

## Effects of inert gas addition, oxygen concentration, and pressure on explosion characteristics of propylene

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**Abstract**—Propylene is used for manufacturing commonly used raw materials and synthetic materials for petrochemical processes. However, it is a volatile and flammable material that poses fire and explosion risks. Nitrogen is inexpensive and can lower the propylene explosion limit because of the dilution effect when used as an inert gas. This study measures the explosion limit, minimum oxygen concentration (MOC), explosion pressure, explosion pressure rise rate, and deflagration index ( $K_g$ ) values for propylene and nitrogen at 25 °C. Results showed that the lower explosion limit of the explosion range did not significantly change with an increase in pressure from 0.10 MPa to 0.25 MPa; however, the upper explosion limit increased significantly. Furthermore, the MOC decreased as pressure increased at 25 °C, while both the maximum explosion pressure and maximum explosion pressure rise rate increased, thereby increasing the explosion risk. The risk of propylene was predicted by the  $K_g$  values determined using the maximum explosion pressure rise rate and volume based on the experimental data. Therefore, through this study, we provide basic data on safety references for preventing fire and explosion accidents.

**Keywords:** Propylene, Explosion Limit, Minimum Oxygen Concentration, Explosion Pressure, Pressure Rise Rate, Gas Deflagration Index ( $K_g$ )

### INTRODUCTION

Propylene is produced by thermal decomposition, a cracking process in oil refining, and is widely used worldwide as a basic raw material after ethylene for making propylene oxide and acrolein.

In the case of gaseous fuels, there is a risk of explosion during the process when the concentration of oxygen is too high due to the formation of a combustible mixer when mixing with a certain proportion of air. If the oxygen concentration is too low, productivity may decrease, so the oxygen concentration must be adjusted [1-3].

In addition, propylene is a flammable gas, and due to an increase in the initial pressure an increase in the amount of combustion per unit volume increases the explosion limit and increases the pressure of the explosion, thereby increasing secondary damage, such as damage to life and property from fire and explosion. In general, the explosive limit depends on the temperature, pressure, and oxygen concentration, and is an experimentally determined value, so experimental research is essential [4,5].

To prevent explosions, it is necessary to use an inert gas such as nitrogen, because it is inexpensive, occupies the largest proportion of air, and can be used in the purge process for discharging flammable gases [6-8]. Much research into the explosive properties of combustible gases has been conducted. Studies on methane-air mixtures include Kundu et al. [9], who studied the explosion limit and flame velocity, and Shen et al. [10], who measured the maximum pressure rise rate and deflagration index. In addition, Li et al. [11] used a methane-hydrogen-air mixture to photograph the flame char-

acteristics according to the initial pressure, and analyzed the sensitivity of the flame through numerical simulation. Giurcan et al. [12] studied the explosion limit, explosion pressure, and explosion pressure rise rate of propane based on initial temperature and pressure using inert gases ( $N_2$ , Ar,  $CO_2$ ). In Zabetakis [13] the characteristics of the explosion were grasped using various variables such as temperature and pressure, depending on the type of hydrocarbons.

On the other hand, some studies have been conducted in which the size and shape of the explosive container affect the explosion [14-18]. Yu et al. [19] measured and compared the upper limit in terms of pressure and temperature using a 1.5 L cylinder and a 20 L spherical container of ethylene and oxygen and ethane and oxygen mixtures, respectively, and obtained almost the same experimental values. In this case, the smaller the container, the more advantageous it is to ensure the efficiency of the experiment per unit time and the convenience and safety of the experiment.

In this study, propylene-nitrogen-oxygen measured the explosion limit, explosion pressure, and explosion pressure rise rate in terms of change in pressure using a 1.1 L cylindrical sealed explosive container to predict the severity and risk of explosion. The deflagration index of the gas was obtained from the ascent rate and the volume of the container. Furthermore, to prevent the propagation of flame during the process, the minimum oxygen concentration causing explosion was measured.

### EXPERIMENTAL SETUP

#### 1. Experimental Samples

Propylene is used as a raw material for the production of synthetic substances, such as polypropylene, acrylic acid, propylene oxide, and the addition polymerization reaction in petrochemical pro-

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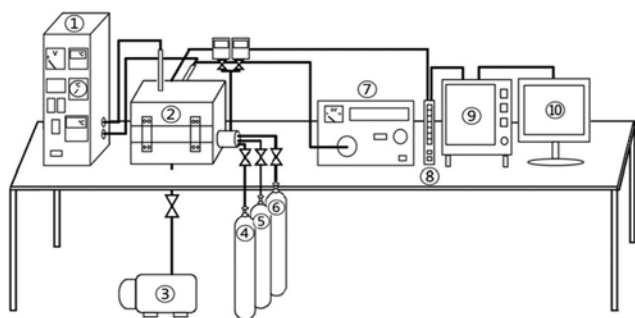


Fig. 1. Schematic diagram of experimental apparatus for explosion measurement.

- |                    |                            |
|--------------------|----------------------------|
| ① Control box      | ⑥ Oxygen bombe             |
| ② Explosion vessel | ⑦ High voltage transformer |
| ③ Vacuum pump      | ⑧ Amplifier                |
| ④ Propylene bombe  | ⑨ Oscilloscope             |
| ⑤ Nitrogen bombe   | ⑩ Computer                 |

cesses. The samples used in this study were 99.9% pure propylene supplied by Seonggwang Special Gas and 99.99% pure  $N_2$  and  $O_2$  provided by Cheonma Industrial Gas Co., Ltd.

## 2. Experimental Setup

### 2-1. Explosive Device

The explosion vessel was made in accordance with the ASTM E 918-83 [20]; Fig. 1 shows its schematic diagram. The experimental setup consists of an explosion vessel with a capacity of 1.1 L and pressure measurement sensors. The explosion vessel, with an external diameter of 148 mm and an internal diameter of 105 mm, consists of a K-type thermocouple with a thickness of 1 mm that is used to check the temperature and an enclosure made of insulation (L 400 mm×W 300 mm×H 330 mm). On the side of the vessel, a pressure sensor (S-1100, Sejin Co., Republic of Korea) capable of measuring pressures between 0 and 10.0 MPa was installed. Inside the vessel, a digital manometer capable of measuring pressures between 0 and 1,000 kPa (PG-200-103GP-S, Copal Electronics, Republic of Korea) was installed to monitor the partial pressure during gas injection. Similarly, a digital manometer capable of measuring pressure between  $-100$  and  $0$  kPa (PG-200-102VP-S, Copal Electronics, Republic of Korea) was installed to measure the vacuum pressure. At the bottom of the vessel, a vacuum pump (08292, Woosung vacuum, Republic of Korea) with a vacuum pressure of  $0.4$  Pa was installed to inject gas into the vessel.

### 2-2. Energy Supply Component

In the energy supply component, a high-voltage device (TOS 5101, Kikusui) operated over a measurement range from  $0$  to  $10$  kV was used. It instantaneously supplies energy to the discharge circuit through the capacitor charged at high voltage.

### 2-3. Explosion Energy Measurement and Storage Component

The data signals obtained from an amplifier (DA-16A, Tokyo Sokki Kenkyujo) capable of amplifying the signal of the pressure sensor in the event of an explosion (DA-16A, Tokyo Sokki Kenkyujo) are measured using an oscilloscope with a frequency of  $100$  MHz (TDS 3014; Tektronix) and stored in a computer.

## 3. Experimental Method

Through the gas regulator at the top of the gas container, the gas entering the explosion vessel was maintained at a constant low

pressure. The inside of the explosion vessel was turned into a vacuum state with a gauge pressure of  $-0.10$  MPa using the vacuum pump.

The amounts of gases required for the experiment were calculated using Dalton's law of partial pressure [21,22]. The gases were injected at a constant pressure maintained by the vacuum gauge installed at the top of the explosive device. In this case, the flow rate was adjusted using a precision valve (NV2H-4T). After the mixing of the gas was completed, the ignition switch was operated to check the pressure through the oscilloscope to determine if there was an explosion. When the experiment was repeated, the inside of the explosion vessel was turned into a vacuum state again, and then the ventilation and air valves were opened for at least  $15$  min before the experiment was repeated.

## RESULTS AND DISCUSSION

### 1. Explosion Limit and MOC According to Pressure

#### 1-1. Explosion Limit

To evaluate the characteristics and risks of explosions according to the pressure, explosion limits were measured according to the amount of  $N_2$ - $O_2$ - $C_3H_6$  injected, and the MOC required for flame propagation was measured. Fig. 2 shows the measured explosion limits at  $25^\circ\text{C}$  while the pressure was varied between  $0.10$  to  $0.15$ ,  $0.20$ , and  $0.25$  MPa. As the pressure increased from  $0.10$  to  $0.25$  MPa, the LEL did not change, but the UEL increased from  $13.5\%$  to  $15.1\%$ . When the pressure increases, the explosion limit appears to be extended because the average intermolecular distance decreases and the effective collision frequency of gas molecules increases, thereby easing flame propagation. Moreover, the UEL rapidly decreased as the oxygen concentration decreased. The explosion limit appears to have decreased because the amount of oxygen required for the explosive reaction between combustibles and oxygen was not sufficient.

#### 1-2. Minimum Oxygen Concentration (MOC)

A minimum oxygen supply is required for flame propagation, and this is referred to as MOC. Fig. 3 shows the variation of the min-

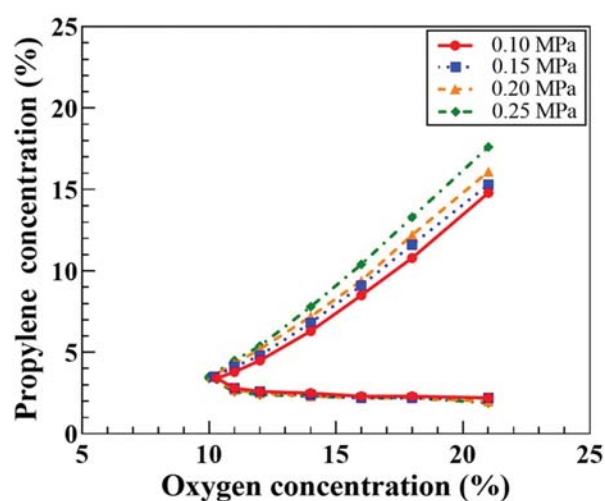


Fig. 2. Explosion limit; Relationship between pressure and oxygen and propylene concentrations at  $25^\circ\text{C}$ .

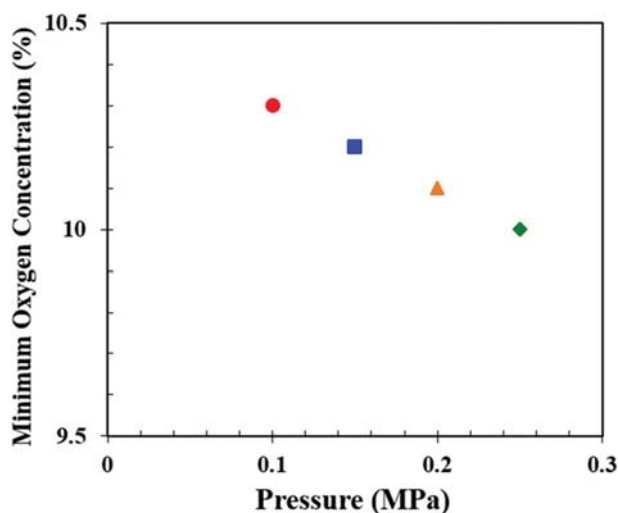


Fig. 3. Relationship between pressure and Minimum oxygen concentration at 25 °C.

imum oxygen concentration with the change of pressure at 25 °C. The minimum oxygen concentration was 11.2% when the pressure was 0.10 MPa and 10.8% when the pressure was 0.25 MPa. Therefore, the MOC decreased by 0.4% as the pressure increased from 0.10 MPa to 0.25 MPa. When the pressure increased, the minimum oxygen concentration decreased, which means that the risk of the process became higher. This is attributed to the fact that the

reaction rate increases as the collision frequency of molecules inside the explosion vessel increases with the rising pressure, which leads to the decrease in the minimum oxygen concentration. Therefore MOC can be used to prevent explosions or to extinguish fires through deactivation, and thus it is used as an important factor in securing safety for a process safety operation.

## 2. Explosion Pressure, Pressure Rise Rate and $K_g$ According to the Pressure at 25 °C

### 2-1. Explosion Pressure

Fig. 4 shows the explosion pressure with pressure change at a propylene concentration of 5% at 25 °C. Fig. 4(a) shows the relationship between time and explosion pressure according to the concentration of oxygen when the pressure is 0.10 MPa, while Figs. 4(b), (c), and (d) represent the explosion pressures at 0.15, 0.20, and 0.25 MPa, respectively. At an oxygen concentration of 21%, the explosion pressure was 2.76 MPa when the pressure was 0.10 MPa and 8.32 MPa when it was 0.25 MPa, showing that the explosion pressure increased three times as the pressure increased.

As the pressure increased from 1.0 bar to 2.5 bar, the maximum explosion pressure increased due to the increase in the mass of the entire combustible gases within the combustible mixer. As the oxygen concentration decreased from 21% to 14% at the same pressure, the explosion pressure decreased, which can be attributed to the fact that the explosion pressure was measured to be low since the amount of oxygen that reacted with the fuel decreased.

### 2-2. Explosion Pressure Rise Rate

Fig. 5 shows the change in pressure rise rate over time.

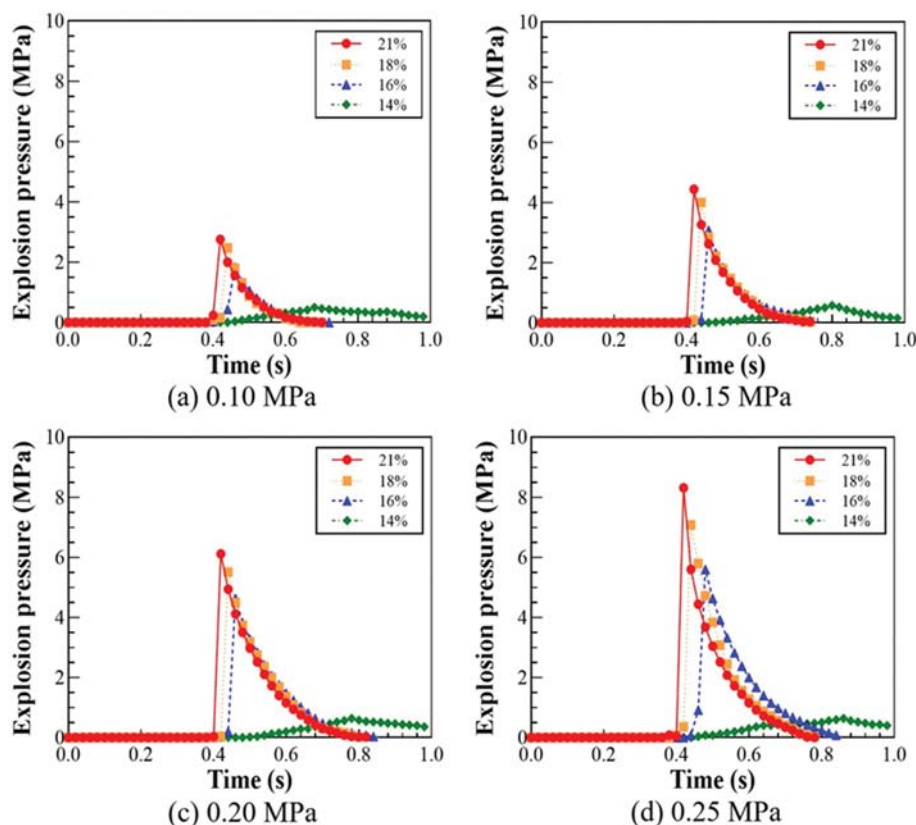


Fig. 4. Explosion pressure of propylene according to the oxygen concentration and time at 25 °C.

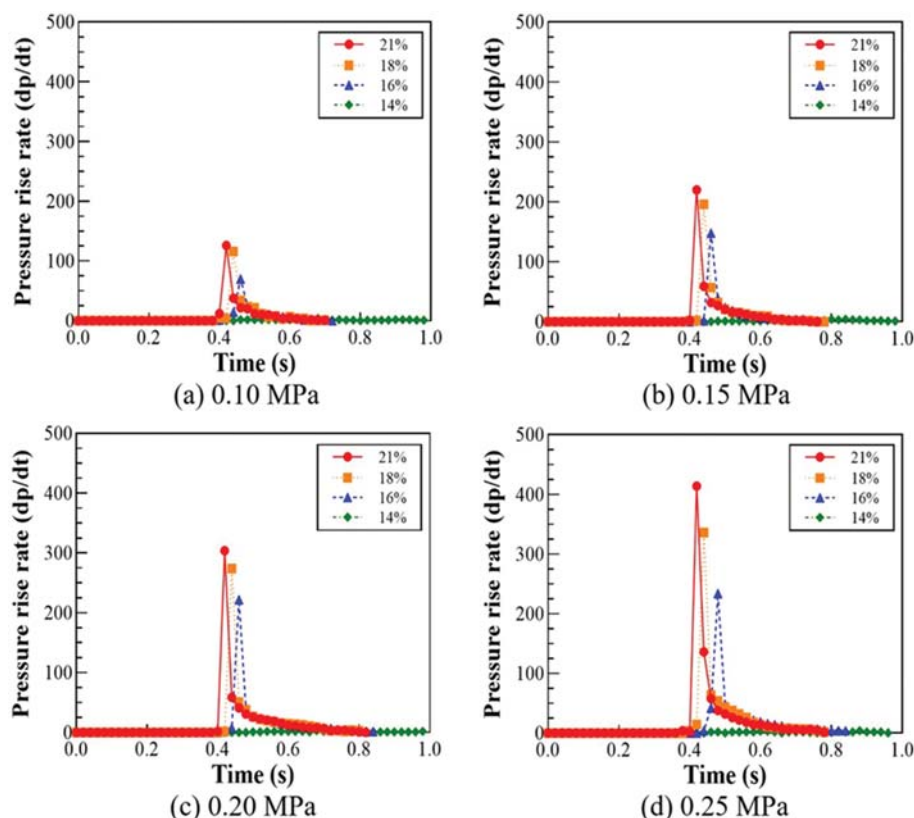


Fig. 5. Explosion pressure rise rate of propylene according to the oxygen concentration and time at 25 °C.

Fig. 5(a) shows the relationship between time and explosion pressure rise rate according to the concentration of oxygen when the pressure is 0.10 MPa, while Fig. 5(b), 5(c) and 5(d) show the explosion pressure rise rates at pressures of 0.15 MPa, 0.20 MPa and 0.25 MPa, respectively. At the oxygen concentration of 21%, the maximum explosion pressure rise rate released from 126 MPa/s at a pressure of 0.10 MPa to 414 MPa/s at 0.25 MPa. As the pressure increased from 0.10 MPa to 0.25 MPa, the explosion pressure rise rate increased by three times. This shows how strong and dangerous the explosion is and confirms that the maximum explosion pressure increases and is affected by the pressure with the increase in the pressure at the same oxygen concentration. In addition, as the oxygen concentration increased at the same pressure, the time to reach the maximum explosion pressure was shortened. Therefore, as the oxygen concentration increases, the explosion delay time decreases, consequently increasing the danger. The main features of the explosion of a closed container are the explosion pressure and the explosion pressure rise rate. The higher the explosion pressure and the rate of explosion pressure rise, the greater the magnitude of secondary damage.

### 2-3. Gas Deflagration ( $K_g$ )

The higher the maximum explosion pressure increase rate and maximum explosion pressure, the stronger the explosion is and the greater the scale and risk of damage.  $K_g$  aims to minimize the damage from explosion by installing openings such as discharge panels.

Thus,  $K_g$  affected by the initial pressure can be obtained using the maximum explosion pressure increase rate and the volume of

the vessel produced in the enclosed space, as shown in Eq. (1), and can be used to determine the required outlet size and thickness to prevent overpressure due to explosion.

Where,  $(dp/dt)_{max}$  is the maximum explosion pressure rise rate and  $V$  is the volume of the sealed vessel ( $0.0011 \text{ m}^3$ ).

$$K_g = \left( \frac{dp}{dt} \right)_{max} \times V^{\frac{1}{3}} \quad (1)$$

Table 1 shows the gas deflagration index with respect to pressure at varied oxygen concentrations. When the oxygen concentration was 21% and the pressure was 0.10 MPa, the deflagration index of the gas was 13.01 m·MPa/s; when the pressure was 0.25 MPa, the deflagration index was 42.74 m·MPa/s.

For the same oxygen concentration, the value of  $K_g$  increased as the pressure increased, and at 0.10 MPa, as the oxygen concentration decreased from 21% to 16%, the deflagration index decreased considerably from 13.01 m·MPa/s to 7.23 m·MPa/s.

Table 1. Gas deflagration index according to the pressure at 25 °C

O <sub>2</sub> [%]	Pressure [MPa]			
	$K_g$ [m·MPa/s]			
	0.10 MPa	0.15 MPa	0.20 MPa	0.25 MPa
21.0	13.01	22.71	31.38	42.74
18.0	11.98	20.23	28.28	34.48
16.0	7.23	15.28	22.92	24.16

Therefore, at the oxygen concentration of 21%, as the reactivity with the combustible gas propylene is high, the gas deflagration index becomes high, leading to the high risk of explosion. At the oxygen concentration of 16%, the oxygen concentration is insufficient, and thus, even if the distance between combustible molecules is close at the high concentration of combustible gases, the reactivity is low due to the lack of oxygen, resulting in the low deflagration index.

## CONCLUSIONS

To obtain the explosion limit and the minimum oxygen concentration (MOC) for the process safety operation of propylene in accordance with the change in pressure, an experiment was performed by varying the oxygen concentration using N<sub>2</sub>, an inert gas. The following conclusions were drawn:

1) At 25 °C, as the pressure increased from 0.10 to 0.25 MPa, the LEL exhibited no change and the UEL increased from 13.5% to 15.1%. Thus, increasing the pressure at the same temperature facilitates the propagation of flames, thereby increasing the risk of explosion limits.

2) The MOC decreased as the pressure increased at 25 °C. Thus, reducing the oxygen concentration below the MOC prevents flame propagation and explosion.

3) When the pressure increased from 0.10 to 0.25 MPa at 25 °C, the explosion pressure increased from 2.76 to 8.32 MPa, while the maximum explosion pressure rise rate increased from 126 to 414 MPa/s at an oxygen concentration of 21%. Thus, the degree and danger associated with the explosion can be determined.

4) It is possible to predict K<sub>st</sub> through the maximum explosion pressure rise rate and volume of vessel. The index is also used to design the size and material of the outlet.

Therefore, in any process using propylene, explosion limit, MOC, explosion pressure, and explosion pressure rise rate must be appropriately considered to prevent any explosions. Furthermore, the results of this study can be utilized as basic data in workplaces that use propylene at high temperatures.

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