ABSTRACT: Air−light hydrocarbon mixing gas with pentane as the main component is recognized as the "fourth urban gas" by the Chinese government. However, leakage may occur because of inadvertent human operation, and in this case, it is very easy to cause explosion. This paper mainly studies the changes in reactants, products, and free radicals during the explosion of pentane, especially the effects of oxygen and carbon monoxide concentrations on human body in this environment. In actual situations, excessive leakage of pentane is predominant. Once an explosion occurs, oxygen will be quickly consumed, and the concentration of carbon monoxide will rise abruptly. The high temperature resulting from the explosion can cause carbon dioxide to rarely react with carbon atoms to form carbon monoxide through the reaction of \( \text{CO}_2 + \text{C} = 2\text{CO}\). The research studies on the three major free radicals including hydrogen radical, oxygen radical, and hydroxyl radical are performed to provide theoretical support for preventing the chain reaction from further expanding the impact of explosion.

1. INTRODUCTION

Energy is the foundation of a modern industrial society, and especially, petroleum resources are the most important reserves of countries in the world. Energy consumption grew by 2.3% in 2018 worldwide, nearly twice the average rate of growth since 2010, driven by a robust global economy and increased heating and cooling needs in some parts of the world. China, the United States, and India together accounted for nearly 70% of the rise in energy demand. In the second half of 2019, the United States used 1.8 million b/d of the new transportation capacity, completely through the bottleneck of shale oil storage and transportation. Shale oil and gas will usher the second wave of revolution, and it is expected that US crude oil production will reach 13 million barrels per day in 2020. As domestic production continues to increase, US crude oil imports continue to decline and will become a net exporter of crude oil in 2020. Exports will reach 4.2 million b/d in 2024, surpassing Russia and approaching Saudi Arabia. In 2019, China’s economy was generally stable, with the GDP growth rate reaching 6.6% and total energy production reaching 3.77 billion tons of standard coal. Energy consumption reached 4.64 billion tons of standard coal, with a growth rate of 3.4%, the highest in five years. Through the energy comparison between China and the United States, the United States is already one of the world’s largest oil exporters, while China is facing a huge energy crisis. Therefore, the development of clean, renewable, recycled, and efficient energy is a major issue that needs increased concern in today’s Chinese society.

In the process of oilfield exploitation, some byproducts are always accompanied, including light hydrocarbon, whose main component is pentane. The previous approach was to burn this part of the fuel directly, but now because of the shortage of energy, light hydrocarbon has regained attention and utilization. Light hydrocarbon can be mixed with air through gasification to obtain air−light hydrocarbon mixing gas, which is clean and is very suitable as a supplementary gas for coal gas and natural gas with high heating value. Therefore, in July 2010, the Ministry of Housing and Urban—Rural Development of China issued the standard for "air−light hydrocarbon mixing gas" (CJ/T 341-2010), which was implemented on January 1, 2011. The standard determines air−light hydrocarbon mixing gas as the "fourth urban gas" after artificial gas, natural gas, and liquefied petroleum gas. However, in the process of using it as a civil fuel, because of the illegal operation, air−light hydrocarbon mixing gas may sometimes leak. The most common inducement of
leakage is operating the gas circuit without following the prescribed operational method, and forgetting to close the air outlet valve after use, causing air—light hydrocarbon mixing gas to remain indoors. In this condition, once the concentration reaches one fixed value, pentane in the air will explode when it encounters an open flame.

At present, the research on pentane explosion is blank, but there are many research studies on the explosion of other fuels, which have reference significance for the research of pentane explosion. Luo et al. studied the evolution characteristics of the flow field inside the duct during the explosion propagation of premixed methane/ethane/air through experimental and simulation methods. The results showed that as the volume fraction of ethane increases, the explosion process of the premixed system is more rapid and violent. Liu et al. studied the characteristics of flame propagation and gas explosion in a propane/air mixture and obtained the variation law of maximum overpressure and maximum temperature with equivalence ratio and discussed the variation law. In a propane/air mixture with an equivalent ratio close to 1.8, two explosions occurred. Tang et al. studied the explosion characteristics of high gas fraction natural gas under different initial conditions in a constant volume combustion vessel. The results showed that with the increase in initial pressure and peak explosion pressure, the mass of combustible gas mixture increases, the heat transfer increases, and the maximum rate of pressure increases accordingly. Wang et al. measured the flammability limit of methane/air mixtures with the addition of gaseous fuel through experiments to study the effect of combustible gas and relative humidity on the flammability limit behavior of methane. The results showed that at the same relative humidity, the addition of gaseous fuel will reduce the lower and upper flammable limits of methane, and these parameters will increase with the increase in relative humidity. The effect of the addition of dimethyl ether (DME) on the explosion of methane/air mixture was studied by Zhang and Ng. Especially, the explosion and deflagration parameters of various CH₄–DME/air mixtures were systematically studied. Lei et al. used chemical dynamics calculation software and a 20 L spherical explosion experimental device to simulate the generation process and formation conditions of H₂ during gas explosion. The experimental results showed that the decomposition of water vapor is the main basic reaction leading to the formation of H₂. Free radical H is the key factor affecting the gas explosion to generate H₂. Luo et al. experimentally studied the pressure and flame emission spectrum characteristics of intermediate products during the explosion of CH₄/C₂H₆/C₂H₄/CO/CH₂O mixtures. Furthermore, the time difference (ΔT) between the peak explosion pressure (Pₚₑₓₘₐₓ) and the peak CH₂O spectral intensity is proposed. The results showed that the effect of system conditions on the formation rate of ΔT and CH₂O is combined, and the correlation between Pₚₑₓₘₐₓ and ΔT can reflect the coupling mechanism between the explosion pressure and the intermediate product. In order to further study the influence of organic combustible gas and inorganic combustible gas on CH₄ explosion, Su et al. experimentally measured the flammability limit and minimum oxygen concentration of CH₄ explosion in a 20 L spherical vessel. The results indicated that the effects of organic and inorganic combustible gases on the flammability limit of CH₄ are significantly different. In order to study the influence of many kinds of gases on the gas combustion process, Jia et al. used CHEMKIN-PRO software to construct a USC Mech 2.0 dynamic model to study the combustion process of C₃H₈/CO₂ gas mixture gas with different components in depth. The C₂H₆/CO₂ gas laminar combustion rate and the volume fraction of CH₄/O radicals in different components were simulated and analyzed, and the sensitivity analysis was performed using the SENKIN program. In order to study the products and types of gas explosions, Nie et al. performed chemical kinetics analysis using a detailed mechanism (GRI-Mech3.0). The closed homogeneous 0-D reactor was used to study the dynamics of gas explosion. At the stoichiometric ratio, the oxygen concentration drops from 19.0 to 2.0%, and cannot support normal breathing after an explosion. In order to study the effect of hydrogenation on the explosion characteristics (explosion pressure and maximum pressure rise rate) of n-hexane/air mixture, Zhang et al. conducted experiments on n-hexane with different initial temperatures of 353–393 K, initial pressures of 60–100 kPa, equivalent ratios of 0.7–1.7, and hydrogen addition range of 0–80% in a cylindrical container with a central ignition. The results showed that the explosion pressure and the maximum pressure rise rate of the lean n-hexane/hydrogen/air mixture increase with the increase in the amount of hydrogen added, and all explosion parameters are closely related to the n-hexane/air ratio, initial pressure, and temperature. Therefore, research on the explosion of a new type of fuel is very important.

This paper mainly studies the changes of reagents and products and the changes of intermediate free radicals after the explosion caused by pentane leakage. The results are meaningful in providing the theoretical basis of chemical kinetics for the prevention of pentane explosion and the control and extinguishment after explosion, which further improve the safe use coefficient of air—light hydrocarbon mixing gas.

2. SPECIFIC SIMULATION MODEL AND COMPUTATIONAL CASES

2.1. Specific Simulation Model. This paper mainly uses the detailed mechanism of pentane to study the chemical reaction during pentane explosion through simulation calculation. Therefore, the previous exploration of the pentane mechanism and the analysis of the fuel chemical reaction are significant in guidance for this study. Bugler et al. perfected the detailed mechanism of pentane by studying the ignition delay time of pentane and the intermediate product of pentane chemical reaction. Ji et al. verified the detailed mechanism of n-pentane by studying the laminar flame speed and extinction strain rate of n-pentane. Chang et al. used the detailed mechanism of aviation kerosene to study its combustion characteristics and emissions. Brower et al. used highly optimized detailed mechanisms of methane to study the chemical reaction and combustion characteristics of methane.

The ignition delay time of pentane with five available chemical kinetic mechanisms that was studied by Jiang et al. and Cheng et al. explored the laminar flame speed of the pentane isomers using a detailed mechanism, and their conclusions both indicated that the simulation results of the NUI Galway pentane isomer model were most consistent with the experimental results. Therefore, in this paper, the NUI Galway pentane isomer model (697 species, 3214 reactions) is used for the study of the pentane explosion process. According to Nie et al.’s simulation study of methane explosion using the closed homogeneous 0-D reactor, it is found that the closed homogeneous batch reactor model in ANSYS CHEMKIN 17.0 is the most suitable for simulating explosions in limited spaces. Combined with the specification of air—light hydrocarbon mixing gas, pentane is a
pentane explosion and is also a strong theoretical support for preventing generation or consumption of components after pentane explosion.

Therefore, the simulation time is set to 0.003 s, which is enough to study the process changes of violent combustion reaction. Therefore, the simulation time is set to 0.003 s, which is enough to study the process changes of violent combustion reaction. Hence, when it comes to the leakage of air—light hydrocarbon mixing gas, pentane and air are leaked at the same time, that is, the proportion of pentane in the air studied in this paper is actually the proportion of pentane in the entire air, which includes the air in the original environment and the leaked air.

There are three types of pentane studied in this paper; the first type is pure $n$-pentane, the second type is the equal mole fraction of $n$-pentane and iso-pentane studied by Fan et al.,$^{25}$ and the third type is a mixture of $n$-pentane, iso-pentane, and neo-pentane provided by Zhong Tong Gas Equipment Science and Technology Company. Table 1 summarizes the computational cases of three different types of pentane leaks that caused the explosion. Pure, whose composition is 1 mol fraction of $n$-pentane, is the first type of pentane. Equal, whose composition is 0.5 mol fraction of $n$-pentane and 0.5 mol fraction of iso-pentane, is the second type of pentane. Mixed, whose composition is 0.81 mol fraction of $n$-pentane, 0.07 mol fraction of iso-pentane and 0.12 mol fraction of neo-pentane, is the third type of pentane. The pentane ratio refers to the percentage of the entire environment at the moment of explosion after the pentane leaks. The pentane ratio of 2.56% is the stoichiometric condition, the pentane ratio of less than 2.56% is the fuel-lean condition, and the pentane ratio of more than 2.56% is the fuel-rich condition.

Sensitivity analysis is helpful in finding solutions to prevent pentane explosion and reduce the secondary impact after pentane explosion. The calculation formulas of sensitivity analysis are shown as follows

$$\frac{d\varphi}{dt} = F(\varphi, t; \alpha)$$

(1)

$$w_{j,i} = \frac{\partial \varphi}{\partial q_i}$$

(2)

$$\frac{dw_{j,i}}{dt} = \frac{\partial F}{\partial \varphi} w_{j,i} + \frac{\partial F}{\partial q_i}$$

(3)

Equation 3 is obtained by differentiating eq 2.

Rate of production (ROP) can quickly extract and analyze the generation or consumption of components after pentane explosion and is also a strong theoretical support for preventing pentane explosion. The calculation formulas of ROP are shown as follows

$$P_k = \sum_{i=1}^{f} v_k q_i$$

(4)

$$C_{k,j}^p = \frac{\max(v_{k,j}, 0) q_j}{\sum_{i=1}^{f} (v_{k,j}, 0) q_i}$$

(5)

2.2. Computational Cases. It should be further clarified that air—light hydrocarbon mixing gas mainly contains a mixture of gasified pentane and air. The air referred to here is the same as the air in the environment, that is, the molar ratio of nitrogen and oxygen is 3.76:1. Hence, when it comes to the leakage of air—light hydrocarbon mixing gas, pentane and air are leaked at the same time, that is, the proportion of pentane in the air studied in this paper is actually the proportion of pentane in the entire air, which includes the air in the original environment and the leaked air.

| pentane type | pentane ratio (%) | $n$-C$_5$H$_{12}$ | iso-C$_5$H$_{12}$ | neo-C$_5$H$_{12}$ | N$_2$ | O$_2$
|--------------|------------------|-----------------|-----------------|-----------------|------|------|
| pure         | 0.80             | 0.0080          | 0               | 0               | 0.7837 | 0.2083 |
|              | 1.30             | 0.0130          | 0               | 0               | 0.7797 | 0.2073 |
|              | 2.56             | 0.0256          | 0               | 0               | 0.7698 | 0.2046 |
|              | 3.70             | 0.0370          | 0               | 0               | 0.7608 | 0.2022 |
|              | 4.90             | 0.0490          | 0               | 0               | 0.7513 | 0.1997 |
| equal        | 0.80             | 0.0040          | 0.0040          | 0               | 0.7837 | 0.2083 |
|              | 1.30             | 0.0065          | 0.0065          | 0               | 0.7797 | 0.2073 |
|              | 2.56             | 0.0128          | 0.0128          | 0               | 0.7698 | 0.2046 |
|              | 3.70             | 0.0185          | 0.0185          | 0               | 0.7608 | 0.2022 |
|              | 4.90             | 0.0245          | 0.0245          | 0               | 0.7513 | 0.1997 |
| mixed        | 0.80             | 0.006480        | 0.000560        | 0.000960        | 0.7837 | 0.2083 |
|              | 1.30             | 0.010530        | 0.000910        | 0.001560        | 0.7797 | 0.2073 |
|              | 2.56             | 0.020736        | 0.001792        | 0.003072        | 0.7698 | 0.2046 |
|              | 3.70             | 0.029970        | 0.002590        | 0.004440        | 0.7608 | 0.2022 |
|              | 4.90             | 0.039690        | 0.003430        | 0.005880        | 0.7513 | 0.1997 |

Table 1. Computational Cases of Three Different Types of Pentane Leaks That Caused an Explosion

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the air at atmospheric pressure.11 The explosion will occur when the pentane concentration is 0.8%, and the oxygen consumption of the three types of pentane will eventually fall to 14.14%. People in this environment will at least face problems in the head, lungs, and circulatory system, not to mention the leakage of high concentrations of pentane. Figure 3 shows the course of the pentane concentration of the three types of pentane with time.

Therefore, it is clarified that when pentane explodes, n-pentane is consumed first, and then its isomers are consumed.

3.2. Explosive Product Profiles. Carbon monoxide is the most harmful to the human body in explosive products. Many casualties in explosions are caused by carbon monoxide secondary injuries. Therefore, this paper mainly discusses the effect of carbon monoxide produced by pentane explosion on the human body. Figure 5 shows the evolution of the concentration of explosive products over time. Obviously, the CO produced by the fuel-rich explosion is much higher than that produced by the fuel-lean explosion. The reason is that there is not enough oxygen to further oxidize CO to CO₂, which is more stable in molecular structures. On comparing the production history and concentration of CO and CO₂, it can be said that the final concentration of CO₂ is the largest under stoichiometric conditions, which is the result of the just complete burning. Most notably, in the range where the pentane leakage concentration is less than 3.7%, the CO concentration first rises and then falls and tends to stabilize, and the CO₂ concentration rises rapidly at a certain moment and then keeps stable. This indicates that in these pentane leakage concentration ranges, the oxide is sufficient when the explosion occurs, CO can be completely converted to CO₂, and the reaction of CO + OH ⇌ CO₂ + H always proceeds to the right product. However, when the pentane leakage concentration is 4.9%, the above situation changes, and the "peak-top" trend in which the CO concentration first increased and then decreased and disappeared, and it becomes a smooth trend directly. On the contrary, the CO₂ concentration shows the "peak-top" trend. The two reactions of 2CO + O₂ = 2CO₂ and CO₂ + C = 2CO in a high-temperature environment can explain this phenomenon.

Because of the excessive concentration of pentane, high temperature is generated after the explosion, and oxygen consumption is exhausted. It is the high-temperature and oxygen-deficient environment that provides a suitable condition for the endothermic reaction of CO₂ with carbon molecules in pentane.

Combined with the previous accidents and simulation results, it is found that excessive pentane leaks are frequent, the explosion hazard is the greatest, and carbon monoxide poisoning is the deadliest, so the following discusses the harm of the carbon monoxide concentration on humans after the pentane fuel-rich explosion. After the explosion of the three types of pentane, as shown in Figure 5a, the rapid generation of carbon monoxide for each of equal and mixed is delayed for a period of time compared to that of pure; however, this time is almost negligible during the explosion, and the concentration of carbon monoxide...
generated by the explosion under all conditions is stable after 0.002 s. The concentration of carbon monoxide produced after the explosion of the three types of pentane is 4.58% under the stoichiometric condition. Table 3 lists the symptoms that occur in humans with the carbon monoxide concentration of parts per million in the air.28−31 When a human is in an environment with a carbon monoxide concentration of 1.28%, the human will lose consciousness after 2−3 breaths and dies in less than 3 min. In summary, the concentration of carbon monoxide produced after the explosion of fuel-rich pentane is higher than 4.58%, which is far higher than the highest threshold of human endurance, that is, it is very easy to kill people in this environment.

Taking the stoichiometric condition as an example, the key reactions that affect the generation rate of carbon monoxide during the explosion of the three types of pentane are studied. The theoretical suggestions are provided to suppress the production of carbon monoxide during pentane explosion. Figure 6 shows the sensitivity coefficients of the top 10 reactions that affect the production of carbon monoxide as a function of time. Figure 7 shows the coefficients of the top 10 reactions for the ROP of carbon monoxide as a function of time. Table 4 summarizes the key reactions that affect the production and annihilation of carbon monoxide. When the explosion of the three types of pentane occurs, the reaction $H + O_2 \rightarrow O + OH$ has the greatest effect on the production and consumption of carbon monoxide. On the whole, the top 10 reactions can be found affecting carbon monoxide reversely beyond a certain time. All the reactions promoting or inhibiting the production of carbon monoxide.

| CO concentration/ppm (% %) | symptoms |
|---------------------------|----------|
| 35 (0.0035, 0.035)        | headache and dizziness within 6−8 h of constant exposure |
| 100 (0.01, 0.1)           | slight headache in 2−3 h |
| 200 (0.02, 0.2)           | slight headache within 2−3 h; loss of judgment |
| 400 (0.04, 0.4)           | frontal headache within 1−2 h |
| 800 (0.08, 0.8)           | dizziness, nausea, and convulsions within 45 min; insensible within 2 h |
| 1600 (0.16, 1.6)          | headache, increased heart rate, dizziness, and nausea within 20 min; death in less than 2 h |
| 3200 (0.32, 3.2)          | headache, dizziness, and nausea in 5−10 min; death within 30 min |
| 6400 (0.64, 6.4)          | headache and dizziness in 1−2 min; convulsions, respiratory arrest, and death in less than 20 min |
| 12,800 (1.28, 12.8)       | unconsciousness after 2−3 breaths; death in less than 3 min |
carbon monoxide before this time turn to inhibit or promote the CO production after this time. Results of ROP indicate that HCO + M ⇌ H + CO + M and CO + OH ⇌ CO2 + H are the fast reactions in producing and consuming CO, respectively.

3.3. Free Radical Profiles during Explosion. Free radicals are a highly active chemical group that can react with other free radicals and molecules, thereby expanding the combustion in the form of a chain reaction. Most combustion reactions do not proceed directly, but through a cyclic chain reaction in which the
intermediate products of radicals and atoms instantaneously proceed. Of particular concern are the hydrogen radical, oxygen radical, and hydroxyl radical. Therefore, capturing and terminating the free radicals generated by the combustion reaction and then reducing the speed and intensity of the combustion reaction are the key to extinguish the fire. The leakage of pentane caused an explosion, and the violent combustion reaction continued, so the study of free radicals is very important to block the chain reaction expansion. Figure 8 shows the evolution of the concentration of the three major free radicals over time. Overall, except for pentane fuel-rich at 4.9%, the increase and decrease in oxygen radical concentration are not obvious, because the oxygen is seriously insufficient, implying that the generation and consumption of oxygen radicals do not form a scale. Under all other conditions, the concentrations of the three major free radicals all show a near-vertical rise at a certain moment and then fall rapidly. The reason is that after the pentane explosion, a large number of free radicals are produced and then quickly react with other atoms and molecules through the chain reaction until they are consumed to a stable level.

Still taking the stoichiometric condition as an example, the key reactions that affect the generation of the hydrogen radical, oxygen radical, and hydroxyl radical during the explosion of the three types of pentane are studied. Figure 9 shows the sensitivity coefficients of the top 10 reactions that affect the production of the three major free radicals as a function of time. Figure 9 shows the sensitivity coefficients of the top 10 reactions that affect the production of the three major free radicals as a function of time. Figure 10 shows the coefficients of the top 10 reactions for the ROP of the three major free radicals as a function of time. Table 5 summarizes the key reactions that affect the production and annihilation of the three major free radicals. In general, when the explosion of the three types of pentane occurs, the reaction \( \text{H} + \text{O}_2 \leftrightarrow \text{O} + \text{OH} \) contributes the most for the formation of the three major free radicals, and the most significant contribution for the suppression of the three major radicals is the reaction \( \text{CH}_3 + \text{H}_2 \text{O} \leftrightarrow \text{CH}_4 + \text{O}_2 \). \( \text{H} + \text{O}_2 \leftrightarrow \text{O} + \text{OH} \) is the fastest reaction to consume the hydrogen radical, and the fastest reaction to produce the oxygen radical and hydroxide radical. \( \text{OH} + \text{H}_2 \leftrightarrow \text{H} + \text{H}_2\text{O} \) is the fastest reaction to produce the hydrogen radical and the fastest reaction to consume the hydroxyl radical. Finally, the fastest reaction to consume oxygen free radicals is \( \text{O} + \text{H}_2 \leftrightarrow \text{H} + \text{OH} \).

4. CONCLUSIONS

In all pentane leakage cases, an explosion situation where the proportion of pentane in the environment is equal to 4.90% is
the most dangerous because in this case, not only an explosion occurs but also a large amount of toxic gas carbon monoxide is generated. In this case, even if not affected by the explosion, because of the consumption of oxygen and the high concentration of carbon monoxide, people may suffer huge injuries or even die in a short time. The reaction $\text{H} + \text{O}_2 \Leftrightarrow \text{O} + \text{OH}$

The coefficients of the top 10 reactions for the ROP of free radicals as a function of time. (a) Pure. (b) Equal. (c) Mixed.

| number | reaction | number | reaction |
|--------|----------|--------|----------|
| R1     | $\text{H} + \text{O}_2 \Leftrightarrow \text{O} + \text{OH}$ | R223   | $\text{C}_3\text{H}_4 + \text{O}_2 \Leftrightarrow \text{C}_3\text{H}_3 + \text{HO}_2$ |
| R2     | $\text{O} + \text{H}_2 \Leftrightarrow \text{H} + \text{OH}$ | R290   | $\text{HCCO} + \text{OH} \Rightarrow \text{H}_2 + \text{CO} + \text{CO}$ |
| R3     | $\text{OH} + \text{H}_2 \Leftrightarrow \text{H} + \text{H}_2\text{O}$ | R291   | $\text{HCCO} + \text{O} \Rightarrow \text{H} + \text{CO} + \text{CO}$ |
| R4     | $\text{O} + \text{H}_2\text{O} \Leftrightarrow \text{OH} + \text{OH}$ | R292   | $\text{HCCO} + \text{H} \Leftrightarrow \text{CH}_3\text{(S)} + \text{CO}$ |
| R12    | $\text{HO}_2 + \text{H} \Leftrightarrow \text{OH} + \text{OH}$ | R301   | $\text{C}_3\text{H}_4 + \text{O} \Leftrightarrow \text{CH}_3 + \text{HCO}$ |
| R28    | $\text{CO} + \text{OH} \Leftrightarrow \text{CO}_2 + \text{H}$ | R302   | $\text{C}_3\text{H}_4 + \text{O} \Leftrightarrow \text{CH}_2\text{CHO} + \text{H}$ |
| R31    | $\text{HCO} + \text{M} \Leftrightarrow \text{H} + \text{CO} + \text{M}$ | R303   | $\text{C}_3\text{H}_4 + \text{O} \Leftrightarrow \text{C}_3\text{H}_3 + \text{H}_2\text{O}$ |
| R74    | $\text{CH}_2\text{O} + \text{H} \Leftrightarrow \text{HCO} + \text{H}_2$ | R328   | $\text{C}_3\text{H}_4 + \text{H} \Leftrightarrow \text{C}_3\text{H}_3 + \text{H}_2\text{(M)} + \text{M}$ |
| R75    | $\text{CH}_2\text{O} + \text{O} \Leftrightarrow \text{HCO} + \text{OH}$ | R334   | $\text{C}_3\text{H}_4 + \text{O} \Leftrightarrow \text{CH}_2\text{CHO} + \text{O}$ |
| R130   | $\text{CH}_4 + \text{OH} \Leftrightarrow \text{CH}_3 + \text{H}_2\text{O}$ | R374   | $\text{C}_3\text{H}_4 + \text{O} \Leftrightarrow \text{CH}_3 + \text{CO}$ |
| R146   | $\text{CH}_2 + \text{HO}_2 \Leftrightarrow \text{CH}_3 + \text{O}_2$ | R375   | $\text{C}_3\text{H}_4 + \text{O} \Leftrightarrow \text{HCCO} + \text{H}$ |
| R147   | $\text{CH}_2 + \text{HO}_2 \Leftrightarrow \text{CH}_3 + \text{O}_2$ | R696   | $\text{C}_3\text{H}_4 + \text{A} + \text{HO}_2 \Leftrightarrow \text{C}_3\text{H}_3 + \text{H}_2\text{O}$ |
| R148   | $\text{CH}_4 + \text{O} \Leftrightarrow \text{CH}_3 + \text{H}_2\text{O}$ | R2304  | $\pi\text{C}_3\text{H}_4 \Leftrightarrow \pi\text{C}_3\text{H}_3 + \text{C}_3\text{H}_3$ |
| R177   | $\text{CH}_2 + \text{O}_2 \Leftrightarrow \text{HCO} + \text{OH}$ | R2310  | $\pi\text{C}_3\text{H}_4 + \text{H} \Leftrightarrow \text{C}_3\text{H}_3 + \text{C}_3\text{H}_3 + \text{H}_2$ |
| R190   | $\text{C}_3\text{H}_4 + \text{H} \Leftrightarrow \text{C}_3\text{H}_3 + \text{H}_2\text{(M)} \Leftrightarrow \text{C}_3\text{H}_3 + \text{H}_2\text{(M)}$ | R2705  | $\pi\text{C}_3\text{H}_4 + \text{H} \Leftrightarrow \text{C}_3\text{H}_3 + \text{C}_3\text{H}_3 + \text{H}_2$ |
| R202   | $\text{C}_3\text{H}_4 + \text{H} \Leftrightarrow \text{C}_3\text{H}_3 + \text{H}_2\text{(M)}$ | R2705  | $\pi\text{C}_3\text{H}_4 + \text{H} \Leftrightarrow \text{C}_3\text{H}_3 + \text{C}_3\text{H}_3 + \text{H}_2$ |
OH is the most important reaction in the pentane explosion process. It plays a key role not only in the formation of carbon monoxide but also in the formation of free radicals and the chain reaction. In practice, compounds containing CO$_3$$^2^-$ and HCO$_3^-$ can be used to neutralize and extinguish the fire. Under the stoichiometric condition, the research on the key reactions of the production and annihilation of free radicals indicates that the reaction that contributed the most to the suppression of the three major free radicals is CH$_4$ + HO$_2$ ⇌ CH$_3$ + O$_2$. The theoretical results of this study are meaningful in blocking the continuation of explosions and preventing secondary disasters caused by explosions and provide constructive suggestions for improving the safe use of pentane.

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