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1	Numerical study on the minimum ignition energy of a methane-air
2	mixture
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10	Abstract
11	In this paper, a semi-detailed mechanism is used to calculate the minimum ignition energy
12	(MIE) of methane-air mixtures, with all calculations conducted using ANSYS Fluent software.
13	Ignition behaviors between success and failure were analyzed, and the effect of isothermal and
14	adiabatic wall condition, equivalence ratio and electrode wall temperature on the MIE were
15	also numerically investigated. From time histories of temperature and species profiles it is easy
16	to determine when a successful ignition occurs. There are big differences between the MIE
17	predictions using the adiabatic wall and isothermal wall conditions. For different equivalence
18	ratio results, we consider our numerical results to be considerably more accurate than previous
19	studies.

20 Keywords: Spark ignition, Methane-air mixture, Minimum ignition energy, Numerical analysis

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21 **1. Introduction**

Despite the rapid development of new alternative sources of energy, fossil fuels still play an important role in energy conversion [1]. Methane (CH₄), which is the main component of natural gas, is a relatively clean fossil fuel compared to large hydrocarbons present in conventional gasoline and diesel fuels. Since it can be made by the anaerobic digestion of biomass, methane is regarded as a renewable energy source and is widely used in industry and in our daily lives [2].

Spark ignition is a complex phenomenon involving the coupling of physical and chemical 28 29 processes. After years of research, the mechanism of ignition is not completely understood. It is known that the formation of the ignition kernel is affected by many factors such as mixture 30 composition, the initial temperature and heat loss to the electrodes. Hill showed that these 31 factors not only change the ignition kernel, but also have an impact on the propagation behavior 32 of a flame [3]. Ballal et al. [4-7] measured the MIE of gaseous and heavy fuels at different 33 34 equivalence ratios, quenching distances, pressures and turbulence intensities. Cui et al. [8] measured the MIE of methane/air mixtures at elevated temperatures and pressures, and 35 determined that the MIE has a high-order linear relationship with $1/p^2$, but has an 36 approximately linear relationship with 1/T. However, there are not enough accurate results for 37 many factors including electrode size, electrode gap distance, and spark duration, among 38 others, and sometimes it is not easy to study these experimentally. Therefore, numerical 39 40 simulation is a good way to capture the transient processes that occur during ignition kernel growth. 41

Several studies have reported on the growth process of the flame kernel. According to Kravchik 42 et al. [9], kernel growth is divided into two phases; in the first short phase, the pressure wave 43 and the expansion of the plasma kernel control the transformation of mass and energy; in the 44 second phase, diffusion and thermal conduction control mass and energy transfer. Ma et al. [10] 45 established a physical model for the spark ignition of combustible gases, and the MIE of 46 combustible mixtures was predicted by numerical analysis. Sarli et al. [11, 12] performed 3-D 47 large eddy simulations and PIV measurements and found that large-scale vortices play a 48 dominant role in the evolution of the flame structure along the path after ignition. Sarli et al. 49 50 also found that unsteady flame propagation is very sensitive to the characteristics of the initial flame kernel, in particular its size and turbulence. Turquand d'Auzay et al. [13] simulated the 51 forced ignition of a methane-air mixture at different turbulence intensities using a three-52 53 dimensional direct numerical simulation method. Han et al. [14] used simulations to study the effect of different parameters on the MIE including electrode size, electrode gap distance, 54 equivalence ratio, and spark duration. For many numerical studies, natural convection, heat 55 56 transfer by radiation and ionic species are ignored as they have little effect on kernel growth and flame propagation [15, 16]. Even though many CFD studies have been conducted, many 57 details still need to be calculated, and more accurate computations performed. There are few 58 simulation papers on the effect of heat loss and electrode wall temperature on the MIE of spark 59 60 ignition. Also, the relative error between simulation and experimental results needs to be further reduced with improved methods and mechanisms. 61

In this study a methane/air mixture was used to computationally investigate the spark ignition
process using a skeletal mechanism reduced from a new chemical kinetic mechanism [17, 18].

The ignition behavior of methane, between success and failure is firstly compared. The effects 64 of several factors on MIE are conducted; (i) isothermal wall condition, (ii) adiabatic wall 65 66 condition, (iii) equivalence ratio and (iv) electrode wall temperature.

67 2. Computational domain and numerical methods

2.1 Governing equations 68

In the spark ignition process, chemical and physical processes are very complex at certain 69 times. To characterize the entire process, the following equations are used. 70

(1) The continuity equation: 71

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v_x) + \frac{\partial}{\partial r} (\rho v_r) + \frac{\rho v_r}{r} = 0$$
(1)

The mass conservation equation is shown in Eq. (1). In Eq. (1), ρ is the density, x is the axial 73 coordinate, r is the radial coordinate, v_x is the axial velocity, and v_r is the radial velocity. 74

75 (2) Momentum conservation equations

$$\frac{\partial}{\partial t}(\rho v_{x}) + \frac{1}{r}\frac{\partial}{\partial x}(r\rho v_{x}v_{x}) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v_{r}v_{x}) = -\frac{\partial p}{\partial x} + \frac{1}{r}\frac{\partial}{\partial x}\left[r\mu\left(2\frac{\partial v_{x}}{\partial x} - \frac{2}{3}(\nabla \cdot \vec{v})\right)\right] + \frac{1}{r}\frac{\partial}{\partial r}\left[r\mu\left(\frac{\partial v_{x}}{\partial r} + \frac{\partial v_{r}}{\partial x}\right)\right]$$

$$\frac{\partial}{\partial t}(\rho v_{r}) + \frac{1}{r}\frac{\partial}{\partial x}(r\rho v_{x}v_{r}) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v_{r}v_{r}) = -\frac{\partial p}{\partial r} + \frac{1}{r}\frac{\partial}{\partial x}\left[r\mu\left(\frac{\partial v_{r}}{\partial r} + \frac{\partial v_{x}}{\partial r}\right)\right]$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left[r\mu\left(2\frac{\partial v_{r}}{\partial r} - \frac{2}{3}(\nabla \cdot \vec{v})\right)\right] - 2\mu\frac{v_{r}}{r^{2}}\frac{2\mu}{3r}(\nabla \cdot \vec{v}) + \rho\frac{v_{z}^{2}}{r}$$

$$(3)$$

78 Where

$$\nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r}$$
(4)

Eqs. (2) and (3) are the axial and radial momentum conservation equations, where μ is the molecular viscosity and *p* is the pressure.

82 (3) Energy conservation equation

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = -\nabla \cdot \left(\sum_{j} h_{j} J_{j}\right) + S_{h}$$
(5)

84 (4) Species mass conservation equation

85
$$\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i$$
(6)

86
$$\vec{J}_i = -\rho D_{i,m} \nabla Y_i - D_{T,i} \frac{\nabla T}{T}$$
(7)

Eqs. (5) and (6) are the energy and species mass conservation equations, respectively, where *E* is the internal energy, S_h is the energy source from heating, Y_i is the local mass fraction of each species *i*, where R_i is the net rate of production of species *i* by chemical reaction and S_i is the rate of creation by addition from the dispersed phase plus any user-defined sources. \vec{J}_i is the diffusion flux of species *i*. In Eq. (7), $D_{i,m}$ is the mass diffusion coefficient for species *i* in the mixture, and $D_{T,i}$ is the thermal (Soret) diffusion coefficient.

93 2.2 Assumptions for simplicity of computations

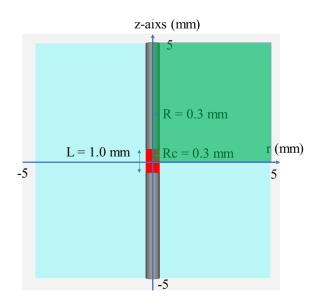
94 To accelerate simulation work and reduce the number of calculation, some assumptions were

made according to the following four assumptions from the work of Han et al. [14].

- 96 (1) The mixture gases are considered as ideal gases
- 97 (2) The Soret, Dufour, and pressure effects are negligible
- 98 (3) The influence of the magnetic and electrical fields can be ignored
- 99 (4) Heat transfer by radiation, ionic and electronic species is neglected
- 100 2.3 Initial and boundary conditions

In this paper, there is no flow before ignition, and the spark in the quiescent combustible 101 mixture is supposed to be cylindrical. If a 3-D simulation were conducted, the differences in the 102 results in the circumferential direction would be negligible. For the 2-D axisymmetric 103 simulations, accurate axial and radial results can be obtained using a reduced number of meshes 104 and with a much shorter computational time. According to Han et al. the initial shape of the 105 flame in gas mixtures is axisymmetric, and the 2-D axisymmetric model in ANSYS Fluent 106 107 software was used [19]. As shown in Fig. 1, the computational region is 5×5 mm in green, the electrode radius R = 0.3 mm, the spark channel radius $R_{\rm C} = R = 0.3$ mm, and the electrode gap 108 distance L = 1.0 mm. According to Sloane et al. [20], when $R_{\rm C}$ is smaller than 0.3 mm, the MIE 109 is almost constant, and so 0.3 mm was chosen for $R_{\rm C}$. 110

The initial gas was a CH₄/air mixture, at an initial temperature of 300 K and at a pressure of 1 atm. For most cases the initial gases were stoichiometric mixtures, and the compositions were changed when equivalence ratios were studied. There were no surface reactions on the electrode boundary, the no-slip condition was used, and all gradients of the species on the surface were set to zero. The temperature of the electrode was changed according to different computational conditions. In this paper, a certain constant ignition energy density q was used to simulate the constant value of the electric power during the ignition process. The ignition energy, Q, was calculated using $Q = q \times \tau_i \times V$, where q is ignition energy density, τ_i is the spark duration and V is the volume of the spark channel. 50 µs was chosen for τ_i for most cases, since an optimum value of the MIE can be obtained for spark durations in the range 3 – 100 µs [21]. The z-axis was considered to axisymmetric, the r-axis was considered as the line of symmetry and other two boundaries were treated as outlets.



124

125

Fig. 1. Scheme of computational domain.

126 2.4 Numerical method

127 A semi-detailed mechanism containing 39 species and 231 reactions was used[18]. The specific 128 heat, thermal conductivity, viscosity and mass diffusivity were calculated using the 129 CHEMKIN-CFD Solver [19], and mixture averaged mass diffusivities for each species were 130 used in the mass diffusivity calculation.

131 In this paper, the ANSYS Fluent software [19] was used, and finite-rate model was conducted

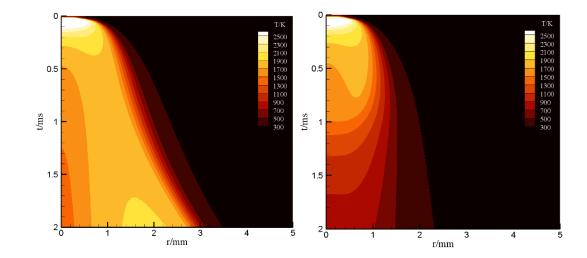
by CHEMKIN-CFD solver in Fluent. For the finite-rate kinetic model, general reaction-rate expressions are used to calculate the chemical source terms. The net source of a chemical species *i* due to reaction is computed as the sum of the reaction sources over the N_R reactions that the species participate in:

$$R_{i} = M_{w,i} \sum_{r=1}^{N_{R}} \hat{R}_{i,r}$$
(8)

137 where $M_{w,i}$ is the molecular weight of species *i* and $\hat{R}_{i,r}$ is the molar rate of reaction/destruction of 138 species *i* in reaction *r*. For more details about finite-rate modeling can be found in the work by Sloane 139 and Rooney [10].

140 The grid size was set at 0.05 mm and the time step to 1 µs according to Han et al. [14, 22]. The 141 coupled method was used to adjust the velocity and pressure fields, and a second-order upwind 142 scheme was employed for convective terms [23].

143 **3. Results and discussion**



144 3.1 Ignition behavior between success and failure

145

146 (a)
$$q = 60 \text{ GW/m}^3$$
 (b) $q = 45 \text{ GW/m}^3$

147 Fig. 2. Time history of temperature at z = 0 mm section.

When computing the MIE, the definition of ignition success is very significant. Successful 148 149 ignition is defined as the time when a flame kernel is formed at a certain place and it can propagate steadily [14]. Based on the temperature time history at the z = 0 mm section, the state 150 of ignition can be judged. On the basis of Fig. 2(a), the high temperature area can expand to the 151 ambient cold region with time using $q = 60 \text{ GW/m}^3$ (Q = 0.848 mJ); Meanwhile Fig. 2(b), 152 using $q = 45 \text{ GW/m}^3$ (Q = 0.636 mJ), shows that it cannot extend and it even shrinks with time 153 (τ) , and moreover the maximum temperature decreases. In this way, the MIE can be simulated 154 in different cases. 155

Maximum temperature histories are shown in Fig. 3. As we can see, the temperature increases quickly with the start of ignition, and after $\tau = 50 \ \mu$ s, it decreases sharply to 2000 K. At $\tau = 2$ ms, the maximum temperature using $q = 45 \ \text{GW/m}^3$ is lower than 1000 K, which means the flame has quenched; while the maximum temperature using $q = 60 \ \text{GW/m}^3$ remains steady at 2000 K.

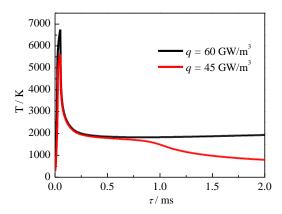
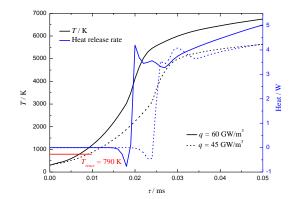




Fig. 3. Maximum temperature history for $q = 60 \text{ GW/m}^3$ and $q = 45 \text{ GW/m}^3$.





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Fig. 4. Maximum temperature and heat release ratio histories during the first 50 µs.

Figure 4 shows the maximum temperature and heat release ratio histories during first 50 µs. 165 The red line shows the temperature (T = 790 K) at which reaction begins. In the initial phase, 166 reaction begins with the reaction $CH_4 + O_2 = \dot{C}H_3 + H\dot{O}_2$, after which, $\dot{C}H_3$ radicals react with 167 O_2 to produce $CH_3\dot{O}_2$ radicals $\dot{C}H_3 + O_2 = CH_3\dot{O}_2$. At low temperatures the reaction $CH_3\dot{O}_2 + O_2$ 168 $\dot{C}H_3 = CH_3\dot{O} + CH_3\dot{O}$ is important in promoting reactivity. The temperature gradually increases 169 due to a constant energy input, before $\tau = 18 \ \mu s$ for $q = 60 \ \text{GW/m}^3$ ($\tau = 24 \ \mu s$ for $q = 45 \ \text{GW/m}^3$) 170 most reactions are endothermic, and the mixture burns at $\tau = 20 \ \mu s \ (\tau = 26 \ us \ for \ q = 45 \ GW/m^3)$ 171 with a sharp increase of heat release ratio. After a few microseconds, a flame front is formed, 172 and propagates steadily towards the unburned mixture region. 173

Figure 5 shows the profiles of some major species in radial direction at different times. At $\tau =$ 40 µs the temperature is high due to heat release. At high temperatures (≥ 2000 K), it is easy to produce radical species such as Ö, ÖH and ĊH₃ in the spark channel. Since there is a difference in energy density, the mass fraction of radical species in the solid lines are higher than the short dashed lines at r = 0 - 0.5 mm. Figure 5(a) shows that the spark kernel of the high energy density ignition can propagate quickly. At $\tau = 1500$ µs the maximum temperature of q = 60GW/m³ is approximately 2000 K, and the flame front propagates to r = 2.2 mm.

From the temperature time history and the profiles of the major species, there are significant differences between successful and failed ignition events, so the state of ignition can be clearly

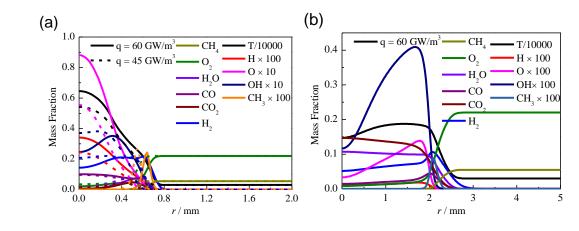
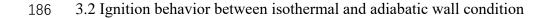




Fig. 5. Profiles of some major species at (a) $\tau = 40 \ \mu s$ and (b) $\tau = 1500 \ \mu s$.



In order to study heat loss during the ignition process, two simulations, Case 1 and Case 2 wereperformed, with details of the conditions given in Table 1.

189

Table 1. Case conditions

Name	Wall condition	MIE / mJ
Case 1	Isothermal, $T = 300 \text{ K}$	0.707
Case 2	Adiabatic	0.254

Figure 6 shows the time histories for these two cases. The flame kernel for Case 1 spreads quickly initially, and at $\tau = 50 \ \mu$ s, the high temperature region expanded at approximately r = 1mm; while the boundary position of the adiabatic flame kernel was approximately $r = 0.4 \ mm$. Adiabatic ignition can propagate stably after $\tau = 50 \ \mu$ s and the temperature of burned region is higher than for isothermal ignition. Figure 7 shows the maximum temperature history and it reflects the different character of these two wall-condition ignitions. Case 1 attains a higher

196 temperature than Case 2 initially, but the temperature in Case 1 falls sharply after the energy 197 supply is stopped.

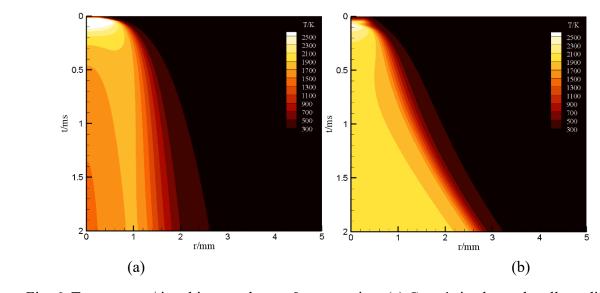
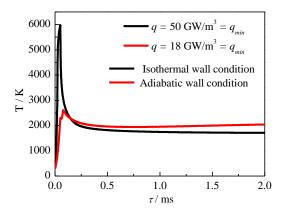


Fig. 6. Temperature/time histor at the z = 0 mm section. (a) Case 1: isothermal wall condition

and (b) Case 2: adiabatic wall condition.



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Fig. 7. Maximum temperature histories for two cases.

Temperature and velocity contours are shown in Fig. 8 and Fig. 9. Initially the energy density of Case 1 is $q_{min} = 50 \text{ GW/m}^3$ which is higher than for Case 2 where $q_{min} = 18 \text{ GW/m}^3$. The high temperature region of Case 1 extends out at high velocity. Due to heat loss from the electrode surface, the fall in temperature in Case 1 was big, and the flame propagation velocity

T/K T/K (b) (a)

Fig. 8. Temperature and velocity contour at $\tau = 40 \ \mu s$. (a) Case 1: isothermal wall condition and

(b) Case 2: adiabatic wall condition.

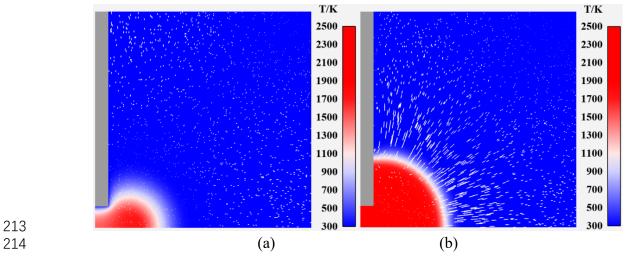


Fig. 9. Temperature and velocity contour at at $\tau = 1500 \ \mu s.$ (a) Case 1: isothermal wall

condition and (b) Case 2: adiabatic wall condition.

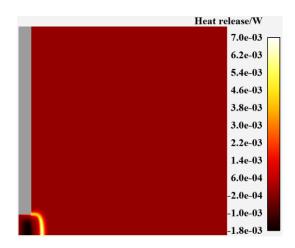




Fig. 10. Heat release contour at $\tau = 40 \ \mu s$ in Case 1: isothermal wall condition.

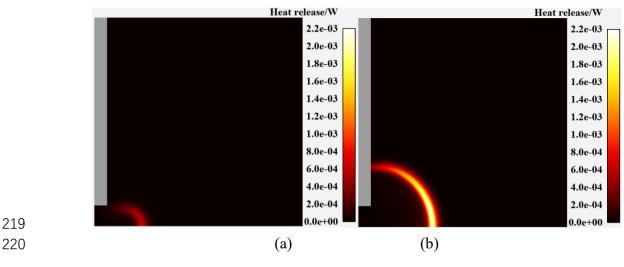
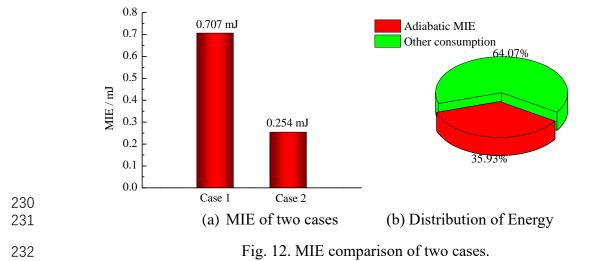


Fig. 11. Heat release contour at $\tau = 1500 \ \mu s.$ (a) Case 1: isothermal wall condition and (b) Case 222 2: adiabatic wall condition.

Figures 10 and Figure 11 show heat release contours at $\tau = 40 \ \mu s$ and $\tau = 1500 \ \mu s$. At $\tau = 40 \ \mu s$, for Case 1 there is a strong heat release, while there is no heat release for Case 2 since the temperature between the electrodes is low. At the propagation phase the heat release become weak for Case 1, while the heat release of Case 2 is very strong.

227 Comparing the MIE for Cases 1 and 2, more energy is consumed for the isothermal wall 228 condition, and the MIE of Case 2 is 35.93% that of Case 1, Fig. 12. Moreover, 64.07% of the



energy consumed is used to heat both the mixture and the electrode wall.

The heat loss and the release rate of both cases are shown in Fig. 13. For the isothermal wall 233 condition the heat release rate and the heat loss rate remain low in the first 3 ms, while it 234 increases rapidly after 1ms for the adiabatic wall condition. The total energy, including heat 235 production and energy input, of the isothermal wall condition ignition is 0.925 mJ over 50 µs, 236 and heat loss is 0.171 mJ. 18.46% of the energy is lost to the wall, with the remaining 81.54% 237 of the energy used to heat and ignite the mixture. Therefore, when designing a spark igniter, an 238 electrode wall composed of a lower thermal conductivity material is more effective in 239 decreasing the MIE and improving ignition performance. 240

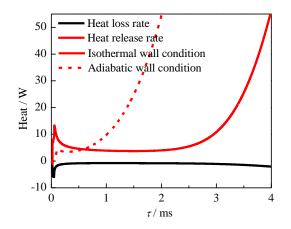
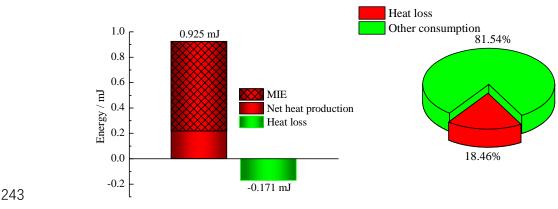


Fig. 13. Heat loss rate and heat release rate of two cases.





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(a) Energy production and loss in 50 μs
 (b) Energy distribution in 50 μs
 Fig. 14. Energy distribution of isothermal wall condition ignition.

246 3.3 Effect of the equivalence ratio on the MIE

Simulations of the effect of equivalence ratio on the MIE were conducted, and these results 247 248 were compared with Han's computations and Lewis' experimental work [14, 24]. For $\varphi = 0.7$, 100 µs was chosen for τ_i to ensure a converged solution, so some numerical problems with 249 high energy density addition for $\tau_i = 50 \ \mu s$ could be avoided. The simulation results in Fig. 15 250 251 show a very good trend compared to the experiment data; the minimum MIE of different 252 equivalence ratios was close to 1.0 in the fuel-lean mixture region. Compared to Han's computation, the simulations in this paper are more accurate. In Han's paper, a simplified 253 transport model was used. The effective thermal conductivity, λ , was calculated from C_p and T 254 255 using a polynomial fit, and the effective diffusivity of species *i* was calculated using the Lewis number. In this paper, for material properties such as specific heat, viscosity, thermal 256 257 conductivity, mass diffusivity and thermal diffusion, they are computed using the CHEMKIN-CFD solver and the mechanism files. Mixture averaged mass diffusivities for each species were 258 used in the calculations. Results are improved using this methodology. 259

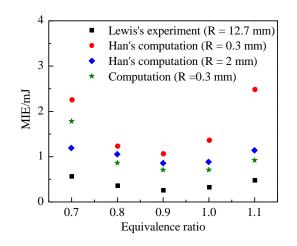
260 Figure 16 shows heat loss ratios of different equivalence ratios. In Fig. 16,

$$Ratio 1 = \frac{q_{Heat \ loss}}{MIE + q_{Heat \ release}}$$

$$(7)$$

$$Ratio \ 2 = \frac{q_{Heat \ loss}}{MIE}$$
(8)

For both Ratio 1 and Ratio 2, minimum values are obtained at $\varphi = 0.9$, with average values of Ratio 1 being about 20% and average values of Ratio 2 are 5% higher than for Ratio 1. Figure 16 indicated that a lower MIE will lose less energy to the electrode wall.



266 267

Fig. 15. Effect of the equivalence ratio on the MIE.

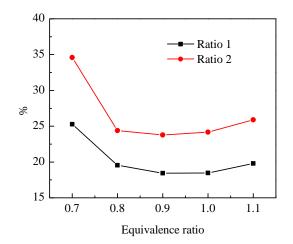


Fig. 16. Heat loss ratios during ignition period.

270 3.4 Effect of the electrode wall temperature on the MIE

Figure 16 shows that 25% of the MIE is consumed by heat loss to the wall, so wall temperature 271 272 effects on the MIE were studied. The effect of wall temperature on the MIE is shown in Fig. 17, and it is observed that as the temperature increases, the MIE decreases. Figure 18 shows the 273 heat loss rate to the wall at wall temperatures of T = 450 K and T = 600 K are higher than for 274 the mixture at temperature of 300 K, because initially heat transfers from the wall to the 275 mixture. When the mixture temperature becomes higher than the wall, energy is transferred 276 back to the wall. At higher wall temperatures, a lower MIE is needed. Moreover, on heating the 277 278 electrode wall, ignition becomes easier. Due to the contribution of the electrode wall temperature, ignition under extreme conditions, such as high altitude relight and plateau 279 280 ignition, can be achieved. So it is much better for a designer to add a heating system on the electrode wall of the spark igniter to decrease the MIE of the mixture and enhance ignition 281 performance. 282

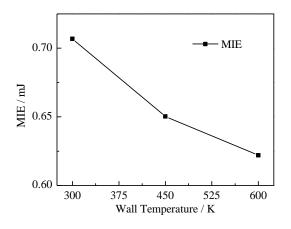
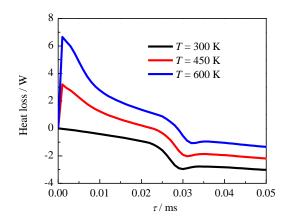


Fig. 17. Effect of the wall temperature on the MIE.



285 286

Fig. 18. Heat loss to the wall at different wall temperatures.

287 4. Conclusions

Ignition behaviors between success and failure were numerically investigated for isothermal and adiabatic wall conditions, at different equivalence ratios and electrode wall temperatures to determine the effect on the MIE for methane/air mixtures. From our computational results, the following conclusions were reached.

(1) Successful ignition can be determined from the temperature/time history at the z = 0 mm section. Maximum temperature histories and species profiles were determined with significant differences being observed between successful ignitions and failures.

(2) For the adiabatic wall condition, ignition costs much less energy than for the isothermal
wall condition. A sharp change in the temperature history was observed for the isothermal
wall condition ignition while in the adiabatic condition it was very flat. For the
stoichiometric methane/air mixture at 1 atm, 18.46% of the energy was taken up by heat
loss to the wall, and the remaining 81.54% was used to heat and ignite mixture. Thus, an
electrode wall with a lower thermal conductivity material is very helpful in decreasing the
MIE required and improving the ignition performance of a spark igniter.

302 (3) At different equivalence ratios, the minimum MIE is close to 0.9, and numerical results
303 with the CHEMKIN-CFD solver and the latest skeletal mechanism are in good agreement
304 with the experiment data and they are better than previous simulation works. A lower MIE
305 will lose less energy to the electrode wall.

306 (4) For higher wall temperatures, a lower MIE is needed. And after heating the electrode, it is
 307 much easier to ignite a mixture. When a heating system is added to the electrode wall of the
 308 spark igniter, the MIE of the mixture is smaller and the ignition performance is enhanced.

The MIE of a methane-air mixture was studied using CFD in this paper. Some methods such as choosing a lower thermal conductivity material and adding a heating system to the electrode wall are proposed to improve ignition performance. However, there are still some factors that affect the MIE such as the ways the energy is discharged, the turbulence intensity and initial conditions of temperature and pressure that should be studied in flow and real engine conditions.

315 Acknowledgements

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