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Inhibition Effect of $KHCO_3$ and KH_2PO_4 on Ethylene Explosion

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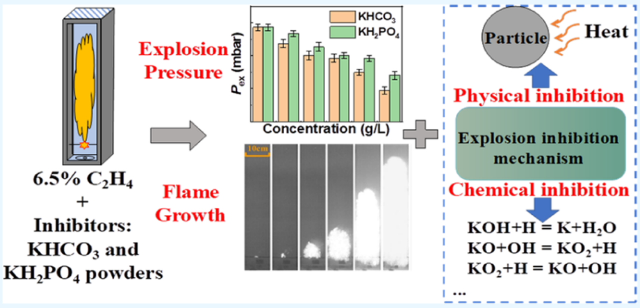

ABSTRACT: The explosion risk of ethylene (C_2H_4) seriously hinders safe development of its production and processing. To reduce the harm caused by C_2H_4 explosion, an experimental study was conducted to assess the explosion inhibition characteristics of $KHCO_3$ and KH_2PO_4 powders. The experiments were conducted based on the explosion overpressure and flame propagation of the 6.5% C_2H_4−air mixture in a 5 L semi-closed explosion duct. Both the physical and chemical inhibition characteristics of the inhibitors were mechanistically assessed. The results showed that the 6.5% C_2H_4 explosion pressure (P_{ex}) decreases by increasing the concentration of $KHCO_3$ or KH_2PO_4 powder. The inhibition effect of $KHCO_3$ powder on the C_2H_4 system explosion pressure was better than that of the KH_2PO_4 powder under similar concentration conditions. Both powders significantly affected the flame propagation of the C_2H_4 explosion. Compared with KH_2PO_4 powder, $KHCO_3$ powder had a better inhibition effect on the flame propagation speed, but its ability to reduce the flame luminance was less than KH_2PO_4 powder. Finally, the inhibition mechanism(s) of $KHCO_3$ and KH_2PO_4 powders were revealed based on the powders' thermal characteristics and gas-phase reaction.

1. INTRODUCTION

C_2H_4 is the primary raw material for most of the chemical and petroleum industry applications. Therefore, its output, production scale, and production technology level become critical indicators to assess the developments in the chemical and petroleum processes.[1,2] Due to the high explosion sensitivity of C_2H_4, it is very easy to cause fire and even explosion accidents during its production and utilization. For example, the explosions of EVAL Plant in the United States in 2018 and that of the Sinopec Maoming Petrochemical Company in 2022 were caused by C_2H_4.[3,4] The explosion risk of C_2H_4 has seriously hindered the development of some specific processes in the chemical and petroleum industries. Therefore, it is imperative to study the inhibition of C_2H_4 explosion to reduce/control personnel and property loss.

According to the wealth of literature on explosion prevention and control, it is clear that explosion inhibitors not only result in a more safe and reliable operation involving certain chemicals but also effectively reduce the explosion intensity and generation of toxic and harmful gases.[5] The commonly used inhibitors include inert gas, powder inhibitors, and water mist.[6] Among them, inert gas mainly inhibits explosions through a physical process, and its application scope is limited.[7] Although the water mist significantly suppresses the explosion and does not cause secondary pollution, its practical application is difficult due to its immature technology.[8] In contrast, powder inhibitors are favored in the chemical industry due to their low price, strong environmental adaptability, and physical and chemical inhibition.[9]

With the improvement of environmental protection policies, there are other characteristics to select appropriate powder inhibitors besides their explosion hindering performance such as their impact on the ecological environment. For instance, halon inhibitors with good fire extinguishing and explosion suppression characteristics have been gradually abandoned, and instead, efficient alkali metal compounds with environmentally friendly characteristics have been utilized over the years.[10] Two alkali metal compounds of $KHCO_3$ and $NaHCO_3$ have been widely studied in the literature.[11,12] Using a modeling approach, Babushok[13] demonstrated that $KHCO_3$ and $NaHCO_3$ particles exhibit better inhibition effects than CF_3Br (halon-1301) under ideal conditions.

The effects of alkali metals on methane explosion inhibition under various factors (i.e., concentration, inhibitor type, and oxygen concentration) have been extensively studied.[14−16] Some studies on flammable gas explosion showed that explosion intensity of olefin gas is often greater than that of alkane gas, with a more complicated explosion process.[17−19] To better ensure safe development of the C_2H_4 industry, it is necessary to study the inhibition mechanisms associated with C_2H_4 explosion. Even though various concentrations of

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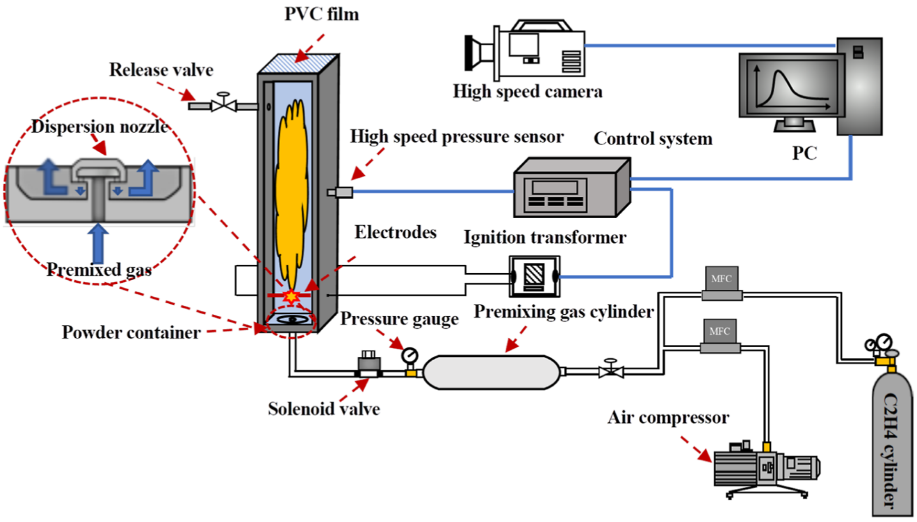

Figure 1. Schematic representation of the experimental apparatus.

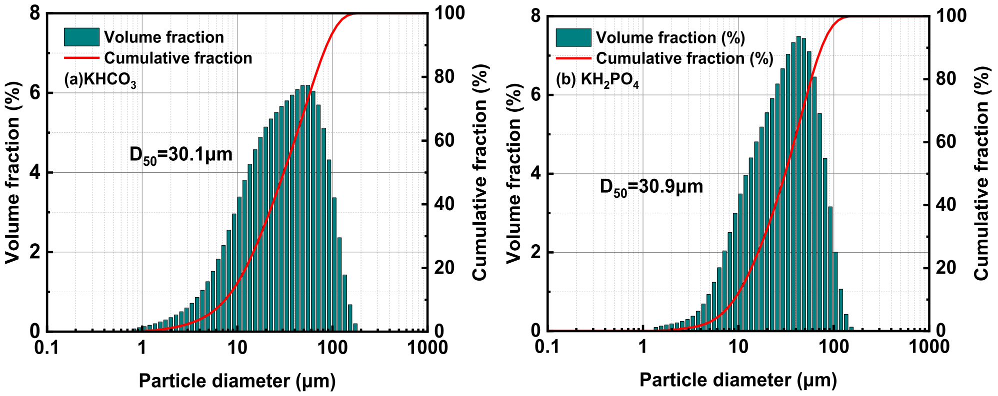

Figure 2. Particle size distribution of two inhibitors: (a) $KHCO_3$ powder and (b) KH_2PO_4 powder.

KH_2PO_4 powder proved to be the best explosion inhibitor for the C_2H_4 system,[20] its performances against other traditional alkali metal inhibitors (i.e., $KHCO_3$ or $NaHCO_3$) have not been studied yet. Since the explosion inhibition characteristics of $KHCO_3$ in the flammable gas systems are generally better than those of $NaHCO_3$,[21] we selected $KHCO_3$ and KH_2PO_4 powder inhibitors in this study in order to explore more ideal C_2H_4 explosion inhibitors.

In the experiments involving C_2H_4 explosion inhibitors, the explosion overpressure and explosion index are mostly used to assess explosion inhibition performance.[22,23] However, the use of the explosion characteristic parameters only cannot reveal the inhibition mechanisms for the C_2H_4 system. Analysis of the explosion inhibition mechanism is generally based on the explosion flame propagation.[24]

In this study, $KHCO_3$ and KH_2PO_4 powder inhibitors were used in C_2H_4 explosion experiments with an equivalent C_2H_4 concentration of 6.5% in a 5 L semi-closed transparent explosion duct. By analyzing the effect of these two explosion inhibitors on the overpressure and flame propagation characteristics of the C_2H_4 system at different concentrations, the explosion inhibition mechanisms of $KHCO_3$ and KH_2PO_4 were revealed considering the combined thermal characteristics of the two inhibitors and the kinetic mechanism of the gas-phase reaction kinetics. The experimental results obtained in this study can be applied to the explosion suppression of C_2H_4 and also provide a theoretical basis for the explosion prevention of the C_2H_4 industry.

2. EXPERIMENTAL SECTION

2.1. Experimental Apparatus. The explosion system used in this study is shown in Figure 1. The explosion system included a 5 L semi-closed explosion duct, an ignition system, a powder dispersion system, a data acquisition system, a high-speed camera, and a time control system. For a detailed description of the experimental apparatus and methodology, please refer to our previous research work.[25]

For the C_2H_4 explosion inhibition experiments, a camera with higher photo-capture frequency and more precise capture quality was used to record the dynamic nature of the process due to rapid propagation of the gas explosion flame. A VEO710 model camera, manufactured by Dantec Dynamics, was used in this study, with 6000 fps and a maximum resolution of 1280 × 800 pixels. To make the powder uniformly dispersed in the duct, a powder dispersion pressure of 0.4 MPa was used in this study, along with an ignition delay time of 600 ms after a series of preliminary tests. The ignition system consisted of a 6 kV high-voltage transformer and ignition electrodes. The ignition electrodes were a pair of tungsten electrode rods set 50 mm above the powder container, with a gap of 4 mm between the two electrodes. The high-voltage transformer was able to generate 30 J sparks.

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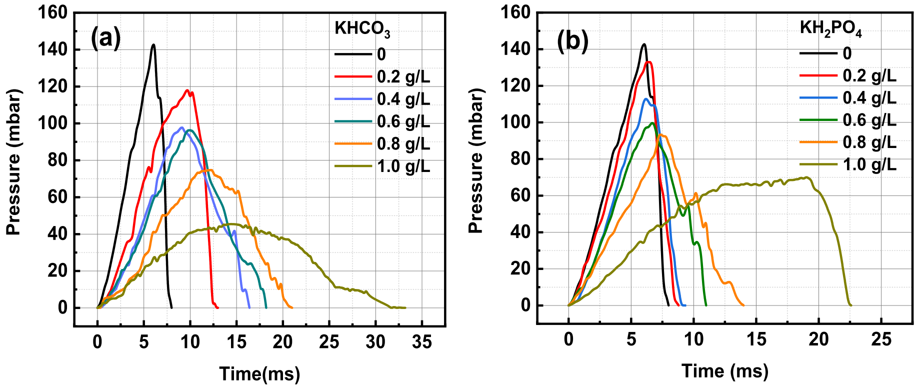

Figure 3. Pressure curves for C_2H_4 explosion in the presence of two inhibitors: (a) $KHCO_3$ powder and (b) KH_2PO_4 powder.

2.2. Experimental Materials. The purity of C_2H_4 used in the experiment was 99.99%. $KHCO_3$ and KH_2PO_4 powders were analytically pure. To avoid the effect of particle humidity and particle size difference on the experiments, the inhibitor powders were placed in a vacuum drying oven at 60 °C for 24 h before the experiments began, and the dried powders were tested using a Malvern laser particle size meter. The results are shown in Figure 2. According to the results, the median particle sizes of $KHCO_3$ and KH_2PO_4 powders were 30.1 and 30.9 μm, respectively, that is, the particle size of the two inhibitor powder types was not much different and can be regarded as the same particle size.

3. RESULTS AND DISCUSSION

3.1. Overpressure Variation of C_2H_4 Explosion in the Presence of Inhibitors. Six different concentrations of inhibitors (i.e., 0.0, 0.2, 0.4, 0.6, 0.8, and 1.0 g/L) were selected, and the effect of inhibitor concentration change on P_{ex} associated with the 6.5% C_2H_4 system was studied. In Figure 3a,b, the pressure curves for C_2H_4 explosion in the presence of two inhibitors are shown, in which the peak value is P_{ex}. It is clear that P_{ex} of C_2H_4 gradually decreased by increasing the inhibitor concentration, that is, both $KHCO_3$ and KH_2PO_4 powders had an excellent inhibition effect on C_2H_4 explosion. The pressure rise phase can also be used to assess the explosion risk.[6] The steeper the rising curve, the greater the explosion risk. In this study, the pressure rise curve gradually became flat with increasing inhibitor concentration, that is, the increasing rate of explosion pressure associated with the C_2H_4 system gradually decreased under the action of two inhibitors.

For precise comparison of the inhibitor effect, the P_{ex} variations under the action of $KHCO_3$ and KH_2PO_4 powders at different concentrations were summarized (Figure 4). P_{ex} associated with C_2H_4 explosion with no inhibitor was 143 mbar. At various $KHCO_3$ powder concentrations, P_{ex} was decreased to 118.4, 100.3, 96.1, 74.8, and 47.2 mbar. The effect of KH_2PO_4 powder on P_{ex} values was weaker, leading to 133.6, 113.4, 100.2, 95.8, and 70.1 mbar values, respectively. It is concluded that $KHCO_3$ powder had a stronger impact on reducing P_{ex}, leading to more effective explosion overpressure inhibition.

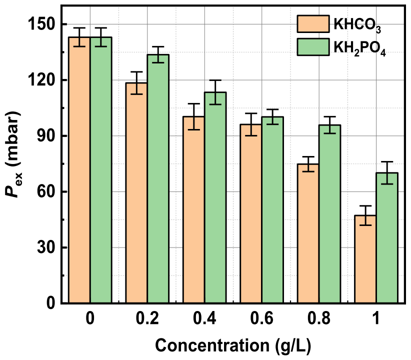

Figure 4. Effect of various inhibitor concentrations on P_{ex} of C_2H_4.

3.2. Flame Propagation Behavior of C_2H_4 Explosion in the Presence of Inhibitors. Through analysis of images captured during the tests, it was found that the explosion flame brightness in the presence of $KHCO_3$ was greater than that of KH_2PO_4 at similar concentrations, which makes it impossible to clearly observe the effect of $KHCO_3$ on the C_2H_4 explosion reaction zone. The reason for this experimental phenomenon is that the content of potassium and its compounds produced by pyrolysis of $KHCO_3$ particles under the same conditions is slightly larger than that of KH_2PO_4 particles, resulting in enhanced flame emissivity and higher brightness.[26,27] Therefore, we selected KH_2PO_4 powder to analyze the flame behavior under various experimental conditions. The flame images associated with various $KHCO_3$ powder concentrations in the C_2H_4 explosion system can be found in the Supporting Information.

In Figure 5, the flame propagation of the 6.5% C_2H_4 explosion system is shown. Clearly, the explosion flame brightness is strong after C_2H_4 was ignited, which is consistent with previous research results.[28,29] The flame propagation process can be divided into two stages: flame growth stage,

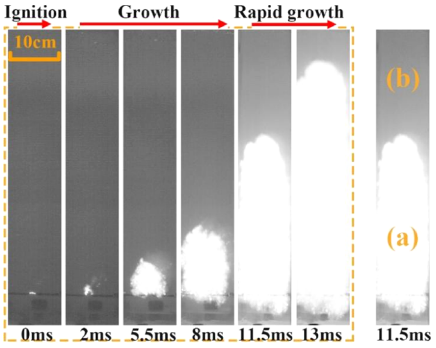

Figure 5. 6.5% C_2H_4 explosion flame propagation: (a) explosion reaction zone and (b) unreacted zone.

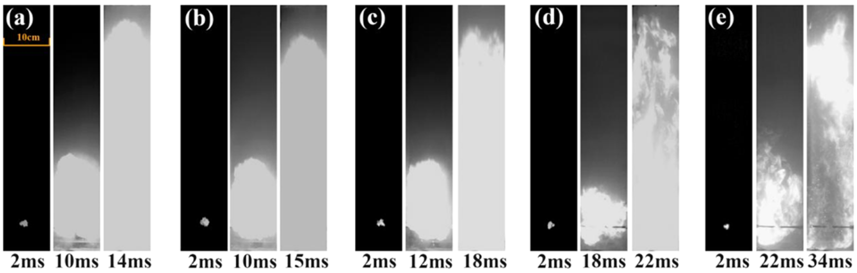

Figure 6. Flame propagation behavior associated with C_2H_4 explosion under different KH_2PO_4 inhibitor concentrations of (a) 0.2, (b) 0.4, (c) 0.6, (d) 0.8, and (e) 1.0 g/L.

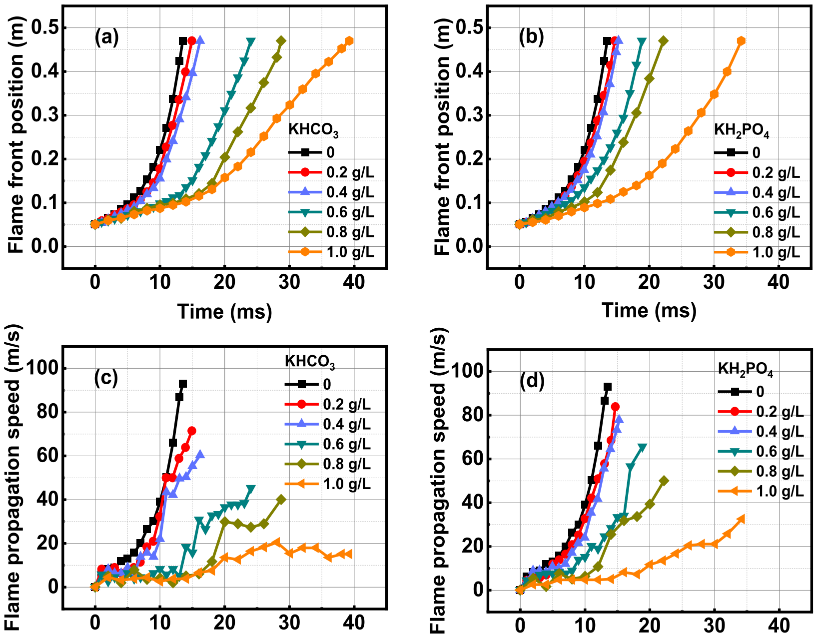

Figure 7. Effects of two different inhibitor concentrations on C_2H_4 explosion flame: (a,b) effects of inhibitors on flame front position and (c,d) effects of inhibitors on flame propagation speed.

during which the flame slowly grew upward and approached the duct wall. The second is the rapid growth stage of the flame during which the flame propagated upward in a finger shape after coming into contact with the duct wall, and the propagation speed was gradually accelerated. During the propagation of the entire explosion flame, we divided the explosion area into an explosion reaction zone and an unreacted zone based on previous research results.[28] The bright flame area in the duct is the explosion reaction area, that is, the (a) area in the figure. The remaining (b) area is unreacted zones. In this study, the effects of different concentrations of inhibitors on the C_2H_4 explosion flame considering these two stages were studied. During the flame propagation process, the irregular shape of the flame front may be caused by factors such as turbulent fields and thermal diffusion instability.[24,30]

In Figure 6, the C_2H_4 explosion flame during two flame propagation stages is displayed after the addition of various KH_2PO_4 concentrations. The first two flame images of each group belong to the first stage. According to this figure, adding a small amount of KH_2PO_4 powder enhanced the flame brightness, resulting in the local changes in the flame that cannot be visually displayed. By increasing the inhibitor concentration, the flame became irregular. At this time, the explosion reaction zone began to appear as a local area with weak brightness. After adding 0.8 g/L KH_2PO_4 powder, the distribution of this area became more obvious in the second stage of the flame, which led to a discrete flame state. When the KH_2PO_4 powder concentration was 1.0 g/L, the flame in the first stage showed an apparent discrete state, and as the flame propagated to the second stage, a large area of weak brightness appeared in the explosion reaction zone. It is generally believed that these areas with weak brightness are originated from inhibition of the explosion flame.[31] From Figure 6, it is observed that the suppression effect of the KH_2PO_4 inhibitor was increased with its concentration.

It is difficult to discuss the effect of $KHCO_3$ powder on C_2H_4 explosion flame behavior, but this does not mean that $KHCO_3$ powder has a weak inhibitory effect on C_2H_4 explosion flame propagation. Since many scholars' research on explosion flame propagation is mainly based on the analysis of flame propagation speed,[32,33] this study mainly compares the effects of two different concentrations of inhibitors on C_2H_4 explosion flame through flame propagation speed.

3.3. Flame Propagation Speed Associated with C_2H_4 Explosion in the Presence of Inhibitors. The effects of $KHCO_3$ and KH_2PO_4 inhibitors on the flame front position and propagation speed of the C_2H_4 explosion flame are

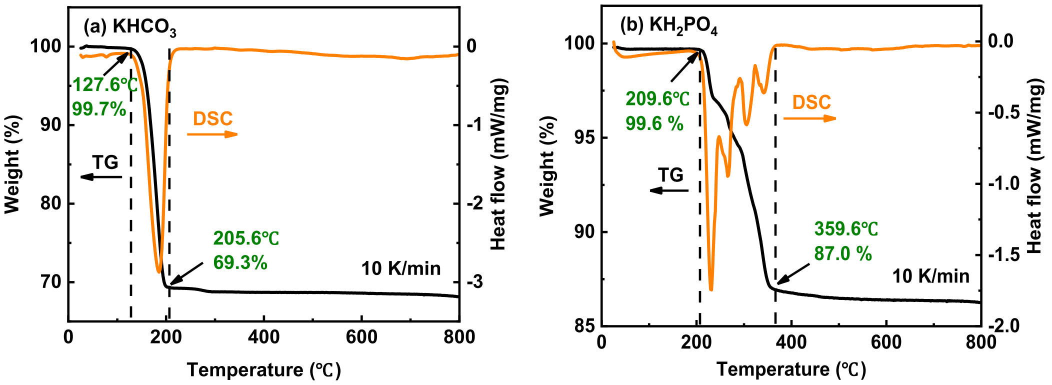

Figure 8. Thermal decomposition characteristics of two inhibitors: (a) $KHCO_3$ powder and (b) KH_2PO_4 powder.

presented in Figure 7. The flame front position is defined as the distance between the highest point of the upward propagating flame and the base of the explosion duct. The flame propagation speed is the ratio of the flame front propagation distance to the propagation time. During explosion flame propagation, the pressure generated by the explosion reaction zone causes the concentrations of C_2H_4 and inhibitors to decrease or close to zero at the proximity of the upper-end opening of the duct. To analyze the variations associated with the flame front position and propagation speed, the 470 mm area above the bottom of the duct was selected. According to Figure 7a,b, the flame generated by C_2H_4 explosion reached the set position in the duct for the shortest time in the absence of any inhibitor, indicating that the average speed associated with C_2H_4 flame propagation was the fastest in this case. With the addition of two different inhibitor concentrations, the average propagation speed associated with C_2H_4 explosion flame was decreased with increasing inhibitor concentration. In Figure 7c,d, the effects of different inhibitors on the flame propagation speed associated with C_2H_4 explosion at different times are displayed. From these figures, it is clear that the relations between the maximum propagation speed associated with C_2H_4 explosion flame and powder concentration also show similar variations. According to the literature, high-quality inhibitors often significantly inhibit the propagation speed associated with explosion flames.[34−37] Clearly, high concentrations of $KHCO_3$ and KH_2PO_4 powders are expected to be influential in inhibiting C_2H_4 explosions.

From Figure 7, it is also observed that the flame propagation time associated with the explosion system in the presence of $KHCO_3$ is longer under similar inhibitor concentration compared to the other inhibitor. This indicates that $KHCO_3$ powder inhibited the C_2H_4 explosion flame better than KH_2PO_4 powder.

4. MECHANISTIC ANALYSIS OF THE C_2H_4 EXPLOSION INHIBITION

It is known that alkali metal compounds inhibit explosions through physical and chemical mechanisms. The physical and chemical reactions are mainly heat absorption and gas-phase reaction, respectively.[38] The inhibition characteristics of $KHCO_3$ and KH_2PO_4 powders were also mechanistically investigated in this research work.

4.1. Physical Inhibition.

Physical inhibition is mainly achieved through heat absorption. In this study, the endothermic mechanism of the two powders was investigated by thermal analysis (Figure 8). From the TG curve presented in Figure 8, it is clear that both $KHCO_3$ and KH_2PO_4 powders had a mass loss stage that occurred in a temperature range of 127.6−205.6 and 209.6−359.6 °C, respectively. The temperature at which $KHCO_3$ powder began to lose mass was less, indicating that the endothermic decomposition temperature of $KHCO_3$ powder was less. The end temperature associated with KH_2PO_4 weight loss was greater, indicating that the end of thermal decomposition for KH_2PO_4 powder required a greater temperature.

As shown in Figure 8, there is an apparent differential scanning calorimetry front curve in the mass loss stage of both inhibitors, which is their endothermic peak. Previous studies have shown that the $KHCO_3$ heat absorption in this stage was mainly decomposed into KOH and CO_2, and then part of KOH reacted with HCO_3^- to form K_2CO_3 and H_2O.[39] Similarly, KH_2PO_4 powder in this stage was mainly decomposed into KPO_3 and H_2O after absorbing the heat.[40] $KHCO_3$ and KH_2PO_4 heat absorption values were 603.4 and 436.2 J/g, respectively. Clearly, $KHCO_3$ powder had better heat absorption characteristics.

The key to explosion inhibition technology is reducing heat transfer from the explosion reaction zone to the unreacted zone.[25] According to the thermal characteristic results of these two inhibitors, the physical inhibition characteristics of $KHCO_3$ for the C_2H_4 explosion were stronger due to its lower trigger thermal decomposition temperature and greater endothermic characteristics. In addition, the H_2O produced by the two inhibitors and the additional CO_2 produced by $KHCO_3$ diluted the oxygen concentration in the explosion system. Other researchers believe that this method has little effect on the explosion;[41,42] therefore, it will not also be discussed in this paper.

4.2. Chemical Inhibition.

Although the physical heat absorption mechanism of the two inhibitors reveals their physical inhibition characteristics, many scholars believe that $KHCO_3$ and KH_2PO_4 powders inhibit gas explosion mainly through gas-phase reaction.[43] In this section, we look further into the explosion inhibition mechanism associated with these two powders through their chemical mechanism.

It is known that the explosion intensity of hydrocarbon fuels depends on how much H and OH radicals participate in the chain reaction during the combustion and explosion processes. One of the main reasons why $KHCO_3$ and KH_2PO_4 powders are effective explosion inhibitors is that the KOH produced by their thermal decomposition can react with these free radicals to form other products, further blocking the explosive chain reaction containing hydrocarbon gases.[9,44] For the case of

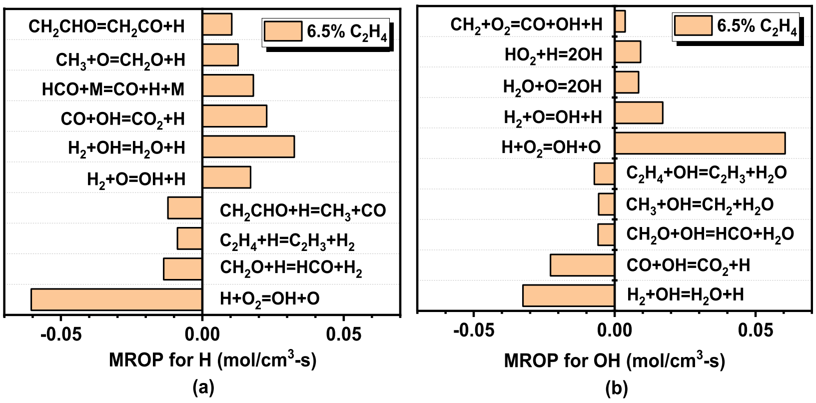

Figure 9. MROP for H (a) and OH (b) radicals of 6.5% C_2H_4 explosion.

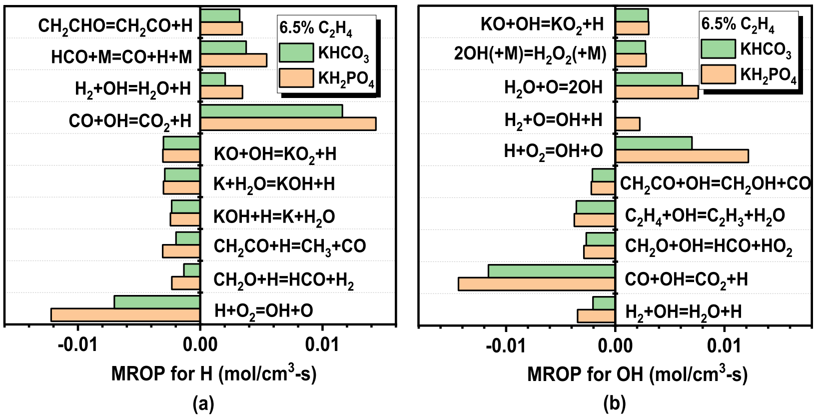

Figure 10. Effect of 1 g/L inhibitors on MROP of H (a) and OH (b).

KH_2PO_4 powder under high-temperature conditions, formation of a large concentrations of KPO_3 does not exhibit any explosion inhibition characteristic.[45] KH_2PO_4 powder can suppress the explosion through pyrolysis by producing a small amount of KOH.[45,46] Previous studies often use reaction kinetics to analyze the flame/explosion inhibition mechanism(s) of alkali metal compounds.[15,38] Constructing complex kinetic models for alkali metal compounds is computationally expensive. Therefore, metal hydroxides have been used as the main kinetic module for simplified calculation, which has proved to have a small effect on the results.[38] Therefore, in our study, only some of the mechanisms of KOH were considered in order to study the inhibition characteristics/mechanisms of $KHCO_3$ and KH_2PO_4.

To reveal the chemical mechanism associated with these two inhibitors, the effect of KOH on H and OH radicals produced by C_2H_4 explosion was considered through reaction kinetics, which has been proven to be a feasible approach in the literature.[44,47,48]

In this study, the effect of KOH on C_2H_4 explosion was investigated using the zero-dimensional homogeneous reactor in CHEMKIN software package. The KOH kinetic module adopts a relatively high degree of recognition between all the kinetic models associated with the K-containing compounds.[49] The C_2H_4 kinetic model uses the San Diego (UCSD) mechanism,[50] which is often used in studying C_2H_4 combustion and explosion in the air medium. All the thermodynamic parameters in this model were from the JANNF thermodynamic database provided by Burcat[51] and the NIST database. The initial temperature and pressure of the numerical simulation were set to 1300 K and 1 atm, respectively. This parameter setting refers to the initial boundary conditions of Wang's[52] numerical simulation model for explosion characteristics of 6.5% C_2H_4.

In addition, it was assumed that the K-compound produced by the rapid pyrolysis of $KHCO_3$ and KH_2PO_4 powders in an ideal high-temperature environment was KOH. It should be noted that in reality, the main product of $KHCO_3$ rapid pyrolysis is KOH, while the rapid pyrolysis of KH_2PO_4 produces less KOH. Therefore, the pyrolysis product in this study was artificially enhanced compared with the real case of application of KH_2PO_4 for C_2H_4 explosion inhibition. To more significantly analyze the effect of KOH on H and OH radicals during C_2H_4 explosion, we selected 1 g/L concentration of $KHCO_3$ and KH_2PO_4 powders in this study.

In the complex reaction system of hydrocarbon fuel, analysis of the maximum rate of production (MROP) is often used to reveal the effect of essential reaction on the formation and consumption of components.[47,48] In this study, the chemical inhibition of the two inhibitors is assessed through their effect on MROP of H and OH radicals. In Figures 9 and 10, variations of the explosion system without and with inhibitors are shown, respectively. From the variations in H and OH radicals in the two figures, the effectiveness of inhibitors is proven. For example, the main reactions of H radical formation and consumption without adding explosion inhibitors are $H_2 + OH = H_2O + H$ and $H + O_2 = OH + O$, and their MROP values are approximately 0.03 and −0.06 mol/cm^3 s, respectively (Figure 9). The MROP of these two reactions are about 0.003 and −0.01 mol/cm^3 s after adding the inhibitors. Similar variations can also be found for the OH radicals. Therefore, $KHCO_3$ and KH_2PO_4 powders are able to inhibit the chain reaction of H and OH radicals during the C_2H_4 explosion, resulting in reduction of the explosion intensity.

As shown in Figure 10, $KHCO_3$ powder has a significant effect on the MROP of H and OH radical inhibition, which is related to the KOH content. For $KHCO_3$ and KH_2PO_4 powders with the same mass, the thermal decomposition of $KHCO_3$ powder produces more KOH because the relative molecular mass of $KHCO_3$ was smaller than that of KH_2PO_4. In addition, previous experimental results showed that KOH was difficult to produce from KH_2PO_4 powder,[42] so the MROP inhibition effect of KH_2PO_4 powder on H and OH radicals is less than the simulation results. However, according to the macroscopic results of overpressure and flame propagation for $KHCO_3$ and KH_2PO_4, the difference in their inhibition performances is not particularly significant. This suggests that during the pyrolysis process of KH_2PO_4, other components except KPO_3 also participated in the chain reaction process. Since P-containing compounds have been also found useful as flame inhibition products, we speculate that a small amount of P-containing components may have been involved in the reaction process. According to the literature, the inhibition effect of $KHCO_3$ is greater than that of KH_2PO_4,[21] which indicates that the P-containing components have no significant explosion inhibition effect. Due to the lack of detailed KH_2PO_4 reaction kinetic equations and thermodynamic parameters, the chemical inhibition mechanism of the two powders should be further studied in the future.

5. CONCLUSIONS

In this study, $KHCO_3$ and KH_2PO_4 powders were used to inhibit the explosion process of 6.5% C_2H_4 in a 5 L semi-closed duct system. The explosion inhibition mechanism of these two powders was studied from both physical and chemical perspectives. The following conclusions are drawn from this study:

(1) After $KHCO_3$ and KH_2PO_4 powders were added to the C_2H_4 explosion system, the P_{ex} of 6.5% C_2H_4 decreased with the inhibitor concentrations, and the inhibition effect of $KHCO_3$ powder on the P_{ex} of C_2H_4 was better than that of KH_2PO_4 powder at similar concentrations.

(2) The average and maximum flame propagation speeds associated with C_2H_4 explosion were decreased by increasing the inhibitor concentration. When the inhibitor concentrations were the same, KH_2PO_4 powder was weaker than $KHCO_3$ powder in reducing the propagation speed of C_2H_4 explosion, but its ability to reduce the luminous brightness of C_2H_4 flame was better than $KHCO_3$ powder.

(3) Compared with KH_2PO_4 powder, $KHCO_3$ powder was superior in physical flame/explosion inhibition due to its lower initial pyrolysis temperature and higher heat absorption.

(4) According to the reaction kinetic model, the chemical inhibition characteristics of $KHCO_3$ powder were better than those of KH_2PO_4 powder. This is due to the production of greater values of KOH from rapid pyrolysis of $KHCO_3$ than KH_2PO_4. Therefore, $KHCO_3$ powder seemed to be a more efficient additive in inhibiting the chain reaction of H and OH radicals.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.2c06894.

Flame propagation behavior associated with C_2H_4 explosion under different $KHCO_3$ inhibitor concentrations, change in species fraction during 6.5% C_2H_4 explosion, and effects of two inhibitors on the C_2H_4 explosion process (PDF)

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Notes

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