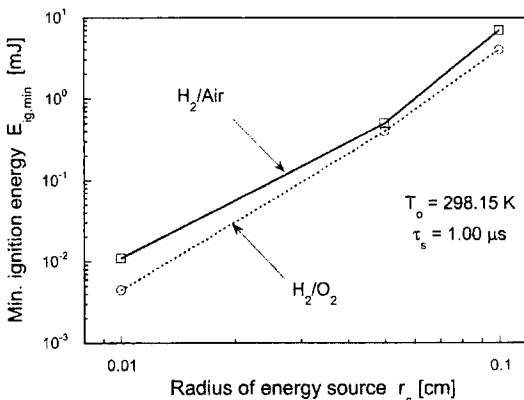


Fig. 3 Variation of minimum ignition energy as a function of radius of energy source for stoichiometric mixture with $T_o=298.15$ K, $p_o=1$ atm, and $\tau_s=1$ μs

3.2 Initial flame kernel size

Based on experiments on minimum ignition energies for hydrocarbon fuels near atmospheric pressure (0.75 and 1.0 atm), Moorhouse et al. (1974) suggested the following empirical relation;

$$E_{ig,min} \sim T_o^{-2} p_o^{-2} \quad (11)$$

Gaydon and Wolfhard (1979) also showed the same dependency of minimum ignition energy on pressure as Eq. (11). This tendency of inversely proportional to the square of pressure does not agree with the numerical results by Maas and Warnatz (1988), since minimum ignition energies have been calculated for a given fixed ignition radius in their work. This indicates that the radius of energy source should be adjusted with pressure.

In electrical spark experiments, the required ignition energy decreases as spark gap distance decreases, then it increases abruptly when the gap distance approaches a quenching distance (Lewis and von Elbe, 1987). Minimum ignition energy can be attained when a spark gap is comparable to the quenching distance or quenching diameter, d_q . Therefore, the radius of energy source, r_s can be correlated with quenching distance.

Previous research (Williams, 1985) showed that d_q is proportional to the flame thickness δ . From the phenomenological analysis of deflagration wave

$$\delta \sim \frac{\lambda}{C_p \rho_o S_L} \sim \frac{\lambda T_o}{C_p M} \frac{1}{p_o} \frac{1}{S_L} \quad (12)$$

where T_o and p_o are the initial temperature and pressure, respectively, and S_L is the laminar burning velocity. Figure 4 plotted the experimentally determined d_q (Lewis and von Elbe, 1987) as a function of pressure together with the two pressure-dependences of d_q , i.e., $d_q \sim (p_o S_L)^{-1}$ and $d_q \sim p_o^{-1}$ where S_L is from Refs. (Peters, 1991; Smooke et al., 1983). As pressure increases, the difference between these two dependences becomes appreciably large, especially for methane.

There are insufficient experimental data of quenching distance, especially at high pressure

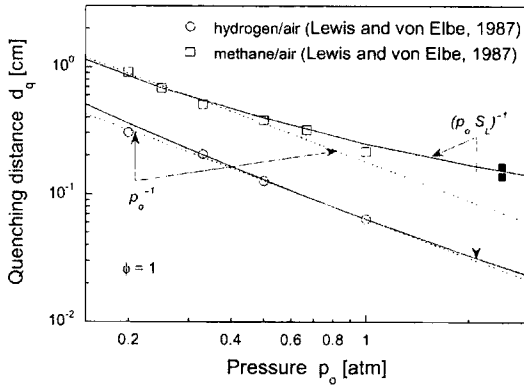


Fig. 4 Quenching distance as a function of pressure ($T_o=298.15$ K, $\phi=1$)

to substantiate the dependence of S_L . The two data for $\phi=0.95, 1.11$ at $p_o=2.5$ atm as closed symbols (Lewis and von Elbe, 1987). Note that since the quenching distance for methane has its minimum shifted toward leaner side, e.g., $\phi=0.85\sim 0.95$ at 1 atm, the value of quenching distance at stoichiometric condition may exist between these two values. Then, the results in Fig. 4 suggest the dependence of S_L on d_q , however further research is needed for high pressure behavior of quenching distances. Note that the subatmospheric data can be reasonably fitted to $d_q \sim p_o^{-1}$.

Assuming that the radius of energy source r_s is proportional to quenching distance d_q , r_s for subatmospheric pressure can be approximated to be inversely proportional to pressure. Then the pressure-dependence of minimum ignition energy can be shown to be consistent with both the empirical relation of Moorhouse et al. (1974) and the concept from Gaydon and Wolfhard (1979); $E_{ig,min}$ is assumed to be proportional to the mass of mixture to be heated such that $E_{ig,min} \sim \rho_o V_o \sim p_o r_s^3$, where V_o denotes mixture volume to be heated by supplied ignition energy. By taking $r_s \sim d_q \sim p_o^{-1}$, $E_{ig,min}$ becomes proportional to p_o^{-2} . In the following, r_s is modeled and correlated with d_q in predicting minimum ignition energies numerically.

3.3 Minimum ignition energy calculation

Minimum ignition energy, $E_{ig,min}$ is calculated

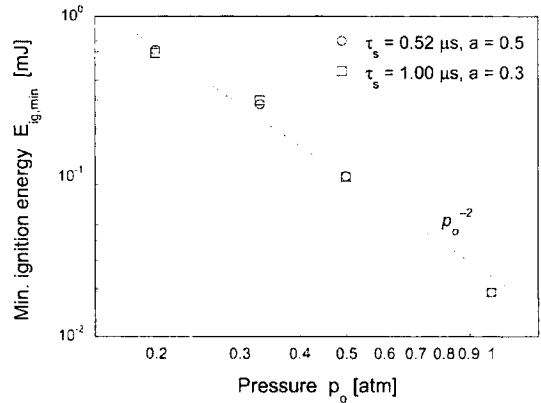


Fig. 5 Comparison between two methods of minimum ignition energies of hydrogen/air mixture as a function of pressure ($T_o=298.15$ K, $\phi=1$)

numerically by solving Eqs. (1)~(5) simultaneously with the aforementioned assumption. First, it has been tested for H_2 /air premixtures with $\phi=1.0$ and $T_o=298.15$ K, in the pressure range of $p_o=0.2\sim 1.0$ atm using the experimental quenching distance from Lewis and von Elbe (1987). For the normalization of the numerical results to be matched with the experimental data at $p_o=1$ atm, two methods were adopted. One is that r_s is adjusted to the value proportional to quenching distance (i.e., $r_s=ad_q$) with the fixed $\tau_s=1$ μ s. The other is adjusting τ_s with the fixed $r_s=d_q/2$. For the H_2 /air mixture with $\phi=1.0$ and $T_o=298.15$ K, it has been found that $a=0.3$ for the fixed $\tau_s=1$ μ s and on the other hand, $\tau_s=0.52$ μ s for $r_s=d_q/2$ to be matched at $p_o=1$ atm. With these constants fixed, the pressure effect has been investigated and the results are shown in Fig. 5. It exhibits that both methods are equally viable in determining minimum ignition energy by using experimental quenching distance data.

The numerical results are compared with the experimental data (Lewis and von Elbe, 1987) for stoichiometric H_2 /air mixtures with $T_o=298.15$ K in Fig. 6 as a function of pressure by adopting $r_s=d_q/2$ and $\tau_s=0.52$ μ s. This result shows that the minimum ignition energy decreases as initial pressure increases, and the numerical data agree well with the experiment. In addition, the numerical results with just utilizing

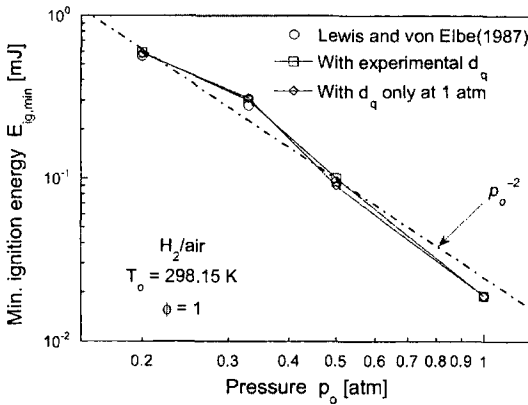


Fig. 6 Minimum ignition energies of stoichiometric hydrogen/air mixture for $T_o=298.15$ K, $r_s=d_q/2$ and $\tau_s=0.52 \mu\text{s}$ as a function of pressure

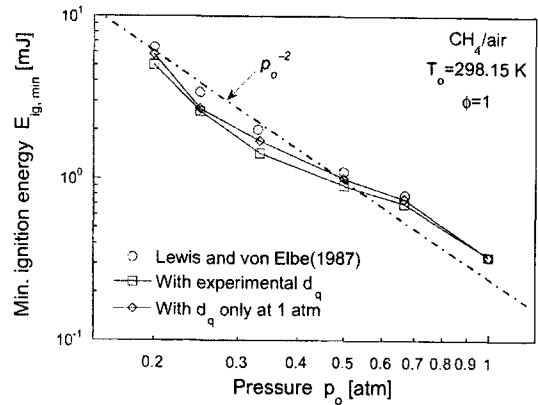


Fig. 8 Minimum ignition energies of stoichiometric methane/air mixture for $T_o=298.15$ K, $r_s=d_q/2$, and $\tau_s=0.60 \mu\text{s}$ as a function of pressure

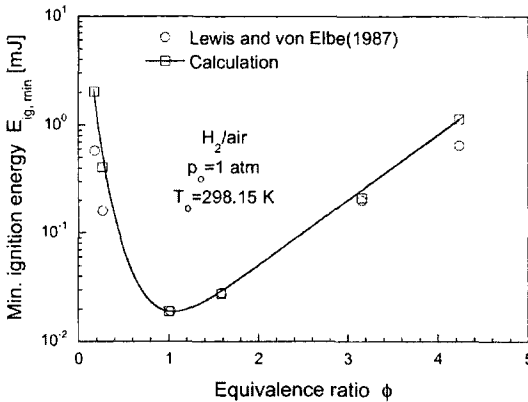


Fig. 7 Minimum ignition energies of hydrogen/air mixture for $T_o=298.15$ K, $p_o=1$ atm, $r_s=d_q/2$, and $\tau_s=0.52 \mu\text{s}$ as a function of equivalence ratio

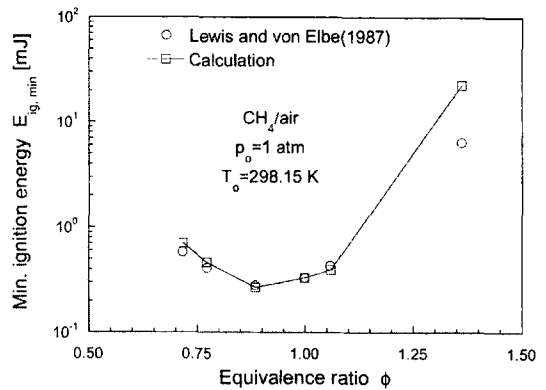


Fig. 9 Minimum ignition energies of methane/air mixture for $T_o=298.15$ K, $p_o=1$ atm, $r_s=d_q/2$, and $\tau_s=0.60 \mu\text{s}$ as a function of equivalence ratio

the quenching distance at $p_o=1$ atm and adopting $d_q \sim p_o^{-1}$ are also shown, which demonstrate reasonable agreement with the experiment.

Numerical determination of minimum ignition energy is further tested by varying the equivalence ratio, ϕ . The results shown in Fig. 7 demonstrate satisfactory agreement in the minimum ignition energy between the numerical and the experimental results (Lewis and von Elbe, 1987). These results for the effects of pressure and equivalence ratio substantiate the validity of the adoption of quenching distance as the radius of ignition energy source in determining the minimum ignition

energy numerically.

The present method to determine minimum ignition energy has been further tested for hydrocarbon fuel of CH_4/air mixtures. The results with $T_o=298.15$ K are shown in Figs. 8 and 9 as functions of pressure and equivalence ratio, respectively. The numerical result also agrees well with the experiment (Lewis and von Elbe, 1987). It is to be noted that $r_s=d_q/2$ and $\tau_s=0.60 \mu\text{s}$ are used for methane.

Figures 6 and 8 demonstrate that $E_{ig,min}$ obtained from the numerical calculation with detailed chemistry is proportional to p_o^{-2} for both

hydrogen and methane fuels, showing that this result is in a qualitative agreement with previous studies (Moorhouse et al., 1974; Gaydon and Wolfhard, 1979). With any kinds of fuel adopted, there are few experimental data on $E_{ig,min}$ at high pressures. Thus, the present method can be applied effectively to extract minimum ignition energies especially at high pressures.

4. Concluding Remarks

Minimum ignition energies for hydrogen/air and methane/air mixtures have been numerically investigated by solving spherically symmetric 1-D conservation equations. The results showed that minimum ignition energy is a sensitive function of radius of ignition energy source in the numerical calculation. The radius of ignition energy source has been correlated with quenching distance and evaluated from experimental values of quenching distance, through which reliable data on minimum ignition energy have been successfully predicted as functions of pressure and equivalence ratio for both hydrogen/air and methane/air mixtures.

Since quenching distance is relatively easier to measure precisely in experiment compared with minimum ignition energy, the present method can be a viable tool in determining minimum ignition energy numerically, especially at high pressures since there are few experimental data for the high-pressure condition.

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