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Experimental Studies and Modeling on Flame Velocity in Turbulent Deflagration in an Open Tube

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Abstract

Studies on flame propagation during turbulent deflagration in a partly opened tube are important in developing explosion protection scheme and suppression technology for industrial process with explosion risk. Gas explosions in coal mines, deflagration in gas transmission tubes and dust explosions in confined working spaces can be simplified by a partly opened tube in studying deflagrations. An experimental rig with a 16 m long open tube of 0.488 m diameter was constructed for studying the flame propagation characteristics of premixed liquefied petroleum gas (LPG) under different mixing ratios with air. The transient flame propagation distance, flame velocity, pressure and temperature were analyzed. A flame velocity model for an explosion in an open tube was proposed and verified by the experimental data. This model was also used to calculate the flame velocity of experiments reported in literature. It is demonstrated that the developed flame velocity model is appropriate for premixed gas deflagrations up to an equivalence ratio of 1 at the initial stage of flame propagation, i.e., with a flame velocity less than 100 m/s.

Keywords: deflagration in tube, flame velocity model, premixed combustion, analytical solution

Nomenclature

A	Area, m^2
$b_{1\sim5}$	Correction factor
c_p	Constant pressure specific heat capacity, J/(kg·K)
$c_{1\sim2}$	Fitting coefficient
D	Tube diameter, m
E	Expansion factor
E_a	Activation energy, kJ/mol
F	Volume force, N
G	Tensile factor
g_{cr}	Critical tensile rate, s^{-1}
H	Generated heat, J
h	Specific enthalpy, J/kg
l	Tube length, m
L	Distance between an axial position and ignition point, m
L_{ch}	Characteristic geometric scale, m
Le	Lewis number
M_i	Molecular weight of the component i, g/mol
$\overline{M}$	Average molecular weight, g/mol
m	Total mass of premixed gas before ignition, kg
n	Amount of material, mol
P	Pressure, Pa
P_r	Reference pressure, Pa
P_m	Adiabatic pressure, Pa
R	Universal gas constant, R = 8.314 J/(mol·K)
R_g	Specific gas constant, $R_g = R / M$， J/(kg·K)
Re	Reynolds number
r	Tube radius, m
S_C	Burning velocity, m/s
S_E	Thermal expansion speed, m/s
S_F	Flame velocity, m/s
$\overline{S}_F$	Average flame velocity, m/s
S_I	Initial velocity, m/s
S_L	Laminar burning velocity, m/s
S_{Lr}	Reference laminar burning velocity, m/s
S_N	Mole increment rate mol/s
S_T	Turbulent burning velocity, m/s

T	Temperature, K
T_m	Adiabatic temperature, K
T_r	Reference temperature, K
U_f	Plane form flame velocity, m/s
$u^{'}$	Turbulence pulsation velocity, m/s
V	Volume, m^3
v	Velocity, m/s
x	Distance between the flame front and the ignition point, m
x_{tip}	Flame front position, m
Y	Mass fraction, %

Greek symbols

α	Temperature index
β	Pressure index
γ	Ratio of specific heat capacities
δ	Laminar flame layer thickness, m
ε	Dissipation rate
κ	Thermal conductivity, W/(m·K)
λ	LPG volume fraction of premixed gas,%
μ	Dynamic viscosity coefficient, N·s/m^2
v	Motion viscosity coefficient, m^2/s
π	Circumference ratio, $\pi = 3.14$
ρ	Density, kg/m^3
ϕ	Equivalence ratio
φ	Diameter, m
φ_i	Volume fraction of component i,%
Ψ	Turbulent burning velocity subrelaxation factor
ψ	Subrelaxation factor index
ω	Rate of chemical reaction, mol/(L·s)

Subscripts

0	Initial state
b	Combustion product
e	Discharge premixed gas
i or α	i species or α species
L	Laminar flow
T	Turbulence
u	Uncombustible premixed gas

1. Introduction

Explosions in industrial processes involving a flammable gas are a threat. Considering the complexity of the problem itself, the flame propagation process is difficult to describe quantitatively. Flame propagation characteristics of the premixed gas in open tubes can be applied to work out a safety scheme on suppressing the flame propagation, reducing the deflagration range and minimizing the chance of a deflagration to detonation transition (DDT). Studies on the explosion of premixed gas in tubes are mainly focused on determining the key factors of flame propagation. Flame velocity in an open tube is an important quantity to study the characteristics of the deflagration flame in a confined space, which directly reflects the intensity and destructive power of the deflagration. A simple model for calculating the flame velocity was developed and reported in this paper. Related experiments were carried out to verify the model and to determine important parameters, such as the exponential relationship between flame propagation distance and time and the limiting factor of the turbulent burning velocity. The model developed is useful for a better understanding of a deflagration from the accidental ignition of the dust in a confined space (Jenkins et al. 2013) and deflagration of leaked flammable refrigerant in a confined space (Chow 2014; Chow and Pang 2012; Huo and Chow 2017; Ng and Chow 2015; Ng et al. 2017). Relevant safety standards and protection measures can then be developed.

Experiments on flame propagation in a tube can be studied by using high-speed photography to capture the transient flame pattern and acceleration more accurately. As reported by Bychkov et al. (2005, 2006) and Akkerman et al. (2007), the premixed gas flow ahead of the flame front caused by the thermal expansion of the combustion products at the initial stage of ignition accelerated the laminar flame. Experiments by Lohrer et al. (2008) on different length-to-diameter ratios (from 3.8 to 143) of tubes for the acceleration of propane air premixed-gas illustrated that the deflagration pressure decreased with the increase of the length-to-diameter ratio when the flame velocity increased. As reported by Chatrathi et al. (2001), experiments on premixed gas of propane, ethylene and hydrogen with air in the tubes with different length-diameter ratios and pipe forms (whether or not there is a bend), the flame velocity and pressure were closely related to the equivalence ratio of the premixed gas. The premixed gas near the upper and lower limit of the deflagration limit would burn slowly without flame acceleration and pressure rise. Besides thermal expansion and equivalence ratio, turbulent flow would also affect the flame propagation. Based on the experimental data of Chatrathi et al. (2001), an empirical formula was proposed by Silvestrini et al. (2008a) for calculating the velocity, pressure and DDT distance in tubes with and without obstacles. The effect of DDT for hydrogen/methane/air premixed gas as a function of blocking ratios and obstacles in a 6-m tube of 0.14 m diameter was reported by Porowski and Teodorczyk (2013).

The critical blocking ratio and the setting distance required for the acceleration of the premixed gas flame to detonation was investigated. A series of analytical expressions for flame acceleration, such as the flame acceleration caused by wall friction of an open tube was reported by Akkerman et al. (2010), the flame acceleration and DDT caused by the obstacles (Valiev et al. 2010) and the effect of the gas compression effect on flame acceleration in a channel with an obstacle (Bychkov et al. 2010). The development of a premixed turbulent flame was studied analytically by Regis et al. (2007) and Kazakov (2012). The destructive effect of the explosion overpressure to a rigid target depends on the angle between the target and the travel direction of the deflagration wave as analyzed by Rigby et al. (2015).

Methods based on Computational Fluid Dynamics (CFD) were also developed and applied to study related problems in this field. A numerical method was applied by Hamlington et al. (2011) to simulate combustion and the interaction between turbulence and the flame in the premixed reaction flow was studied.

The above studies focused on determining the key factors of flame propagation, proposing the mechanism of flame acceleration, a qualitative description of the process of flame propagation, and a better understanding on the causes of DDT. It is observed from the results that the velocity of flame propagation is mainly affected by the flammable gas, the initial conditions (such as pressure and temperature), the properties of the premixed gas (equivalence ratio) and turbulence. However, it is complicated to establish a theoretical model including chemical reactions and turbulence accurately to study the change of flame propagation velocity with propagation distance (or time) during the deflagration of premixed gases. In order to obtain enough experimental data to support the establishment of a flame velocity model, deflagration experiments in an open tube were carried out to provide more data.

An experimental rig was built to carry out experimental studies on the flame propagation characteristics of a premixed gas in an open tube. Premixed liquefied petroleum gas (LPG) and air was used in this study. A 16 m-long circular straight tube was used to study flame propagation. Effects of surface roughness and obstacles were not included. One end of the tube was closed and the other end, open. Key parameters such as the deflagration pressure, flame propagation distance, flame velocity and temperature were measured. The variation of the flame propagation distance and velocity with equivalence ratio was studied.

Equations describing the flame propagation process in an open tube were reviewed. Acceleration mechanisms of the flame propagation process were analyzed. An analytical solution of the flame velocity of the premixed gas in the tube was obtained. A mathematical model for calculating the flame velocity was proposed. Experimental data of the tube experiments were used to correct and verify the velocities calculated.

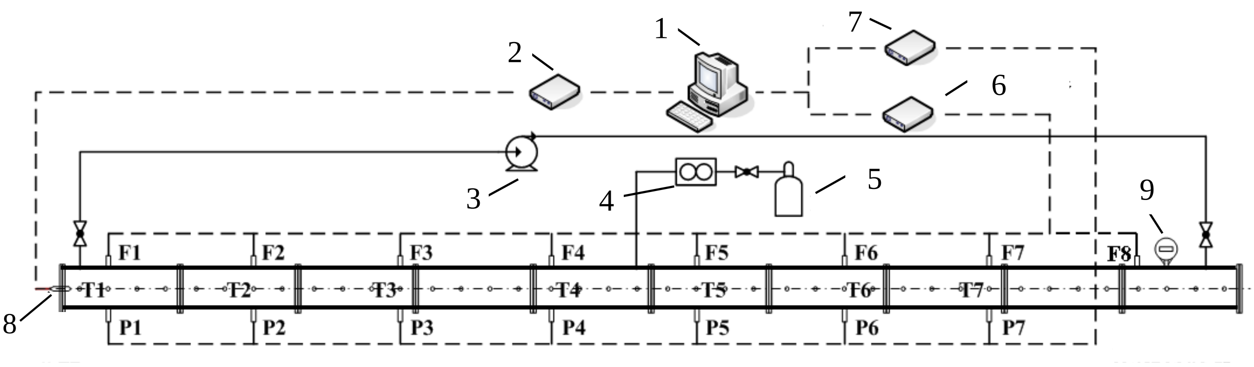
As the flame velocity is affected by combustion and turbulent flow simultaneously, there is a coupling relationship between them. The state equation and conservation equation of the flame propagation process were established by simplifying the physical model to deduce the flame propagation velocity. The formula of flame velocity was corrected by experimental data, and then verified by experiments published in literature.

Ambient conditions of the experiment were normal temperature and pressure. The deflagration was initiated by a weak ignition source which was a high voltage spark with an ignition energy of 20 J. The initial state of the premixed gas was stagnant with initial turbulence ignored.

The laminar burning velocity depends on the equivalence ratio of the premixed gas under the given temperature and pressure conditions. The equivalence ratio of the premixed gas and laminar burning velocity may be combined into a single variable.

2. Experimental Rig

An experimental rig was built to study gas deflagration in an open tube. A tube of length *l* (16 m) was constructed from 10 shorter tubes with an internal diameter *d* of 488 mm and a length of 1.6 m as shown in Figure 1(a). One end of the tube was sealed by a steel plate. The other end was sealed by a plastic film which was taken out before ignition according to the experimental condition. A spark igniter was installed at the center of the closed end. A photograph of the tube is shown in Figure 1(b).



1: Computer 2: Ignition controller 3: Circulating Pump 4: Flow meter
5: LPG storage tank 6: Flame and temperature data collector
7: Pressure data collector 8: Electric igniter 9: LPG concentration sensor

F - Flame velocity sensors; P - Pressure sensors; T - Temperature sensors

(a) Schematic diagram

(b) Photograph of the tube

Fig. 1: The experimental rig

The gas distribution system was composed of an LPG storage tank, flow meters, a gas sensor measuring LPG volume fraction and a circulation pump. The volume fraction sensor was a HR100L-GAS Sensor and produced by Shenzhen Huaruixiang Technology Co., Ltd of China. The gas injection inlet was in the middle of the tube. LPG was injected slowly into the tube with the concentration monitored by the LPG volume fraction sensors. After the gas filling process was completed, the circulation was continued for over 30 minutes to ensure that the gas in the tube was evenly mixed. To eliminate the effect of initial turbulence on flame propagation, the experiment was started after another 30 minutes. The composition of the LPG used in this paper is shown in Table 1. The average molecular weight of the premixed gas under different equivalence ratios is shown in Table 2.

Table 1: LPG composition

LPG component	H_2	CH_4	C_2H_6	C_3H_8	C_3H_6	C_4H_{10}	C_4H_8
volume fraction/%	5	10	5	20	10	45	5

Table 2: Average molecular weight of premixed gas

LPG volume fraction λ vol%	3	4	5	6	7	8
Equivalence ratio ϕ	0.73	0.97	1.21	1.45	1.69	1.93
$\overline{M}_{LPG-air}$ g/mol	29.469	29.619	29.767	29.911	30.053	30.193

Seven pressure sensors with a measurement range from 0 to 1.0 MPa and with an error range 0.25% were used. Eight home-made flame sensors with light-sensitive diodes to capture the light signal of the explosion were used to measure the transient flame front positions. Seven K type 0.1-mm thermocouple bare wires were used to measure the temperature. In the data acquisition device, temperature data was collected by a data acquisition card. Another data acquisition card was used to collect the pressure and flame front position data. Both cards had a sampling frequency of 5 kHz. The data acquisition equipment was equipped with a unified controller to realize synchronous ignition and data acquisition. The positions of pressure (P), flame (F) and temperature (T) sensors are shown in Table 3.

Table 3: Transducers arrangement

Pressure sensor	P1	P2	P3	P4	P5	P6	P7	—
Flame sensor	F1	F2	F3	F4	F5	F6	F7	F8
Temperature sensor	T1	T2	T3	T4	T5	T6	T7	—
Distance from the ignition end (m)	0.6	2.6	4.6	6.6	8.6	9.6	11.6	13.6

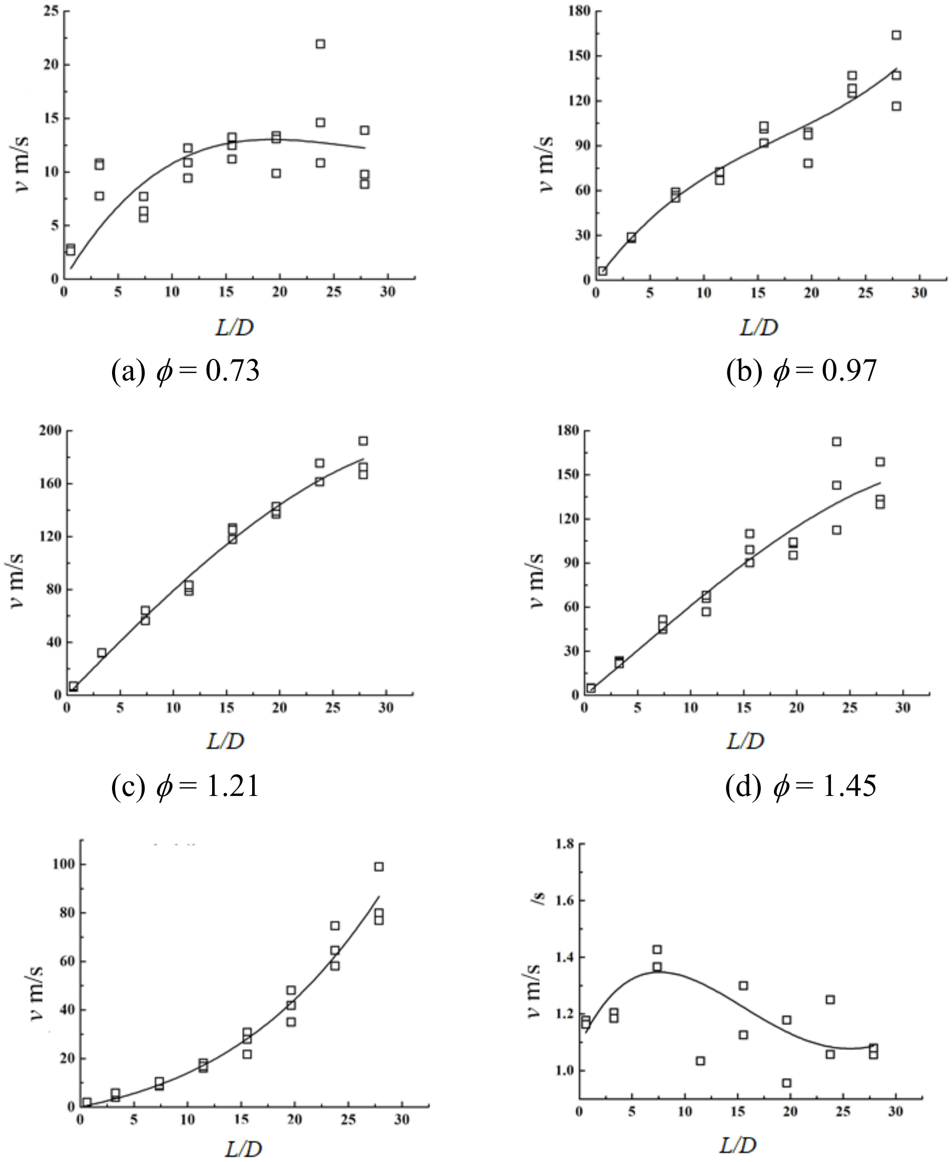
In the experiment, the premixed gas equivalence ratio was varied, and the flame propagation speed, pressure and temperature characteristics were measured. The experimental conditions are shown in Table 4. Each working condition was repeated at least 3 times. Repeatability of the experimental results was ensured by getting at least 2 sets of experimental data for each condition.

Table 4: Equivalence ratios of the premixed gas in experiments (Electric ignition)

LPG volume fraction λ vol%	3	4	5	6	7	8
Equivalence ratio ϕ	0.73	0.97	1.21	1.45	1.69	1.93

3. Flame Propagation Velocity

The flame velocity under different equivalence ratios of premixed gas was calculated quantitatively by the transient flame front positions recorded by the flame sensor. The sensor can only receive light in the incident range of ±10°, and most of the reflected light with large incident angle is shielded. In addition, the magnitude of the voltage signal recorded by the sensor is also one of the criteria for judging the flame signal. The flame velocity was taken as the average velocity over the distance between two adjacent sensors and was plotted against a dimensionless distance (*L/D*) in Figure 2. Values of *L/D* corresponding to each sensor location is shown in Table 5.



(a) $\phi = 0.73$ (b) $\phi = 0.97$

(c) $\phi = 1.21$ (d) $\phi = 1.45$

(e) $\phi = 1.69$ (f) $\phi = 1.93$

□ Experimental data – polynomial fitting

Fig. 2: Flame velocity v of various equivalence ratios in an open-end tube as a function of distance travelled

Table 5: Propagation distances and corresponding dimensionless distance (*L/D)*

Distance/m	0.3	1.6	3.6	5.6	7.6	9.6	11.6	13.6
Ratio of distance to diameter *L/D*	0.61	3.28	7.38	11.48	15.57	19.67	23.77	27.87

The arithmetic means of flame velocities of three repeated experiments in Figure 2 were calculated and plotted in Figure 3. In plotting flame velocity as a function of equivalence ratio, the flame velocities v were less scattered for equivalence ratio φ between 0.97 and 1.69. On the other hand, for φ equal to 0.73 and 1.93, the flame velocity was not monotonically increasing, due to the approximation of the equivalence ratio to the lower and upper deflagration limits, respectively. For $\varphi = 0.73$, flame velocity slightly increased to 12 m/s, and for $\varphi = 1.93$, it was less than 1.5 m/s. All indicating that the experimental data for $\varphi = 0.73$ and $\varphi = 1.93$ were not useful for developing a flame velocity model in the process of flame acceleration in an open tube.

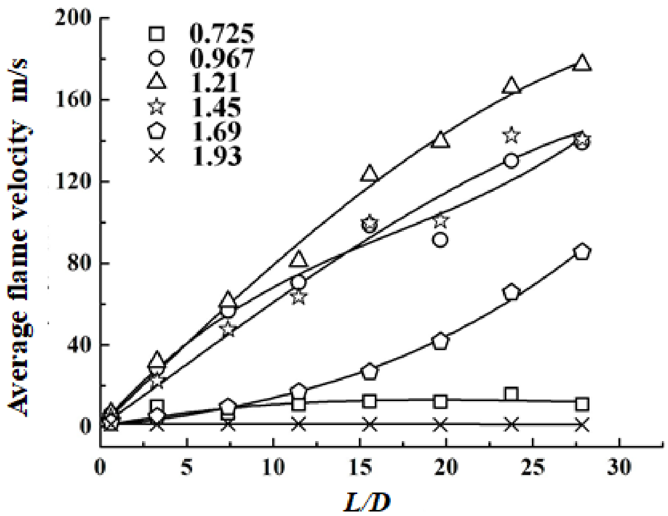
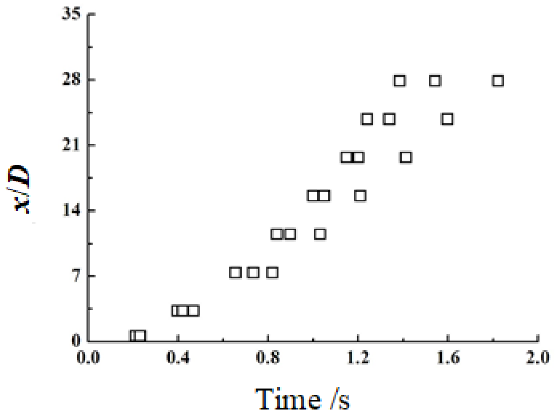


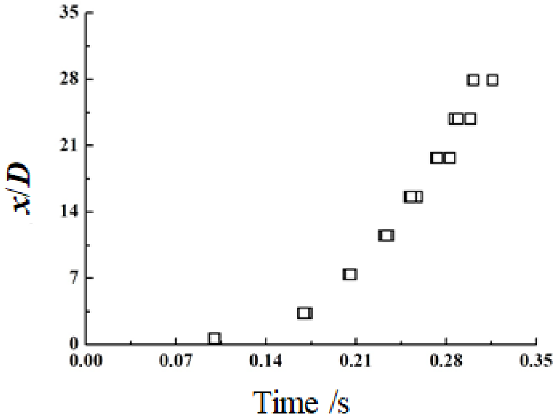
Fig. 3: Average flame velocity in three repeated experiments of various equivalence ratios

4. Flame Propagation Distance

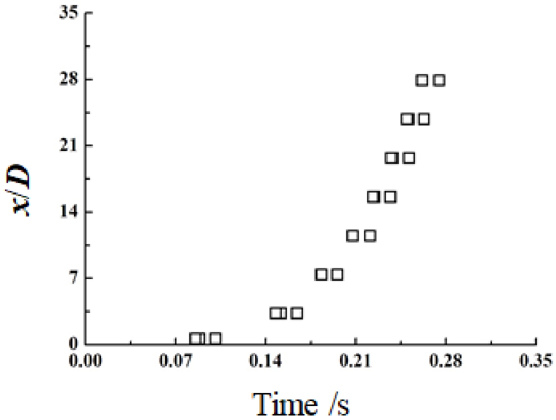
In addition to flame velocity, the distance travelled by the flame from the ignition end is another important parameter to characterize the flame propagation process. Transient variation of flame propagation distance in the tube under different premixed gas equivalence ratios is shown in Figure 4.



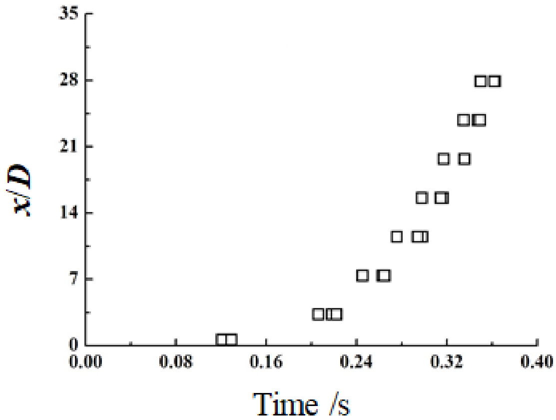
(a) ϕ = 0.73



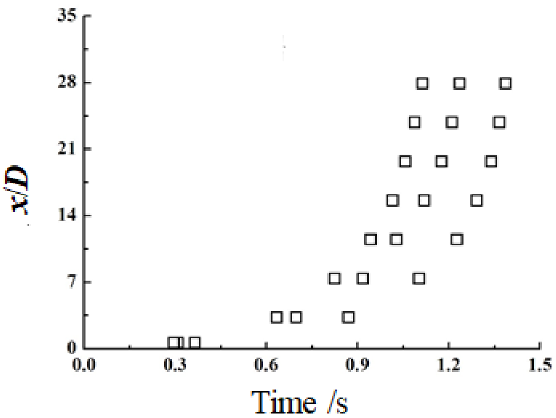
(b) ϕ = 0.97



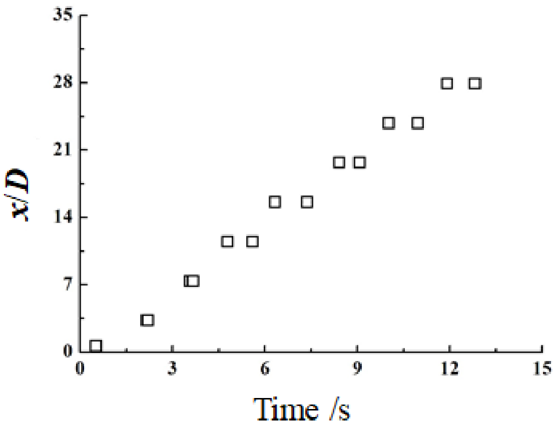
(c) ϕ = 1.21



(d) ϕ = 1.45



(e) ϕ = 1.69



(f) ϕ = 1.93

Fig. 4: Dimensionless flame propagation distance versus time for various equivalence ratios

By simplifying the flame propagation process, an analytical expression for the flame propagation distance as a function time can be deduced.

The flame in the tube is simplified to a cylindrical flame surface with a radius r equal to the radius of the tube *R* ($r \approx R$), as in Figure 5.

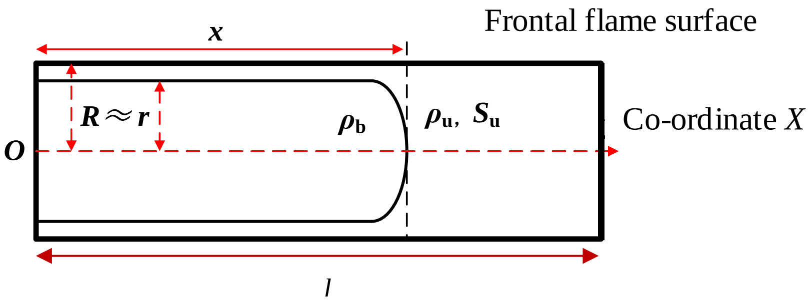


Fig. 5: Schematic of the simplification of the flame front propagation

In the process of flame propagation, the transient change of volume *V* of combustion products can be expressed in terms of the expansion ratio *E*, cylindrical flame surface area *A*, and frontal surface flame velocity U_f (Figure 6).

$$\frac{\mathrm{d}V}{\mathrm{d}t} = EAU_\mathrm{f} \tag{1}$$

Taking *x* to represent the distance from the flame front to the ignition end, then the area of the cylindrical flame surface *A* and the volume of the combustion product *V* are given by $A \approx 2\pi Rx + \pi R^2$ or $A \approx 2\pi Rx$ assuming that $R << x$, and $V \approx \pi R^2 x$. Equation (1) can be written as:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = 2E\frac{U_\mathrm{f}}{R}x \tag{2}$$

The solution of equation (2) is

$$x \propto \exp\left(\frac{2EU_\mathrm{f}}{R}t\right) \tag{3}$$

This means that the relationship between the propagation distance of the flame front and time is consistent with the exponential relation based on the natural number. The exponent proportional relation expressed in equation (3) is written in terms of correction coefficients c_1 and c_2 as:

$$x = c_1 \exp(c_2 t) \tag{4}$$

The factor $(2EU_f / R)$ in equation (2) is included in c_2 in equation (4). Equation (4) was used to fit the experimental data of flame propagation distances. As there were three replicate experiments for each value of ϕ, the arithmetic averages of three experimental results were used for curve fitting. The fitting curves are shown in Figure 6. The fitting results are shown in Table 6.

The fitting results suggest that the exponential relation can be used to express the variation of the propagation distance of the flame front with time. It is acceptable to simplify the flame front to a cylindrical surface in the tube with a large length-to-diameter ratio considered in this work.

Table 6: Fitting results of dimensionless distance with time

$x/D = c'_1 \exp(c_2 t)$, $c_1 = c'_1 D$						
Equivalence ratio ϕ	0.73	0.97	1.21	1.45	1.69	1.93
c'_1	1.281	0.205	0.147	0.116	0.225	0.275
c_2	2.031	16.300	19.937	15.456	4.046	1.150
Goodness of fit	0.907	0.967	0.985	0.986	0.989	0.979

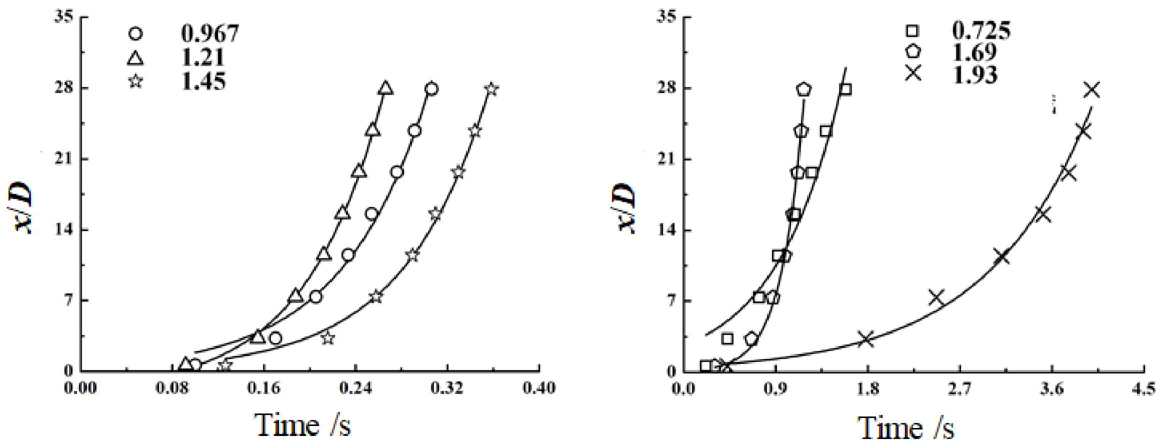


Fig. 6: Dimensionless flame propagation distance versus average time for selected values of ϕ

5. Empirical Model

The open tube can be taken as a container with a pressure relief so that flame gas is released directly into the atmosphere without any obstruction. The overpressure in containers with unconfined outlets in most process industries is less than 0.1 MPa. The gas flow is then subsonic in the pressure relief (Nagy 1983). Consider the premixed gas deflagration and pressure relief process in a tube with a volume of V as shown in Figure 7. The premixed gas before deflagration is shown by the dotted line. In the process of deflagration, the combustion products, the unburnt premixed gas in the tube and the discharged premixed gas are included, expressing density, pressure, temperature, volume, amount of material in number of moles and average molecular weight of the premixed gas and combustion products with ρ, P, T, V, n and $\overline{M}$, respectively. The subscripts b, u, e and 0 describe the combustion products, the unburned premixed gas in the tube, the discharged premixed gas and the initial parameters. Assume the total mass of premixed gas in the tube before ignition to be *m*, and the initial deflagration pressure and temperature to be the same as the ambient pressure and temperature, P_0 (1.01325 x 10^5Pa) and T_0 (298K) respectively. The closed end of the tube is the ignition end, and at the other end there is a pressure relief port with an area of A_V.

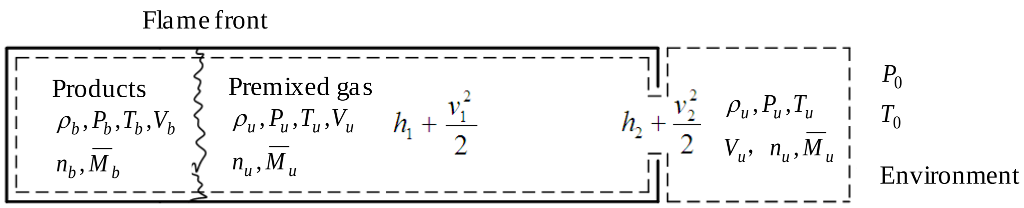


Fig. 7: Pressure relief in an open tube

Assuming isothermal conditions, for the deflagration stage in the tube, the pressure produced by the combustion can quickly be released into the environment through the opening, neglecting the compression effect of the premixed gas in front of the flame. The temperature rise of the premixed gas in front of the flame is not very high (Nagy 1983), which does not exceed 10% of the initial temperature actually when the premixed gas passes through the pressure relief position at a subsonic velocity. It can be approximated by taking the temperature of the premixed gas in front of the flame to be constant, and equal to the initial temperature, i.e., $T_u = T_0 = 295$ K. The temperature of the combustion products T_b is also not affected by compression for an isothermal process, and is equal to the flame adiabatic temperature T_m, that is, $T_b = T_m$.

The equation of state is applied to the premixed gas in front of the flame. Taking the derivative of this equation with respect to time t gives:

$$P\frac{\mathrm{d}V_{\mathrm{u}}}{\mathrm{d}t}+V_{\mathrm{u}}\frac{\mathrm{d}P}{\mathrm{d}t}=RT_{\mathrm{u}}\frac{\mathrm{d}n_{\mathrm{u}}}{\mathrm{d}t} \tag{5}$$

$\mathrm{d}n_u/\mathrm{d}t$ is the rate of change of the amount of unburned premixed gas in the tube.

From equation (5), the number of moles premixed gas in front of the flame is affected by two factors:

- The first term on the left side of equation (5), represents the volume change of the premixed gas caused by the flame propagating through the premixed gas.
- The second term on the left side represents the change caused by compression, which is weak for the open tube, and can be neglected. Equation (5) is then simplified to:

$$P\frac{\mathrm{d}V_{\mathrm{u}}}{\mathrm{d}t}\approx RT_{\mathrm{u}}\frac{\mathrm{d}n_{\mathrm{u}}}{\mathrm{d}t} \tag{6}$$

Putting $V_{\mathrm{u}}=A(l-x)$ into equation (6) as in Figure 6 gives:

$$-AP\frac{\mathrm{d}x}{\mathrm{d}t}=RT_{\mathrm{u}}\frac{\mathrm{d}n_{\mathrm{u}}}{\mathrm{d}t} \tag{7}$$

The implicit expression of the flame front velocity $S_F=\mathrm{d}x/\mathrm{d}t$ can be obtained from Eq. (7), with *P* and ($\mathrm{d}n_u/\mathrm{d}t$) unknown, so the expressions of *P* and $\mathrm{d}n_u/\mathrm{d}t$ must be derived first.

6. Derivation of Pressure

In deflagration with pressure relief, the conservation equation of mass gives:

$$m = n_{\mathrm{u}} \overline{M}_{\mathrm{u}} + n_{\mathrm{b}} \overline{M}_{\mathrm{b}} + n_{\mathrm{e}} \overline{M}_{\mathrm{u}} \tag{8}$$

In equation (8), m is the total mass of the premixed gas before ignition. Equations of state for combustion products, premixed gas and vented premixed gas in tube are given by:

$$PV_{\mathrm{b}} = n_{\mathrm{b}} RT_{\mathrm{b}} \tag{9}$$

$$PV_{\mathrm{u}} = n_{\mathrm{u}} RT_{0} \tag{10}$$

$$PV_{\mathrm{e}} = n_{\mathrm{e}} RT_{0} \tag{11}$$

Substituting equations (9) to (11) into equation (8) for n_b, n_u and n_e gives:

$$m = \overline{M}_{\mathrm{u}} \left(\frac{PV_{\mathrm{u}}}{RT_0} + \frac{P_0 V_{\mathrm{e}}}{RT_0} \right) + \overline{M}_{\mathrm{b}} \frac{PV_{\mathrm{b}}}{RT_{\mathrm{b}}} \tag{12}$$

The initial-state premixed gas and the final-state combustion product satisfy the equation of state and mass conservation through the maximum pressure of deflagration, P_m (in Pa), and the maximum temperature of deflagration T_{m} (in K):

$$P_0 V = \frac{m}{\overline{M}_{\mathrm{u}}} RT_0 \tag{13}$$

$$P_{\mathrm{m}} V = \frac{m}{\overline{M}_{\mathrm{b}}} RT_{\mathrm{m}} \tag{14}$$

Equations (13) and (14) give:

$$\frac{P_0}{P_{\mathrm{m}}} = \frac{\overline{M}_{\mathrm{b}}}{\overline{M}_{\mathrm{u}}} \frac{T_0}{T_{\mathrm{m}}} \tag{15}$$

Dividing equation (11) by $\overline{M}_{\mathrm{b}}$, multiplying by RT_m, and combining equations (14) and (15) gives:

$$P_m V = \frac{P_m}{P_0}\left(PV_u + P_0 V_e\right) + PV_b \tag{16}$$

In equation (16), V_e is the volume of the premixed gas discharged from the moment the vent opens, which is caused by the joint action of the thermal expansion velocity and the molar increment velocity, defined as S_E and S_N, which can be expressed as:

$$V_e = \left(S_E + S_N\right)At \tag{17}$$

In the time interval Δt, the volume increment caused by the change of the average molar mass of the combustion products is $\Delta V^{'} = A\Delta x^{'}$, and the corresponding volume change rate is expressed by the equation of state.

$$\frac{\Delta V'}{\Delta t} = \frac{\Delta x + \Delta x'}{\Delta t}A - \frac{\Delta x}{\Delta t}A = \frac{RT_u}{P}\frac{\Delta n_b}{\Delta t} - \frac{RT_u}{P}\frac{\Delta n_u}{\Delta t} \tag{18}$$

$\Delta x^{'}$ is the increment of the flame distance caused by the change of the molar mass of the products.

The premixed gas generates combustion products, following the conservation of mass:

$$\Delta m = \overline{M}_u \Delta n_u = \overline{M}_b \Delta n_b \tag{19}$$

Putting equation (19) into equation (18), the molar increment velocity $S_N = \Delta x^{'} / \Delta t$ can be expressed as

$$S_N = \frac{RT_u}{AP}\left(1 - \frac{\overline{M}_b}{\overline{M}_u}\right)\frac{\Delta n_b}{\Delta t} \tag{20}$$

The chemical reaction transforms the premixed gas with a mass of Δm to an equal mass of combustion products, and the temperature rises from T_u to T_b. The volume increment caused by thermal expansion is $\Delta V^{''} = A\Delta x^{''}$, similar to that of equation (18), and the corresponding volume change rate is

$$\frac{\Delta V''}{\Delta t} = \frac{R}{P}\left(T_{\mathrm{b}} - T_{\mathrm{u}}\right)\frac{\Delta n_{\mathrm{b}}}{\Delta t} \tag{21}$$

The thermal expansion velocity $S_E = \Delta x''/\Delta t$ can be expressed as

$$S_{\mathrm{E}} = \frac{R}{AP}\left(T_{\mathrm{b}} - T_{\mathrm{u}}\right)\frac{\Delta n_{\mathrm{b}}}{\Delta t} \tag{22}$$

Putting equations (20) and (22) into equation (17), and combining with equation (15) gives:

$$V_{\mathrm{e}} = \left(\frac{P_{\mathrm{m}}}{P_0} - 1\right)S_{\mathrm{T}}At \tag{23}$$

Putting equation (23) into equation (16) and taking P as

$$P = \frac{l - \left(\frac{P_{\mathrm{m}}}{P_0} - 1\right)S_{\mathrm{T}}t}{\frac{l}{P_0} + \left(\frac{1}{P_{\mathrm{m}}} - \frac{1}{P_0}\right)x} \tag{24}$$

Equation (24) contains the flame propagation distance x and the time t. An empirical formula describing the relation of x and t is given by equation (4), which can be rewritten as:

$$t = \frac{1}{c_2}\ln\left(\frac{x}{c'_1 D}\right) \tag{25}$$

The values of $c_1^{'}$ and c_2 are shown in Table 6, and D is the tube diameter. Putting equation (25) into equation (24) gives:

$$P = \frac{l - \frac{S_{\mathrm{T}}}{c_2}\ln\left(\frac{x}{c'_1 D}\right)\left(\frac{P_{\mathrm{m}}}{P_0} - 1\right)}{\frac{l}{P_0} + \left(\frac{1}{P_{\mathrm{m}}} - \frac{1}{P_0}\right)x} \tag{26}$$

Equation (26) can be used for calculating the deflagration pressure P of premixed gas in an open tube.

7. Derivation of the Rate of Change of Flammable Gas

Taking the derivative of equation (8) with respect to time *t* will give the change rate of the amount of unburned premixed gas material in the tube in equation (7):

$$\frac{\mathrm{d}n_{\mathrm{u}}}{\mathrm{d}t} = -\frac{\mathrm{d}n_{\mathrm{b}}}{\mathrm{d}t}\frac{\overline{M}_{\mathrm{b}}}{\overline{M}_{\mathrm{u}}} - \frac{\mathrm{d}n_{\mathrm{e}}}{\mathrm{d}t} \tag{27}$$

$\mathrm{d}n_u/\mathrm{d}t$ can be determined from $\mathrm{d}n_b/\mathrm{d}t$ and $\mathrm{d}n_e/\mathrm{d}t$.

In deriving $\mathrm{d}n_e/\mathrm{d}t$, the premixed gas released from the tube due to the deflagration is taken as one-dimensional isentropic flow with conservation equations in terms of density ρ (in kg/m^3), tube cross section area A (in m^2), speed v (in m/s), specific enthalpy h (in J/kg) and gas constant R_{g} (in J/ (kg K)), where $R_{\mathrm{g}} = R/M$.

Continuity equation:

$$\frac{\mathrm{d}\rho}{\rho} + \frac{\mathrm{d}v}{v} + \frac{\mathrm{d}A}{A} = 0 \tag{28}$$

Momentum equation:

$$v\mathrm{d}v = -\frac{1}{\rho}\mathrm{d}p \tag{29}$$

Energy equation：

$$h + \frac{v^2}{2} = \text{constant} \tag{30}$$

State equation:

$$P = \rho R_{\mathrm{g}} T \tag{31}$$

With subscripts 1 and 2 considering the premixed gas before and after opening of the tube the energy equation satisfies

$$h_1 + \frac{v_1^2}{2} = h_2 + \frac{v_2^2}{2} \tag{32}$$

The enthalpy of an ideal gas has the following relation with pressure and volume in terms of the ratio of the specific heat capacities of the premixed gas γ:

$$h = \frac{\gamma}{\gamma - 1}\frac{P}{\rho} \tag{33}$$

Putting equation (33) into equation (32) gives:

$$\frac{v_2^2}{2} = \frac{v_1^2}{2} + \frac{\gamma}{\gamma - 1}\left(\frac{P_1}{\rho_1} - \frac{P_2}{\rho_2}\right) \tag{34}$$

The isentropic equation of an ideal gas is

$$P_2 / \rho_2^{\gamma} = P_1 / \rho_1^{\gamma} \tag{35}$$

Putting equation (35) into equation (34) gives:

$$\frac{v_2^2}{2} = \frac{v_1^2}{2} + \frac{\gamma}{\gamma - 1}\frac{P_1}{\rho_1}\left[1 - \left(\frac{P_2}{p_1}\right)^{\frac{\gamma - 1}{\gamma}}\right] \tag{36}$$

In the time interval Δt, the mass of the gas passing through the opening area A_V at speed v_2 is m_e, giving

$$\frac{\mathrm{d}m_{\mathrm{e}}}{\mathrm{d}t} = \frac{A_{\mathrm{V}} v_2}{1/\rho_2} \tag{37}$$

Putting equations (35) and (36) into equation (37) gives:

$$\frac{\mathrm{d}n_{\mathrm{e}}}{\mathrm{d}t} = \frac{A_{\mathrm{V}} P_1}{\overline{M}_{\mathrm{u}} (R_g T_1)^{1/2}} \left\{ \frac{v_1^2}{R_g T_1}\left(\frac{P_2}{P_1}\right)^{2/\gamma} + \frac{2\gamma}{\gamma - 1}\left[\left(\frac{P_2}{P_1}\right)^{2/\gamma} - \left(\frac{P_2}{P_1}\right)^{(\gamma+1)/\gamma}\right]\right\}^{1/2} \tag{38}$$

Equation (38) can be arranged as:

$$\frac{\mathrm{d}n_{\mathrm{e}}}{\mathrm{d}t}=\frac{A_{\mathrm{v}}P_2}{\overline{M}_{\mathrm{u}}\left(R_gT_1\right)^{1/2}}\left\{\frac{v_1^2}{R_gT_1}\left(\frac{P_1}{P_2}\right)^{\frac{2\gamma-2}{\gamma}}+\frac{2\gamma}{\gamma-1}\left[\left(\frac{P_1}{P_2}\right)^{\frac{2\gamma-2}{\gamma}}-\left(\frac{P_1}{P_2}\right)^{\frac{\gamma-1}{\gamma}}\right]\right\}^{1/2} \tag{39}$$

Air in the premixed gas is mainly composed of oxygen and nitrogen, so $\gamma=1.39$ is used. The pressure increase during the explosion satisfies (Nagy 1983) the following:

$1\le P_1/P_2\le 2$

This gives:

$$\left(\frac{P_1}{P_2}\right)^{\frac{2\gamma-2}{\gamma}}=\left(\frac{P_1}{P_2}\right)^{0.56}=\left[1+\left(\frac{P_1}{P_2}-1\right)\right]^{0.56}\approx 1+0.56\left(\frac{P_1}{P_2}-1\right) \tag{40}$$

$$\left(\frac{P_1}{P_2}\right)^{\frac{\gamma-1}{\gamma}}=\left(\frac{P_1}{P_2}\right)^{0.28}=\left[1+\left(\frac{P_1}{P_2}-1\right)\right]^{0.28}\approx 1+0.28\left(\frac{P_1}{P_2}-1\right) \tag{41}$$

The exact and approximate values estimated by equations (40) and (41) are compared in Figure 8. As the error does not exceed 7% for equation (40), and not exceed 6% for equation (41), the approximation is acceptable.

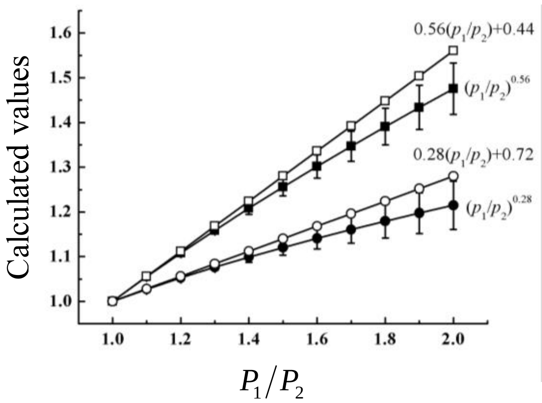


Fig. 8: Results of approximation using formula (40) and (41)

Putting equations (40) and (41) into equation (39) gives:

$$\frac{\mathrm{d}n_{\mathrm{e}}}{\mathrm{d}t}=\frac{A_{\mathrm{v}}P_2}{\overline{M}_{\mathrm{u}}\left(R_gT_1\right)^{0.5}}\left[\left(\frac{0.56v_1^2}{R_gT_1}+2\right)\left(\frac{P_1}{P_2}\right)+\left(\frac{0.44v_1^2}{R_gT_1}-2\right)\right]^{0.5} \tag{42}$$

The temperature of the premixed gas in front of the flame is $T_1 = T_u$, P_1 is the pressure inside the tube and v_1 is the velocity of premixed gas in front of the flame.

The volume change of premixed gas participating in the reaction is ΔV in time interval Δt. The premixed gas having a mass of Δm involved in the reaction is expressed with the number of moles as Δn_u. Using the state equation to express the volume change rate of premixed gas participating in the reaction gives:

$$\frac{\Delta V}{\Delta t} = \frac{RT_{\mathrm{u}}}{P}\frac{\Delta n_{\mathrm{u}}}{\Delta t} \tag{43}$$

In the above equation, R is the universal gas constant, 8.314 J/(mol·K), T_u (in K) is the premixed gas temperature, p (in Pa) is the pressure, and V (in m^3) is the volume.

Under given pressure and temperature conditions, the premixed gas volume entering the flame front per unit area per unit time is constant as pointed out by Nagy et al. (1969) and expressed by Khitrin (1962) as:

$$\frac{1}{A}\frac{\Delta V}{\Delta t} = k'_{\mathrm{r}} \tag{44}$$

In the above equation, k'_{r} has the dimension of velocity in m/s. Experimental results show that the analytical expression of k'_{r} is very complicated in relation to the change of temperature and pressure of the premixed gas. An empirical expression based on the experimental data is:

$$k'_{\mathrm{r}} = k_{\mathrm{r}}\left(\frac{T}{T_{\mathrm{r}}}\right)^{\alpha}\left(\frac{P_{\mathrm{r}}}{P}\right)^{\beta} \tag{45}$$

In the above equation, T_r is the reference temperature, 298 K, P_r is the reference pressure, 101325 Pa, k_{r} has the dimension of m/s at the given reference temperature and pressure, α is the temperature index, and β is the pressure index. k'_{r} and k_{r} are laminar burning velocities of premixed gas at the actual temperature and pressure conditions and the reference temperature and pressure conditions, defined as S_L and S_{Lr} respectively.

Studies were carried out to determine the value or empirical formula for α and β in equation (45) for the laminar burning velocity under different temperatures and pressures using different combustibles (Dahoe 2005; Liao et al. 2007; Kuznetsov et al. 2011; Tang et al. 2008;

Jerzembeck et al. 2009). In this paper, the premixed gas formed by liquefied petroleum gas and air was studied. Expressions of α and β were reported by Huzayyin et al. (2008) experimentally in terms of the equivalence ratio of the premixed gas ϕ.

$$\alpha = 2 + 2.75\phi - 2.13\phi^2 \tag{46}$$

$$\beta = -0.137 + 0.029\phi - 0.026\phi^2 \tag{47}$$

Variations of α and β with ϕ are shown in Figure 9.

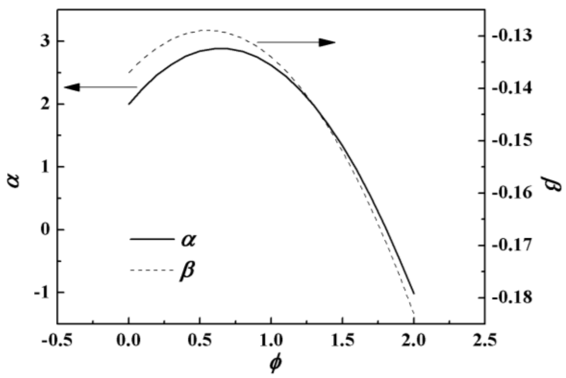


Fig. 9: Temperature and pressure indices as a function of ϕ

An equation for $\Delta n_b/\Delta t$ can be derived from equations (43), (44) and (19),

$$\frac{\mathrm{d}n_\mathrm{b}}{\mathrm{d}t} = S_\mathrm{Lr}\left(\frac{T}{T_\mathrm{r}}\right)^{\alpha}\left(\frac{P_\mathrm{r}}{P}\right)^{\beta}\frac{AP}{RT}\frac{\overline{M}_\mathrm{u}}{\overline{M}_\mathrm{b}} \tag{48}$$

Putting (48) and (42) into (27) gives:

$$\frac{\mathrm{d}n_\mathrm{u}}{\mathrm{d}t} = -S_\mathrm{L}\frac{AP}{RT_\mathrm{u}} - \frac{A_\mathrm{v}P_0}{\overline{M}_\mathrm{u}\left(R_gT_\mathrm{u}\right)^{0.5}}\left[\left(\frac{0.56v_1^2}{R_gT_\mathrm{u}}+2\right)\left(\frac{P}{P_0}\right)+\frac{0.44v_1^2}{R_gT_\mathrm{u}}-2\right]^{0.5} \tag{49}$$

8. Flame Velocity

With a deflagration, the initial condition is a laminar flame, and this develops quickly into a turbulent flame. Therefore, the turbulent flame velocity S_T is introduced here by putting equation (49) into equation (7):

$$S_{\mathrm{F}} = \frac{\mathrm{d}x}{\mathrm{d}t} = S_{\mathrm{T}} + \frac{A_{\mathrm{v}}}{A}\frac{P_0}{P}\left[\left(0.56v_1^2 + 2R_g T_{\mathrm{u}}\right)\frac{P}{P_0} + 0.44v_1^2 - 2R_g T_{\mathrm{u}}\right]^{0.5} \tag{50}$$

Multiplying equation (26) by $\frac{1}{P_0}$ gives:

$$\frac{P}{P_0} = \frac{l - \frac{S_{\mathrm{T}}}{c_2}\ln\left(\frac{x}{c'_1 D}\right)\left(\frac{P_{\mathrm{m}}}{P_0} - 1\right)}{l + \left(\frac{P_0}{P_{\mathrm{m}}} - 1\right)x} \tag{51}$$

The expansion ratio E of the density of the unburned premixed gas to the density of the combustion products is used to characterize the thermal expansion of the combustion products. E was found (Nagy and Verakis 1983) to be approximately equal to the ratio of the maximum overpressure P_m of the adiabatic deflagration to the initial pressure P_0:

$$E = \frac{P_{\mathrm{m}}}{P_0} \tag{52}$$

The pressure ratio P / P_0 is defined as G and is given by:

$$G = \frac{P}{P_0} = \frac{(E+1)\left[l - \frac{S_{\mathrm{T}}E}{c_2}\ln\left(\frac{x}{c'_1 D}\right)\right]}{E(l-x)+l} \tag{53}$$

Equation (50) can be expressed as:

$$S_{\mathrm{F}} = S_{\mathrm{T}} + \frac{H}{G}\left[(0.56G + 0.44)v_1^2 + 2(G-1)R_g T_{\mathrm{u}}\right]^{0.5} \tag{54}$$

Taking into account the initial velocity of premixed gases ($S_{\mathrm{I}} \neq 0$), the flame velocity for an open tube is:

$$S_F = S_T + \frac{H}{G}\left[(0.56G + 0.44)v_1^2 + 2(G-1)R_g T_u\right]^{0.5} + S_I \quad (55)$$

The first term on the right side of equation (55) is the turbulent burning velocity, which can be calculated from the laminar burning velocity from equations (56) to (61). The second term corresponds to the effect of thermal expansion on the velocity of the flame, which includes the contribution of the combustion products expansion to flame acceleration and the contribution of the premixed gas before the flame to flame acceleration, reflected in the pressure ratio G and the speed v_1, respectively. v_1 represents the flow velocity of premixed gas in front of the flame, and it is also the initial velocity of the premixed gas that is about to be introduced into the flame front. The third term, the initial velocity, is determined from the initial conditions. The independent variable of equation (55) is the distance between the flame front and the ignition end x. The flame velocity at different positions of the tube can be calculated.

No mathematical model is available to simulate all phenomena, because of the nonlinear relationship between the turbulent burning velocity and the turbulent flow field. A simple analytical approach is reported in this paper. Turbulent burning velocity models are reported in the literature (Gülder Ömer 1991; Bray 1990, 1996; Bradley 1992; Veynante and Vervisch 2002). Equation (56) is used as the model for calculating the turbulent burning velocity. Turbulent burning velocity is calculated using the widely used model proposed by Ciccarellia and Dorofeev (2008).

$$\frac{S_T}{S_L} = b_1 + b_2\left(\frac{u'}{S_L}\right)^{b_3}\left(\frac{L_{ch}}{\delta}\right)^{b_4} \mathrm{Le}^{b_5} \quad (56)$$

In the above equation, b_1 to b_5 are correction factors and shown in Table 7. u' (in m/s) is the turbulence pulsation velocity, L_{ch} (in m) is the characteristic geometric scale, δ (in m) is the laminar flame layer thickness, and Le is the Lewis number.

Table 7: Turbulent burning velocity correction factors

Correction factors	b_1	b_2	b_3	b_4	b_5
Bray (1990)	0	1.8	0.412	0.196	0
Gülder (1991)	1	0.7	3/4	1/4	0
Bradley (1992)	0	1.53	0.55	0.15	-0.3
Shy et al. (2000)	1	0.05	0.39	0.61	0

The laminar thickness of the laminar flame layer δ can be calculated in terms of the kinematic viscosity coefficient of the premixed gas ν (in m^2/s):

$$\delta = \frac{\nu}{S_{\mathrm{L}}} \tag{57}$$

The Lewis number is defined in terms of thermal diffusivity χ (in m^2/s) and mass diffusivity D_i (in m^2/s) as:

$$\mathrm{Le} = \frac{\chi}{D_i} \tag{58}$$

It is believed that the thermal diffusivity of the premixed gas is comparable to that of mass diffusion ($Le = 1$).

Putting equation (57) into equation (56) by taking $Le = 1$ gives:

$$S_{\mathrm{T}} = b_1 S_{\mathrm{L}} + b_2 (u')^{b_3} \left(\frac{L_{\mathrm{ch}}}{\nu} \right)^{b_4} S_{\mathrm{L}}{}^{1-b_3+b_4} \tag{59}$$

The turbulent flame velocity S_T can be calculated from equation (59) using the laminar flame velocity S_L . The turbulence fluctuating velocity u' is modeled (Silvestrini et al. 2008b) in terms of the premixed gas velocity in front of the flame U (in m/s) and Reynolds number, Re:

$$u' = 0.16U\ \mathrm{Re}^{-0.125} \tag{60}$$

Re is given by:

$$\mathrm{Re} = \frac{UL_{\mathrm{ch}}}{\nu} \tag{61}$$

In the premixed gas deflagration experiments with equivalence ratios of 0.97, 1.21, 1.45 and 1.69, the flame accelerations were intense. These experimental data were used to justify the flame velocity model in the open tube. Figure 10 shows the process of calculating flame propagation velocity.

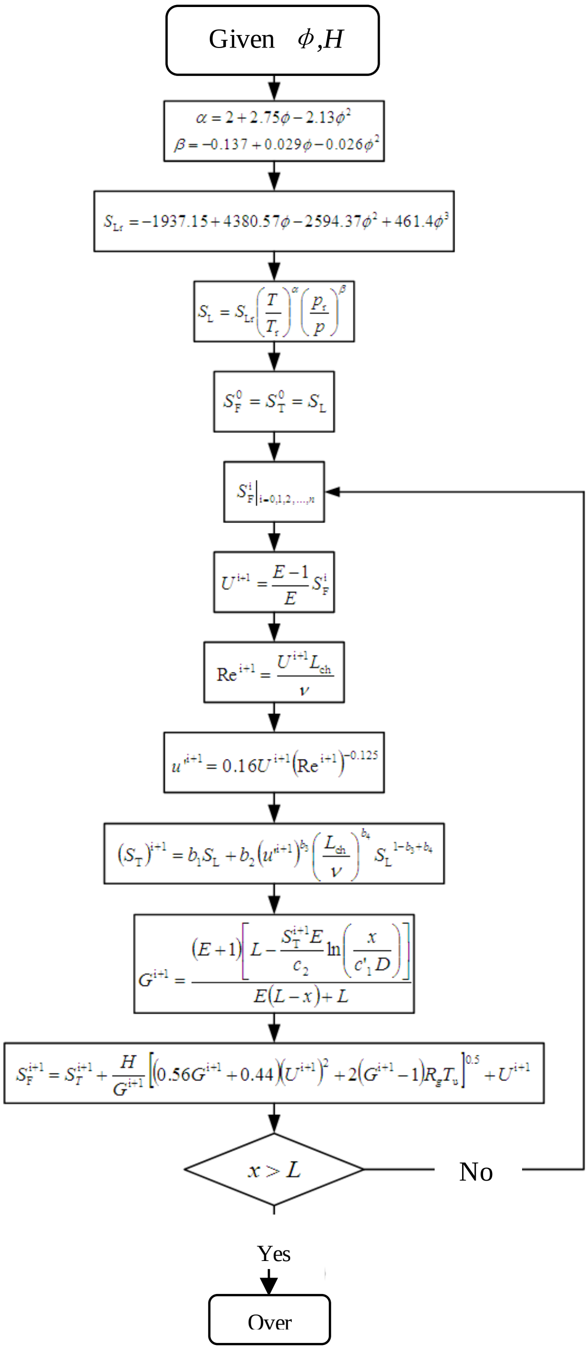


Fig. 10: Calculation process of flame velocity model

Parameters are calculated as follows:

- Laminar Burning Velocity

Based on the experimental data of the laminar burning velocity of the LPG-air premixed gas measured by Huzayyin et al. (2008) and Razus et al. (2007) under standard conditions, using the empirical formula of the polynomial form proposed by Huzayyin et al. (2008), the reference value of the laminar burning velocity of LPG-air premixed gas with different equivalence ratios under standard conditions is obtained using the model.

$$S_{\mathrm{Lr}} = -1937.15 + 4380.57\phi - 2594.37\phi^2 + 461.4\phi^3 \quad (62)$$

Before calculating the laminar burning velocity of LPG- air premixed gas under non-standard conditions, equation (62) is used to calculate the reference value of the laminar burning velocity under standard conditions. The laminar burning velocity of LPG- air premixed gas under non-standard conditions can then be calculated using equations (45) to (47). According to the experimental conditions in this work, using equations (45) to (47) and (62), the laminar combustion velocities at equivalence ratios of 0.97, 1.21, 1.45 and 1.69 were calculated, as shown in Table 8. The equivalence ratios in the experiments carried out by Huzayyin et al. (2008) and Razus et al. (2007) are different from that used in this work. Therefore, the experimental data of the literature are not compared in Table 8. Nevertheless, the fitting formula, equation (62), based on a large number of experimental data is reliable (Huzayyin et al. 2008).

Table 8: Laminar burning velocity (m/s) of LPG-air premixed gas at different equivalence ratios

ϕ	0.97	1.21	1.45	1.69
α	2.6675	2.2090	1.5092	0.5640
β	-0.1333	-0.1400	-0.1496	-0.1622
S_{Lr}	0.291	0.382	0.367	0.283
S_{L}	0.294	0.386	0.369	0.283

Calculated at T_r = 298K, T = 300K, P_r = 1.01325×10^{5}Pa, P = 0.9851×10^{5}Pa

- Expansion ratio E

The values of the expansion ratio E obtained in the experimental results were used to calculate the flame velocity. According to the maximum pressure data of the premixed gas deflagration in the closed tube, as shown in Figure 11, the expansion ratios of the premixed gas with equivalence ratios of 0.97, 1.21, 1.45, and 1.69 are $E_{0.97} = E_{1.45} = 3.6$, $E_{1.21} = 4$, $E_{1.69} = 3.3$, respectively.

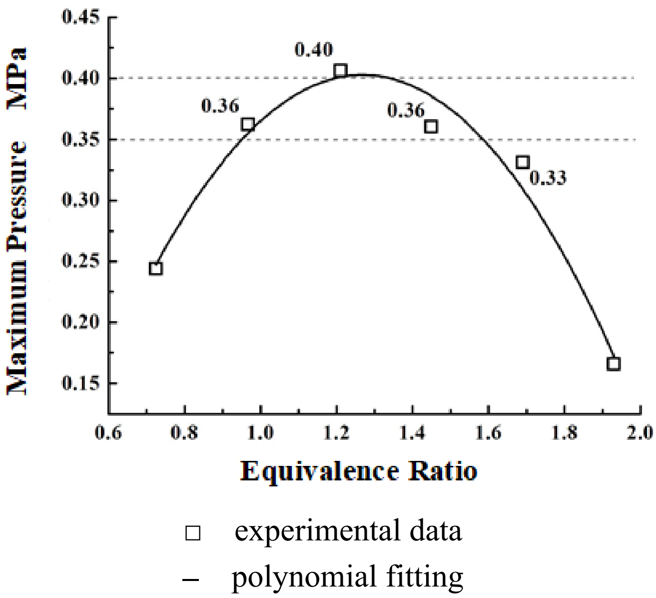


Fig. 11: Maximum pressure of various equivalence ratios gas in closed-end tube

- Because the air in the premixed gas is more than 90% of the volume fraction, the motion viscosity of the premixed gas takes as that from air, and its value is $\nu = 1.461\times10^{-5}\,\mathrm{m^2/s}$.

- In Table 7, the correction factors of four turbulent burning velocity models are given. The different values will affect the calculation results of the flame velocity, so the different correction factors were used to calculate the flame velocity, and then the differences between the results were compared.

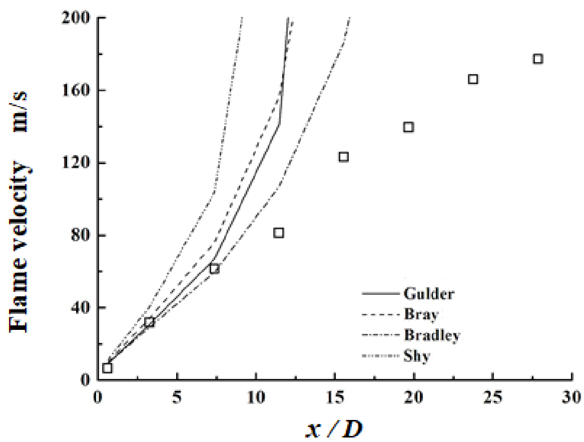
- Values of $c_1^{'}$ and c_2 in the pressure expressions are shown in Table 6 (See equation (4)). For the open tube, the pressure relief ratio $A_V/A = 1$.

9. Turbulent Burning Velocity

Under the experimental conditions in this work, the flame propagation velocity is the fastest when the equivalence ratio of the premixed gas is 1.21 (as shown in Figure 3). The flame acceleration with an equivalence ratio of 1.21 was calculated by using the flame velocity model to study the effect of turbulent burning velocity.

The deflagration flame velocity of the premixed gas with an equivalence ratio of 1.21 was calculated, with the results shown in Figure 12. The calculated values using the flame velocity model are higher than the experimental values and the flame acceleration is also too big. In the calculation with the increase of flame propagation distance x, the ratio of the deflagration pressure to the initial pressure $G < 0$ appeared in equation (53), causing errors in the calculation. Through the analysis of equation (53), G < 0 is caused by the increase of the turbulent burning velocity S_T.

The experimental results (Ciccarelli and Dorofeev 2008) showed that the turbulent burning velocity S_T increases with the increase of turbulence fluctuating velocity u', given in equations (59) and (60), and subsequently levels off with the increase of Reynolds number. The range of S_T was found to be a function of u' by Bradley et al. (1992) and Shy et al. (2000) through experiments. Their experimental results and the calculation results of the turbulent burning velocity S_T by equation (59) are shown in Figure 13. In the overlapping part of the Bradley region and Shy region, the maximum value of S_T is about 12 times the laminar burning velocity S_L. The calculated results of equation (59) exceeded this limit, which led to the errors.



□ experimental data

Fig. 12: Flame velocity computation for flammable mixture with ϕ =1.21

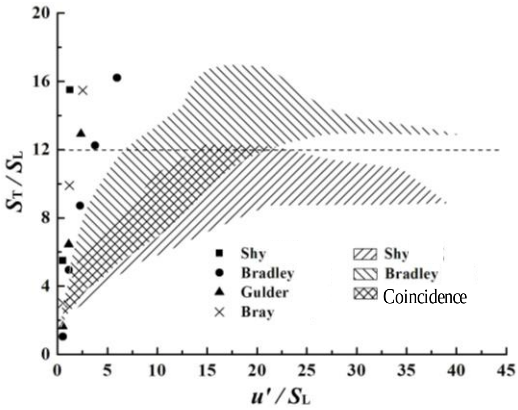


Fig. 13: Changes of S_T with turbulent intensity

In order to solve the problem in having too high a turbulent burning velocity S_T as turbulent fluctuating velocity u' increases, a correction factor is introduced to limit the increase rate of S_T.This factor increases with the increase of Re and subsequently levels off, which represents the maximum turbulent burning velocity S_T in flame acceleration. The factor ψ is labelled as "sub relaxation factor of turbulent burning velocity".

$$\Psi(S_T) = \min\left(\tanh\left(\mathrm{Re}^{\psi}\right)S_T, 12S_L\right) \quad (63)$$

In the above equation, the hyperbolic tangent function was selected, its range is (-1,1), and it increases monotonously. In addition, when the independent variable is greater than zero, the slope of the curve decreases with the increase of the independent variable, which meets the requirements of the factor. The exponential form of Re is used as the independent variable of the hyperbolic tangent function to ensure that the dependent variable of the function can obtain a large range of variation. At the same time, it should be ensured that the corrected turbulent burning velocity can reduce the error of flame velocity calculation. For these two reasons, $\psi = -0.125$.

When the turbulent fluctuating velocity of the premixed gas flow in front of the flame is large, the turbulent burning velocity is equal to $12S_L$. The value of ψ is used to calculate the turbulent burning velocity of the premixed gas with an equivalence ratio 1.21 as shown in Figure 14. The rate of increase in turbulent burning velocity, after the correction using the sub relaxation factor, is reduced. Comparing the four turbulence models, values predicted by the modified Shy model and the Gulder model are closer to the experimental values. The predicted values are basically in the Shy region. The turbulent burning velocities calculated by the Bray model and the Bradley model are lower than the experimental values.

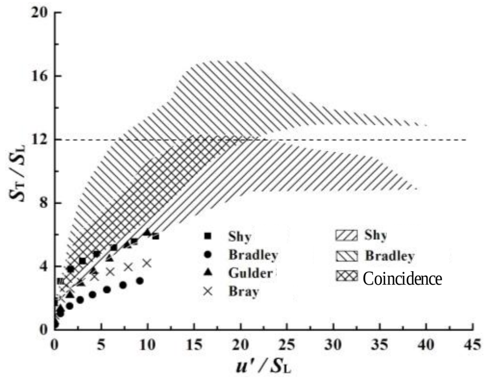


Fig. 14: Turbulent burning velocity modified with the sub-relax factor

In summary, the turbulent burning velocity S_T, predicted by four empirical models, develops too fast compared with the experimental results. A sub-relaxation factor was introduced in this work based on the experimental results obtained by Bradley et al. (1992) and Shy et al. (2000). This factor limits the increasing rate of S_T to the normal range and gives the maximum value, which makes the empirical models more in line with the actual physical law.

10. Comparison with Experiments

The modified turbulent burning velocity model was applied to equation (55), the flame velocity model of the open tube. The flame velocity under gas equivalence ratios of 0.97, 1.21, 1.45 and 1.69 was calculated. The flame velocity and experimental values calculated by different turbulent burning velocity models in Table 7 are shown in Figure 15.

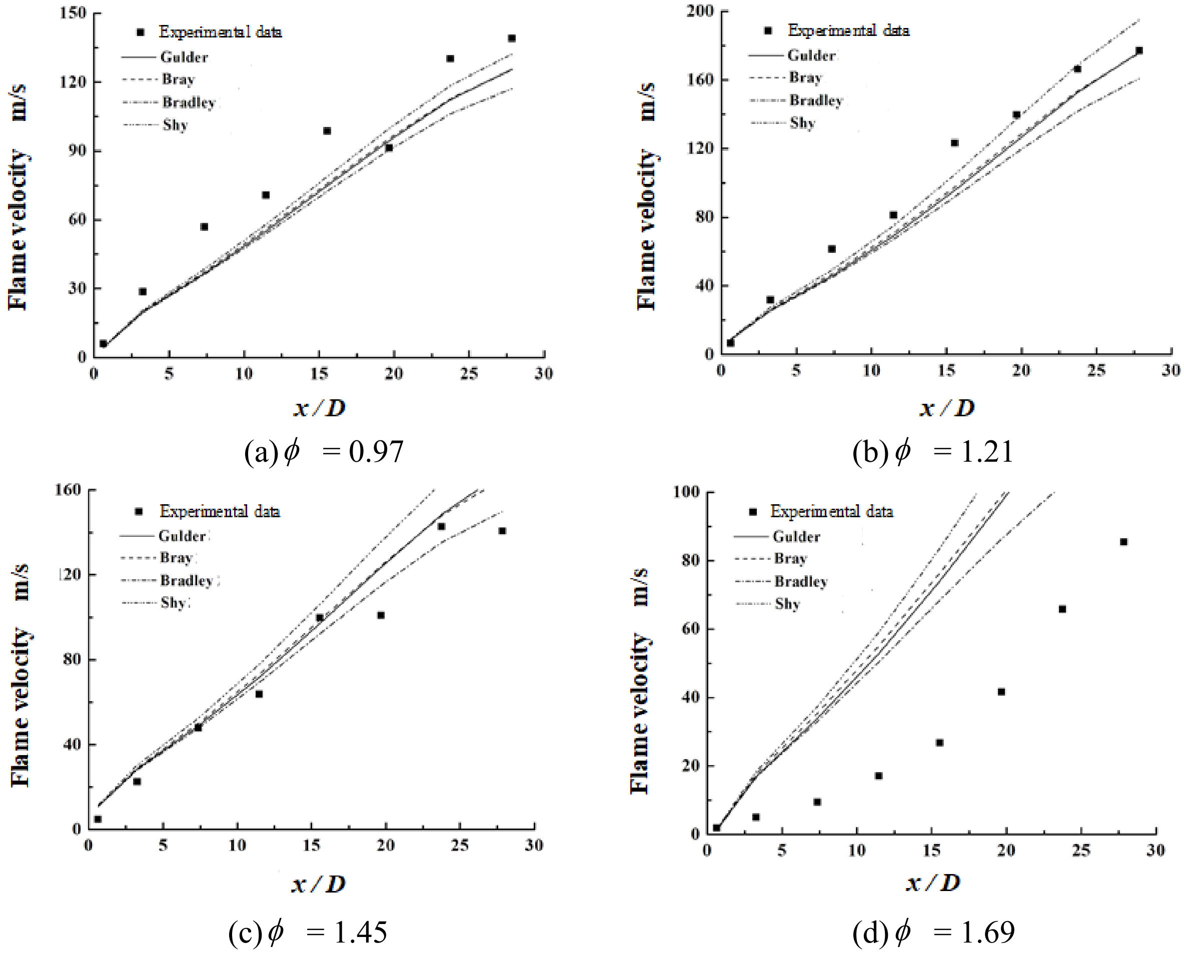
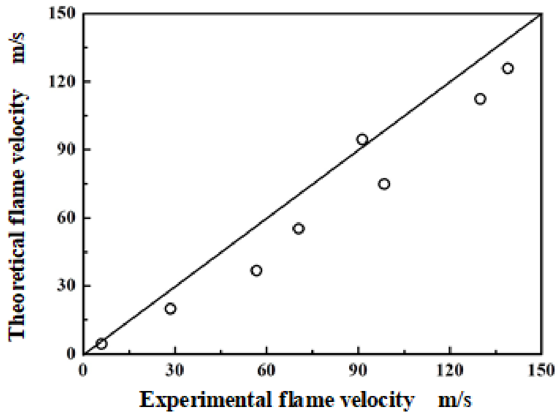


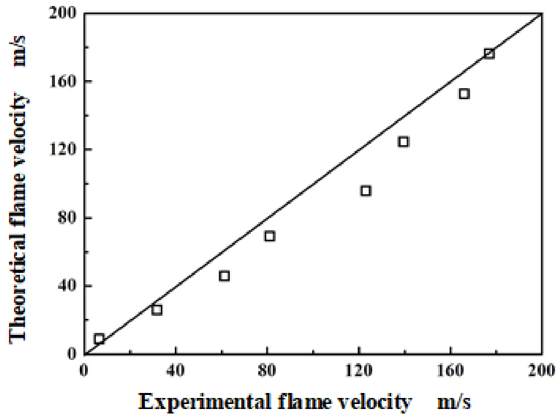
Fig. 15: Comparing flame velocities calculated with models with experimental values

For the premixed gas with equivalence ratio of 0.97, 1.21 and 1.45, the calculated values of the flame velocity agree with the experiment. The calculated value of the flame velocity of the premixed gas with the equivalence ratio of 1.69 is significantly higher than that of the experimental value. The empirical flame velocity model established by theoretical analysis is suitable for the calculation of the flame velocity of the premixed gas with an equivalence ratio in the range from 0.97 to 1.45, corresponding to the volume fraction of LPG from 4% to 6%. When the equivalence ratio is 1.69, the volume fraction of LPG is 7%, which is close to the upper explosion limit of 8%-9% (Mishra and Rahman, 2003), the turbulent burning velocity modified by the sub-relaxation factor may still have its limitations. Comparing the calculated results with different turbulent burning velocity models, Gulder's turbulent burning velocity model are applied to the proposed flame velocity model.

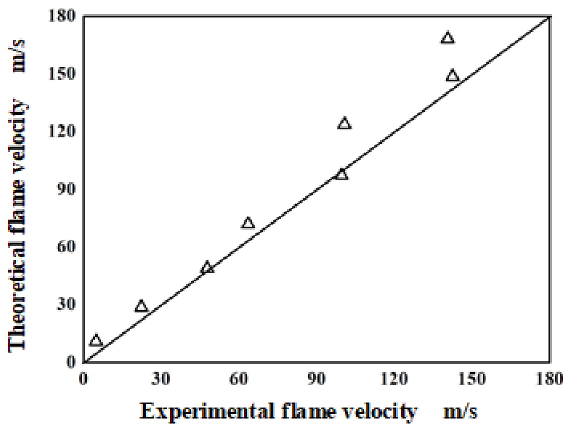
The flame velocities of premixed gas with the equivalence ratio of 0.97, 1.21, and 1.45 calculated using the Gulder turbulent burning velocity model is compared with experimental values, as shown in Figure 16, with the data are shown in Table 9.



(a) ϕ = 0.97



(b) ϕ = 1.21



(c) ϕ = 1.45

Fig. 16: Comparing flame velocities calculated by the model using Gülder coefficients and experimental values

Table 9: Flame velocity values calculated using Gülder model and experimental results

Equivalence ratio φ \ x/D		0.6	3.3	7.4	11.5	15.6	19.7	23.8	27.9
0.97	Experimental value	6.0	28.6	56.8	70.5	98.6	91.4	130.0	139.0
	Calculated value	4.4	19.9	36.8	55.2	74.8	94.6	112.4	125.7
	Relative error/%	26.7	30.4	35.2	21.7	24.1	3.5	13.5	9.6
1.21	Experimental value	6.6	31.8	61.3	81.1	123.1	139.6	166.0	177.1
	Calculated value	8.9	25.9	45.8	69.1	95.8	124.5	152.7	176.2
	Relative error/%	34.8	18.6	25.3	14.8	22.2	10.8	8.0	0.5
1.45	Experimental value	4.8	22.4	47.7	63.5	99.7	100.8	142.5	140.6
	Calculated value	10.9	28.6	48.8	71.8	97.1	123.6	148.5	168.1
	Relative error/%	127.0	27.7	2.3	13.1	2.6	22.6	4.2	19.6

The results show that the calculation of the deflagrative burning velocity of the premixed gas with an equivalence ratio close to 1 is in line with the actual process of accelerated flame propagation. When the equivalence ratio is 0.97, 1.21 and 1.45, the average errors of the experimental and calculated values are 20%, 16% and 27%, and the standard deviations are 10%, 10% and 38%, respectively. The open-tube flame velocity model, equations (53), (55) and (63), is suitable for predicting the development trend of accelerated flame propagation and approximate range of flame velocity.

11. Effect of Expansion Ratio

The expansion ratio E is a measure of the thermal expansion of the combustion products. In the analysis of equation (55), the second item on the right side of equation (55) represents the effect of thermal expansion on flame acceleration, which is one of the main factors affecting flame acceleration. The effect of the expansion ratio on the flame velocity can be analyzed using the Gülder model.

The flame velocity calculated from the Gülder model with an expansion ratio of 3 to 8 is plotted in Figure 17.

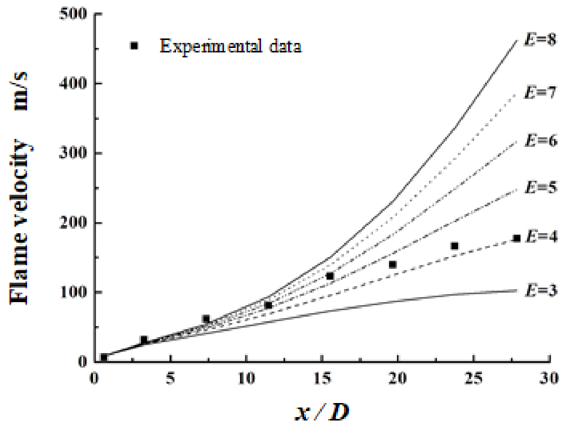


Fig. 17: Flame velocity calculated using Gülder coefficients under various expansion ratios

The calculation of expansion ratio E requires the maximum deflagration pressure under closed vessel conditions, which makes it difficult to apply the flame velocity model in actual tubes, because the maximum deflagration pressure is often unknown. The maximum pressure of deflagration in a constant volume container is between 0.7 to 0.8 MPa (Nagy and Verakis 1983), so the upper limit of the expansion ratio is fixed to 8. By comparing the results of flame velocities under different expansion ratios between 3 to 8 in Figure 17, the maximum difference of flame velocities is not more than 10 m/s when x/D is less than 10. That is, in the tube with x/D less than 10, the expansion ratio has little effect on the flame velocity model, and can be flexibly selected within range of 3 to 8 without depending on the closed deflagration experiments. However, the flame velocity model is suitable for calculating the flame velocity with an equivalence ratio of about 1, where the flame acceleration and pressure rise are very intense. In order to avoid too conservative estimation for flame velocity, the expansion ratio can be taken as 8.

12. Verification of the Flame Velocity Model

In order to further verify the prediction capability and effectiveness of the flame velocity model in an open tube, the experimental data in literature (Chatrathi et al. 2001) was used to calculate the flame velocity under similar experimental conditions.

A 15-m long tube with an inner diameter *D* of 0.1524 m was used by Chatrathi et al. (2001). The ignition end was closed and the other end was open. A Propane/air mixture (volume fraction 4% and equivalence ratio $\phi = 1$) and an ethylene/air mixture (ethylene volume fraction 6.5% and equivalence ratio $\phi = 1$) were used.

The experimental data of the flame velocity along the length of the tube reported by Chatrathi et al. (2001) are summarized in Table 10.

Table 10: Experimental results of flame velocity (m/s) of propane and ethylene in air (Chatrathi et al. 2001)

Distance /m	0.61	1.68	2.29	3.81	5.33	7.16	9.14	10.06	11.13	11.89	12.65	13.72
x/D	4	11	15	25	35	47	60	66	73	78	83	90
Flame velocity of propane air mixture (m/s)	4.1	8.3	11.3	30.2	42.9	64.8	125.6	222.5	299.5	373.6	483.4	579.5
Flame velocity of ethylene air mixture (m/s)	5.6	12.2	19.5	28.6	56.4	74.0	111.5	225.1	412.5	460.0	684.6	885.7

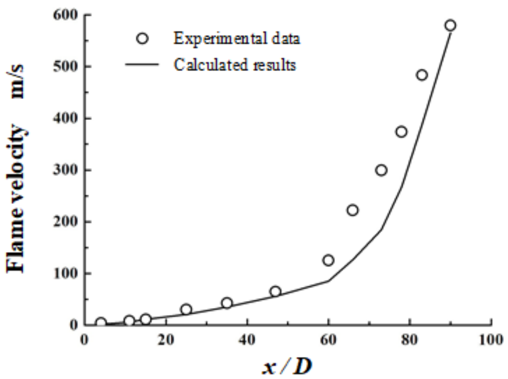
The laminar burning velocities of propane/air and ethylene/air premixed mixtures with an equivalence ratio $\phi = 1$ are 0.392 m/s and 0.445 m/s, respectively, based on the fitting of experimental data (Hermanns and Konnov 2010; Konnov et al. 2001; Metghalchi and Keck 1980; Razus et al. 2010; Vagelopoulos et al. 1994; Zhao et al. 2004). The expansion ratio is $E = 8$. The turbulent burning velocity was calculated using the Gulder model, with $b_1 = 1$, $b_2 = 0.7$, $b_3 = 0.75$, $b_4 = 0.25$.

The empirical coefficients $c_1^{'}$ and c_2 take the average value of the empirical coefficient with equivalence ratios of 0.97, 1.21 and 1.45 in Table 6, that is, $c_1^{'} = 0.16$, $c_2 = 17$.

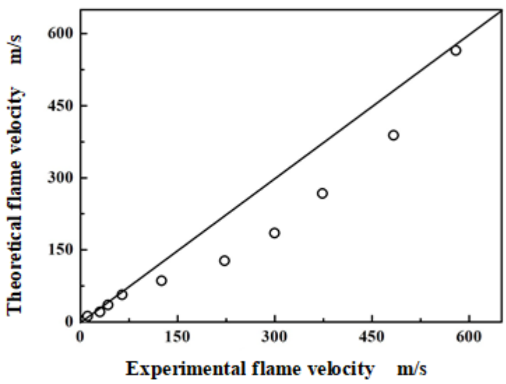
The results of the flame velocity of propane/air and ethylene/air calculated by the open tube flame velocity model, equations (53), (55) and (63), are shown in Table 11, and the comparison between the calculated results and the experimental results is given in Figure 18.

Table 11: Experimental results of (Chatrathi et al. 2001) compared with the calculated flame velocity (m/s)

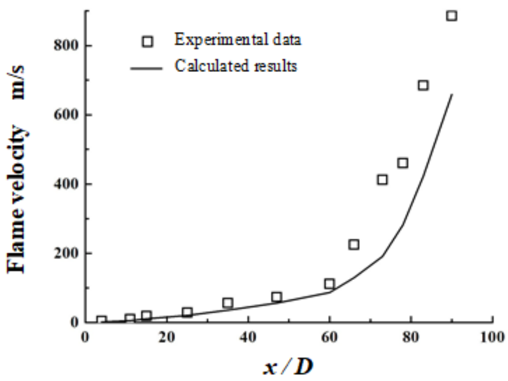
x/D	4	11	15	25	35	47	60	66	73	78	83	90
Propane experimental	4.1	8.3	11.3	30.2	42.9	64.8	125.6	222.5	299.5	373.6	483.4	579.5
Calculated value	2.2	5.8	11.5	20.7	35.0	56.1	85.2	126.7	184.6	267.4	388.6	565.0
Relative error /%	46.3	30.1	1.8	31.5	18.4	13.4	32.2	43.1	38.4	28.4	19.6	2.5
Ethylene experimental	5.6	12.2	19.5	28.6	56.4	74.0	111.5	225.1	412.5	460.0	684.6	885.7
Calculated value	2.1	5.7	11.4	20.6	35.1	56.5	86.4	129.6	191.2	282.0	423.0	657.7
Relative error /%	62.5	53.3	41.5	28	37.8	23.6	22.5	42.5	53.6	38.7	38.2	25.7



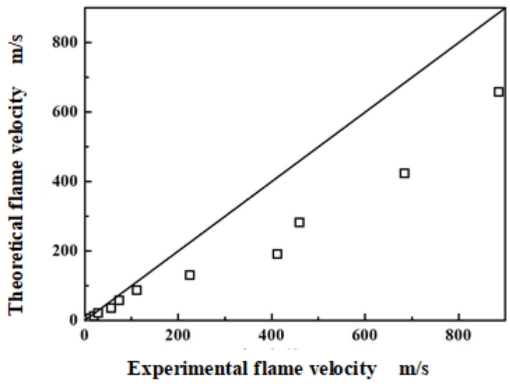
(a) Flame velocity of propane/air



(b) Theoretical and experimental flame velocity of propane / air



(c) Flame velocity of ethylene/air



(b) Theoretical and experimental flame velocity of ethylene / air

Fig. 18: Comparison of theoretical and experimental results of the flame velocity of propane/air and ethylene/air

From the trend of the calculated values of the flame velocity model in Figure 18, the model can reasonably predict the slow and fast acceleration stages during flame propagation. Some slight differences can be observed. The transformation of the slow and fast acceleration stages from the model lags behind the experiment, and the increase of the flame velocity in the fast acceleration stage is less compared with the experimental results. The results of (Chatrathi et al. 2001 and Shy et al. 2000) show that the turbulent burning velocity dominates the flame acceleration in the "slow acceleration stage", while the influence of the turbulent burning velocity is weakened in the "fast acceleration stage". In the flame velocity model, the maximum turbulent burning velocity is determined by the empirical coefficient "Ψ", which makes the calculation results of flame velocity in the "fast acceleration stage" smaller than the experimental results. The average relative errors of the flame velocity of the premixed gases formed by propane/air and ethylene/air are 25.5% and 38.9% respectively, and the standard deviations are 14.0% and 18.2% respectively, which indicates that there is a certain gap in the calculation of the flame velocity at the specified position. In spite of this, considering the complexity of the flame propagation in a tube and the approximation and hypothesis in the establishment of the flame velocity model, the flame velocity model of the open tube can predict the flame acceleration propagation process and the model is suitable for the calculation of the flame velocity at the initial stage of deflagration. In this phase, with the flame velocity less than 100 m/s, the difference between the calculated value and the experimental value is basically in the 10 m/s range. When the flame velocity exceeds 100 m/s, the effect of the flow field on flame propagation is significant and greatly increases the flame velocity. As for the flame acceleration caused by the flow field when the deflagration flame propagates at high speed (over 100 m/s), the model cannot provide accurate values, but it can predict the development trend and approximate range of flame velocity.

13. Conclusions

A flame velocity model for a partially open tube (0.488 m in diameter and 16 m length) was established, and deflagration experiments with LPG/air premixed gas were carried out. The reliability of the flame velocity model was verified by experiments available in literature.

The exponential relationship between flame propagation distance and time was proposed, which was used to establish the flame velocity model. In the final model validation, the exponential relationship makes the calculated results agree well with the experimental results. Based on the analysis of the physical process, there is a relationship between the flame propagation distance and the deflagration pressure and temperature. However, the time-dependent exponential relationship cannot be fully explained in theory.

Compared with the experimental results in this work, the traditional empirical formulas are not accurate enough to predict the increase of the turbulent burning velocity. A "sub-relaxation factor" was introduced to make the empirical formulas more consistent with the actual physical law, whose physical meaning is to limit the maximum range of the turbulent burning velocity.

The validity and accuracy of the flame velocity model were verified by experimental results and data retrieved from the literature. The results show that in the initial stage of flame acceleration (flame velocity less than 100 m/s), the flame velocity model can accurately calculate the flame acceleration. After the flame velocity exceeds 100 m/s, the model can predict the development trend and approximate range of the flame velocity. The flame velocity model can predict better the deflagration flame with high acceleration with the equivalence ratio close to 1. These conditions are dangerous in industrial processes. Besides the LPG/air premixed gas, the model is also applicable to study associated problems for propane/air and ethylene/air.

Declarations of Interest

None.

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