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Effect and mechanism of C_2HF_5 on premixed flame of runaway gas (syngas) in lithium-ion batteries

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Abstract. Lithium-ion battery is a new type of clean energy. Due to manufacturing defects, improper use, unexpected accidents and other reasons, lithium-ion battery thermal runaway fire and explosion accidents are frequently re-ported, and its safety has become an important issue to be solved. In this paper, the effect of second-generation halon substitute C_2HF_5 on runaway gas premix flame of lithium-ion battery are studied by experiments and numerical simulations.The bunsen burner was used to measure the changing trend of the premixed flame velocity of the runaway gas/air under different equivalent ratios and different concentrations of C_2HF_5. The results show that the flame velocity is in good consistency with the model under the conditions of lean flame and low inhibitor addition.The promotion effect of inhibitors on combustion has been verified by bunsen flame. Compared with CH_4, C_2HF_5 is more suitable for inhibiting syngas flame of lithium-ion batteries, and the effect on the rich flames is better than lean flames.

1 Introduction

With the development of industrialization worldwide, human society has become increasingly dependent on fossil fuels. The resulting problems such as excessive greenhouse gas emissions, environmental pollution, and energy shortages have seriously threatened the sustainable development of human society. As a new type of renewable and clean energy, lithium-ion batteries has received widespread attention due to its environmental protection and high efficiency characteristics, and has been applied in many fields such as power source of battery powered vehicles and hybrid electric vehicles [1]. However, in the actual application process, the storage and use of lithium-ion batteries are dangerous. Factors such as manufacturing defects, overcharge, impact, and short circuit can easily cause thermal runaway of lithium-ion batteries and release high heat [2]， and generate a large amount of toxic and combustible gas mixture[3]. Therefore, it is necessary to propose corresponding solutions to improve the safety and reliability of lithium-ion batteries.

The fire extinguishing mechanism of halon extinguishing agent (1211,1301,2402) widely used in the early days is chemical fire extinguishing. However, at the same time, halon was banned in 1987 due to its destructive effect on the ozone layer [4].

C_2HF_5 is a new halon replacement product developed by dupont of the United States, with zero ODP and low GWP and ATL values, listed in NFPA-2001(2018)[5] and ISO 14520 (2015)[6] standards. At room temperature and pressure, C_2HF_5 is a colorless, almost odorless, non-conductive, no residual clean gaseous chemical extinguishing agent that is compatible with rubber and plastic sealing materials. Due to the advantages of low boiling point and low potential greenhouse effect, short atmospheric survival time and superior fire extinguishing performance, the U.S. Department of Defence chose C_2HF_5 as the fire protection for aircraft engines.

The FAA conducted aerosol tank tests on C_2HF_5 found that when the amount of added C_2HF_5 was lower than its inert concentration (8.9%), the explosion pressure was 2.6 times higher than that in the dry test[7,8], and the flame combustion was strengthened. This phenomenon of enhanced combustion has attracted the attention of scholars. Pagliaro et al. [9] measured the flame velocity and pressure changes of methane/air premixed laminar flow with different amounts of added C_2HF_5 using a constant volume burner. Babushok et al. [10] established a model and found through simulation calculation that the addition of C_2HF_5 promoted combustion in the lean combustion side. NIST's Takahash et al. [11] tested with a cup burner and found that the addition of a certain amount of C_2HF_5 would increase the heat release rate, thus promoting combustion.

The syngas fuel used to simulate the thermal runaway of lithium-ion batteries is mainly composed of H_2 and CO, and may also contain N_2, CO_2, water vapor (H_2O), hydrocarbons and other substances, such as CH_4. The effect of syngas combustion composition ratio on the minimum ignition energy, flame velocity and flame stability is the current research hotspot, but there are few studies on the effect of halon replacement on the

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combustion rate of syngas. In particular, the composition ratio of syngas used in this paper is based on the composition of the thermal runway gas of lithium ion battery measured in the experiment.

Based on the Bunsen burner method, this article studies the influence of the amount of C_2HF_5 on the adiabatic temperature and flame velocity in the mixed gas/air laminar premix flames with different equivalence ratios. The first purpose of current work is to reproduce the experimental phenomenon of FAA-ACT in Bunsen burner experiment. To test the performance of C_2HF_5 as an inhibitor, and to discuss the feasibility of application. The second purpose of this paper is to enrich the experimental values of the laminar flame velocity of syngas in lithium-ion batteries.

2 Experimental methodology

2.1 Experimental setup

The content and composition of the fuel was the same as in our previous research [12], i.e., H_2-29.6%, CO-22.3%, CO_2-35.5%, CH_4-6.9%, and C_2H_4-5.7%.

Four combustion diameters (diameter 8, 10, 12, and 15mm) are designed for the nozzle of the tubular burner, and the pipe length is designed to be 900mm, all of which are made of stainless steel. At the same time, the smoothness of the nozzle edge of the burner is improved to ensure that the air flow at the outlet of the nozzle of the burner is within the laminar flow state range. In order to reduce the influence of flame stretch and curvature on the measurement of flame velocity, different nozzle diameters are set to ensure flame stability at low equivalence ratio. The experimental data in this paper are mainly obtained at 10mm and 12mm diameters (8mm flame has poor stability, and 15mm is limited by gas velocity). When $\varphi \geq 1$, the measurement uncertainty of 12mm and 10mm nozzles is consistent [13]. The system diagram of the experimental device is shown in Fig. 1.

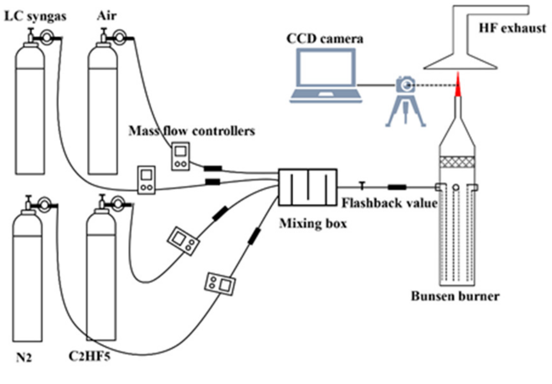

Fig. 1. Schematic diagrams of the experimental apparatus.

Mass flowmeter should be used in gas pipeline control (FLOWS INSTRUMENT company Dmass mass flowmeter, the entire range accuracy of ±1.0% in the range, repeatability of ±0.1%). Before the trial of the syngas are collected and used to use GC-MS INSTRUMENT analysis, ensure that each group of experimental mixed gas composition error less than 0.1% (21% of synthetic air is 79% N_2, O_2). In the experiment, the flame height maintained was 2 to 3 times of the nozzle diameter of the burner. Excessively low flame would increase the heat loss of the burner [13], and excessively high flame would have an effect on the elongation rate. The flame image was captured by a 105mm, f / 4.5 UV lens with a resolution of 2320 × 1720 and a pixel size of 7μm × 7μm with a shooting speed of 500FPS with a high-speed CCD camera. 500 images were taken in each experimental group and averaged to reduce the influence of disturbance caused by the surrounding environment. All experiments were carried out at standard atmospheric pressure, and the temperature of the unburned mixture was 298±2K.

In the experiment, the uncertainty of gas mix ratio comes from the uncertainty of fuel component measurement and gas flow velocity measurement, which is about 0.002-0.004. The total uncertainty of S_L obtained by the test is about 1.5-3.0cm/s.

2.2 Laminar flame velocity measurement method and flame stability analysis

Laminar flame velocity was measured using a Cone Angle Method (Fig. 2.) in which the flame propagated to unburned mixture at an Angle α/2. The calculation formula of laminar flame velocity is as follows:

$$Su = U \sin\alpha/2 \tag{1}$$

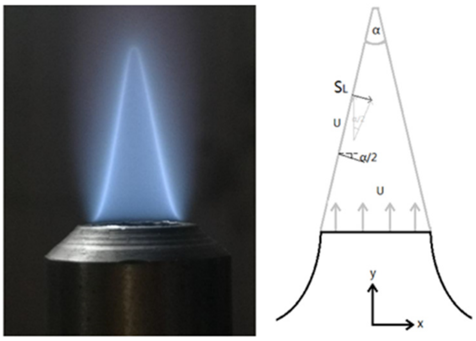

Fig. 2. Measure laminar flame velocity (angle method).

The stable flame morphology is related to the nozzle velocity, combustion velocity, effective Lewis number and environmental conditions. The instability of gas flow and the stretching phenomenon of flame will greatly affect the flame stability of tubular burner. In the process of premixed gas combustion, the ratio of heat transfer to mass diffusion plays a decisive role in flame morphology and stability, and the effective Lewis number is the key parameter of flame stability. In order to reduce the influence of these factors, the method of quantifying the effective Lewis number at different equivalence ratios is adopted. In the study of this paper, the effective Lewis number is first calculated for any working condition to ensure that it is within the stable range. When the effective Lewis number is approximately 1, the flame can be considered stable.

Based on Lapalme's [14] method for determining the effective Lewis number of multi-component mixed-gas fuel, according to the composition of syngas, the effective Lewis number is calculated at different equivalence ratios [15,16]:

$$Le_{f/O_2} = 1 + \frac{(Le_{exc}-1)+(Le_{def}-1)A_1}{1+A_1} \tag{2}$$

Where, $Le_{f/O2}$ is the effective Lewis Numbers of syngas/oxygen, Le_{exc} is the effective Lewis Numbers of reactant excess and Le_{def} is the effective Lewis Numbers of reactant shortage.Parameters $A_1 = 1 + Ze(\Phi - 1)$, Φ as reactant under the condition of excess and deficiency relative to the quality of the chemical equivalence ratio (when $\varphi \leqq 1$, $\Phi = 1/\varphi$;When the $\varphi > 1$, $\Phi = \varphi$), Ze for Zel' dovich number, expression is:

$$Ze = E_a(T_{ad} - T_u)/(RT_{ad}^2) \tag{3}$$

Where R is the general gas constant, E_a is the activation energy, and the expression is:

$$E_a = -2R\partial\, ln(rS_L)/\partial(1/T_{ad}) \tag{4}$$

Based on the method of Sun [17], the sensitivity of laminar flame velocitys to flame temperature was obtained to determine the value of E_a under the condition of not changing the mixture equivalence ratio by making small adjustments to the content of CO_2.

2.3 Modeling

The simulation was carried out by CHEMKIN-PRO program group [18-20]. The Back Diffusion ffect, Heat Diffusion Soret effect and Molecular Diffusion effect of gas inlet boundary were taken into account in the setting. The mixture of syngas and air was calculated in the Mixture-averaged method. The simulated environmental conditions were normal temperature and pressure (298K, 0.101Mpa), and the air composition was the same as that of the synthetic air. The design parameters CURV were set as 0.05 and 0.05 respectively, and the generated mesh quantity ranged from 350 to 500. The mesh quantity met the requirements of grid independence, and the absolute error of laminar flame velocitys was < 1%.

3 Results and discussion

3.1 Experimental validation

In order to evaluate the reliability of the experimental device, the premixed flame velocity of CH_4/air and syngas/air within a certain equivalent range (298K, 0.1 MPa) was measured, and compared with the literature and model values. The results are shown in the Fig. 3.

For the CH_4/air premixed flame, as shown in Fig. 3., due to the different research methods of scholars, different mixing ratios and measurement errors, the data points are relatively scattered. But in general, each data point is consistent with the laminar flame velocity variation trend simulated by the model. The maximum value of CH_4/air laminar flame velocity occurs between 1.0 and 1.2, with a velocity distribution of 35~41cm/s. The maximum laminar flame velocity obtained by the author is 40.3cm/s (φ=1.1), and the value is within a reasonable range. Between mixed gas φ=0.8~1.1 and other scholars use different methods to measure the data is relatively close, especially in the lean flame (φ≤1.0).

The study of Burbano [21] showed that the prediction ability of different hydrocarbon combustion mechanism models was consistent when the equivalence ratio was less than 1.5, which was also the focus of this paper. At present, the obtained experimental data is slightly higher than the research results of other scholars (only lower than the Lintercis data), which is highly consistent with the model used in the whole range.

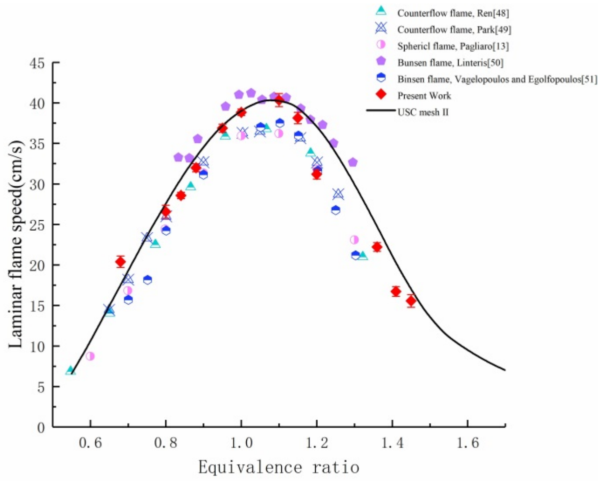

Fig. 3. Flame velocity and calculated adiabatic flame temperature of premixed CH_4/air flames with added C_2HF_5 for different initial equivalence ratios; line: simulations using detailed mechanism.

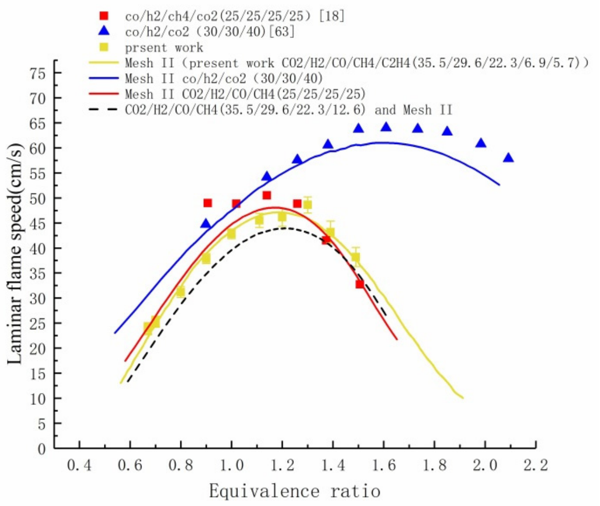

Fig. 4. Laminar flame velocity of syngas/air (298K, 0.1MPa) and previously corresponding published results.

No measurements have been made for the combustion of syngas (component) in lithium ion batteries. According to Le-Chatelier formula [22], the flammable limit calculated in normal conditions (298K, 0.1mpa) syngas/ air in a certain equivalence ratio range is 7.6%~52.5%. The corresponding equivalence ratio is φ=0.22~2.99. Experimental measurement and model simulation were carried out within the range of equivalence ratio, and the results were compared with the research conclusions of other scholars on syngas with similar components, Fig. 4.

As shown in Fig. 4, the experimental value of wang [23] has a large error in the rich combustion area of φ>1.4, and the experimental value has a good consistency with the simulation results under other working conditions. Lapalme [24] showed that the increase of CO_2 and CH_4 content in syngas would reduce the flame velocity and lead to the reduction of the equivalent ratio of the maximum flame velocity. The flame velocity curve moved to the lean flame side, which was more sensitive to CH_4 content. The CO_2 content in the syngas component of the lithium ion battery used is higher than 25%, the CO content is lower than 25%, and the CH_4 content is between 0 and 25%. As a result of the component change, the inhibition effect on flame velocity is enhanced and the promotion effect is weakened, making the experimental and simulated values lower than Lapalme experimental conditions. While in the case of φ>1.4, a situation occurred in which the experimental speed of synthetic gas used was higher than Lapalme experimental condition, which can be explained by the use of synthetic gas H_2:CO>1:1, H_2 in the rich combustion region has a greater impact on the flame velocity[16].

In conclusion, the simulation and experimental results of CH_4/air and syngas/air premixed laminar flames are in good agreement with the research conclusions of other scholars. The verification experiment shows that the device and model can get reasonable experimental results. Although the verification experiment was carried out before adding C_2HF_5, it was inserted into the overall experiment process to ensure the reliability of the device and the repeatability of the experiment.

3.2 Analysis of laminar flame velocitys variation

The USC Mech Version II model has achieved good consistency in the CH_4/ air premix flame process without adding C_2HF_5, but its application in the synthesis gas of lithium ion batteries is unknown. In the current study, the equivalence ratio (not adding inhibitor) within the range of 0.6 ~1.2 add C_2HF_5 (X_a = 0%~5%, within the scope of the published data is more, at the same time, this paper mainly focus on lean burn condition add trace inhibitor changes in the velocity of the flame) of CH_4/air. Premixed flame of synthetic gas/air has carried on the experiment and simulation, C_2HF_5 mechanism research needs based on the experiment the Bunsen burner flame. Inhibitor addition is carried out under the condition of determining the ratio of fuel to air. The initial conditions are T_0=298±2K and P_0= 0.1Mpa. The addition of inhibitors is carried out in the form of the volume proportion in the mixture:

$$X_a = X_{(agent)}/\left[X_{(fuel)} + X_{(air)} + X_{(agent)}\right] \qquad (5)$$

Where X (agent) is the mole number of inhibitor components in the mixture. Novec 1230 was selected as the research baseline because its experimental fire-extinguishing concentration was low, and it was also the second generation of halon substitute product, so the data was of certain comparative significance. At the same time, the simulated and experimental values of N_2 only playing a thermal role were set as the background baseline, as shown in Fig. 5.

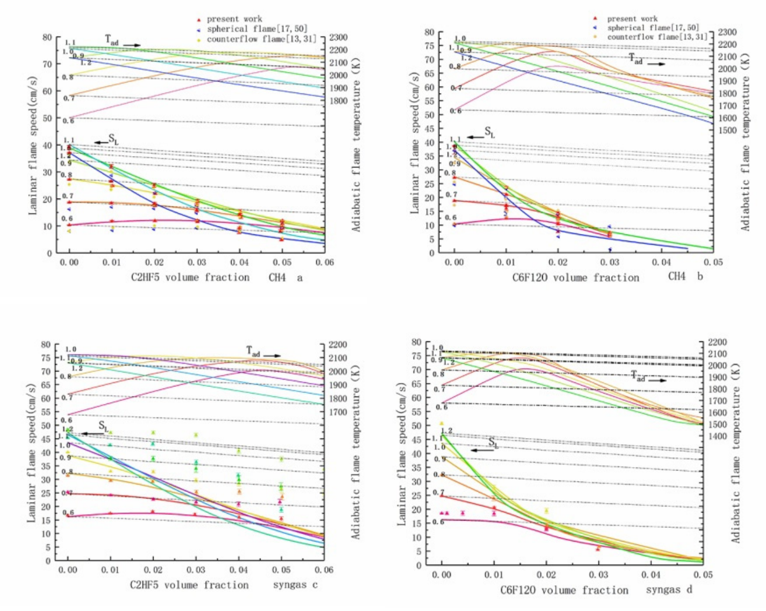

Fig. 5. Flame velocity and calculated adiabatic flame temperature of premixed CH_4/air (a,b) syngas/air (c,d) flames with added $C_6F_{12}O$ (Novec 1230) for different initial equivalence ratios; lines: simulations using detailed mechanism；symbols: experimental data.

Compare methane/air premixed flame velocitys (C_2HF_5 Fig. 5a and Novec 1230 Fig. 5b) measurement value, the predicted values and the published experimental measurement data hedge flame compare, it can be found that the data is very close. That further prove that adopted by the numerical model of equivalence ratio in range of 0.6 ~ 1.2 can better predict inhibitors added case flame properties change. At the equivalent of close to the combustion limit (φ=0.6), the model predicted value is slightly higher than the experimental value. For example, when C_2HF_5 X_a=0.02, the simulated value was 2.6% higher than the experimental value (Bunsen burner flame), and when Novec 1230 X_a=0.02, the simulated value was 30% higher than the experimental value. This is due to the limitation of flame combustion experiment in lean flame side. Compared with other equivalent experiments, flame velocity is lower and flame radiant heat loss is greater. With the increase of gas equivalence ratio, the gap between experimental value and simulated value is further narrowed. From the overall trend, the burnt-out side has a good fitting degree in the range of φ=0.7~1.0. In the condition of rich combustion-side (φ>1), the simulated value showed a trend of being lower than the experimental value, and the inhibitory effect of the inhibitor was overestimated. When φ=1.2, C_2HF_5 X_a=0.02, the simulated value is lower than the experimental value 3.38%, 1230 X_a=0.02, the simulated value is lower than the experimental value 12.25%. This is caused by the entrainment of ambient air by the Bunsen burner flame in an open environment (further burning of excess fuel). However, with the further increase of inhibitor addition, the consistency between the simulated and experimental values became better.

As for premixed syngas/air lean flame at φ= 0.6 (C_2HF_5 Fig .5c, Novec1230 Fig. 5d). The flame velocity increases first and then decreases with the increase of the addition amount of inhibitor (experimental and simulation). Such as relative to add C_2HF_5 flame velocity, the size of the X_a is respectively 1%, 1.5%, 2%, 2.5%, 3% of the cases, the flame velocity increased by 6.32%, 7.38%, 7.13%, 5.48%, 1.99%. When X_a=0.001 and 0.004, the combustion rate increased by 1.8% and 3.9%. The corresponding promotion effect was more obvious in methane flame (ab). Subsequently, the flame velocity decreased with the increase of addition amount. Previous studies have involved the analysis of the reasons for promoting flame combustion [9, 25-28], which is caused by the competitive relationship between the thermal effect of the inhibitor itself as a fuel combustion and the flame inhibition effect of the contained F element. And in the equivalence ratio of φ>0.67 showed inhibitory effect, chemical equivalent and more sensitive to the addition of inhibitors, in the case of φ=0.7, 1.0, 1.2, add C_2HF_5 X_a=0.01, flame velocity reduced by 4.73%, 6.17%, 27.89%, this is because at this time inhibitor containing F inhibition is stronger than its thermal effect as fuel.

However, at the range of 0.6~1.0 equivalence ratio, the consistency between the simulation and the experimental values becomes worse with the increase of inhibitor addition. Respectively, when the equivalence ratio was 0.6, 0.7, 0.8, 0.9, 1.0, and the addition amount of C_2HF_5 X_a=2%, the difference between the experimental and simulated values was 3.42%, 0.9%, 7.13%, 9.22%, and 28.44%. This is due to the limitations of the Bunsen flame and the nature of the syngas itself. The reaction rates of combustible gas components in syngas and oxygen in ambient gas are different, furthermore, under the action of extinguishing agent, the combustion equilibrium of syngas was broken. Nevertheless, the numerical model ignores the large error caused by the flame disturbance caused by the high addition of extinguishing agent. The addition of Novec 1230 also has similar conclusions, but the simulation conclusion of the model is more consistent than that of C_2HF_5.

Further discussion on temperature change. At the lean flame and chemical equivalent flame (φ=0.6~1.0), laminar adiabatic flame temperature with low addition of inhibitor will lead to an increase in temperature. Under the condition of the same proportion of inhibitor addition, the temperature rise of adiabatic flame temperature increases with the lower the fuel equivalent ratio (0.6, X_a (C_2HF_5, Novec 1230)=0.01). Compared with C_2HF_5, the rise of flame temperature is more sensitive to the addition of Novec 1230. Novec 1230 can make the adiabatic flame temperature reach the peak faster at the same low amount of premixed gas. This provides a certain basis for the explanation of the increase of fire speed. Temperature has a particularly significant influence on the fire speed. Previously, some scholars have put forward relevant conclusions about the relationship between temperature and flame velocity [29].

In the process of experimental simulation, it was found that if the flame velocity of 5cm/s (premixed gas φ=0.55) as the laminar flame limit flame velocity[30,31], when mixed gas φ=0.5, using the model is not able to calculate. When adding C_2HF_5 X_a=0.01, laminar flame velocity is 10cm/s. From the perspective of simulation, this indicates that the addition of inhibitors with fuel properties will expand the combustion limit of mixed gas [9,12,32,33]. Previously, some scholars used constant volume incendiary bombs to conduct experiments and obtained similar conclusions[10], which further supported the conclusion of promoting combustion with low equivalence ratio and low addition, and verified the numerical simulation results in this article.

For the premixed syngas used, USC Mech Version II model can obtain better simulation results in the case of mixed gas in the lean combustion side and adding low inhibitory dose. Even in the case of poor consistency in the rich combustion side simulation, but in the case of φ>1, inhibitors show inhibitory effect, which is not the focus of this paper. Compared with previous applications of CH_4 and C_3H_8 flame[9,10], C_2HF_5 and Novec 1230 are more suitable for the flame generated by uncontrolled heat gas in lithium ion batteries. In fact, from the comparison of data in ac and bd graph, we can see that under the condition of φ=0.6 and the addition of inhibitor X_a=0.01, the combustion rate of methane flame increased by 10.93% (C_2HF_5) and 17.43% (Novec 1230). For the gas distribution flame, the flame velocity increased by 6.32% (C_2HF_5) and decreased by 1.51% (Novec 1230) with the same amount of additive. The different flame promotion effect is related to the fuel properties of the inhibitors used. With the same addition amount, Novec 1230 can make the flame temperature reach the peak earlier, and the peak value moves to the rich combustion side. In terms of the flame promotion effect on the poor combustion side, Novec 1230 promotes the peak flame velocity more than C_2HF_5 (methane flame).

For the condition of rich combustion (as shown in Fig. 6), the simulation results can be compared. When the same amount of inhibitor was added, the inhibitory effect of Novec 1230 was better than that of C_2HF_5 (as can be seen from the tangent slope of the curve in the Fig. 6.).

For φ =1.0~1.6, the initial flame velocity and temperature is still at a high value, when adding a small number of inhibitors can quickly get a better control. With the gradual increase of inhibitor addition, the slope of laminar flame velocitys and temperature change gradually decreases, and finally reaches a stable value at a high dosage, which is consistent with the description of inhibitor saturation effect in literature [34,35]. Therefore, the focus of this paper is still a discussion on the demarcation point of promoting and inhibiting the burnt-out side.

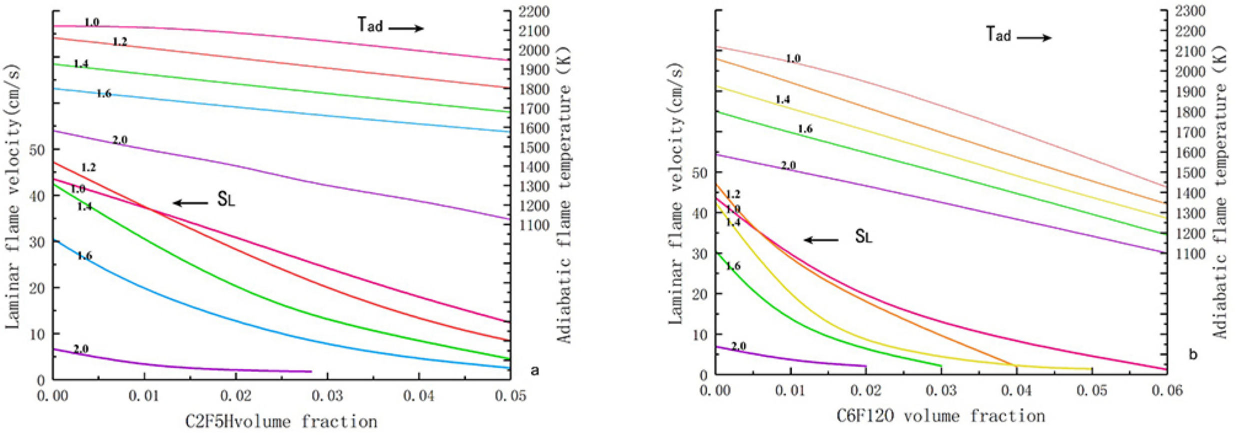

Fig. 6. Burning velocity and calculated adiabatic flame temperature of premixed syngas/air (a,b) flames(φ≥1) with added C_2HF_5 (Novec 1230) for different initial equivalence ratios; lines: simulations using detailed mechanism.

3.3 Changes of flame morphological photographs

In previous studies on the application of halon substitutes, many scholars used pool fire experiments or cup-burner experiments loaded on the oxidant end, which would generate similar diffusion flames similar to the actual flames. Therefore, the experimental conclusions are often used to guide practical engineering applications. However, the mechanism and efficiency of action of inhibitor and fuel gas in premixed condition are different, so it is necessary to conduct Bunsen burner flame experiment. For the measurement of laminar flow velocity in premixed combustion, strict experimental conditions are required for the analysis of instantaneous schlieren images obtained from constant volume incendiary bomb experiments. However, the structure of the opposed flame is different from the actual flame because it is a one-dimensional plane flame.

With the inhibition of syngas/ air flame as an example, Fig. 7. shows the equivalence ratio of φ=0.6, added C_2HF_5 (added amount X_a=0~0.04) and $C_6F_{12}O$ (added amount X_a=0~0.02) syngas/air premixed flame photos (inhibitor involved in CH_4/air premixed flame combustion process chemical thermodynamics and kinetic mechanism has been confirmed).

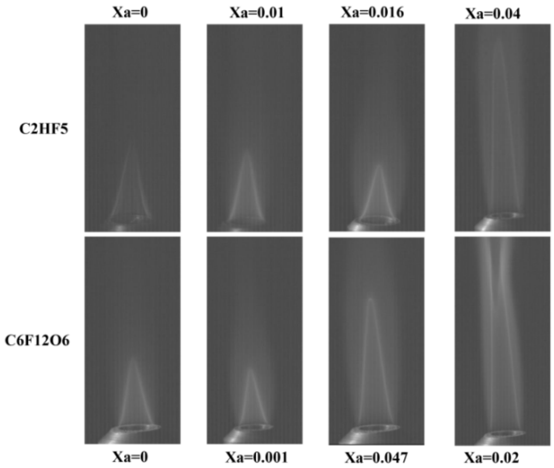

Fig. 7. Morphological photographs of the premixed syngas/air (φ=0.6)Bunsen flames with the addition of 0~0.02 $C_6F_{12}O$(upper flames) and 0~0.04 C_2HF_5(lower flames); conditions: (298K, 0.1MPa).

When no inhibitor was added, the conical flame was light blue with obvious contour. When the trace inhibitor was added (C_2HF_5 X_a=0.005, Novec 1230 X_a=0.001, which showed the effect of promoting flame combustion), the flame turned bright blue and the reaction area was thickened. With the increase of the amount of inhibitor, the flame length was further shortened (the combustion rate was increased). When the C_2HF_5 was X_a=0.016 and the $C_6F_{12}O$ was X_a=0.0047, the flame combustion rate reached the extreme value of the promotion effect under this equivalent. At this time, the flame was the most active and brighter, reflecting a significantly larger area (compared with the condition without inhibitor). This is because the inhibitor C_2HF_5, Novec 1230) itself, as part of the fuel, participates in the combustion process, consumes oxygen and produces a heating reaction, which promotes combustion and expands the flame reaction area. When the amount of inhibitor was further increased, the flame brightness decreased while the length was lengthened. As the condition for the existence of the conical stable flame of Bunsen burner is that the flame combustion velocity is equal to the airflow velocity, when the flame velocity decreases, the root of the flame tends to break away from the edge of the burner under the action of no gas (on the contrary, it is tempering). In fact, at this time, the premixed flame has reached the point where it can be extinguished at random under certain concentration of inhibitor (that is, small changes in air flow may cause the flame to blow off). In addition, as the density of combustion gas decreases under the action of heat, the flame will be aggravated by the influence of buoyancy, which will also lead to the extinction of the flame.

Bunsen burner flame (low yield, low inhibitory concentration to promote combustion) can clearly reproduce the phenomenon of flame intensification in the FAA-ACT experiment, and can intuitively observe the stable and bright conical premixed flame. At the same time, under the action of inhibitor, the flame burning speed, thermal diffusion and frontal position will change. Therefore, the application of premixed flame test equipment of tubular burner can also be used to deeply understand the phenomenon of flame intensification in FAA-ACT experiments.

4 Conclusions

The promotion/inhibition properties of the second generation halon replacement extinguishing agent C_2HF_5 (Novec 1230 and N_2 as pairs) on the heat runaway gas syngas flame (CH_4/ air premix flame as contrast) of the lithium ion battery were studied by Bunsen burner experiment. The parameters of laminar flame velocity and adiabatic flame temperature with addition of C_2HF_5 (X_a=0~0.06), Novec 1230 (X_a=0~0.05) and N_2 were studied and simulated in the range of equivalence ratio φ =0.6~1.2. The cone Angle method was used to measure the flame velocity, and the USC Mech Version II model was experimentally verified. With a low additive amount on the lean side (φ=0.6~1.0, the inhibitor additive amount range was related to the nature of the inhibitor used), a good consistency was obtained, and a large deviation was observed in the simulation on the rich combustion side.

In terms of laminar combustion velocity, compared with previous applications of CH_4 and C_3H_8 flame, C_2HF_5 and Novec 1230 are more suitable for the flame generated by thermal runaway gas in lithium ion batteries. With φ =0.6 and inhibitor addition X_a=0.01, the combustion rate of methane flame increased by 10.93% (C_2HF_5) and 17.43% (Novec 1230). For the gas distribution flame, the flame velocity increased by 6.32% (C_2HF_5) and decreased by 1.51% (Novec 1230) with the same amount of additive. According to the kinetic model analysis, the inhibitor will promote the reactivity under the condition of low equivalent and low addition, and then increase the flame burning speed.

Bunsen flame reappeared the flame intensification phenomenon in the FAA-ACT experiment with low equivalent and low inhibitory concentration, and the flame intensification effect could be clearly observed through the change of flame shape, position and color. The results show that the flame height decreases with the increase of laminar flame velocity. When the flame is promoted by the inhibitor, the flame is brighter and a lot of heat is released. The success of Bunsen flame experiment provides a convenient experimental approach for further analysis of combustion products. In practical engineering application, the dosage of inhibitor is usually higher than the designed concentration. However, in the case of low concentration addition, the role of promoting combustion cannot be ignored, and this characteristic also exists in the case of premix of other fluorocarbon inhibitors and hydrocarbon fuels. Current experiments show that it is feasible to use Bunsen burner flame to study the flame promotion/inhibition effect of inhibitors.

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References

1. Martínez C.M, Hu X, Cao D, Velenis E, et al. IEEE Trans. Veh. Technol **66**, 1-16 (2016)
2. Feng X, Fang M, He X, et al. J. Power Sources **255**, 294-301 (2014)
3. Koch S, Fill A, Birke KP. J. Power Sources **398**, 106-112 (2018)
4. Benedick. Int. N. **1**, 231-246 (1987)
5. Association NFP. NFPA 2001 (2018 Edition). MA 021692018.
6. Standardization IOf. ISO14520-1(Third edition 2015-12-01). 2015.
7. Reinhardt J.W. Behavior of bromotrifluoropropene and pentafluoroethane when subjected to a simulated aerosol can explosion. In: Administration FA, editor. Washington,D.C. USA2004.
8. Reinhardt J.W. Aircraft cargo MPS test of FK-5-1-12. In: Administration FA, editor. International Aircraft Systems Fire Protection Working GroupOctober 25-26, 2006.
9. Pagliaro J.L, Linteris G.T, Sunderland P.B, et al. Combust. Flame **162**, 41-49 (2015)

10. Babushok V.I, Linteris G.T, Burgess Jr. D.R, et al. Combust. Flame **162**, 1104-1112 (2015)
11. Takahashi F, Katta V.R, Linteris G.T, et al. Proc. Combust. Inst. **35**, 2741-2748 (2015)
12. Liu L, Du Z, Zhang T, et al. Int. J. Hydrogen Energy **44**, 22282-22300 (2019)
13. Bouvet N, Chauveau C, Gkalp I, et al. Int. J. Hydrogen Energy **36**, 992-1005 (2011)
14. Linteris G.T, Babushok V.I, Sunderland P.B, et al. Proc. Combust. Inst. **34**, 2683-2690 (2013)
15. Addabbo R, Bechtold J.K, Matalon M. Proc. Combust. Inst. **29.2**, 1527-1535 (2002)
16. Bechtold J.K, Matalon M. Combust. Flame **127**, 1906-1913 (2001)
17. Sun C.J, Sung C.J, He L, et al. Combust. Flame **118**, 108-128 (1999)
18. Kee RJ, Rupley FM, Miller JA. Chemkin-II: A Fortran chemical kinetics package for the analysis of gas-phase chemical kinetics. United States1989.
19. CHEMKIN-PRO 15101. Reaction design: San Diego, CA; 2013.
20. Kee RJ, Warnatz J, Miller JA. Fortran computer-code package for the evaluation of gas-phase viscosities, conductivities, and diffusion coefficients. [CHEMKIN]. United States1983.
21. Burbano H.J, Pareja J, Amell A.A. Int. J. Hydrogen Energy **36**, 3232-3242 (2011)
22. Lau L.J. J Econ Theory. **12**, 131-163 (1976)
23. Wang Z.H, Weng W.B, He Y, et al. Fuel. **141**, 285-292 (2015)
24. Lapalme D, Seers P. Int. J. Hydrogen Energy **39**, 3477-3486 (2014)
25. Moffat R.J. Exp. Therm Fluid Sci. **1**,3-17(1988)
26. Pagliaro J.L, Linteris G.T. Fire Saf. J. **87**,10-17 (2017)
27. Wu, Xu, Yong, et al. J. Fire Sci. **34**, 289-304 (2016)
28. Ren X, Jiang Y, Xu W. J. Fire Sci. **34**,416-430(2016)
29. Stephen R. An Introduction to Combustion: Concepts and Applications. Boston2000.
30. Egerton A, Thabet S.K. Proc. R. Soc. London, ser. A. **211**, 445-471 (1952)
31. Westbrook C.K. Combust. Sci. Technol. **34**, 201-225 (1983)
32. Shebeko Y.N, Azatyan V.V, Bolodian I.A, et al. Combust. Flame **121**, 542-547 (2000)
33. Azatyan V.V, Shebeko Y.N, Shebeko A.Y, et al. Russ. J. Phys. Chem. A **4**, 760-768 (2010)
34. Noto T,Babushok V,Hamins A, et al. Combust. Flame **112**, 147-160 (1998)
35. G.T. Linteris AM, Tsang W. Halon Replacements ACS Symposium Series 611: American Chemical Society; p. 260-274(1995).