



Research Paper

Coupling effects of mineral components on arsenic transformation during coal combustion

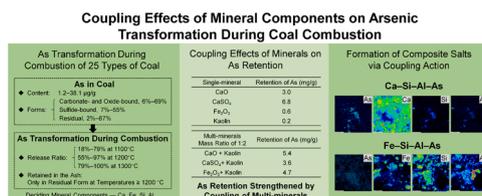
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HIGHLIGHTS

- Arsenic (As) transformation during combustion of 25 coal samples was studied.
- The release ratios of As during combustion vary in a wide range of 18–100%.
- As is only retained as residual form in the ash at combustion temperatures ≥ 1200 °C.
- Multi-minerals retain As as Ca–Si–Al–As and Fe–Si–Al–As composite salts.
- Coupling of Ca/Fe, Si and Al strengthens As retention and its mechanism is proposed.

GRAPHICAL ABSTRACT



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ABSTRACT

Exploring arsenic (As) transformation during coal combustion is beneficial for reducing its pollution. Herein, combustion experiments were developed at 1100–1300 °C in a fixed-bed experimental system with 25 types of coal samples. The occurrences of As in coal and combustion products were characterized. All the original forms of As in coal were found to be unstable during combustion. As retained in ash existed as water-soluble and ion-exchangeable and residual forms, but only as residual form at combustion temperature above 1200 °C. The distribution of As in gaseous and solid combustion products varied widely by coal types, which resulted from the coupling effects of multi-minerals in coal. Co-combustion experiments were conducted using As model compounds and pure minerals, by which the interaction of Ca, Fe, Si and Al minerals to retain As was elucidated. The As transformation during coal combustion was primarily attributed to the coupling action of Ca, Fe, Si and Al minerals in coal. As a result, As was retained as Ca–Si–Al–As and Fe–Si–Al–As composite salts in the ash, which have little environmental hazard. Utilizing the coupling effects of multi-minerals during combustion help reduce As pollution from coal-fired plants.

1. Introduction

Coal combustion is a significant source of atmospheric arsenic (As) (H.Z. Tian et al., 2015; Zhang et al., 2016). As is a semi-volatile element

during coal combustion. After being discharged into the environment, As can enter the human respiratory system or accumulate in the food chain and cause serious harm to human health (Finkelman, 2004; Yang et al., 2021), which has attracted widespread attention. Therefore, limits

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for As emissions from coal-fired installations have been set in some countries (U.S Environmental Protection Agency, 2012; European Union, 2016). After coal combustion, most As existing in coarse particles is removed by dust removal devices and through wet flue gas desulfurization, and remaining As in fine particles and in the gas phase is discharged into the atmosphere with the flue gas (Zhao et al., 2017a, 2017b; Wang et al., 2019). The transformation of As during coal combustion must be extensively investigated to develop novel control technologies and improve the current ones.

As migration in coal-fired systems is divided into two stages: the coal combustion and post-combustion stages (Seames and Wendt, 2000). During the coal combustion stage, part of the As in the solid matrix is decomposed and released into the flue gas (Liu et al., 2009; Zhou et al., 2019). The rest is retained in the solid phase because of thermal stability or interaction with other components in coal (Cao et al., 2020; Song et al., 2021), resulting in the final distribution of As in the gas and solid phase. Upon cooling the flue gas during the post-combustion stage, gaseous As in the flue gas migrates to fly ash particles through chemical reactions over the medium- and high-temperature range and via adsorption and condensation in the low-temperature range (Wang et al., 2020; Xu et al., 2021). The transformation characteristics of As and corresponding critical factors affecting As behavior during these two stages are different.

Many studies have been conducted on As transformation in coal-fired systems (Zhao et al., 2017a, 2017b; Wang et al., 2019), and As distribution undergoing the two stages has been extensively investigated. However, research on the transformation of As during the coal-combustion stage was limited. Previous studies indicated that the ratios of As released into the gas phase after coal combustion varied widely for different researches. The experimental methods, combustion conditions, and coal types affected As release. Ji et al. (2019) used three types of coal to carry out combustion experiments and determined that the release ratios of As at 1300 °C ranged between 53% and 71%. Zou et al. (2017) subjected six types of coal to carry out combustion experiments and found that the As release ratio at 1300 °C was between 55% and 90%. Liu et al. (2016) used eight types of coal to carry out combustion experiments and found that the As release ratio at 1500 °C was 53–99%. Under identical combustion conditions, the As release ratios of some coal types were similar whereas those of other coal types were significantly different. The key influencing factors that caused such differences remained unclear due to limited coal types used in previous researches (Ji et al., 2019; Zou et al., 2017; Liu et al., 2016).

The distribution of As in the high-temperature coal combustion products depends on the original As forms in coal and the chemical reactions during combustion (Liu et al., 2009; Zou et al., 2017; Chen et al., 2019). Coal contains various forms of As. According to Finkelman et al. (2018) and Senior et al. (2000), As forms in coal can be divided into water-soluble and ion-exchangeable, oxide-bound, sulfide-bound, organic-bound, and residual forms. Zou et al. (2017) analyzed six kinds of China's steam coal and found that As was primarily present as the sulfide-bound form (54.3–74.5%), followed by the residual form (12.0–45.7%) and organic-bound form (0–16.7%). The thermal stabilities of various forms of As were significantly different. Liu et al. (2009) used the extraction residue of Yima coal, which contained a single form of As, to perform pyrolysis experiments at 1000 °C. They demonstrated that residual As was partially released, whereas As in the carbonate- and oxide-bound, sulfide-bound, and organic-bound forms was completely released. Zou et al. (2017) analyzed the forms of As in combustion products of the six kinds of coal mentioned before, and demonstrated that at 1000 °C, organic-bound As disappeared, sulfide-bound and residual As decreased, and ion-exchangeable As appeared. These results indicated that each form of As was released because of thermal instability during the coal combustion stage, and there may also be mutual transformations among these forms. Figuring out the transformation of As in different forms helps predicting As distribution during high-temperature coal combustion, and provides theoretical support for

reducing environmental hazard of by-products in coal-fired plants. According to He et al. (2020), the bioavailability and environmental risks of residual As was much lower than other As forms. Transferring As into residual form in ash is beneficial for reducing the leaching toxicity of by-products in coal-fired plants. However, the conversion of As forms during the high-temperature coal combustion stage has not been reported to date.

The migration of As during the coal combustion stage depends on the As form distribution in coal and the contents of mineral and non-mineral components in coal. The minerals with the most significant effects on As migration can be determined through the distribution characteristics of As in fly ash. Seames and Wendt (2007) suggested that As content depended significantly on the Ca and Fe contents in fly ash particles. Luo et al. Luo et al. (2011) reported that As was primarily presented as $\text{Ca}_2\text{As}_2\text{O}_7$ in fly ash using X-ray Absorption Fine Spectroscopy. Fu et al. (2021) found that the spatial distribution of As in the fly ash was consistent with Fe. These results indicated that Ca and Fe played the primary roles in retaining As owing to the reactions between As and the Ca- and Fe-containing compounds in coal during the post-combustion (Li et al., 2020; Yu et al., 2021; Hu et al., 2021) or high-temperature coal combustion stage (Cao et al., 2020; Song et al., 2021). Because of the complexity of components in coal, pure substances were used in previous studies to explore the reactions between minerals and As. Cao et al. (2020), He et al. (2021) and B. Song et al. (2020) analyzed the adsorption of As_2O_3 using Ca-based minerals in the temperature range of 1000–1300 °C, and determined that CaO, CaSiO_3 , and CaSO_4 retained gaseous As as $\text{Ca}_3(\text{AsO}_4)_2$. Song et al. (2021) found that Fe_2O_3 adsorbed As_2O_3 to form FeAsO_4 in the temperature range of 1000–1300 °C. Moreover, the aforementioned Ca and Fe oxides and sulfates were converted into aluminosilicates in the presence of the Si and Al components of coal during combustion (Wen et al., 2016). Morphological changes of Ca and Fe components can lead to differences in the retention abilities of As (Zha et al., 2018). The effects of multi-minerals in coal on As transformation need to be clarified. Besides, blending coal combustion and in-furnace injection of sorbents have been proven to be effective ways to inhibit As release from coal combustion (Song et al., 2021; B. Zhao et al., 2021). Exploring the interaction between As and multi-minerals is beneficial for optimization of these control technologies. The effects of the non-mineral components of coal on As migration under high-temperature conditions are limited. Chen et al. (2015) studied the effect of SO_2 on As adsorption by CaO and determined that SO_2 inhibited the retention of As through competitive reactions; however, this inhibitory effect was no longer observed at temperatures higher than 900 °C. Fu et al. (2019) demonstrated that Cl compounds could convert As_2O_3 into AsCl_3 , thus promoting As release. However, the thermodynamic equilibrium calculations performed by Zhang et al. (2020) indicated that AsCl_3 was unstable at temperatures higher than 1000 °C, suggesting that Cl did not affect As migration during high-temperature coal combustion.

As transformation during coal combustion is a complex process that depends on the coal type and combustion conditions. However, the transformation mechanism of As is of great interest for the development of environmental control technologies. In this study, 25 coals were used as raw materials, and coal combustion experiments were performed in the temperature range of 1100–1300 °C in a fixed-bed experimental system. The As release characteristics were obtained by measuring the As contents in coal and combustion products. The sequential extraction method was used to analyze As forms before and after coal combustion, and the migration pathways of As during coal combustion were explored. Correlation analysis was conducted between the As release characteristics and the mineral components in multiple coals. Co-combustion experiments were conducted on As model compounds and minerals, namely CaO, CaSO_4 , Fe_2O_3 and kaolin. The As retention abilities of single- and multi-minerals were compared. The phase composition, elemental distribution at the microscopic level, and X-ray photoelectron spectroscopy (XPS) profiles of As were analyzed. The

coupling effects of mineral components on As transformation during coal combustion were elucidated.

2. Experimental

2.1. Sample

To comprehensively understand the transformation characteristics of As during coal combustion, 25 types of coal from different regions of China and with significant differences in As content and coal quality, numbered A1–25, were used. Before the experiment, the coal was ground and sieved to obtain a powder with a particle size of 74–96 μm and was dried at 105 $^{\circ}\text{C}$ for 10 h for later use. The results of industrial and elemental analysis of the coal samples are summarized in Tables S1 and S2. The contents of mineral components in the coal sample were analyzed by X-ray fluorescence spectroscopy (XRF; ARL PERFORM'X, Thermo Fisher Scientific, USA). Slow-ashing of the coal samples were conducted in a muffle furnace. Coal (2 ± 0.1 g) was weighed, placed in a crucible, and then sent into the constant temperature zone of the muffle furnace at room temperature. The furnace temperature was increased to 500 $^{\circ}\text{C}$ within 30 min and kept constant for 30 min. Next, the temperature was increased to 815 $^{\circ}\text{C}$ and kept constant for 2 h. After cooling to room temperature, the ash was collected for analysis. Based on the XRF results, Eq. (4) was used to calculate the mass fraction of each mineral element converted to raw coal (w_M ; M = Si, Al, Ca, Fe, Mg, Na, or K). The results are summarized in Table 1. An atomic fluorescence spectrophotometer (AFS; AFS-9320, Jitian, China) instrument was used to analyze the As content of the coal samples.

$$w_M = w_{MO} \times \frac{MW_M}{MW_{MO}} \times A_{ash} \times 100\% \quad (1)$$

where w_{MO} (%) is the mass fraction of the mineral oxides determined using XRF. MW_M and MW_{MO} are the relative atomic and relative molecular masses of the corresponding mineral oxides, respectively, and A_{ash} (%) is the ash content.

2.2. Experimental setup

The coal combustion experiment was conducted in a fixed-bed experimental system (Fig. 1). The fixed-bed reactor, which was heated

Table 1
Contents of mineral components and As in coal samples (wt% ad).

Coal	Si	Al	Fe	Ca	Mg	Na	K	As ($\times 10^{-4}$)
A1	8.39	5.95	0.72	1.09	0.10	0.07	0.34	1.5
A2	14.10	7.74	0.67	2.73	0.34	0.09	1.54	1.2
A3	9.64	7.83	0.93	1.87	0.17	0.08	0.41	1.4
A4	5.30	4.69	1.01	1.36	0.09	0.12	0.25	1.3
A5	10.23	5.29	0.63	1.72	0.18	0.12	0.73	1.2
A6	7.68	5.91	1.32	1.97	0.27	0.20	0.51	3.0
A7	2.38	5.59	1.49	0.42	0.04	0.01	0.07	12.0
A8	5.96	5.37	1.32	2.56	0.12	0.08	0.30	4.1
A9	8.39	5.45	0.76	1.78	0.20	0.07	0.45	38.1
A10	8.31	2.79	0.57	0.56	0.10	0.08	0.39	11.0
A11	10.41	4.12	0.77	1.20	0.14	0.14	0.83	22.2
A12	7.22	3.87	1.43	2.21	0.26	0.21	0.76	9.0
A13	7.54	4.42	2.53	2.14	0.41	0.11	0.37	3.5
A14	10.26	5.20	1.21	2.55	0.48	0.11	0.99	5.6
A15	9.16	5.35	2.08	1.80	0.35	0.19	0.64	3.5
A16	7.94	4.16	0.54	2.57	0.36	0.23	0.97	3.2
A17	2.13	1.23	0.32	0.20	0.04	0.09	0.12	3.5
A18	6.81	5.14	1.65	2.00	0.38	0.19	0.56	20.4
A19	4.22	2.45	1.95	1.83	0.28	0.17	0.42	3.2
A20	5.23	3.95	1.42	3.26	0.10	0.10	0.18	20.4
A21	2.18	1.70	0.95	0.75	0.17	0.10	0.18	15.4
A22	5.39	2.66	0.91	1.86	0.23	0.13	0.39	5.7
A23	2.18	1.73	1.04	0.81	0.18	0.09	0.17	2.7
A24	2.90	1.39	1.90	1.52	0.04	0.04	0.04	3.2
A25	6.53	3.00	0.69	2.32	0.20	0.14	0.52	1.3

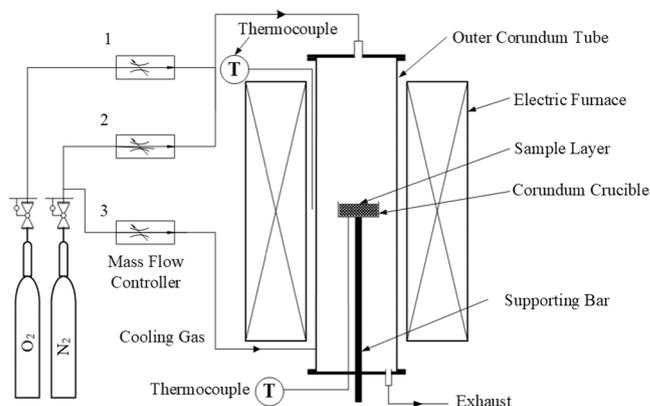


Fig. 1. Schematic of the fixed-bed reactor system.

by a resistance furnace, consisted of an outer tube made of corundum, a supporting bar, and a crucible. The diameters of the outer tube of the reactor and the crucible were 50 and 25 mm, respectively. The crucible was fixed on the upper end of the supporting bar. The reaction gas comprised 21% O_2 and 79% N_2 by volume. Mass flow controllers were used to control the flow rates of N_2 and O_2 . The total gas flow rate was set to 500 mL/min. In the experiment, the temperature of the constant temperature zone in the reactor was increased to the set temperature (1100, 1200, and 1300 $^{\circ}\text{C}$) by heating in a resistance furnace. The reaction gas was introduced from the top and discharged from the bottom of the reactor. After 30 min of continuous ventilation, the temperature and atmosphere in the reactor were completely stable. Next, a crucible with 0.8 g of a coal sample was quickly inserted into the reactor from the bottom to the top, and the crucible was placed in the constant temperature zone in the reactor. After the set reaction time was reached, the crucible was removed and the sample was cooled and collected for analysis.

2.3. Methods

2.3.1. Coal combustion experiments

Twenty-five types of coal were subjected the combustion experiments in the temperature range of 1100–1300 $^{\circ}\text{C}$ using corundum crucibles that can withstand high temperatures. However, corundum cannot be processed into sieves with fine holes. Thus, the reaction gas was flow around the crucible surface. Coal combustion was limited by mass transferability in the crucibles, and significant time was required for the complete burning of coal. The CO_2 concentration in the outlet gas generated during the combustion experiments was determined, and the results indicated that each coal type was completely burned at 1100 $^{\circ}\text{C}$ over 45 min. Therefore, the reaction time was set to 45 min. The As contents and forms in the coal and ash samples removed from the crucible after combustion were analyzed.

The coal and ash samples were digested as follows (Ji et al., 2019; Song et al., 2019). First, 50 mg of the sample was placed in a digestion tank. Then, 10 mL of an aqueous solution of HNO_3 (65–68%), 1 mL of an aqueous solution of H_2O_2 (30%), and 1 mL of an aqueous solution of HF (30%) were added in sequence. The tank was placed in a microwave digestion apparatus (Milestone ETHOS UP, Italy) and digested at 240 $^{\circ}\text{C}$ for 40 min. The digestion solution was then filtered through a 0.22 μm syringe filter, and the As concentration was measured by AFS. The release ratio of As (R_{As}) during coal combustion was calculated using Eq. (2).

$$R_{As} = \left(1 - \frac{m_p \times c_p}{m_c \times c_c}\right) \times 100\% \quad (2)$$

where m_c and m_p (g) are the masses of the coal used in the experiment and the residual ash in the crucible after combustion, which were

obtained by weighing the coal and ash samples before and after the experiment. c_c and c_p ($\mu\text{g/g}$) are the As content in the experimental coal and ash samples, respectively.

The form analysis of As in the coal and ash samples was conducted by modifying a four-step chemical extraction method reported by Finkelman et al. [Finkelman et al. (2018)] and G.C. Song et al. (2020). The forms of As were divided into five types: the water-soluble and ion-exchangeable form (F1), carbonate- and oxide-bound form (F2), sulfide-bound form (F3), organic-bound form (F4), and residual form (F5). The extractant and extraction times used for each extraction step are listed in Table 2.

The extraction operation process was described in detail in our previous study (G.C. Song et al., 2020). AFS was used to determine the content of As in the extractant of each extraction step, and the proportions of the As forms in the coal and ash samples were obtained. The proportions of As in F1, F2, F3, and F4 (P_{s,F_j}), where the s subscript denotes coal or ash sample) were calculated using Eq. (3). The fraction of As in F5 in coal ($P_{\text{coal},F5}$) and ash ($P_{\text{ash},F5}$) was calculated using Eqs. (4) and (5), respectively.

$$P_{s,F_j} = \frac{M_{s,F_j}}{M_r} \times 100\% \quad (3)$$

$$P_{\text{coal},F5} = 100\% - \sum_{j=1}^4 P_{\text{coal},F_j} \quad (4)$$

$$P_{\text{ash},F5} = 100\% - R_{As} - \sum_{j=1}^4 P_{\text{ash},F_j} \quad (5)$$

where M_{s,F_j} (μg) is the amount of As in the F_j form in the coal or ash samples, and M_r (μg) is the total amount of As in coal. The recovery rates were 96.1–101.7% for As in coal and 97.6–102.5% for As in ash.

2.3.2. Co-combustion experiments of As model compounds and minerals

As is present in small amounts in coal and coal combustion products; therefore, its direct characterization is difficult. Moreover, the retention of As on specific minerals was hard to clarify because the mineral composition of coal is complex. Herein, the As model compound and pure minerals were subjected to co-combustion to explore the retention mechanism of As by several minerals. The As model compound comprised a mixture of cellulose and p-aminophenyl arsenic acid. The As content was determined to range between 3.06% and 3.16% (average value 3.12%, relative deviation within 5%) by three parallel measurements, proving that the samples were evenly mixed. CaO, CaSO₄, Fe₂O₃, and kaolin were used as model compounds for the minerals in coal. The reasons for selecting these minerals are discussed in detail in Section 3.1. Co-combustion experiments were performed at 1200 °C using the As model compound and mineral mixtures with mass ratios of 1:1. The CO₂ concentration in the outlet gas was determined, and the results indicated that the samples were burned completely after 10 min therefore, the reaction time was set to 10 min. The amount of As retained by each mineral (W_{As} , mg/g) was calculated as follows.

$$W_{As} = \frac{m_{\text{mi,p}} \times C_{\text{mi,p}}}{m_{\text{mi,r}}} \quad (6)$$

where $m_{\text{mi,r}}$ and $m_{\text{mi,p}}$ (g) are the masses of minerals before and after the reaction, respectively. $C_{\text{mi,p}}$ (mg/g) is the As content of the solid

Table 2

Extracts used for sequential chemical extraction.

Form of As	Extracts	Time
Water-soluble and ion-exchangeable	1 mol/L CH ₃ COONH ₄	20 min
Carbonate- and oxide-bound	3 mol/L HCl	60 min
Sulfide-bound	2 mol/L HNO ₃	40 min
Organic-bound	2 mol/L HNO ₃ + 5% H ₂ O ₂	60 min

product. The procedure used to measure the As content is described in Section 2.3.1.

CaO, CaSO₄, Fe₂O₃ were used individually or as 1:2 (w/w) mixtures with kaolin. The amounts of As retained by each mineral were compared, and the coupling effects of multi-minerals were evaluated. The compositions of the raw materials used under different experimental conditions are listed in Table 3. The products were heated under the same atmosphere for 10 and 30 min, and then the As content was analyzed to determine the stability of the retained As.

X-ray diffraction (XRD; D8 Discover, Bruker, Germany) instrument was used to analyze the phase compositions of the reactants and products. The XRD patterns of all the samples were obtained in the 2 θ range of 5°–80° at a resolution of 0.02°.

An X-ray photoelectron spectrometer (XPS; ESCALAB 250Xi, Thermo Fisher, U.K.) apparatus with an Al K α anode was used to analyze the binding energy of As_{2p} in the retention products. The XPS profiles were obtained at a narrow-spectrum scan resolution of 0.05 eV and a transmission energy of 30 eV. All the XPS profiles were calibrated using the C 1s (284.8 eV) profile.

An electron probe microanalysis (EPMA; JXA8230, JEOL, Japan) system, which featured a LaB6 electron gun and a wavelength dispersive spectrometer and was operated in the sample-stage scanning mode, was used to analyze the elemental distributions of the samples at the microscopic level. The experiments were conducted at an acceleration voltage of 20 kV and a current of 1×10^{-8} A. The resolution in the X and Y directions was 0.28 μm , and the analysis point interval was 10 ms. For the fixed-point qualitative analysis experiments, the accelerating voltage, current, and beam spot diameter were 20 kV, 1×10^{-8} A, and 1 μm , respectively.

3. Results and discussion

3.1. Transformation characteristics of As during coal combustion

The As release ratios of the 25 types of coal during combustion at 1100, 1200, and 1300 °C are summarized in Table 4. For each type of coal, the As release ratio increased with increasing temperature, and the average values at 1100, 1200, and 1300 °C were 51%, 82%, and 96%, respectively. The As release ratios of different coal samples were considerably different. At 1100 °C, the A1 and A25 coal samples presented the lowest and highest As release ratios of 18% and 79%, respectively. At 1200 °C, the A2 and A17 coal samples presented the lowest and highest As release ratios of 55% and 97%, respectively. At 1300 °C, the A2 coal sample presented the lowest As release ratios of 79%, whereas the As release ratios for the other coal samples exceeded 90%. Moreover, at 1300 °C, the As release ratios of six coal samples exceeded 99%.

The distributions of As forms in the 25 coal samples are presented in Fig. 2. The primary As forms in these 25 coal samples are carbonate- and oxide-bound, sulfide-bound, and residual As. The average proportion of carbonate- and oxide-bound As was approximately 38% of the As amount in the coal samples, ranking first among all forms. The A15 and A17 coal samples contained the highest and lowest proportions of carbonate- and oxide-bound As of 69% and 6%, respectively. The average

Table 3

Compositions of the sample used for the co-combustion experiments.

Sample	As model compound (g)	CaO (g)	CaSO ₄ (g)	Fe ₂ O ₃ (g)	Kaolin (g)
1	0.15	0.15	–	–	–
2	0.15	–	0.15	–	–
3	0.15	–	–	0.15	–
4	0.15	–	–	–	0.15
5	0.15	0.05	–	–	0.10
6	0.15	–	0.05	–	0.10
7	0.15	–	–	0.05	0.10

Table 4
Release ratios of As during coal combustion at 1100, 1200 and 1300 °C (%).

Coal	1100 °C	1200 °C	1300 °C
A1	18 ± 1	63 ± 2	95 ± 2
A2	25 ± 2	55 ± 2	79 ± 3
A3	26 ± 2	83 ± 3	99 ± 1
A4	31 ± 3	84 ± 4	98 ± 1
A5	32 ± 2	74 ± 1	95 ± 2
A6	36 ± 3	90 ± 3	99 ± 1
A7	37 ± 1	89 ± 2	95 ± 2
A8	40 ± 2	78 ± 2	96 ± 2
A9	43 ± 1	88 ± 2	95 ± 2
A10	48 ± 3	81 ± 2	93 ± 1
A11	49 ± 3	72 ± 3	95 ± 2
A12	53 ± 2	90 ± 2	91 ± 2
A13	55 ± 1	75 ± 1	96 ± 1
A14	55 ± 2	75 ± 3	93 ± 1
A15	57 ± 1	82 ± 3	97 ± 1
A16	57 ± 3	87 ± 2	95 ± 2
A17	60 ± 2	97 ± 1	100
A18	60 ± 3	77 ± 4	100
A19	61 ± 2	78 ± 1	100
A20	63 ± 2	91 ± 5	97 ± 1
A21	66 ± 1	77 ± 2	100
A22	71 ± 3	92 ± 3	98 ± 1
A23	72 ± 4	80 ± 2	97 ± 1
A24	74 ± 2	89 ± 4	95 ± 1
A25	79 ± 3	96 ± 2	98 ± 1

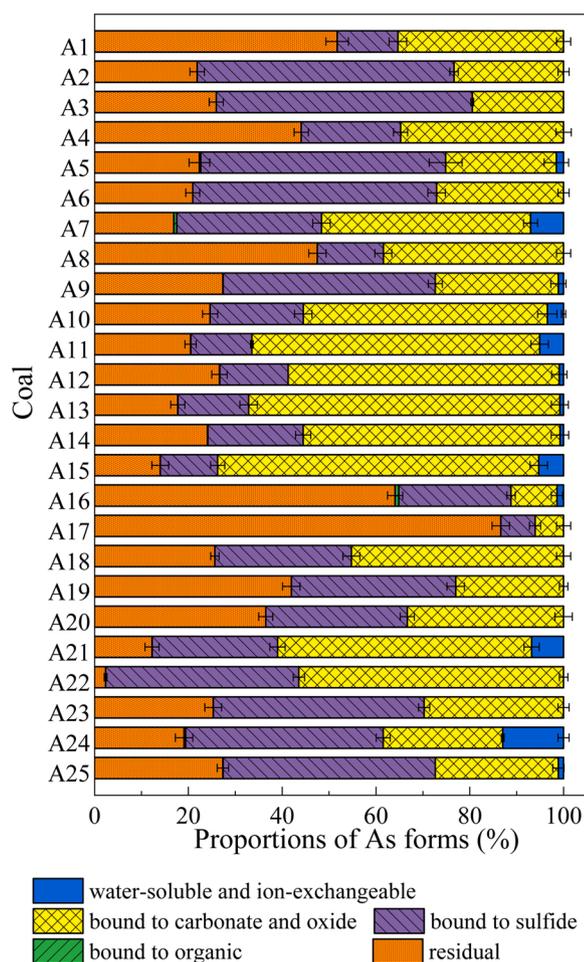


Fig. 2. Distribution of As forms in coals.

proportion of sulfide-bound As in the coal samples was 30%. The A2 and A17 coal samples presented the highest and lowest sulfide-bound As proportions of 55% and 7%, respectively. The average proportion of residual As in the coal samples was 30%. The A17 and A22 coal samples contained the highest and lowest proportions of residual As of 87% and 2%, respectively. Some coal samples contain small amounts of water-soluble and ion-exchangeable As accounting for no more than 13% of the total As. Significant differences were observed in As form distribution in various types of coal. However, the stability of each form of As during high-temperature coal combustion was not reported yet. It is essential to discover the transformation of As in different forms, especially the primary forms of As in coal, which were carbonate- and oxide-bound, sulfide-bound, and residual As.

Among the coal samples, A5, A10 and A22 coals with significant differences in As release characteristics were selected to analyze the form distribution of As in the ash produced at 1100, 1200, and 1300 °C. The distribution of As forms in A5 coal and its ash are illustrated in Fig. 3 (a). As in A5 coal was primarily in the sulfide-bound, carbonate- and oxide-bound and residual forms, accounting for 52%, 24% and 22% of the total As amount, respectively. After combustion at 1100 °C, 32% of As was released into the gas phase, whereas 35%, 27% and 6% of As remained in the ash as water-soluble and ion-exchangeable form, residual form and carbonate- and oxide-bound form, respectively. Upon increasing the combustion temperature to 1200 and 1300 °C, almost the entire amount of As in the ash was residual As; however, the proportions of residual As obtained at 1200 and 1300 °C were only 23% and 5%, respectively. The distribution of As forms in A10 coal and its ash are presented in Fig. 3 (b). The primary forms of As in the A10 coal samples were carbonate- and oxide-bound, residual, and sulfide-bound As, accounting for 52%, 25%, and 20%, respectively. After combustion at 1100 °C, 48% of As was released into the gas phase, and 24%, 17% and 11% of As remained in the ash in the water-soluble and ion-exchangeable form, residual form and carbonate- and oxide-bound form, respectively. When the combustion temperature was increased to 1200 °C, residual As basically remained unchanged while other forms disappeared. The proportion of residual As was decreased to 7% at 1300 °C. The distribution of As forms in A22 coal and its ash are illustrated in Fig. 3 (c). As in the coal was primarily in the carbonate- and oxide-bound and sulfide-bound forms, accounting for 56% and 41% of the total As, respectively. After combustion at 1100 °C, 71% of As was released into the gas phase, whereas 23% of As remained in the ash as the residual form. When the combustion temperature was increased to 1200 and 1300 °C, the proportions of residual As were decreased to 8% and 0, respectively.

The stability of the original As forms in coal was analyzed by comparing the As form distribution in coal and its combustion products. The proportions of carbonate- and oxide-bound and sulfide-bound As decreased significantly upon burning A5, A10, and A22 coal samples at 1100 °C, and were 0 for the samples burned at 1200 °C. These results suggested that these two forms of As were thermally unstable and could be completely released during coal combustion at high temperatures. The proportion of residual As in the combustion product of A10 coal decreased by 61% at 1100 °C, indicating that the original residual As in the coal was thermally unstable. Similar results were obtained for the other coal samples. For example, the proportion of residual As in A17 coal was 87%, and the As release ratio exceeded 97% at 1200 °C, suggesting that the residual As in the coal was almost completely released.

Because the original forms of As in coal were thermally unstable, they were either released into the gas phase or converted into stable forms, which were retained in the solid phase. The proportions of residual As in the combustion products of A5 and A22 coals at 1100 °C were 0.2 and 8.8 times higher, respectively, than those of the corresponding coal samples, indicating the transformation of other forms of As into residual As. The proportions of water-soluble and ion-exchangeable As in the combustion products of A5 and A10 coals at 1100 °C were higher than those of the corresponding coal samples,

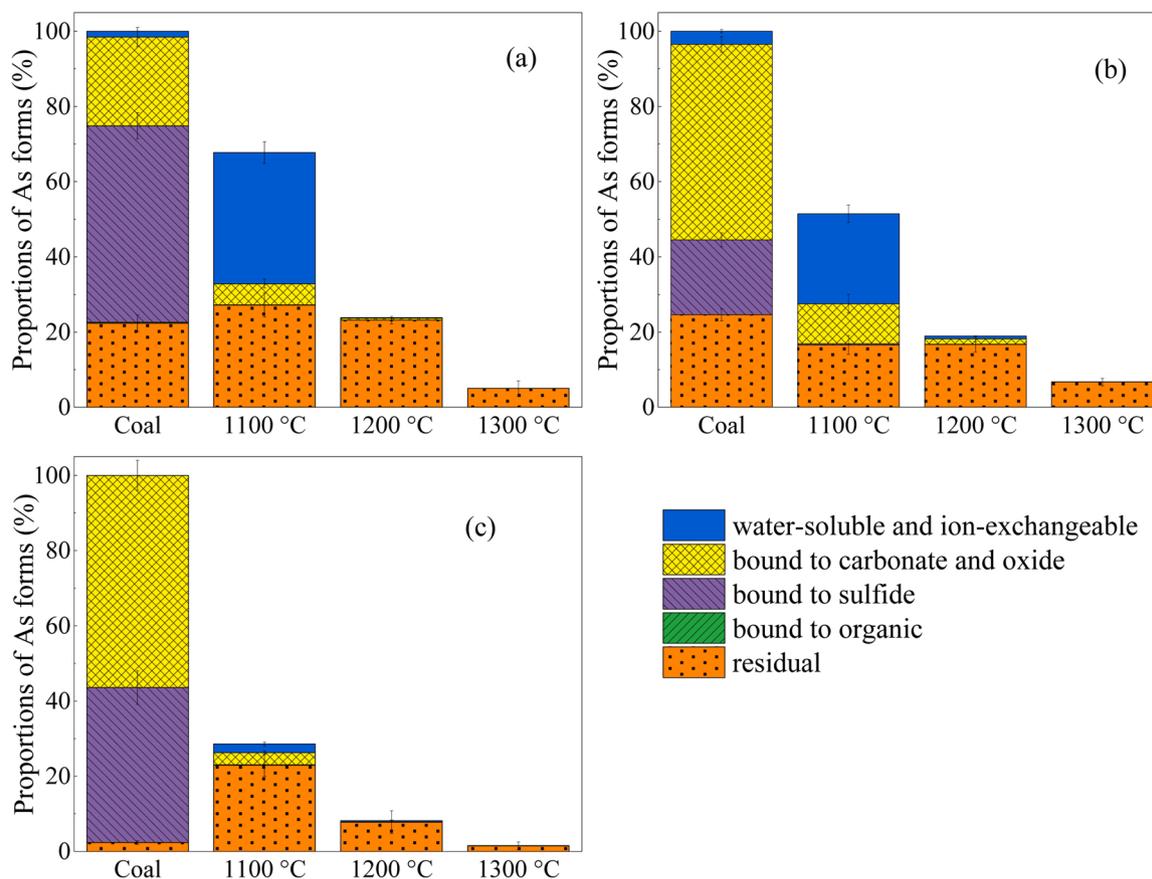


Fig. 3. Distribution of As forms in the coal and combustion products: (a) A5 coal; (b) A10 coal; (c) A22 coal.

suggesting the transformation of other forms of As into water-soluble and ion-exchangeable As. Only residual As was present in the ash samples obtained by burning the A5 and A10 coal samples at 1200 and 1300 °C.

It was inferred that the difference in As release characteristics of different coal types were attributed to the influence of two factors: (1) the distribution of As forms differed with coal types and the stability of each form of As was different during coal combustion; (2) the mineral components in coal affected the conversion of As in coal to the water-soluble and ion-exchangeable and residual As in the ash. According to Fig. 2, the primary As forms in coal were carbonate- and oxide-bound form, sulfide-bound form, and residual form. It can be seen that all the three forms of As were thermally unstable and could be completely

released from coal during combustion at temperatures ≥ 1200 °C. The minerals present in the coal samples were the primary factor that caused the differences in the As release ratios among various coal types.

According to previous studies (Seames and Wendt, 2007; Luo et al., 2011; Fu et al., 2021), Ca and Fe played the primary role in retaining As during coal combustion, which converted As into $\text{Ca}_3(\text{AsO}_4)_2$ and FeAsO_4 , respectively. Taking oxides as an example, the reactions between CaO, Fe_2O_3 and As_2O_3 can be described as follows:



The mass ratios of As to Ca and Fe in the products were 1.25:1 and

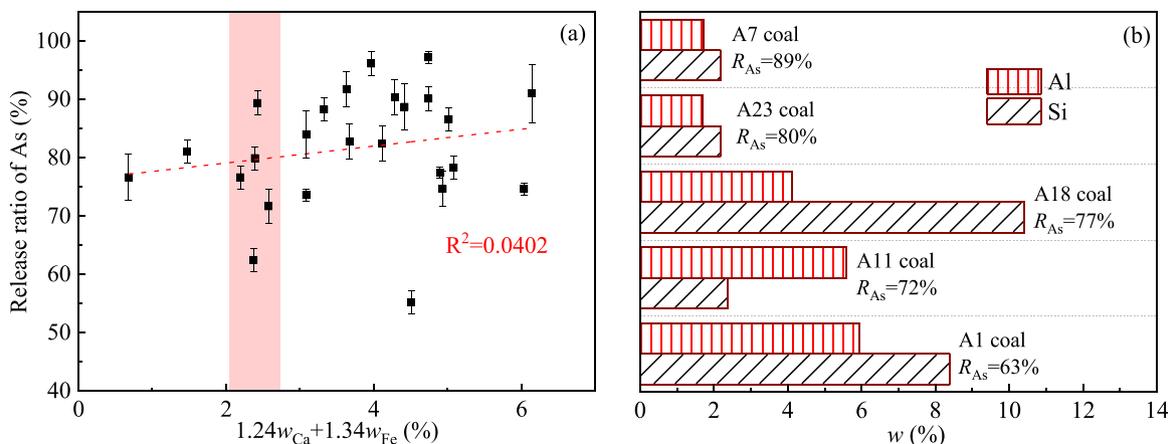


Fig. 4. (a) correlation analysis between release ratio of As and contents of Ca, Fe; (b) comparison of Al and Si content in A1, A11, A18, A23, A7 coals.

1.34:1, respectively. Assuming that during coal combustion at 1200 °C, both Ca and Fe existed as oxides to retain As, and then they retained up to 1.25 and 1.34 times their own masses of As, respectively. Therefore, the release ratios of As during the combustion of different coal types should be negative with "Ca content \times 1.25 + Fe content \times 1.34" in coal. However, no significant correlation was observed between the two variables as shown in Fig. 4(a). This was ascribed to the dependence of the retention abilities of minerals for As on the contents of Ca and Fe and also on the forms of Ca and Fe present in the coal samples.

Numerous researchers studied the transformation of the Ca and Fe forms during coal combustion. The Ca compounds in coal included calcite (CaCO₃), dolomite (CaMg(CO₃)₂), gypsum (CaSO₄), and organic-bound Ca (i.e., -(COO)₂Ca), etc. (Matsuoka et al., 2008). The decomposition of carbonates, combustion of organic matter and the reactions between Ca and silico-alumina minerals occurred during coal combustion (Tian et al., 2018; Akar et al., 2013; Wang et al., 2017). The primary forms of Ca in the ash were CaO, CaSO₄ and aluminosilicates (such as CaAl₂Si₂O₈, Ca₄Al₆O₁₂(SO₄)₂) (Tian et al., 2018; Akar et al., 2013; Wang et al., 2017). The primary Fe compounds in coal were hematite (Fe₂O₃), siderite (FeCO₃), green vitriol (FeSO₄) and pyrite (FeS₂) (Wen et al., 2016). Fe was converted into hematite (Fe₂O₃), magnetite (Fe₃O₄) and aluminosilicates during coal combustion (Sefidari et al., 2020; Anshits et al., 2020). Wen et al. (2016) performed combustion experiments on three types of coal at 1300 °C using a drop tube furnace. They determined that the predominant form of Fe in the ash was iron aluminosilicate (40–90%), followed by iron oxides, whereas Ca was predominantly present as aluminosilicates. Tian et al. (Tian et al., 2015) and Yang et al. (2021) conducted coal combustion experiments at 1250 °C and found that iron aluminosilicate and iron oxides accounted for approximately 32% and 68%, respectively, of the Fe in the collected ash. These findings suggested that calcium and iron aluminosilicates were the primary forms of Ca and Fe, respectively, in the ash.

Five coals with similar total Ca and Fe contents but significantly different As release characteristics were selected. A negative correlation was obtained between the Si and Al contents in coals and the corresponding As release ratios (Fig. 4(b)). These results indicated that the Si and Al components could increase As retention by changing the forms of Ca and Fe in coal. Therefore, to study the retention mechanism of minerals on As during high-temperature coal combustion, the coupling effects of multi-mineral components in coal were considered, which will be discussed in Section 3.2.

3.2. Coupling effects of mineral components on As transformation

The primary forms of Ca and Fe in ash were aluminosilicates, which were primarily formed via the reactions of CaO, CaSO₄, and Fe₂O₃ with Si and Al minerals, including kaolin, during coal combustion (Sefidari et al., 2020). Herein, pure CaO, CaSO₄, Fe₂O₃, and kaolin were used to simulate the complex reactions of Ca and Fe minerals during coal combustion. The direct characterization of the As forms present in coal and combustion products was challenging because of their low contents. Moreover, it was difficult to evaluate the retention of As on specific minerals because of the complexity of the mineral components of coal. The mixture of cellulose and p-aminophenyl arsenic acid was used as the As model compound to conduct co-combustion experiments with

various minerals. The retention amounts of As by different minerals at 1200 °C are presented in Table 5. The amounts of As retained by CaO and CaSO₄ (3.0 and 6.8 mg/g, respectively) were significant. In contrast, the As retention abilities of Fe₂O₃ and kaolin were poor (0.6 and 0.2 mg/g, respectively). The retention capacities of CaO, CaSO₄, and Fe₂O₃ mixtures with kaolin with mass ratios of 1:2 reached 5.4, 3.6 and 4.7 mg/g, respectively. These values were significantly higher those obtained via the linear superposition of the retention capacities of the individual minerals (1.1, 2.4, and 0.3 mg/g, respectively). These results indicated that the retention of As was enhanced by the coupling of CaO, CaSO₄ and Fe₂O₃ with kaolin. The products were heated for 10 and 30 min and the relative change in As content was within 3.7%, suggesting that the retained As was thermally stable.

To explore the As retention mechanism under the coupling of kaolin and CaO, the XRD, XPS and EPMA experiments were performed. The data for the products of CaO and (CaO + kaolin) were compared. The phase compositions of the two retention products are illustrated in Fig. 5 (a). A fraction of CaO reacted with kaolin to form aluminosilicate minerals, such as gehlenite (Ca₂Al₂SiO₇) and anorthite (CaAl₂Si₂O₈). The product also contained unreacted CaO and mullite, which was the thermal conversion product of kaolin. The diffraction peaks of As compounds were not present in the XRD patterns of the retention products. This was ascribed to the low As contents or poor crystallinity of the As compounds. The As_{2p} XPS profiles of the retention products were used to analyze the morphology of As in the retention products. As reacted with CaO to form Ca₃(AsO₄)₂, as previously reported in the literature (Cao et al., 2020), and the corresponding peak of Ca₃(AsO₄)₂ was observed at 1327.45 eV (Fig. 5(b)). However, the peak of As in the XPS profile of the retention product of (CaO + kaolin) downshifted by approximately 1 eV. This indicated that As did not form Ca₃(AsO₄)₂ in the presence of (CaO + kaolin). Owing to the limited studies on the electron binding energy of the 2p orbital of As, the As compounds present in the retention products could not be identified using XPS peak fitting. However, the spatial distribution of elements in the retention products, which was obtained using EPMA, facilitated understanding the occurrence of As. The distributions of As, Ca, Si, and Al in the retention product of (CaO + kaolin) are presented in Fig. 5(c). The brighter the color, the higher the element content in the area. The areas with high As contents significantly overlapped with the areas with high Al and Si contents; moreover, Ca was also distributed in these areas. The three areas with the highest As contents were subjected to qualitative analysis. The Ca:Al:Si atomic ratios in those areas were 1:0.66:0.76, 1:0.60:0.67, and 1:0.61:0.62, indicating that As was enriched in calcium aluminosilicates and Ca–Si–Al–As composite salts were formed. CaO was the primary component in the area with a high Ca content and low Al and Si contents. The As content in this area was relatively low, which confirmed that the retention ability of CaO for As was significantly lower than that of (CaO + kaolin).

Three pathways were proposed for the formation of Ca–Si–Al–As composite salts: (1) As reacted directly with CaO and kaolin, and AsO₄³⁻ formed in the calcium aluminosilicate lattice (Z.W. Zhao et al., 2021), (2) gaseous As₂O₃ was adsorbed by the calcium aluminosilicate formed via the reaction of CaO with kaolin, and (3) the As retention product of CaO, Ca₃(AsO₄)₂, underwent a solid–solid reaction with kaolin to form a eutectic. In the absence of kaolin, the amount of As retained by CaO was 3.0 mg/g. When CaO was mixed with kaolin with mass ratios of 1:2, the amount of As retained via pathway (3) did not exceed 1.0 mg/g, which was significantly lower than the actual As retention amount of 5.4 mg/g. These results indicated that pathway (3) was not the primary As retention mechanism for (CaO + kaolin). To explore the significance of pathways (1) and (2), CaO and kaolin were reacted at 1200 °C for 40 min to convert a fraction of CaO into calcium aluminosilicate. The product was then co-fired with the As model compound, and an As retention amount of 3.6 mg/g was achieved. The XRD pattern revealed the presence of calcium aluminosilicate, unreacted CaO, and mullite in the product. The As retention amount of 3.6 mg/g was ascribed to the

Table 5
Retention of As by various mineral components.

Minerals	Retention of As (mg/g)
CaO	3.0 ± 0.2
CaSO ₄	6.8 ± 0.4
Fe ₂ O ₃	0.6 ± 0.1
Kaolin	0.2 ± 0.1
1/3 CaO + 2/3 Kaolin	5.4 ± 0.3
1/3 CaSO ₄ + 2/3 Kaolin	3.6 ± 0.2
1/3 Fe ₂ O ₃ + 2/3 Kaolin	4.7 ± 0.1

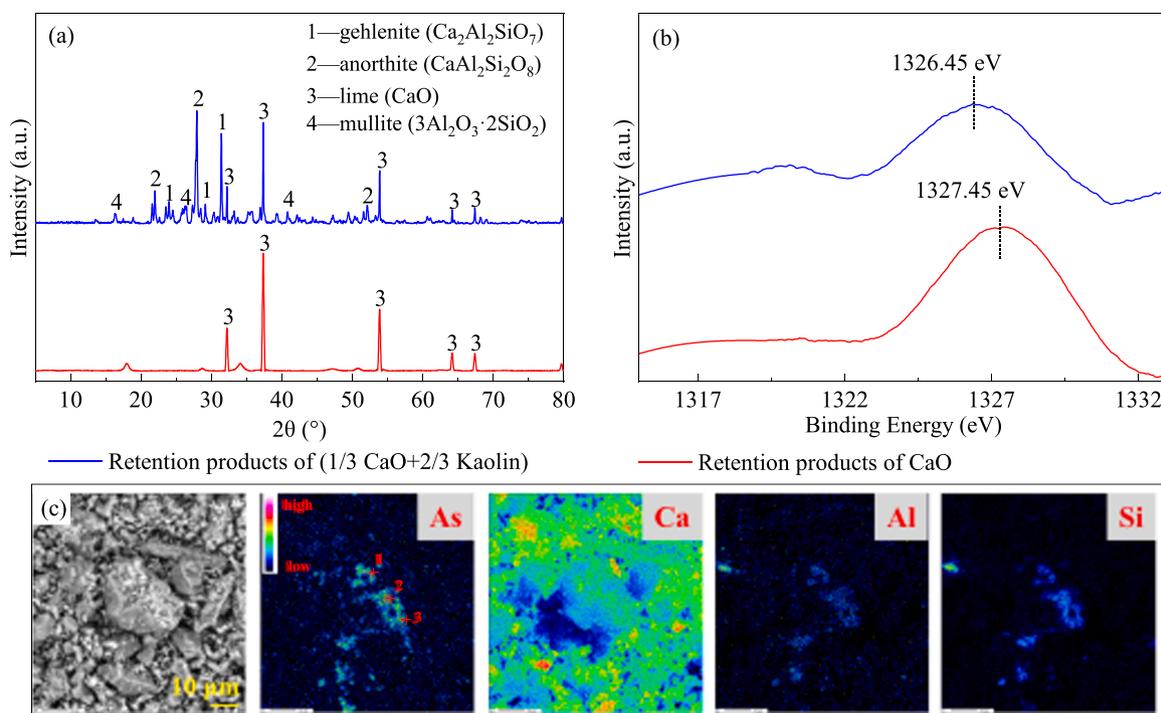


Fig. 5. (a) XRD patterns of retention products; (b) XPS spectrum of As_{2p} in retention products; (c) elemental mapping of retention products of (1/3 CaO+2/3 Kaolin).

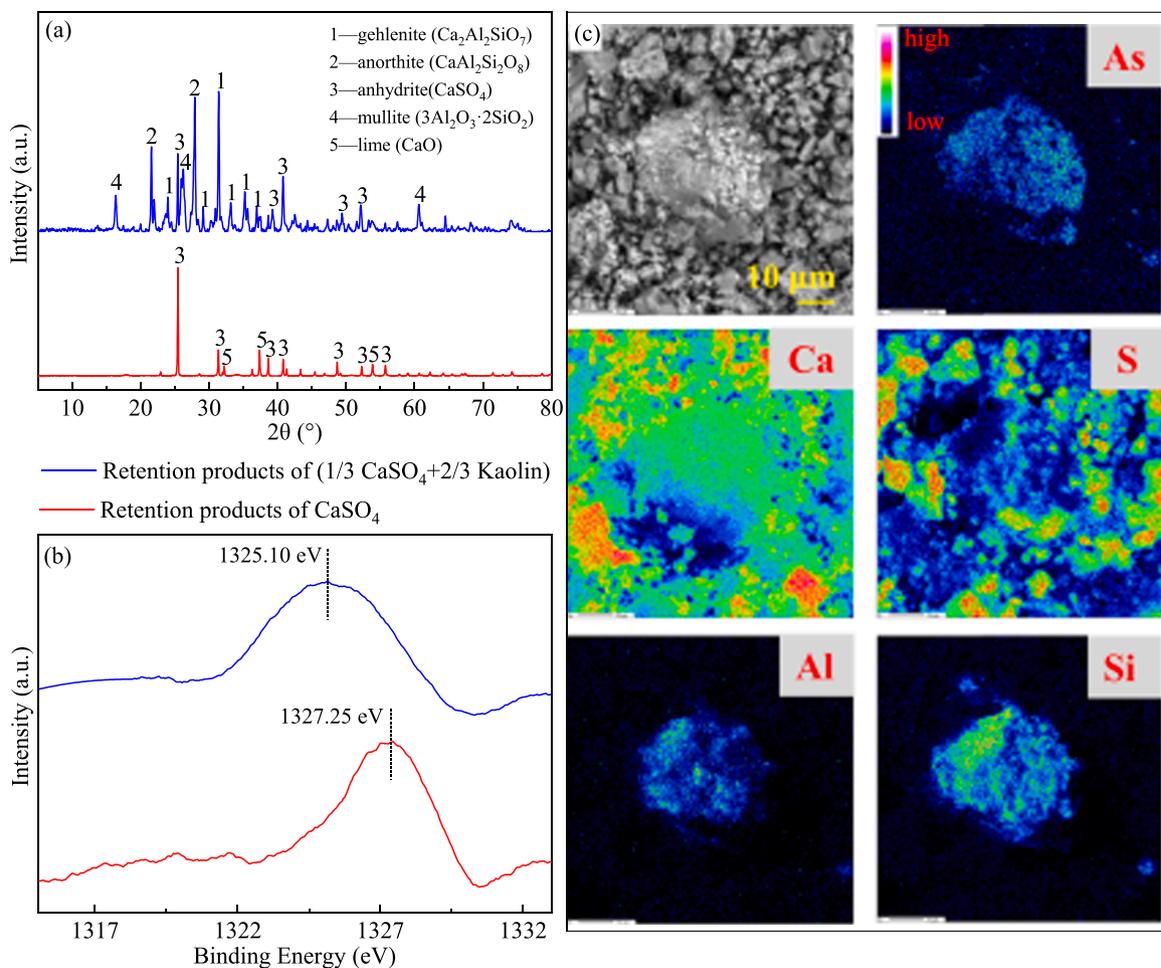


Fig. 6. (a) XRD patterns of retention products; (b) XPS spectrum of As_{2p} in retention products; (c) elemental mapping of retention products of (1/3 CaSO₄+2/3 Kaolin).

combined contributions of CaO, calcium aluminosilicate, and mullite. This value was higher than that obtained via the linear superposition of the individual As retention amounts of CaO and kaolin (1.0 mg/g), indicating that pathway (2) was plausible and the retention ability of calcium aluminosilicate for As_2O_3 was higher than that of CaO. However, the aforementioned As retention amount was lower than that of unreacted (CaO + kaolin) (5.4 mg/g), suggesting that the amount of As retained via the direct reaction of As with CaO and kaolin (pathway (1)) was the highest.

The XRD, XPS, and EPMA data for products of CaSO_4 and (CaSO_4 + kaolin) were analyzed. The phase compositions of the retention products are presented in Fig. 6(a). A fraction of CaSO_4 reacted with kaolin to form aluminosilicates. The retention products also contained unreacted CaSO_4 , its decomposition product, CaO, and mullite. As reacted with CaSO_4 to form $\text{Ca}_3(\text{AsO}_4)_2$, as previously reported in the literature (B. Song et al., 2020), and the corresponding XPS peak of $\text{Ca}_3(\text{AsO}_4)_2$ was observed at 1327.25 eV (Fig. 6(b)), which was close to that of the As retention product of CaO. However, the XPS peak of the As retention product of (CaSO_4 + kaolin) downshifted by approximately 2.15 eV, suggesting a change in the As form. The spatial distributions of As, Ca, Si, and Al in the As retention products of (CaSO_4 + kaolin) are illustrated in Fig. 6(c) and were similar to those of the As retention products of (CaO + kaolin). The As-rich area overlapped significantly with the Ca-, Al-, and Si-rich areas, indicating that the coupling effect of CaSO_4 and kaolin for As retention was similar to that of CaO, that is, Ca–Si–Al–As composite salts were formed.

Three pathways similar to those proposed for CaO were suggested for As retention by coupling of CaSO_4 and kaolin. CaSO_4 and kaolin were reacted at 1200 °C for 40 min, such that a fraction of CaSO_4 was converted into calcium aluminosilicate. The product was then co-fired with the As model compound, and an As retention amount of 3.2 mg/g was achieved. This amount was higher than the As retention amount obtained via the linear superposition of the individual As retention amounts of CaSO_4 and kaolin (2.3 mg/g), indicating that the As retention ability of calcium aluminosilicate was higher than that of CaSO_4 . Therefore, the As retention amount associated with pathway (2) was higher than that associated with pathway (3). The amount of As retained

by unreacted (CaSO_4 + kaolin) was 3.6 mg/g, which was higher than that retained by reacted (CaSO_4 + kaolin), suggesting that the amount of As retained via pathway (1) was higher than that retained via pathway (2).

The XRD, XPS, and EPMA data for products of Fe_2O_3 and (Fe_2O_3 + kaolin) were analyzed. The phase compositions of the two retention products are illustrated in Fig. 7(a). A fraction of Fe_2O_3 reacted with kaolin to form $\text{Fe}_2\text{Al}_4\text{Si}_5\text{O}_{18}$. As was retained by Fe_2O_3 to form FeAsO_4 as previously reported in the literature (Song et al., 2021), and the corresponding peak was observed at 1326.30 eV from Fig. 7(b). However, the peak of As in the XPS profile of the retention product of (Fe_2O_3 + kaolin) shifted by approximately 2.4 eV. This indicated that As did not form FeAsO_4 . The areas with high As contents significantly overlapped with the areas with high Al and Si contents as shown in Fig. 7(c). The three areas with the highest As contents were subjected to qualitative analysis. The Fe:Al:Si atomic ratios in those areas were 1:1.35:0.64, 1:0.45:0.37, and 1:1.05:1.50, indicating that As was enriched in ferric aluminosilicates and Fe–Si–Al–As composite salts formed.

Three pathways were proposed for As retention using (Fe_2O_3 + kaolin). The As retention amount of Fe_2O_3 was 0.6 mg/g. Therefore, the amount of As retained via pathway (3) was lower than 0.2 mg/g when using the mixture of Fe_2O_3 and kaolin with mass ratios of 1:2. This amount was significantly lower than the total retention amount (4.7 mg/g), suggesting that the amount of As retained via pathway (3) was low. Fe_2O_3 and kaolin were reacted at 1200 °C, such that a fraction of Fe_2O_3 was converted into ferric aluminosilicate. The As retention amount of iron aluminosilicate was 3.3 mg/g, which was lower than that of unreacted (Fe_2O_3 + kaolin). This suggests that most As was retained via the direct reaction of As with Fe_2O_3 and kaolin, which led to the formation of AsO_4^{3-} in the ferric aluminosilicate lattice. The secondary pathway involved the adsorption of gaseous As_2O_3 by ferric aluminosilicate.

3.3. Mechanism analysis of As transformation during coal combustion

As discussed in Section 3.2, CaO, CaSO_4 , and Fe_2O_3 could retain As at high temperatures, and the As retention amounts of the combinations of

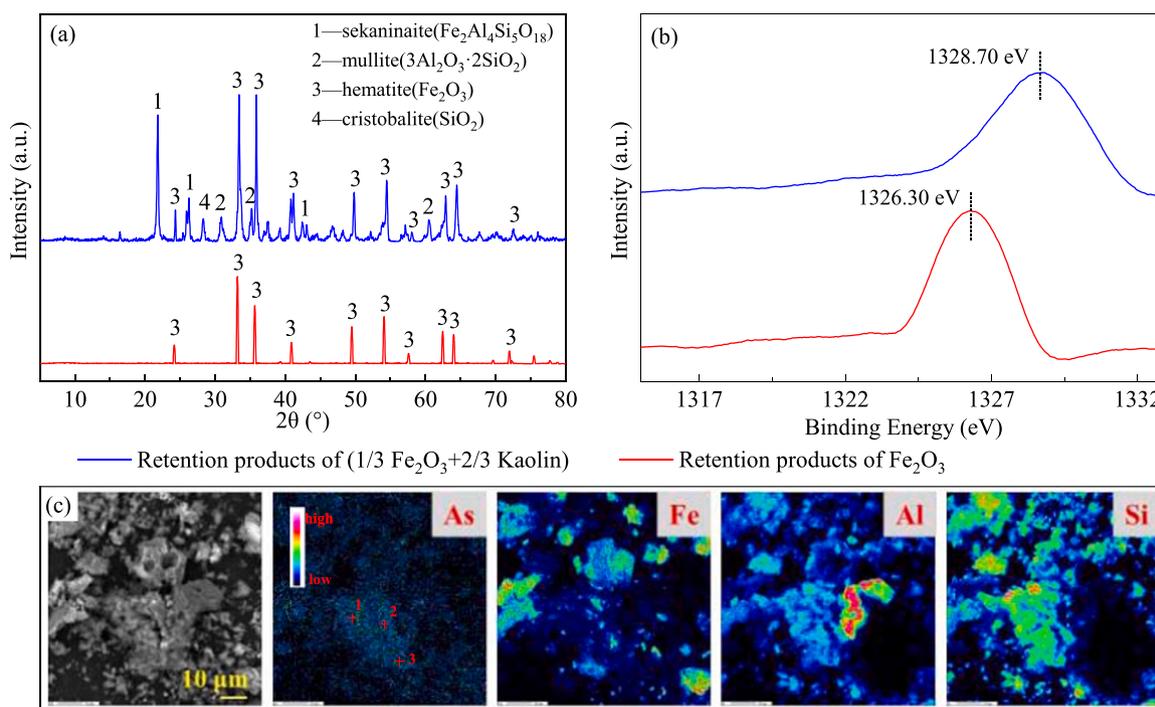


Fig. 7. (a) XRD patterns of retention products; (b) XPS spectrum of As_{2p} in retention products; (c) elemental mapping of retention products of (1/3 Fe_2O_3 +2/3 Kaolin).

CaO, CaSO₄, and Fe₂O₃ with kaolin were significantly higher than those of CaO, CaSO₄, and Fe₂O₃, respectively, suggesting that the As retention abilities were improved by the coupling effects. The XPS and EPMA profile indicated that upon its retention by combinations of CaO, CaSO₄, and Fe₂O₃ with kaolin, As formed Ca–Si–Al–As and Fe–Si–Al–As composite salts. Three pathways were suggested for the formation of these composite salts: (1) As reacted directly with CaO/CaSO₄/Fe₂O₃ and kaolin, and AsO₄³⁻ formed in the aluminosilicate lattice, (2) gaseous As₂O₃ was adsorbed by the aluminosilicate formed via the reaction of CaO/CaSO₄/Fe₂O₃ with kaolin, and (3) the products of As retained by CaO/CaSO₄/Fe₂O₃, which were Ca₃(AsO₄)₂ and FeAsO₄, underwent a solid–solid reaction with kaolin to form eutectics. Unlike direct co-firing, when CaO/CaSO₄/Fe₂O₃ and kaolin were pre-reacted to form aluminosilicate, which was then used for the retention of As, this process did not include pathway (1). The contents of Ca and Fe remained unchanged; however, the amount of retained As decreased, indicating that the contribution of pathway (1) was higher than that of pathway (2). The occurrence of pathway (3) depended on the amounts of As retained by CaO/CaSO₄/Fe₂O₃, which were lower than those retained by the calcium and ferric aluminosilicates with the same Ca and Fe contents. The contribution of pathway (2) was higher than that of pathway (3). Therefore, the primary As retention mechanism of multi-minerals is as follows. As reacts with the mixtures of Ca and Fe minerals with kaolin, forms AsO₄³⁻ in the aluminosilicate lattices, and generates Ca–Si–Al–As and Fe–Si–Al–As composite salts, respectively.

According to the As retention mechanism by multi-minerals, the mechanism of As transformation during high-temperature coal combustion could be further developed. As discussed in Section 3.1, As existed in various forms in coal, and all original forms of As in coal were thermally unstable and could be completely released during coal combustion at temperatures ≥ 1200 °C. The original Ca and Fe components in coal, such as CaO and Fe₂O₃, reacted with Si/Al components including kaolin. Meanwhile, the As in gas phase was partially retained by Ca, Fe, Si and Al components through pathway (1) or (2) mentioned before. For coal samples with similar contents of Ca and Fe, the coal with higher contents of Si and Al had stronger ability to retain As owing to the coupling mechanism. The retained As were insoluble Ca–Si–Al–As and Fe–Si–Al–As composite salts rather than soluble Ca₃(AsO₄)₂ and FeAsO₄, and thus As was only retained as residual form in ash at combustion temperatures above 1200 °C.

The above-proposed mechanism of As transformation during coal combustion is important for As pollution control. As we know, the gaseous As released into the flue gas after combustion is much more difficult to remove than that in the solid phase (Wang et al., 2019). If more As is retained in solid combustion products under the coupling action of multi-minerals, the As emission from coal-fired plants can be reduced. This has been manifested efficiently in blended coal combustion (B. Zhao et al., 2021) and in-furnace injection of mineral sorbents (Song et al., 2021; He et al., 2021). Moreover, the As is retained in ash as residual form during high-temperature coal combustion, which is the most stable form of As with low leaching toxicity (He et al., 2020). Utilizing the coupling effects of multi-minerals during coal combustion can reduce the environmental hazard of by-products from coal-fired plants.

4. Conclusions

The transformation characteristics of As during combustion of 25 types of coal were obtained. The release ratio of As increased with increasing temperature and varied widely with the coal type. At 1100 °C, 18–79% of As in coal was released. The release ratios increased to 55–97% at 1200 °C. As was almost completely released from most coal samples at 1300 °C. The primary forms of As in the 25 coal samples were carbonate- and oxide-bound, sulfide-bound, and residual forms. These As forms were unstable during coal combustion. A fraction of As was released into the gas phase, whereas the rest of As was converted

into more stable water-soluble and ion-exchangeable and residual As forms in the ash. The only form of As present in the ash obtained by burning coal at temperatures above 1200 °C was residual As.

The coupling effects of the multi-mineral components in coal was the deciding factor for the differences in the As release ratio among coal samples. The CaO, CaSO₄, Fe₂O₃ and kaolin in coal could retain As at high temperatures, and the amounts of As retained by CaO and CaSO₄ were the highest. The amounts of As retained by mixtures of kaolin with the aforementioned Ca and Fe minerals were significantly higher than the linear superpositions of the retention amounts of the individual minerals. This indicated that the As retention capacities of the mineral combinations were higher than those of the individual minerals. Three As retention pathways were proposed for coupling mechanism of multi-mineral combinations. The primary pathway involved the reaction of As with CaO/CaSO₄/Fe₂O₃ and kaolin, and AsO₄³⁻ formed in the aluminosilicate lattices. The other pathways involved the adsorption of gaseous As₂O₃ by the aluminosilicates formed via the reactions of the Ca and Fe minerals with kaolin. Besides, the products of As retained by CaO/CaSO₄/Fe₂O₃, which were Ca₃(AsO₄)₂ and FeAsO₄, underwent a solid–solid reaction with kaolin to form eutectics. Lastly, As was retained as Ca–Si–Al–As and Fe–Si–Al–As composite salts.

The mechanism of As transformation during coal combustion was proposed considering the coupling action of Ca, Fe, Si and Al minerals. It provides theoretical support for developing As emission control technologies, such as blended coal combustion and in-furnace injection of mineral sorbents.

Environmental implication

Coal combustion is a significant source of atmospheric arsenic (As), which is highly toxic. As transformation characteristics during combustion of 25 coal samples were reported in this paper, which are helpful for further understanding the As distribution in different coal combustion systems. The coupling effects of Ca/Fe, Si and Al components were identified as the deciding factor for As retention. The results provide theoretical support for developing methods of minimizing As pollution, including coal blending and preparation of adsorbents.

CRedit authorship contribution statement

Guo-chang Song: Conceptualization, Methodology, Formal analysis, Investigation, Writing – original draft. **Wen-ting Xu:** Methodology, Validation, Writing – review & editing, Resources, Visualization. **Xing-yu Yang:** Methodology, Validation, Writing – review & editing. **Qiang Song:** Writing – review & editing, Supervision, Project administration, Funding acquisition.

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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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.jhazmat.2022.129040](https://doi.org/10.1016/j.jhazmat.2022.129040).

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