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Thermal–oxygen evolution and atmospheric pollutant emission characteristics during the vertical propagation of underground coal fires

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Abstract

Underground coal fire propagation is concealed and difficult to monitor, while the resulting atmospheric pollution poses persistent environmental risks. However, the coupled evolution of the temperature field, oxygen concentration, and pollutant emissions during vertical propagation remains insufficiently understood. In this study, a self-developed physical similarity simulation experimental system was used to conduct a physical similarity simulation experiment from ignition to extinction. The temperature field, oxygen concentration, CO₂, CO, CH₄, C₂H₆, PM_{2.5}, PM₁₀, and total suspended particles were monitored continuously. The results showed that thermal–oxygen evolution could be divided into five stages: incubation, rapid heating, intensive reaction, rapid cooling, and burnout. Clear depth-dependent differences were observed: C1–C2 were dominated by burnout, C3–C5 constituted the principal sustained-reaction zone, and C6 exhibited oxygen-limited attenuation. Responses in the overlying strata and at the ground surface lagged behind those within the coal seam. CH₄, C₂H₆, and particulate matter were released mainly during the early stage, whereas CO₂ and CO dominated the middle and later stages. CH₄ and C₂H₆ were concentrated within the first 40–60 h and approached background levels after approximately 80 h. The atmospheric pollution assessment indicated predominantly moderate-to-severe pollution, with CO as the principal contributor. These findings clarify the stage-dependent and depth-dependent coupling among heat transfer, oxygen consumption, and

pollutant emissions during the vertical propagation of underground coal fires, providing a basis for monitoring, risk assessment, and mitigation.

Keywords:

underground coal fire; vertical propagation; temperature field; oxygen concentration; atmospheric pollution; physical similarity simulation experiment

1 Introduction

Underground coal fires, typically associated with coal spontaneous combustion (CSC), represent one of the most common, complex, and hazardous thermodynamic disasters during coal resource exploitation. In shallow-buried or exposed coal seams, natural or anthropogenic disturbances can induce stress redistribution in the overlying strata. This process promotes the development of extensive fractures and air leakage pathways. As a result, the coal seam remains in prolonged contact with oxygen, leading to continuous low-temperature oxidation and heat accumulation. Once the temperature reaches a critical threshold, concealed combustion may initiate and subsequently propagate along the coal seam or fracture networks (Liang et al. 2023). The heat released from coal oxidation has dual effects. On the one hand, it weakens the mechanical strength of the coal–rock mass and induces multiple types of interconnected fractures, resulting in the formation of complex convective pathways that increase the oxygen supply. On the other hand, large quantities of gaseous pollutants and suspended particulate matter generated during combustion can migrate through fracture networks and be emitted into the atmosphere. These emissions pose persistent threats to mine safety, surface geological stability, and the regional ecological environment (Liu et al. 2024). Fire source propagation determines the spatial evolution pathway of underground coal fires. The evolution of thermal–oxygen conditions during propagation constitutes the fundamental driving mechanism for fire persistence. Moreover, pollutant emissions have external impacts on the atmosphere and ecological environment. These three aspects represent not only the primary focus of existing studies but also the core elements integrated within a unified experimental framework in this work.

In terms of the propagation mechanisms of underground coal fires, existing studies have systematically investigated fracture structures, oxygen supply modes, and driving mechanisms (Torero et al. 2020; Wang et al. 2025). Mathematical models for underground smouldering fires based on coal pyrolysis and carbon oxidation reactions have revealed the oxygen-supply control mechanism of fire propagation under oxygen-limited conditions (Song 2022; Zhu et al. 2025). Physical and numerical studies have analysed the effects of fracture-channel geometry on airflow and oxygen transport (Li et al. 2023; Wang et al. 2022). Numerical and experimental results further indicated that oxygen supply, thermal circulation, heat losses, and non-uniform air flux are key factors controlling the persistence and propagation of underground coal fires and smouldering fronts (Wessling et al. 2008; Rashwan et al. 2021). Controlled experiments have established multi-parameter experimental frameworks for underground coal fires. By adjusting fire depth, coal particle size, and fissure size, these studies systematically analysed the propagation characteristics of the drying, pyrolysis, and oxidation fronts (Song et al. 2019; Zhang et al. 2019). Their findings indicated that ventilation during the smouldering stage is driven primarily by the buoyancy of hot flue gases.

With respect to the thermal–oxygen coupling mechanism, previous studies have demonstrated that thermal–

oxygen conditions are critical for controlling the initiation, propagation, and attenuation of smouldering combustion (Beamish and Theiler 2019). Experimental and numerical studies have investigated the vertical migration of high-temperature zones in underground coal fires and reported nonlinear propagation characteristics, with characteristic temperatures generally decreasing with depth (Bustamante Rúa et al. 2019; Zhao et al. 2023a). Studies of coal-fire propagation depth and direction have further indicated that fire spread depends on oxygen availability and preferentially follows the dip direction of coal seams, while structural discontinuities can alter the propagation pathway (Bustamante Rúa et al. 2019; Singh et al. 2021). Furthermore, Wang et al. (2017) developed a coupled heat-transfer model that incorporates conduction, convection, radiation, and finite-rate oxidation reactions for spontaneous combustion in porous coal and rock strata.

In terms of atmospheric pollutants, underground coal fires release mainly gaseous pollutants, including CO₂, CO, CH₄, and C₂H₆ (Engle et al. 2012), as well as suspended particulate matter (Li K et al. 2022; Reisen et al. 2017), such as PM_{2.5}, PM₁₀, and total suspended particles (TSPs). Jia et al. (2022), on the basis of the theory of CSC, systematically elucidated the generation processes and mechanisms of major gaseous products during coal combustion. Zhao et al. (2019) classified the CSC process into different stages and highlighted the significance of gas composition evolution with respect to reaction stages. Low-temperature oxidation experiments have demonstrated that the concentrations of CO, CO₂, CH₄, and C₂H₆ vary systematically with temperature, with some gases increasing rapidly after the onset of coal cracking (Ma et al. 2020; Wang et al. 2023; Yan et al. 2022; Chen et al. 2022); at the near-surface scale, CO₂ diffusion and CO₂ and CO fluxes are affected by surface temperature, wind, meteorological conditions, and soil properties (Zhang et al. 2025; Xing et al. 2023). With respect to particulate matter, Li et al. (2022) quantitatively evaluated the emissions of CO₂, CO, and PM_{2.5} from underground coal fires and characterized the physicochemical properties and toxicity of PM_{2.5}. Field measurements by Reisen et al. (2017) further revealed that coal fires can lead to severe exceedances of PM_{2.5} and CO concentrations over spatial scales ranging from hundreds of metres to several kilometres.

However, most existing studies are based on constant-temperature oxidation experiments, small-scale bench tests, or macroscopic emission statistics. Systematic experimental investigations under conditions simulating the vertical propagation of underground coal fires are still lacking. In particular, there is still a lack of integrated experimental systems that enable the simultaneous monitoring and coupled analysis of the temperature field, oxygen concentration, and typical atmospheric pollutants. Moreover, the complete chain of “propagation–temperature–oxygen concentration–gaseous pollutants–particulate matter,” as well as the multilayer interactive responses between the coal seam and the overlying strata, remains insufficiently constrained by quantitative evidence derived from a unified physical similarity simulation platform.

On this basis, a physical similarity simulation experimental system for the vertical propagation of underground coal fires was established in this study. The temperature transfer, oxygen supply mechanism, and emission behaviour of typical pollutants were taken as the primary research focuses. Systematic analyses were conducted on the thermodynamic evolution during different stages of vertical fire propagation, the concentration evolution of atmospheric pollutants, and their effects on air quality. The results contribute to a deeper understanding of the development mechanisms of underground coal fires. They also clarify the emission characteristics of different pollutants and their controlling factors during fire propagation. Furthermore, this study provides a theoretical basis for the prevention and control of coal fire hazards, as well as for ecological and environmental management in

mining areas.

2. Experimental methods

2.1 Construction of the physical similarity simulation experimental system for underground coal fire propagation

On the basis of the principle of physical similarity, a physical similarity simulation experimental system for underground coal fire propagation was constructed in this study. Key parameters, including geometric dimensions and medium density, were designed according to similarity criteria. The developed system can simulate the vertical propagation process of underground coal fires from ignition to extinction under controlled conditions. It also enables the acquisition of high temporal resolution data for the temperature field, oxygen concentration, and typical pollutants.

The combustion furnace of the simulation system is a rectangular chamber with dimensions of 30 cm× 30 cm× 60 cm. With the exception of the top surface, all the other sides of the furnace are lined with thermally insulated bricks to simulate the insulating effect of the surrounding rock. The interior of the furnace is divided into eight layers along the vertical direction, with each layer having a height of 7.5 cm. Layers C1–C6 represent the coal seam space, while the upper two layers are filled with soil to simulate the overlying strata. Considering both the mining conditions and the scale of the experimental system, the similarity constants were determined according to Eqs. (1)–(4).

The calculated geometric similarity ratio for the thickness of the overlying strata is as follows:

$$\alpha_l = \frac{L_p}{L_m} = 1/50 \quad (1)$$

where L_p represents the thickness of the overlying strata designed in the experimental system (m), and L_m represents the average thickness of the overlying strata in the actual mining area (m).

The calculated geometric similarity ratio for the coal seam thickness is as follows:

$$\alpha_l = \frac{L_p}{L_m} = 1/5 \quad (2)$$

where L_p represents the thickness of the coal seam designed in the experimental system (m), and L_m represents the average thickness of the coal seam in the actual mining area (m).

The similarity ratio for the bulk density of the overlying strata is as follows:

$$\alpha_\gamma = \frac{\gamma_p}{\gamma_m} = 1/1 \quad (3)$$

where γ_p represents the soil density designed in the experimental system (g/cm³), and γ_m represents the actual surface soil density above the coal seam in the mining area (g/cm³).

The similarity ratio for the bulk density of the coal seam is calculated as follows:

$$\alpha_{\gamma} = \frac{\gamma_p}{\gamma_m} = 1/1.2 \quad (4)$$

where γ_p represents the density of coal particles designed in the experimental system (g/cm^3), and γ_m represents the density of the coal seam in the actual mining area (g/cm^3).

To achieve synchronous monitoring of multiple parameters during the propagation of underground coal fires, the system was equipped with three subsystems: temperature measurement, gas analysis, and particulate matter monitoring (Figure 1). The temperature measurement system is based on a self-developed digital display platform, which is connected to temperature sensors for real-time monitoring. The gas analysis system is centred on a gas chromatograph. Gas samples are extracted from different positions within the furnace through sampling pipelines. The concentrations of typical gases, including CO_2 , CO , CH_4 , C_2H_6 , and O_2 , are quantitatively analysed to characterize the oxygen consumption and gas emission behaviours of the coal sample at different stages. The particulate matter monitoring system employs a pump-suction particle monitor to measure the concentrations of suspended particles with different size ranges in the air environment.

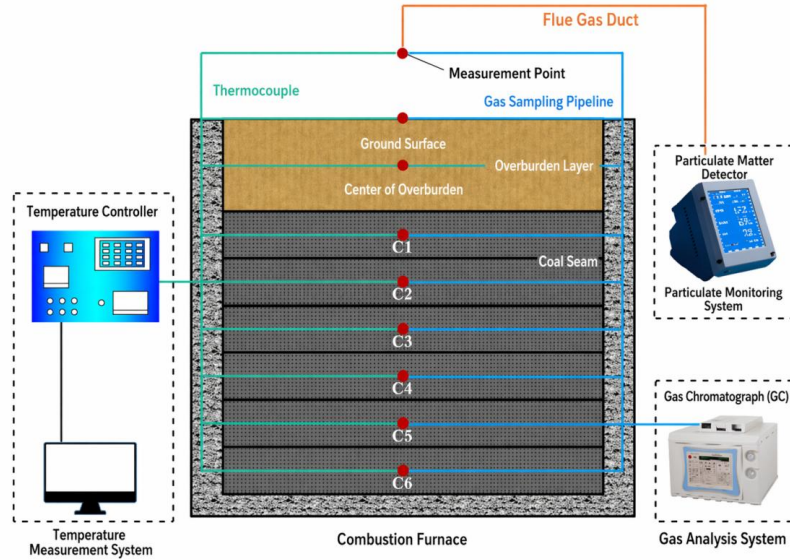


Fig. 1. Principle and experimental system of the physical similarity simulation for underground coal fire propagation

2.2 Experimental conditions

The coal samples and overlying soil used in the experiments were collected from the Shendong coalfield. The coal samples were not washed and were sealed and transported to the laboratory after collection. To simulate the actual structure of underground coal seams, coal particles with a size range of 7–10 mm were used in the experiments. To characterize the material properties of the coal samples and ensure the reproducibility of the results, proximate analysis and ultimate analysis were conducted. The results are presented in Table 1 and Table 2.

Table 1 Proximate analysis of coal samples

item	M_{ad}	A_{ad}	V_{ad}	FC_{ad}
raw coal	9.75	22.14	25.33	42.78

bottom ash	1.3	87.67	2.57	8.46
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Table 2 Ultimate analysis of coal samples

item	C	H	O	N	S
content	71.74	4.50	23.36	0.16	0.28

As shown in Table 1, the relatively high fixed carbon content ($FC_{ad} = 42.78\%$) and a certain amount of volatile matter ($V_{ad} = 25.33\%$) indicate that the coal sample can sustain oxidation reactions under increasing temperature conditions. Combined with the relatively high oxygen content ($O = 23.36\%$) in Table 2, the coal sample is more prone to incomplete oxidation under oxygen-limited conditions, resulting in the formation of gaseous products represented by CO. After the experiment, the ash content of the bottom ash increases significantly ($A_{ad} = 87.67\%$), while a certain amount of fixed carbon ($FC_{ad} = 8.46\%$) remains. This suggests that although most combustible components have been consumed, residual carbon still exists. This behaviour reflects the incomplete combustion characteristics of smouldering under oxygen-limited conditions and provides support for the subsequent analysis of stage-dependent oxygen consumption and pollutant emission patterns.

Approximately 3.5 kg of coal samples were evenly packed layer by layer into the six coal seam compartments (C1–C6), ensuring consistent packing density and heat accumulation conditions for each layer at the initial stage. To simulate the heat transfer environment between the underground coal seam and the overlying strata, the upper two compartments were filled with soil. These layers function to restrict heat dissipation and regulate oxygen transport during the subsequent propagation process.

After the coal samples were filled, a heating rod was placed at the geometric centre of layer C1 for active heating at a heating rate of $5\text{ }^{\circ}\text{C}/\text{min}$. To avoid local temperature overshoot caused by excessive heating rates and to improve reproducibility, the final temperature of the heating rod was controlled at $350\text{ }^{\circ}\text{C}$. This ensured that the coal entered a stage of enhanced exothermic reactions and stably triggered self-heating runaway. The onset of a noticeable temperature rise in layer C2 was taken as the indicator of ignition in layer C1, at which point the power supply to the heating rod was turned off. The experiment then entered the underground coal fire propagation stage. Data acquisition was terminated when all monitored parameters returned to their initial ambient levels.

During the propagation stage, the experimental system operated continuously for approximately 1100 h. The experiment was terminated when the temperature of layer C6 decreased to ambient temperature. The temporal evolution curves of all the parameters were subsequently extracted for analysis. The reported data represent the mean values of three repeated experiments, and the maximum relative deviation among the repeated measurements was within $\pm 5\%$.

3. Results and discussion

3.1 Temperature evolution characteristics and stage division of fire propagation

Temperature is a direct indicator of heat release during underground coal fire processes, and its variation reflects the progression of coal seam combustion. As shown in Figure 2, under continuous heating conditions, first, the temperature of layer C1 rapidly increases. Heat is then transferred downwards through conduction and radiation, driving a sequential temperature rise in layers C2–C6 and forming a depth-dependent temperature field structure. The heating stages of each coal layer are generally short in duration and quickly reach peak temperatures. This finding indicates that once sufficient heat accumulation and oxygen supply conditions are satisfied, the fire can

propagate rapidly towards deeper coal seams within a relatively short period.

Layers C1 and C2 are characterized by rapid heating followed by rapid cooling. However, the cooling process in layer C2 lags behind that in layer C1, which is attributed mainly to its greater burial depth and relatively lower heat dissipation rate. Layers C3–C5 exhibit a typical increase in secondary temperature, and this phenomenon becomes more pronounced with increasing depth. This is because deeper coal samples maintain higher temperatures during the same period, continuously transferring heat and radiation to adjacent layers, which induces reignition of the overlying residual coal. Although a secondary temperature increase is also observed in layer C6, its second peak is significantly lower than that of layer C5 because of oxygen-limited conditions. This finding indicates that the vertical propagation of the coal fire is restricted at greater depths.

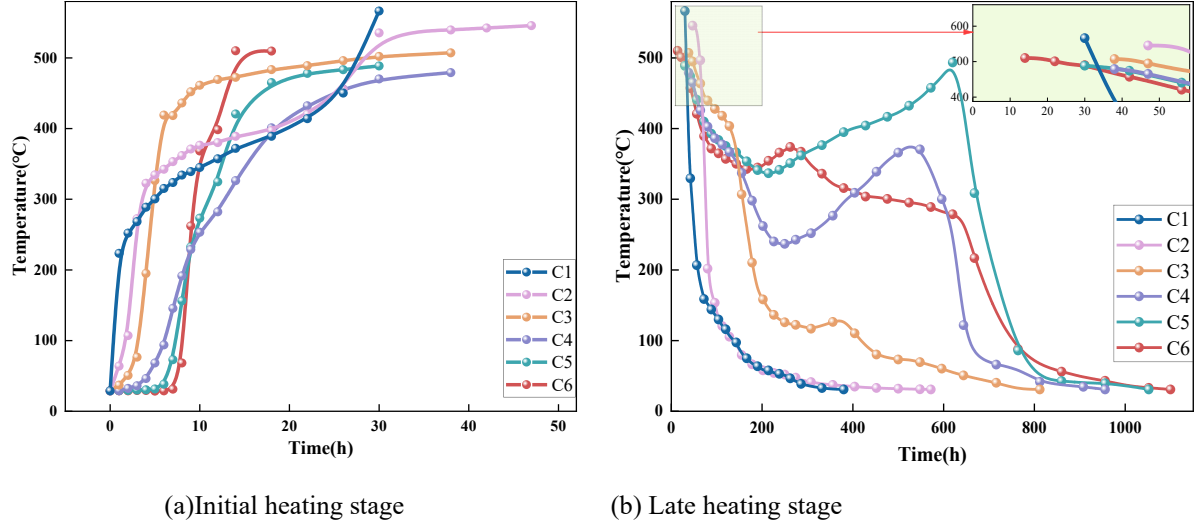


Fig. 2. Variation of temperature with time in different coal layers

In this study, the propagation stages were systematically divided on the basis of the characteristics of the first- and second-order derivatives of the temperature–time curves for different coal layers. Taking layer C4 as an example (Figure 3), the inflection point $f'(t_1) = 0$ is used to distinguish the incubation stage (I) from the rapid heating stage (II). The first local maximum, $f'(t_2) = 0$, defines the boundary between the rapid heating stage (II) and the intensive reaction stage (III). The second local maximum, $f'(t_3) = 0$, separates the intensive reaction stage (III) from the rapid cooling stage (IV). Finally, the inflection point $f'(t_4) = 0$ is used to distinguish the rapid cooling stage (IV) from the burnout stage (V).

By applying the same method to the temperature curves of the remaining layers, the stage division characteristics for different coal seams can be obtained, as summarized in Table 3. The temporal distribution of each stage significantly varies with burial depth. The incubation, rapid heating, and rapid cooling stages account for relatively small proportions across all the layers. This finding indicates that once a spontaneous combustion point is formed, the temperature evolution rapidly enters a relatively stable high-temperature and attenuation process. The vertical differences are governed primarily by the intensive reaction stage and the burnout stage. The results further reveal a systematic depth-dependent transition in stage duration. In layers C1 and C2, which are close to the surface and subject to strong heat dissipation, the intensive reaction stage is absent, and the process is almost entirely dominated by the burnout stage (>86%). Layers C3–C5 constitute the main heat-release zone, where the intensive reaction stage has the highest time proportion (42.12–53.80%). In contrast, layer C6 exhibits attenuation characteristics of fire propagation because of insufficient oxygen supply.

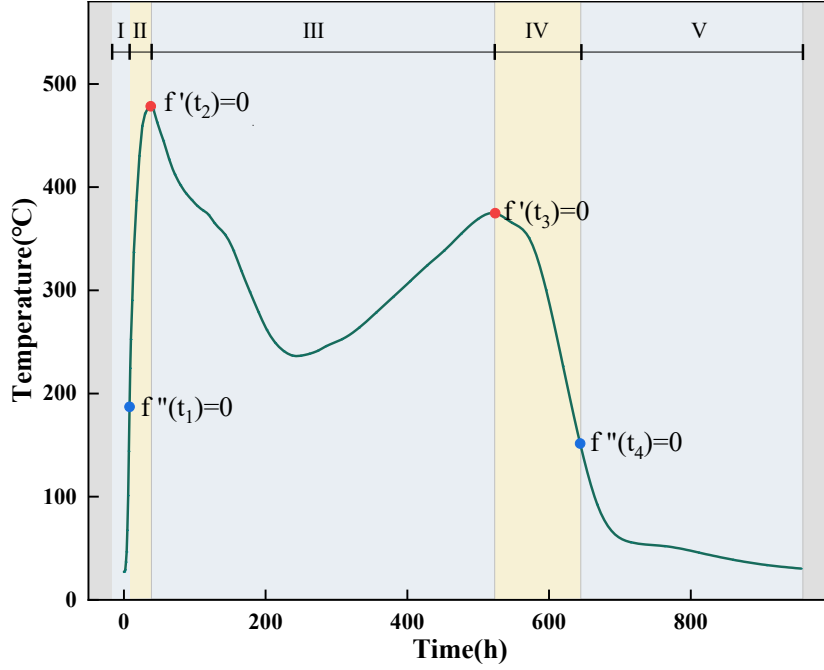


Fig. 3. Criteria for stage division of underground coal fire propagation

Table 3 Stage classification of temperature evolution characteristics for different coal layers during underground coal fire propagation

coal layer	incubation stage(%)	t1 (h)	rapid heating stage(%)	t2 (h)	intensive reaction stage(%)	t3 (h)	rapid cooling stage(%)	t4 (h)	burnout stage(%)
C1	0.39	1.5	7.5	30			3.16	42	88.95
C2	0.52	3	7.69	47			5.77	80	86.02
C3	0.62	5	4.06	38	42.12	380	14.78	500	38.42
C4	0.84	8	3.14	38	50.84	524	12.55	644	32.63
C5	0.76	8	2.28	30	53.80	596	6.84	668	36.32
C6	0.82	9	0.82	18	22.18	262	4.18	308	72

The vertical propagation of coal seam temperature manifests as a synchronous response in the overlying strata and ground surface, although with an overall slight delay. As shown in Figure 4, the temperatures of the overlying strata and the ground surface reach their first peaks at approximately 30 h (201 °C and 72.8 °C, respectively). When secondary temperature increases in layers C3–C5, a corresponding minor secondary temperature increase is observed in the overlying strata and ground surface before 600 h (60.2 °C and 38.1 °C, respectively). This behaviour reflects the layer-by-layer heat transfer characteristics within porous media. Owing to the relatively rapid heat dissipation of the overlying strata and the ground surface, it is difficult for them to form a stable heat accumulation platform. As a result, their peak temperatures remain significantly lower than those within the coal seam. Nevertheless, they maintain an anomalous temperature increase throughout the entire fire development process, indicating that heat from underground coal fires can effectively propagate upwards and potentially adversely impact the surface environment.

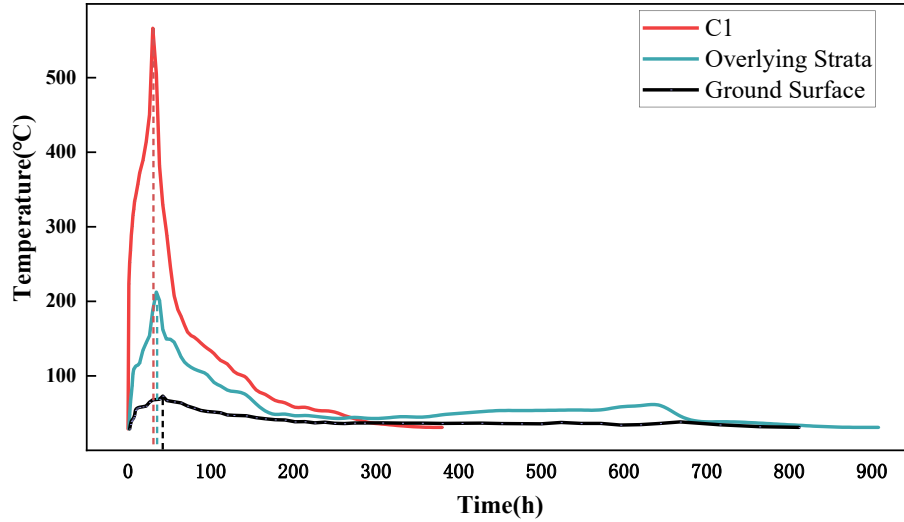
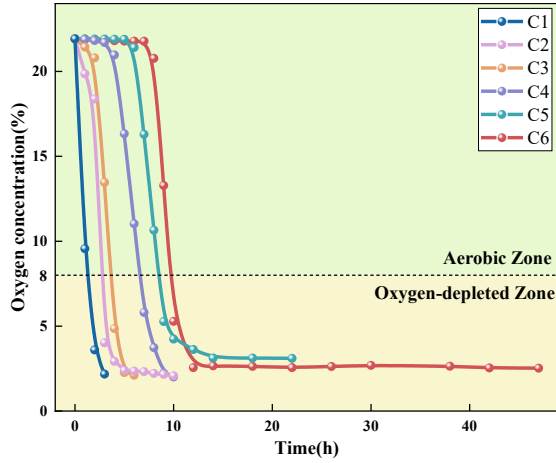


Fig. 4. Variation of temperature with time at the overlying strata and ground surface

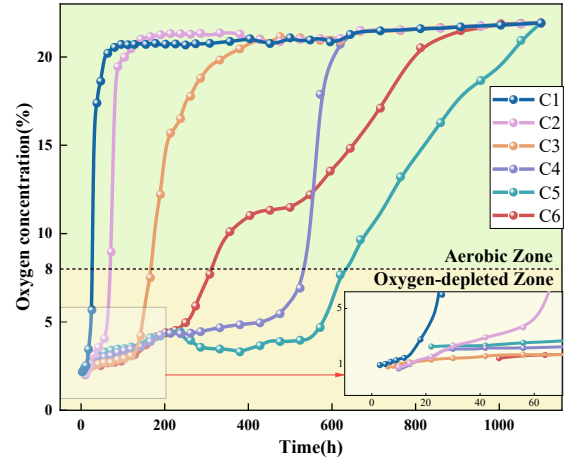
3.2 Evolution characteristics of the oxygen concentrations and oxygen supply limitations

The influence of air on underground coal fires is reflected primarily by the oxygen concentration under smouldering conditions (Deng et al. 2019; Wojtacha-Rychter and Smoliński 2020). As shown in Figure 5, the oxygen concentration in each layer decreases rapidly after heating. With increasing temperature, the oxygen concentration decreases sharply layer by layer, reflecting rapid oxygen consumption associated with coal–oxygen reactions during the initial heating stage. After the minimum level is reached, the recovery rate of the oxygen concentration varies among the different layers. Layer C1, which is close to the ground surface, can obtain oxygen from the external environment, allowing its oxygen concentration to recover to near ambient levels within a relatively short time. In contrast, the recovery rate of layers C2–C5 decreases with increasing depth. In particular, the oxygen concentration in layer C5 fluctuates around the minimum level before 600 h, indicating that the duration of smouldering is greatest under oxygen-limited conditions.

In layer C6, the oxygen concentration initially increases slowly during the recovery stage. After approximately 200 h, a short period of rapid increase is observed, indicating that the underground coal fire begins to show signs of extinction and that the demand for oxygen starts to decrease. However, from 400–600 h, the oxygen concentration ceases to increase. This can be attributed to two factors. First, the temperature remains relatively high and decreases slowly during this stage. Owing to the sufficient availability of coal, the layer still maintains a certain demand for oxygen. Second, layers C3–C5 experience a secondary temperature increase during this period, and the elevated temperatures further sustain the combustion state in layer C6. Beginning from layer C6, the vertical propagation of underground coal fires attenuates. Therefore, this layer is defined as the transition layer marking the onset of propagation attenuation.



(a) Early stage of the experiment



(b) Late stage of the experiment

Fig. 5. Variation of O_2 concentration with time in different coal layers

To compare the evolution characteristics of the oxygen concentration across different stages, the oxygen concentration curves of each coal layer were divided into stages on the basis of the previously established propagation stage classification method, as shown in Table 4. The first and second stages account for less than 5% of the total duration in all the layers. These stages mainly correspond to the rapid oxygen consumption caused by coal self-adsorption and initial oxidation. Once a spontaneous combustion point is formed, the internal oxygen concentration of the coal rapidly decreases from ambient levels to an oxygen-limited state within a very short time, resulting in a limited early intervention window. The third and fourth stages represent the primary recovery phases of oxygen concentration, and the recovery rate decreases with increasing depth. In particular, layer C5 remains in a stable oxygen-limited environment for an extended period, serving as the main oxygen consumption zone sustaining smouldering combustion. Compared with the other layers, layer C6 exhibits distinct behaviour. After the third stage, the oxygen concentration recovers rapidly, and the sharp reduction in oxygen consumption further confirms the attenuation of fire propagation in this layer. The proportion of the fifth stage generally decreases with depth. Layers C1 and C2 have higher proportions and faster recovery, whereas layer C5 does not exhibit typical fifth-stage characteristics, further indicating its prolonged smouldering duration and slow oxygen concentration recovery.

Table 4 Stage classification of oxygen concentration evolution characteristics for different coal layers during underground coal fire propagation

Coal layer	Stage I (%)	t1	Stage II (%)	t2	Stage III (%)	t3	Stage IV (%)	t4	Stage V (%)
C1			0.27	3	2.09	26	10.64	143	87
C2	0.18	2	0.73	10	5.64	72	12.91	214	80.54
C3	0.27	3	0.27	6	15.64	178	38	596	45.82
C4	0.55	6	0.36	10	48.91	548	24	812	26.18
C5	0.73	8	1.27	22	63.73	723	34.27		
C6	0.82	9	3.45	47	23.73	308	62.63	997	9.37

As shown in Figure 6, compared with normal levels, the oxygen concentrations in the atmospheric environment and near-surface region exhibit only minor variations. Owing to the dilution effect of gases escaping through fractures on near-surface air, the surface oxygen concentration remains slightly lower than that of the ambient

atmosphere. The variation in oxygen concentration within the overlying strata tends to be similar to that in layers C1 and C2. In brief, oxygen-limited conditions occur in the overlying strata at approximately 3 h, with the oxygen concentration decreasing to a minimum of 7.531%. This reflects the rapid adsorption and continuous consumption of oxygen by the underlying coal during the initial stage of spontaneous combustion.

Before 30 h, the oxygen concentration in the overlying strata decreases rapidly, which is followed by recovery. This behaviour results from the combined effects of oxygen consumption and dilution by generated gases. In the early stage, oxygen consumption by coal self-adsorption is dominant. In the later stage, as the combustion products accumulate, the gas dilution effect is enhanced and becomes the primary controlling factor. The coal fire subsequently enters a relatively stable stage, during which the oxygen concentration in the overlying strata fluctuates slightly below that of the ambient atmosphere. These findings indicate that the combined effects of an oxygen-limited environment and anomalous temperature increase may threaten biological survival in the overlying strata and adversely impact the near-surface ecological environment.

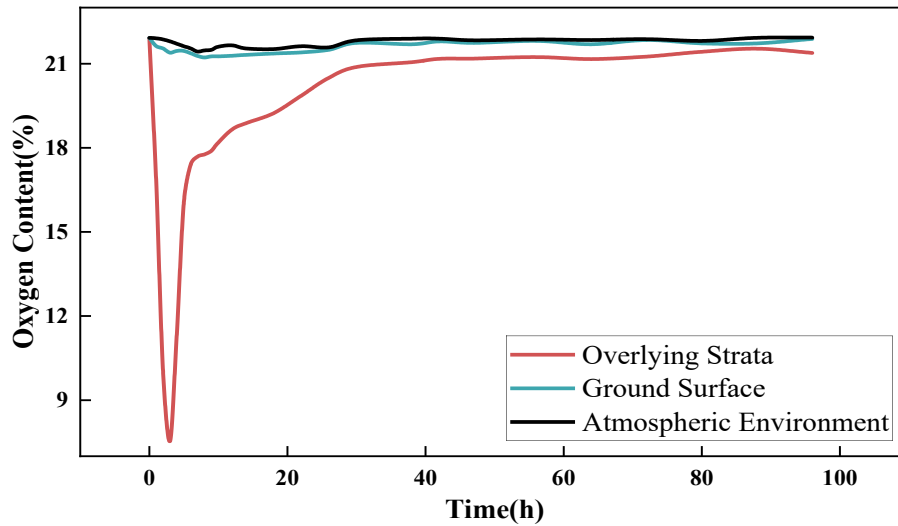


Fig. 6. Variation of O₂ concentration with time at the overlying strata, ground surface, and atmospheric environment

3.3 Emission characteristics of typical pollutant gases

During the propagation of underground coal fires, large quantities of typical atmospheric pollutants, which are primarily carbon oxides (CO₂ and CO) and reducing hydrocarbon gases (CH₄ and C₂H₆), are released. The generation mechanisms, emission timings, and depth distributions of different gases significantly differ. These characteristics are coupled with the evolution of coal seam temperature and oxygen supply conditions, forming stage-dependent and layer-dependent emission patterns of pollutants.

3.3.1 Evolution of CO₂ concentrations

The temporal evolution of the CO₂ concentration in different coal layers during underground coal fire propagation is shown in Figure 7. In the initial stage, CO₂ release exhibits a depth-dependent lag, and all layers reach their first peak at approximately 14 h. Subsequently, the concentration decreases overall because of stage-dependent cooling. In layers C1–C3, the CO₂ concentration shows a single-peak decay pattern, and the rate of decrease slows with increasing depth. This behaviour can be attributed to two factors: the direct generation of CO₂

from high-temperature coal pyrolysis and the further oxidation of the intermediate product CO (Zhao et al. 2023b). In contrast, layers C4–C6 exhibit multiple periodic fluctuations in CO₂ concentration. Although C4 and C5 experience a temporary decrease at approximately 350 h, sufficient heat accumulation enables continuous carbon chain cracking and recombination with O₂, leading to renewed increases in the CO₂ concentration and the formation of the second and third peaks. These findings indicate that these layers maintain strong oxidation and heat release capacity over an extended period. By comparison, layer C6 shows a rapid decline after the second peak. This is attributed to both the weakening thermal influence from the overlying coal layers and insufficient local temperature and oxygen supply to sustain continuous CO₂ generation.

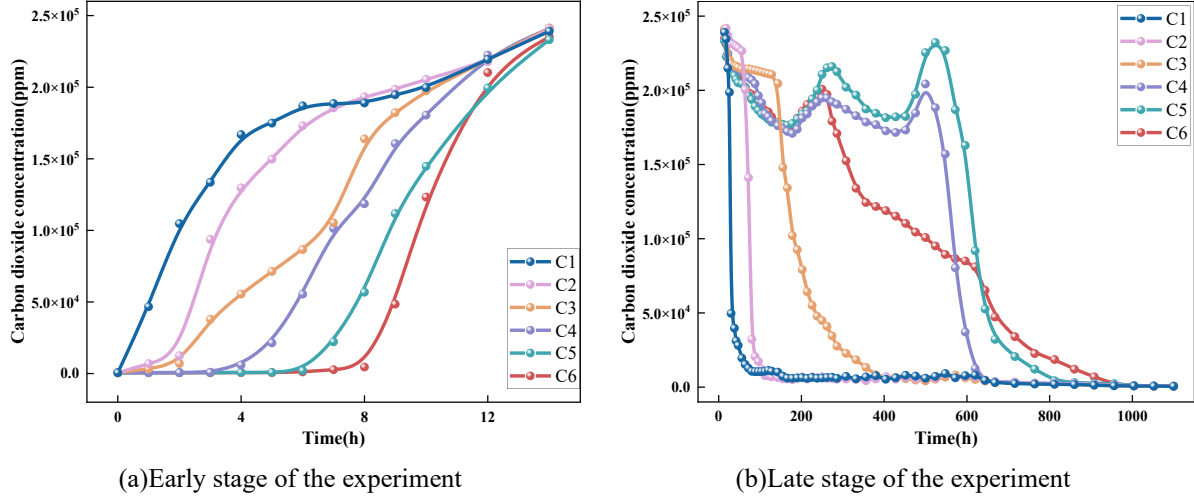


Fig. 7. Variation of CO₂ concentration with time in different coal layers

On the basis of the three local maxima, the CO₂ emission process is divided into four stages, as summarized in Table 5. The first stage is very short in duration, with no significant differences among layers, corresponding to the initial accumulation of CO₂. In the second stage, layers C3–C6 maintain relatively high CO₂ concentrations for an extended period after the first peak, whereas layer C1 exhibits weaker sustained release because of strong heat dissipation. The third stage appears only in layers C4 and C5 and corresponds to multippeak behaviour, indicating that these layers act as the dominant zones for concentrated CO₂ release during the middle and later stages. The fourth stage accounts for the greatest proportion of time across all layers, and its duration generally decreases with increasing depth. However, this trend is not observed in layer C6, where fire propagation is restricted.

Table 5 Stage classification of CO₂ concentration for different coal layers

Coal layer	Stage I (%)	t1	Stage II (%)	t2	Stage III (%)	t3	Stage IV (%)
C1	1.27	14					98.73
C2	1.27	14	3.01	47			95.72
C3	1.27	14	10.36	128			88.37
C4	1.27	14	21.45	250	22.73	500	54.55
C5	1.27	14	23.64	274	22.73	524	52.63
C6	1.27	14	21.45	250			77.28

The responses of CO₂ in the overlying strata, ground surface, and atmospheric environment are shown in Figure 8. Gas diffusion within the overlying strata is hindered by pore structures and experiences the weakest dilution effect, whereas in the ground surface and atmospheric environment, gases are subject to strong dilution. In the initial stage

of the experiment, the CO₂ concentrations at all monitoring points increase sharply. The CO₂ concentration in the overlying strata reaches its first peak at approximately 3 h, while the peak occurrence at the ground surface and in the atmosphere is significantly delayed and accompanied by much lower peak concentrations.

The CO₂ concentration in the overlying strata subsequently decreases during two cycles, followed by an increase during the middle and later stages, corresponding to the multipeak behaviour observed in layers C4 and C5. This phenomenon can be explained by the further oxidation of CO to CO₂ under high-temperature conditions within the upward gas flow, leading to a secondary increase in the CO₂ concentration in the overlying strata during certain periods. In contrast, as gases migrate upwards and enter the atmosphere, they are continuously weakened and diluted. As a result, similarly pronounced secondary peaks are not observed at the ground surface or in the atmospheric environment. Therefore, the multipeak evolution and attenuation patterns of CO₂ across different coal layers and overlying media reveal that the oxidation process of underground coal fires is jointly controlled by heat accumulation conditions and oxygen supply capacity in both temporal and spatial dimensions.

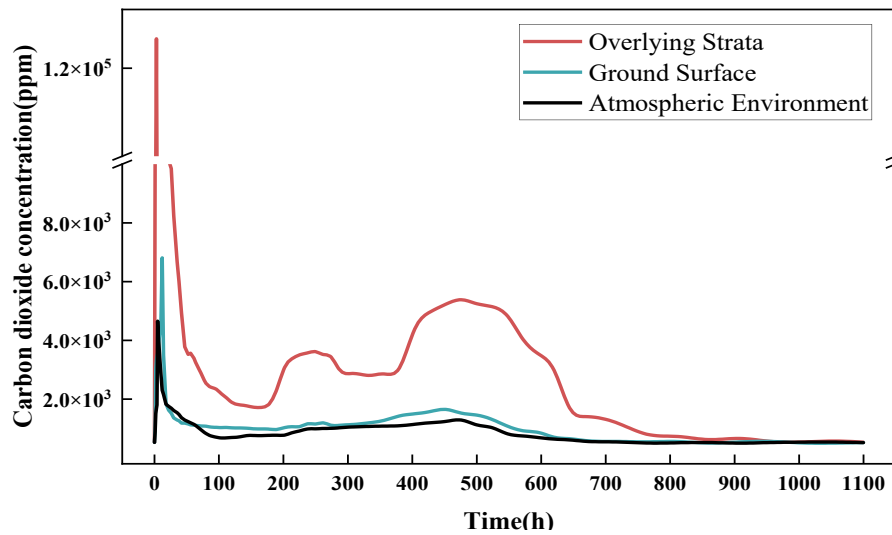


Fig. 8. Variation of CO₂ concentration with time at the overlying strata, ground surface, and atmospheric environment

3.3.2 Evolution of CO concentrations

When heat is transferred to each coal layer, the CO concentration increases rapidly and peaks first. Layers C1–C3 respond almost synchronously, whereas layers C4–C6 exhibit a depth-dependent lag. Subsequently, the CO concentrations in all the layers decrease overall because of cooling. Layers C1 and C2, characterized by weak heat accumulation conditions, show monotonic decay after the first peak. In layer C3, the absence of a pronounced secondary temperature rise results in a relatively rapid attenuation of the CO concentration. In contrast, layers C4 and C5 exhibit a multipeak pattern of “decrease–increase–decrease” under conditions of strong heat accumulation and sufficient oxygen supply, making them the dominant zones for sustained CO emission. Although a secondary peak is observed in layer C6, its amplitude is low and decays rapidly, indicating that fire propagation in deeper coal seams is constrained by both the oxygen supply and temperature and that smouldering tends towards termination.

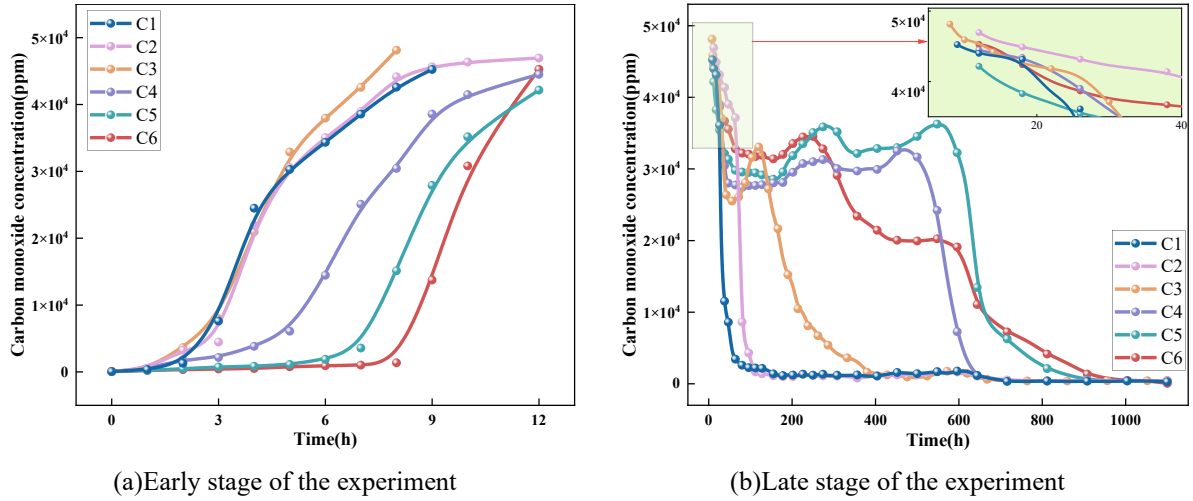


Fig. 9. Variation of CO concentration with time in different coal layers

As shown in Table 6, the CO concentration curves are divided into several stages. The results indicate that the first stage has the shortest duration and ends at the first peak. The second and third stages constitute relatively small proportions of the total time but exhibit the highest concentration levels, representing the main CO emission period. In the second stage, starting from layer C3, the time proportion increases with depth. A similar trend is observed from layer C4 onwards in the third stage. This reflects that deeper coal is more prone to generating incomplete oxidation products during the intermediate stage. The fourth stage has the longest duration, and its proportion decreases progressively with depth. This finding indicates that although all layers remain in a state of slow cooling with low-to-moderate CO concentrations during the later stage of spontaneous combustion, the CO emission capacity in deeper layers declines earlier than that in shallow layers.

Table 6 Stage classification of CO concentration for different coal layers

Coal layer	Stage I (%)	t1	Stage II (%)	t2	Stage III (%)	t3	Stage IV (%)
C1	0.82	9					99.18
C2	1.09	12					98.91
C3	0.73	8	10.18	120			89.09
C4	1.09	12	23.82	274	18.36	476	56.73
C5	1.09	12	24.91	286	23.82	548	50.18
C6	1.09	12	20.55	238	28.18	548	50.18

The response characteristics of CO in the overlying strata, ground surface, and atmospheric environment are shown in Figure 10. Because gas diffusion is faster than heat transfer, an increase in CO concentration can be detected at all three monitoring locations shortly after the experiment begins, and peak values are reached within a short period. This finding indicates that the CO generated by underground coal fires can rapidly migrate to the surface through fractures in the overlying strata. The peak concentrations decrease in the order of the overlying strata, ground surface, and atmospheric environment, which is consistent with the progressive dilution and attenuation of gases during upward transport. After the peak, the CO concentrations at all monitoring points decrease rapidly, indicating that the oxidation state of the coal gradually increases. After approximately 300 h, a slight increase in CO concentration is observed in the overlying strata, suggesting that the temperature at this stage can only drive limited coal pyrolysis to produce small amounts of CO. Compared with CO₂, CO is more sensitive to

temperature fluctuations and local variations in oxygen supply, making it an important indicator of the development stage and reaction intensity of underground coal fires.

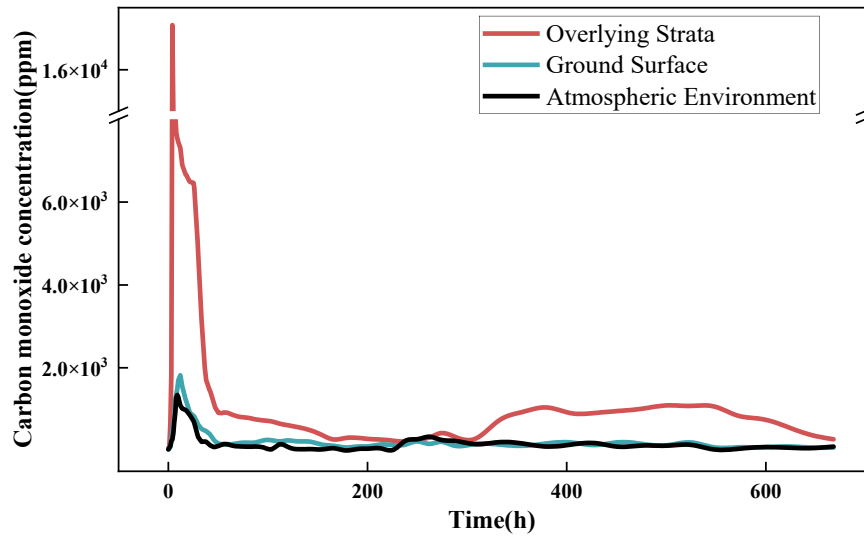


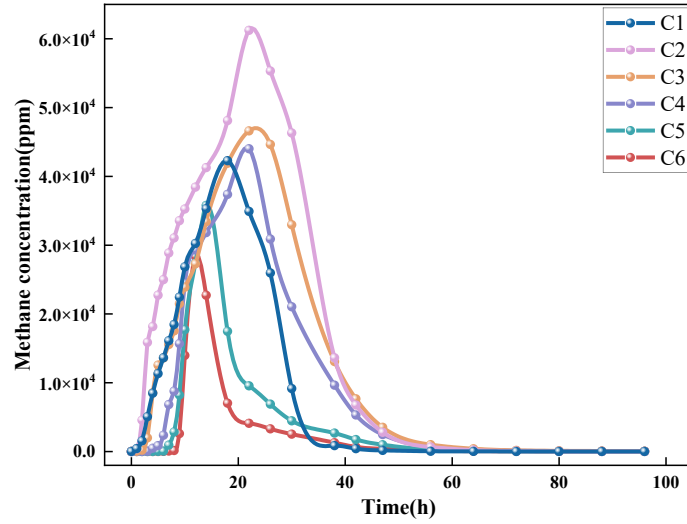
Fig. 10. Variation of CO concentration with time at the overlying strata, ground surface, and atmospheric environment

3.3.3 Evolution of CH₄ and C₂H₆ concentrations

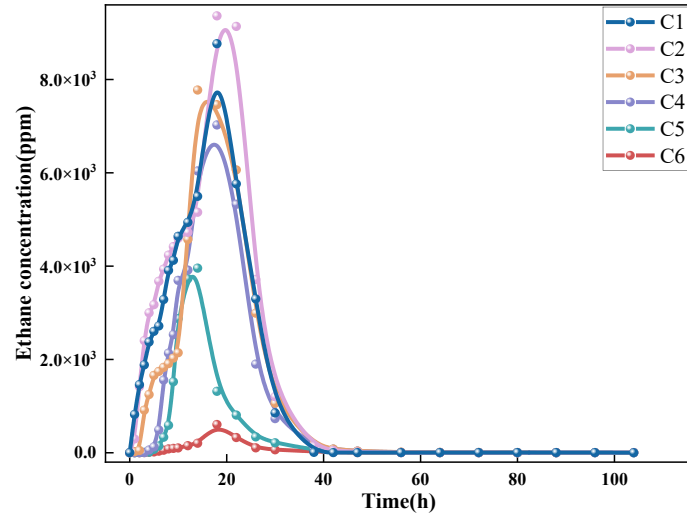
Compared with those of CO₂ and CO, the concentration variations in CH₄ and C₂H₆ are relatively simple. As shown in Figure 11, both gases exhibit a single-peak pattern in the early stage within the coal seam, with highly concentrated release periods. As a major greenhouse gas during CSC, CH₄ is mainly released within the first 60 h. After a brief period of slow variation, the concentration in each coal layer increases rapidly to a single peak, followed by a sharp decline and stabilization. The peak concentration of CH₄ in layers C2–C6 generally decreases with increasing depth, whereas the peak occurrence time appears earlier with increasing depth. This finding indicates that temperatures below 500 °C represent the dominant range for CH₄ release during smouldering. Moreover, deeper coal layers exhibit lower temperatures and limited generation rates. As the temperature further increases and the system enters the intensive reaction stage, CH₄ is readily oxidized into more stable products. Consequently, CH₄ concentrations in all layers decrease rapidly and generally fall below 100 ppm after approximately 80 h, followed by a gradual decline towards background levels as the coal fire attenuates.

The formation of C₂H₆ is more strongly associated with low-temperature and incomplete oxidation conditions. Its main high-concentration interval across different coal layers is consistently within approximately 40 h, and all the layers exhibit a single-peak structure. With the exception of layer C1, which is directly heated, the peak concentration of C₂H₆ decreases with depth, and the peak occurrence time slightly advances. As the temperature continues to increase and oxidation becomes more complete, the C₂H₆ concentrations decrease rapidly in all layers. After approximately 60 h, the concentrations decrease below 10 ppm and cease sequentially from the shallow to deep layers. This finding indicates that C₂H₆ is associated mainly with the incubation and rapid heating stages of CSC and is rarely generated during the intensive reaction stage.

A combined analysis of the temporal characteristics of CH₄ and C₂H₆ shows that both gases act as early-release and early-decay indicator gases. However, compared with CH₄, C₂H₆ corresponds to a lower degree of oxidation, presents an earlier peak occurrence, and is more sensitive to the initial stage of incomplete reactions.



(a) Variation of CH₄ concentration with time in different coal layers



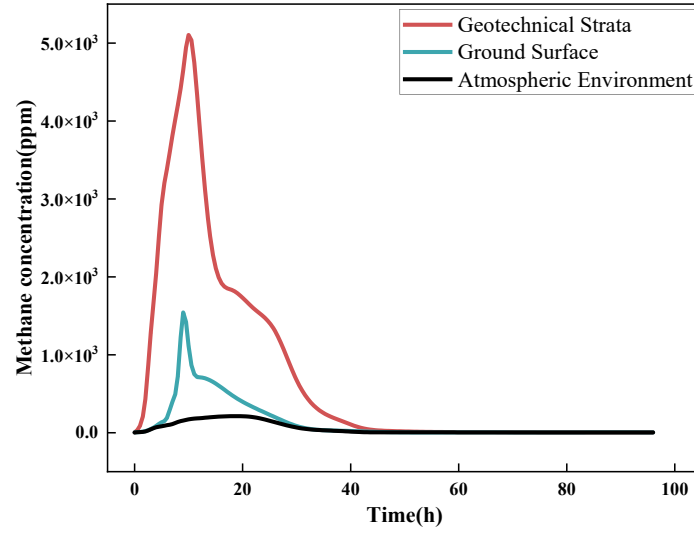
(b) Variation of C₂H₆ concentration with time in different coal layers

Fig. 11. Variation of CH₄ and C₂H₆ concentrations with time in different coal layers

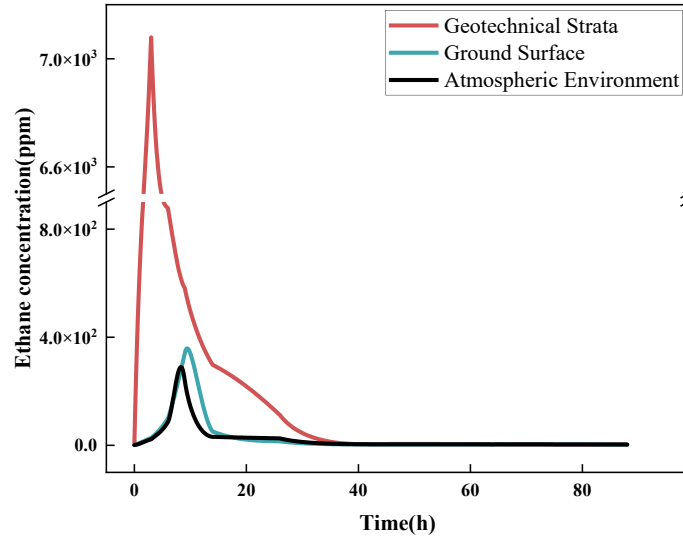
In the overlying strata, ground surface, and atmospheric environment, CH₄ and C₂H₆ also exhibit early-stage concentrated release characteristics. The peak concentrations decrease sequentially from the overlying strata to the ground surface and then to the atmospheric environment, while the peak occurrence times show a slight delay, reflecting the effects of diffusion and dilution during upward migration. The peak occurrence times of C₂H₆ are approximately 3 h in the overlying strata, 10 h at the ground surface, and 8 h in the atmospheric environment, which are generally earlier than those of CH₄. This further confirms that C₂H₆ is more sensitive to low-temperature and incomplete oxidation stages. After approximately 80 h, the concentrations of both gases approach background levels, indicating that hydrocarbon gases contribute little once the CSC process enters the intensive oxidation and later attenuation stages.

Overall, CH₄ and C₂H₆ reflect the release behaviour of organic components during the initial smouldering and low-temperature pyrolysis stages of underground coal fires. These gases can provide important supplementary information for the early detection of spontaneous combustion and monitoring during the incubation period. However, in the middle and later stages of coal fire development, diagnostic analysis should rely more on oxidation

products such as CO_2 and CO .



(a) Variation of CH_4 concentration with time in the overlying strata, ground surface, and atmospheric environment



(b) Variation of C_2H_6 concentration with time in the overlying strata, ground surface, and atmospheric environment

Fig. 12. Variation of CH_4 and C_2H_6 concentrations with time in the overlying strata, ground surface, and atmospheric environment

3.4 Emission characteristics of suspended particulate matter

To reveal the impact of underground coal fire propagation on atmospheric particulate load and air quality, concentration–time curves of $\text{PM}_{2.5}$, PM_{10} , and total suspended particles (TSPs) were obtained at the atmospheric monitoring point. On the basis of these data, their contributions to the air quality index were evaluated. As shown in Figure 13, both $\text{PM}_{2.5}$ and PM_{10} significantly increase during the early stage of fire development. Shortly after the experiment begins, the concentrations increase rapidly to the first peak, followed by a slight decrease, and then reach a second, higher peak at approximately 20 h. The first peak corresponds to incomplete combustion when the

shallow coal layers enter the initial smouldering stage, during which large amounts of fine particles are emitted with flue gases. As the fire propagates deeper, coal samples at greater depths successively participate in incomplete combustion. The superposition of particulate emissions from multiple layers results in a second peak that exceeds the first. As each coal layer gradually enters the intensive reaction stage, the degree of combustion becomes more complete, leading to a significant reduction in fine particle generation. As a result, the $PM_{2.5}$ and PM_{10} concentrations decrease rapidly and remain relatively low.

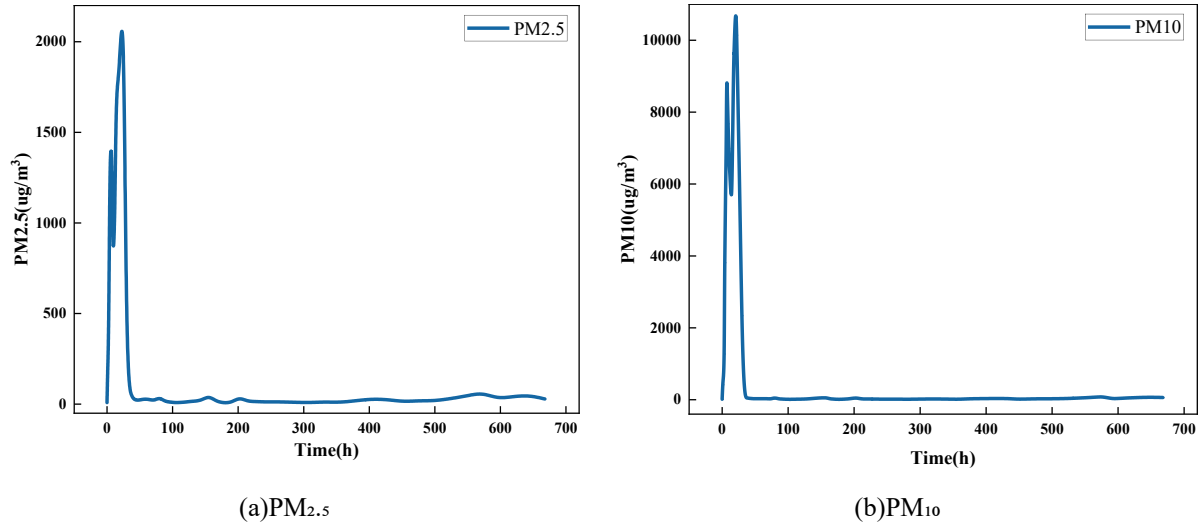


Fig. 13. Variation of $PM_{2.5}$ and PM_{10} concentrations with time in the atmospheric environment

As shown in Figure 14, the evolution of the TSP concentration is generally consistent with that of $PM_{2.5}$ and PM_{10} . Two distinct peaks appear in the early stage of propagation, and their occurrence times are nearly identical to those of $PM_{2.5}$ and PM_{10} . This finding indicates that both coarse and fine particles are released mainly within the first 40 h of incomplete combustion. A comparison of the peak concentrations reveals that $PM_{2.5}$ and PM_{10} account for a relatively small proportion of TSPs, suggesting that suspended particles generated by underground coal fires are dominated by coarse particles with diameters greater than $10\ \mu m$. However, from a health risk perspective, fine particles remain the primary concern.

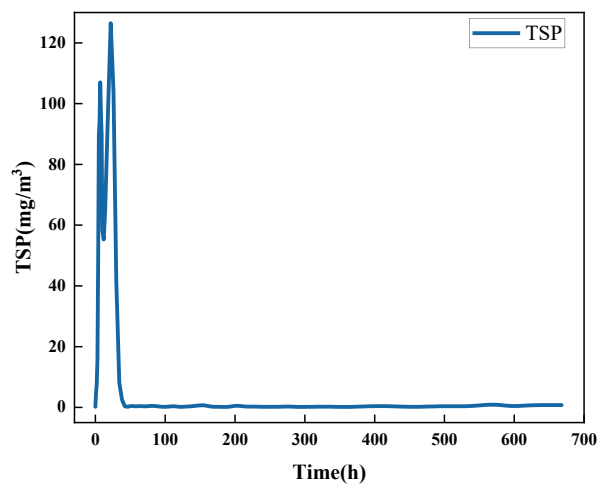


Fig. 14. Variation of TSP concentration with time in the atmospheric environment

3.5 Atmospheric pollution characteristics during underground coal fire propagation

In terms of the air quality assessment, CO, PM_{2.5}, and PM₁₀ were selected as representative indicators in this study. In accordance with the Technical Regulation on Ambient Air Quality Index (AQI) (Trial) (HJ 633—2012) and the Ambient Air Quality Standards (GB 3095—2012), the individual air quality index (IAQI) for each pollutant was calculated. The overall air quality index (AQI) was then determined on the basis of these values.

The concentration limits corresponding to different IAQI levels are listed in Table 7. For PM_{2.5} and PM₁₀, the 24 h average concentration classification provided in the standard was adopted. The CO concentration was converted from ppm to mg/m³ using Equation (5), and its IAQI was subsequently calculated by linear interpolation between adjacent concentration breakpoints using Equation (6). For each evaluation period, the IAQI values of the three pollutants were calculated separately, and the maximum value among them was taken as the overall AQI for that period.

$$C_m = \frac{ppm \times M}{24.45} \quad (5)$$

where C_m represents the mass concentration (mg/m³), ppm denotes the concentration in parts per million, M is the molar mass of CO (28.01 g/mol), and 24.45 is the molar volume of gas under standard conditions (L/mol).

Table 7 Pollutant concentration limits corresponding to individual air quality index levels

Individual Air Quality Index (IAQI)	Pollutant Concentration Limits			
	PM ₁₀ (24 h average, μg/m ³)	PM _{2.5} (24 h average, μg/m ³)	CO (24 h average, mg/m ³)	CO (1 h average, mg/m ³)
0	0	0	0	0
50	50	35	2	5
100	150	75	4	10
150	250	115	14	35
200	350	150	24	60
300	420	250	36	90
400	500	350	48	120
500	600	500	60	150

In the air quality calculation method, the IAQI of pollutant P is calculated as follows:

$$IAQI_P = \frac{IAQI_{Hi} - IAQI_{Lo}}{BP_{Hi} - BP_{Lo}} (C_P - BP_{Lo}) + IAQI_{Lo} \quad (6)$$

where $IAQI_P$ represents the individual air quality index of pollutant P, and C_P represents its mass concentration. BP_{Hi} is the upper breakpoint concentration corresponding to C_P in Table 7, and BP_{Lo} is the lower breakpoint concentration. $IAQI_{Hi}$ and $IAQI_{Lo}$ are the corresponding IAQI values associated with BP_{Hi} and BP_{Lo} , respectively. When C_P exceeded the highest breakpoint in Table 7, the highest breakpoint interval was linearly extrapolated to obtain an extended IAQI. All values above 300 were classified as Level VI severe pollution.

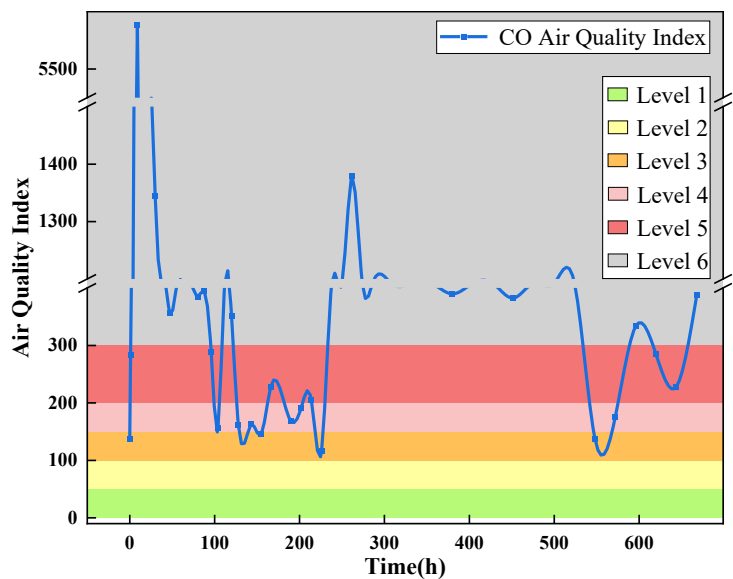
The AQI is calculated as follows:

$$AQI = \max \{IAQI_1, IAQI_2, IAQI_3, \dots, IAQI_n\} \quad (7)$$

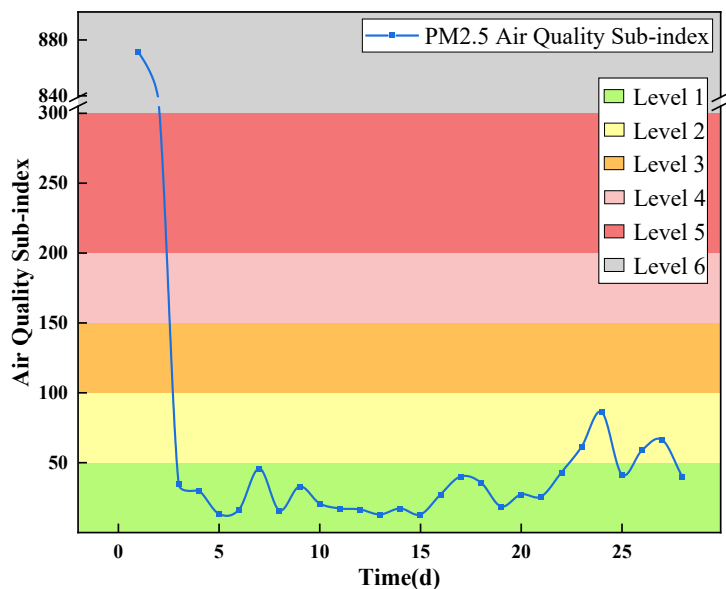
where IAQI represents the individual air quality index, and n denotes the number of pollutants.

The evaluation results for individual pollutants are shown in Figure 15. The IAQI of CO remains at Level III

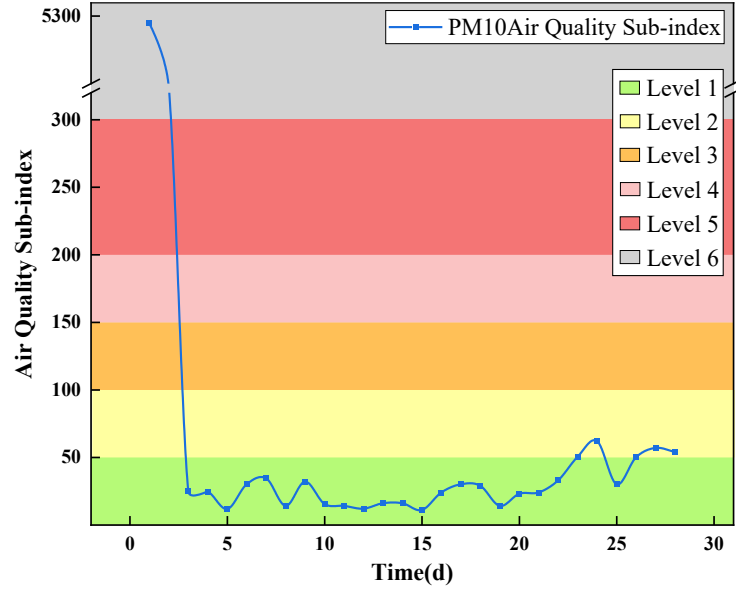
(light pollution) or higher throughout the entire experiment and reaches that of Level VI (severe pollution) during most periods. The high-value intervals correspond well with the stages of concentrated CO release in the coal seam. In contrast, the IAQI values of $PM_{2.5}$ and PM_{10} increase significantly, mainly during the early stage of the experiment. As the coal layers gradually enter the intensive reaction stage, the combustion becomes more complete, and the IAQI values of the particulate matter decrease rapidly to the excellent–good range. Only minor rebounds are observed during certain periods, which may be attributed to the dispersion of lighter ash particles from the large amount of bottom ash produced during coal combustion. These particles are transported outwards by thermal buoyancy under residual heat conditions.



(a)CO



(b) $PM_{2.5}$



(c)PM₁₀

Fig. 15. Individual air quality indices and pollution levels of CO, PM_{2.5}, and PM₁₀

Using Equation (7), the overall air quality index (AQI) considering the combined effects of CO, PM_{2.5}, and PM₁₀ can be further obtained. On the basis of the classification criteria, a comprehensive evaluation of the pollution levels is conducted, as shown in Figure 16. The entire coal fire propagation process is dominated by heavy to severe pollution, with only a few periods falling into light or moderate pollution levels. The dominant pollutant contributing to the AQI shifts from PM₁₀ in the early stage to CO in the middle and later stages. Overall, underground coal fires cause pronounced particulate pollution in the early stage and sustain severe air quality deterioration dominated by CO over an extended period. This poses a persistent threat to the surrounding environment and public health in mining areas.

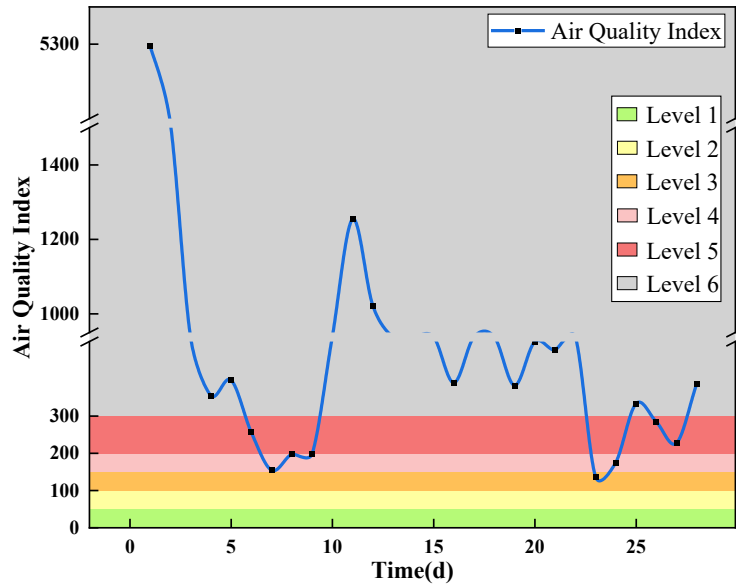


Fig. 16. Air quality and classification during underground coal fire propagation

4 Mechanistic interpretation and diagnostic implications of vertical underground coal fire propagation

The results show that the vertical propagation of underground coal fires is not governed by heat transfer alone. Instead, it is a transient process jointly controlled by heat accumulation, oxygen transport, coal–oxygen reactions, and pollutant migration. In C1 and C2, strong heat exchange with the surroundings limits long-term heat retention. Although O₂ concentrations recover relatively rapidly, high-temperature reactions persist for only a short period. C3–C5 have more favorable heat-retention conditions and receive a sustained oxygen supply. They therefore form the principal sustained-reaction zone and exhibit pronounced secondary heating and multi-peak CO₂ and CO release patterns. C6 receives heat transferred from the overlying coal layers. However, the longer oxygen-transport pathway increasingly restricts oxygen supply. The dominant control on the reaction consequently shifts from thermal driving to oxygen limitation. This transition is accompanied by declining temperature, reduced oxygen consumption, and attenuated pollutant release. Overall, vertical coal-fire propagation does not intensify or weaken monotonically across the different layers. Instead, the dominant control mechanism shifts from heat-loss control to coupled thermal–oxygen maintenance and, finally, to oxygen-limited attenuation.

The sequence of pollutant release further reveals the stagewise transition in the coal-fire reaction state. CH₄, C₂H₆, PM_{2.5}, PM₁₀, and TSP are released predominantly during the early stage of the experiment. This pattern reflects short-lived, concentrated emissions associated with coal heating, volatile release, and incomplete oxidation. As the coal–oxygen reaction intensifies, hydrocarbon gases and particulate matter decline rapidly, whereas CO₂ and CO gradually become the dominant gaseous products. In C4 and C5, the secondary temperature rise coincides with multi-peak responses of CO₂ and CO. This correspondence indicates that pollutant release during the middle and late stages is not controlled solely by the instantaneous temperature. It is also influenced by prior heat accumulation, localized oxygen replenishment, and the continued transport of reaction products. By contrast, the response in C6 decays rapidly after the secondary peak. This finding further confirms that elevated temperature alone is insufficient to sustain coal-fire development. Oxygen availability is therefore a critical constraint on the persistence of the reaction. Meanwhile, the temperature and gas-concentration peaks measured in the overlying strata, at the ground surface, and in the ambient atmosphere are generally delayed and attenuated relative to those within the coal seam. Surface observations therefore represent an integrated response to in-seam reactions, transport through the overlying medium, and atmospheric dilution. They should not be interpreted directly as the instantaneous reaction intensity within the coal seam.

These results indicate that underground coal-fire diagnosis should adopt a multi-parameter framework tailored to the different stages of fire evolution. During the early stage, a rapid decrease in O₂, accompanied by concentrated releases of CH₄, C₂H₆, and particulate matter, can indicate low-temperature pyrolysis and incomplete oxidation. During the sustained-reaction stage, attention should be focused on the coupled variations in temperature, O₂ depletion, and multi-peak or persistently elevated CO₂ and CO concentrations. These indicators can be used to identify the principal reaction layers and assess the persistence of the reaction.

During the attenuation stage, declining temperature, O₂ recovery, and sustained CO release should be jointly evaluated to determine whether the coal fire has been fully extinguished or remains in an oxygen-limited smouldering state. Future studies will integrate field measurements of temperature, gas concentrations, surface emission fluxes, and fracture structures. These data will be used to evaluate the scale applicability of the thermo–oxygen–pollutant coupling relationship under different geological conditions.

5 Conclusions

On the basis of a physical similarity simulation experimental platform for underground coal fire propagation, this study systematically investigated the characteristics of temperature transfer, oxygen concentration evolution, and the release behaviour of typical atmospheric pollutants and suspended particulate matter during the vertical propagation process. The main conclusions are as follows.

(1) The vertical propagation of underground coal fires exhibits distinct thermal–oxygen stratification characteristics. The evolution of coal seam temperature and oxygen concentration can be divided into five stages: incubation, rapid heating, intensive reaction, rapid cooling, and burnout. Layers C1 and C2 are almost entirely dominated by the burnout stage, layers C3–C5 constitute the main heat-release zone, and layer C6 exhibits propagation attenuation because of insufficient oxygen supply. The temperature and oxygen concentration responses in the overlying strata and ground surface lag those in the coal seam.

(2) The release of typical pollutant gases shows stage-dependent concentration and depth-dependent variability. CO₂ and CO exhibit multistage fluctuations during fire development, with more complex temporal responses at greater depths. CH₄ and C₂H₆ are mainly released within the first 40–60 h under incomplete oxidation conditions and then rapidly decay during the intensive reaction stage. The gas concentrations in the overlying strata and at the ground surface generally lag behind those within the coal seam.

(3) Suspended particulate matter is predominantly released during the early stage of propagation, and air quality is characterized mainly by moderate to severe pollution levels, with CO as the dominant controlling factor. PM_{2.5}, PM₁₀, and TSP exhibit two distinct peaks during the initial stage of fire development, reflecting concentrated emissions during incomplete combustion. According to the air quality index evaluation, most periods of the experiment fall within heavy or more severe pollution levels. The dominant pollutant shifts from PM₁₀ in the early stage to CO in the subsequent stages.

In summary, the propagation of underground coal fires is a coupled process involving heat transfer, oxygen consumption, and pollutant generation and emission. It clearly exhibits stage dependence, depth-dependent variability, and temporal lag characteristics. These findings provide important scientific support for understanding the mechanisms of vertical coal fire propagation, predicting fire development trends, and formulating monitoring and mitigation strategies.

CRedit authorship contribution statement

Jingyu Zhao: Supervision, Validation, Investigation, Funding acquisition. **Tianlan Chen:** Conceptualisation, Data curation, Writing original draft. **Jiajia Song:** Resources, Writing – review and editing, Project administration. **Shikui Jin:** Formal analysis. **Zhijin Yu, Biao Zhou:** Funding acquisition. **Chang Su, Yanwei Hou:** Writing-review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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