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Calcium and Arsenic Interaction during Leaching Process of Coal Fly Ash: Analysis by FactSage

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Abstract

Analysis of interaction between calcium compound and arsenic (As) in fly ash generated a combustion process have been investigated through using thermodynamic calculation, FactSage. This study was employed to theoretically predict the possibly As-bearing compounds and its distribution in leaching process of two fly ashes under four different kind of calcium compounds (CaO, $Ca(OH)_2$, $CaCO_3$ and $CaSO_4$) as inhibitor. The influence of different mass addition of each inhibitors in the range of 0 to 1 gram with data search FactPS and FToxid were evaluated. The analysis indicated that, on combustion process $AlAsO_{4(s)}$ was the most probably specie resulting compound from interaction of arsenic with fly ash components. CaO and $Ca(OH)_2$ have an effect on leaching process of arsenic in fly ash due to the reaction of predicted arsenic with those calcium compounds than other inhibitors. This reaction was largely dependent on the pH of the leachate to study the leaching performance. CaO and $Ca(OH)_2$ preferentially generate high-pH leachate on leaching process and encourage the reaction of calcium and arsenic to form precipitate $Ca_3(AsO_4)_2$. The application of this inhibitors in leaching process was a promising method to prevent the arsenic compounds into environment and minimize its leachability from fly ash.

1 Introduction

Coal power plants generate large volumes of coal combustion products such as flue gas desulfurization materials, bottom ash coal fly ash, etc. Coal fly ash is the most hazardous coal combustion products because contains environmentally significant quantities of hazardous leachable trace elements such as As, Mo and Se [1]. During combustion process, the organic matter in coal destroyed and as result the concentration of trace elements in coal fly ash enhanced relative to the source coal [2]. Arsenic (As) released from combustion is one of the most environment concern due to its toxic, potential carcinogenic propensities and high volatility. In generally, coal fly ash derived from coal combustion is subjected to disposal and reuse. The leaching of arsenic will cause potential hazard on aquifer systems and soil, which thus cause a critical environmental problem. With increase in awareness of the public in environment impact of the combustion of coal, it is vital to control the emission of arsenic during coal combustion and its leaching during fly ash treatment. The development of inhibitors for inhibit the leaching of the trace element into the environment, previous study experimentally was found that calcium has positive effect in decreasing trace element leaching concentration, [3]. FactSage, facility for the analysis of chemical thermodynamic, was conducted to predict the formation of arsenic-bearing species, previous research was found calcium is the most influential factor on arsenic transformation. The presence of calcium in coal fly ash play an important role in leaching process behavior of arsenic, which abundance of free CaO generates an alkaline leachate during leaching test and successively reduces arsenic leaching since the precipitate was preferentially occurred via the reaction of arsenic with calcium at high pH leachate [4]. This study aims to evaluate the influence of different calcium components as inhibitor and mode of occurrence of trace elements in leaching process by using factsage software. The application of this inhibitors in leaching process was a promising method to prevent the arsenic compounds into environment and minimize its leachability from fly ash.

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2 Experimental

2.1 Coal Fly Ash Samples

Coal Fly ash samples which used in this research was obtained from different coal-fired power plants in Japan, namely FA AC and FA AD.

Components	Coal Fly Ash Samples	
	FA AC	FA AD
Chemical Composition (%)		
SiO_2	68.98	64.01
Al_2O_3	22.53	24.04
TiO_2	1.07	1.34
Fe_2O_3	3.80	4.43
CaO	0.78	2.27
MgO	0.51	0.48
Na_2O	0.45	0.35
K_2O	1.21	1.26
P_2O_5	0.18	1.27
MnO	0.04	0.04
V_2O_5	0.02	0.01
SO_3	0.44	0.49
Total	100	100
Trace Element (mg/kg)		
Arsenic (As)	14.58	5.53

Table 1: Chemical composition of coal fly ashes by XFR analysis

The chemical composition of these fly ash samples was determined by X-ray fluorescence analysis (WDXRF S8 TIGER, Bruker AXS). Table 1 shows the chemical composition of coal fly ash samples which used in this study. Calcium content in FA AD is 2.27 % whereas only 0.78 % calcium is in FA AC. On the other hand, arsenic concentration in FA AC and AD are 14.58 mg/kg and 5.53 mg/kg, respectively.

2.2 Thermodynamic equilibrium analysis

In this study, thermodynamic equilibrium was carried out using FatSage 7.2 software to predict the possible As-bearing compounds in coal fly ash and its distribution under different calcium compounds as inhibitor during leaching process. The data search used in this analysis include FactPS and FToxid. On combustion process, the elemental composition of ash was used as input data. The calculation were performed in different temperatures interval between 100 to 1600 °C, at atmospheric pressure. For leaching process, the predicted arsenic compound and different calcium compounds as inhibitors (CaO, $Ca(OH)_2$, $CaCO_3$ and $CaSO_4$) with mass in addition interval between 0 and 1 gram at room temperature, atmospheric pressure were used as input data. During simulation analysis on combustion and leaching process, aqueous, gases and solid species are chosen as output.

3 Results and Discussion

3.1 Interaction of Arsenic with Fly Ash Component during Combustion Process

Interaction of arsenic with fly ash components favors the formation of arsenate compound due to reaction interaction with gas phase compounds and fly ash particles. On studying the formation of As-bearing compound during combustion process was conducted by FactSage software. The prediction introduced in Fig. 1, it clearly sign that $AlAsO_4$ (Aluminum arsenate) was the most probably predicted compound forming during combustion process, indicated $AlAsO_4$ was compound contain in fly ash samples. This process can be explained by the following reaction to generate $AlAsO_4$ through Eq. (1).

$$Al_2O_3 + As_2O_3 + O_2 \rightarrow 2AlAsO_4 \quad (1)$$

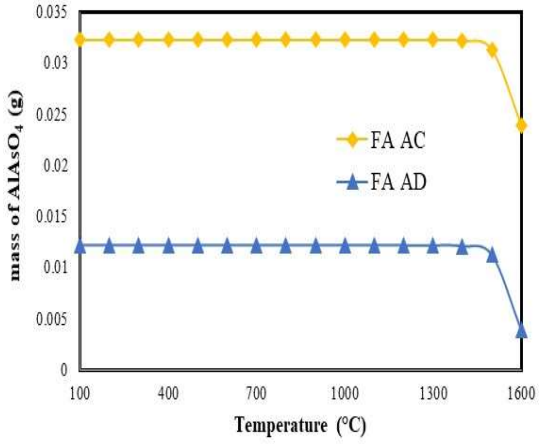


Figure 1: Prediction of As-bearing compound during combustion of Fly ash AC and AD

The amount of predicted compound of arsenic in FA AC was higher than that in FA AD because of higher arsenic content in coal fly ash samples (see Table 1). However, variations on arsenic concentration do not modified the distribution of arsenic compound on analysis process.

3.2 Effect of Inhibitors on Leaching Analysis of Predicted Arsenic Compound

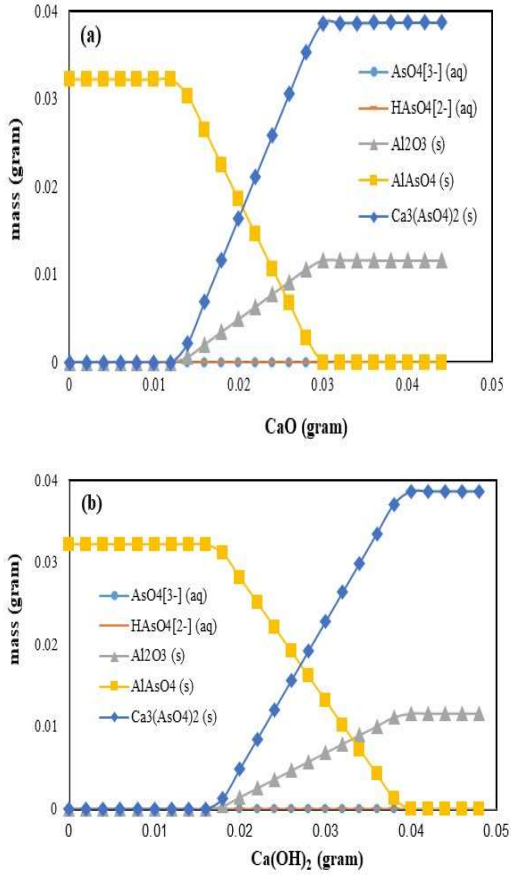
FactSage 7.2 was conducted to predict the formation of arsenic-bearing species during leaching process under different calcium compounds as inhibitors. As illustrated in Fig. 2, the leaching of predicted arsenic in the coal fly ash collected from combustion of arsenic with coal fly ash components.

Here, the leaching analysis with CaO and $Ca(OH)_2$ have an effect on leaching process of arsenic in coal fly ash due to the reaction of predicted arsenic with those calcium compounds to form precipitate $Ca_3(AsO_4)_2$. On the other hand, $CaCO_3$ and $CaSO_4$ were not give an effect on leaching process of arsenic. The formation of $Ca_3(AsO_4)_2$ with CaO and $Ca(OH)_2$ can be explained by the following reaction (2) and (3).

$$2AlAsO_4 + 3CaO + H_2O \rightarrow Ca_3(AsO_4)_2 + Al_2O_3 + H_2O \quad (2)$$

$$2AlAsO_4 + 3Ca(OH)_2 + H_2O \rightarrow Ca_3(AsO_4)_2 + Al_2O_3 + 4H_2O \quad (3)$$

In addition, the solubility of $Ca_3(AsO_4)_2$ in water is enough low to avoid leachability of arsenic from ash [5]. The solubility of $Ca_3(AsO_4)_2$ is 0.04g/L.



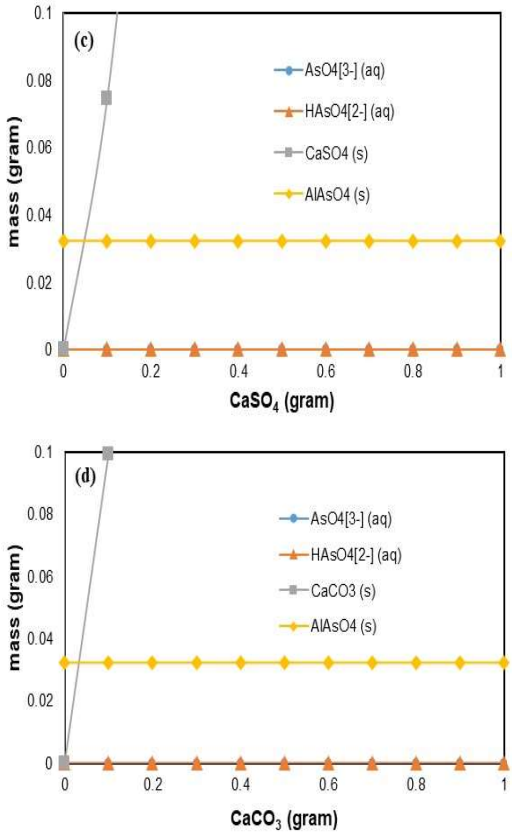


Figure 2: Effect of calcium compounds into arsenic leaching process on FA AC at 25 °C atmospheric condition (a) CaO, (b) $Ca(OH)_2$ (c) $CaSO_4$ and (d) $CaCO_3$

3.3 Effect of pH on Leaching Analysis of Predicted Arsenic Compound

According to the above results, $Ca_3(AsO_4)_2$ is the predicted specie resulting from As-Ca interaction during leaching process. Effect of inhibitors into leachate pH on arsenic on leaching process illustrated in Fig 3. Increase in the addition ratio of inhibitors (CaO and $Ca(OH)_2$) caused the increase of leachate pH and in formation of $Ca_3(AsO_4)_2$. The formation of $Ca_3(AsO_4)_2$ indicates that successively reduces of arsenic in leaching process since the precipitate was preferentially occurred via the reaction of arsenic with calcium compound at alkaline pH leachate. To better understand the effect of different coal fly ash on formation of $Ca_3(AsO_4)_2$ in leaching process shown in Table 2.

Inhibitor	Coal l Fly Ash Sample			
	FA AC		FA AD	
	pH	$Ca_3(AsO_4)_2$ formed (gr)	pH	$Ca_3(AsO_4)_2$ formed (gr)
CaO	12.30	0.0387	12.11	0.0147
$Ca(OH)_2$	12.16	0.0387	11.97	0.0147
$CaCO_3$	9.93	-	9.93	-
$CaSO_4$	7.12	-	7.12	-

Table 2: Effect of different coal fly ash samples on arsenic leaching process at 25 °C atmospheric condition

The amount of formation of $Ca_3(AsO_4)_2$ in FA AC was higher than that in FA AD because of higher predicted arsenate compounds forming after combustion process. Although CaO content in FA AD was higher than that in FA AC, the formation of $Ca_3(AsO_4)_2$ in FA AC was higher than that in FA AD, indicating that leaching process of arsenic from coal fly ash is reduced via the combustion process (see Table 1). However, variations on arsenic concentration do not modified the distribution of arsenate compound on leaching analysis process.

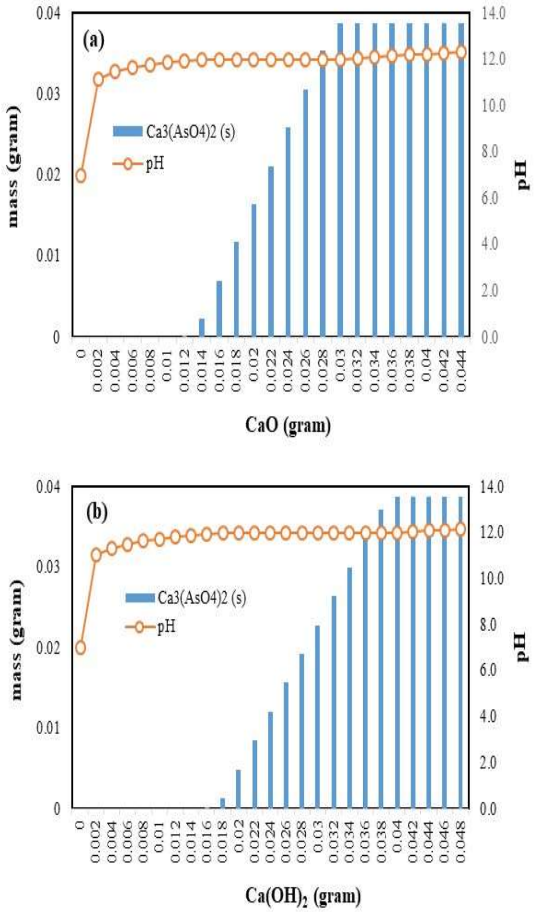


Figure 3: Effect of inhibitors into leachate pH on arsenic leaching process on FA AC at 25 °C atmospheric condition (a) CaO and (b) $Ca(OH)_2$

4 Conclusions

Leaching analysis of arsenic and different calcium compounds was carried out by FactSage 7.2, then the results confirmed that interaction between arsenic and the main fly ash, arsenic element preferentially formed mainly $AlAsO_4$ after combustion process. $Ca_3(AsO_4)_2$ was predicted to be arsenate compound forming in leaching process of coal fly ash with CaO and $Ca(OH)_2$ as inhibitor. Arsenic leaching process optimally working at alkaline pH during leaching test and successively reduces arsenic leaching since the precipitate was preferentially occurred via the reaction of arsenic with calcium compound at alkaline pH leachate.

5 Acknowledgment

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