

Effect of Cl/S Molar Ratio on Theoretical Partitioning of Heavy Metals under Waste Combustion Conditions

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Abstract—A simulation calculation was carried out to predict the behavior of heavy metals during waste incineration according to the variation of chlorine content by using a thermodynamic equilibrium model. To predict the behavior of heavy metals in incineration of wastes, chlorine content in wastes was changed up to 3.00 on a Cl/S molar ratio basis. Then the partitioning characteristics of heavy metals with Cl/Metal molar ratio were investigated as solid, liquid, and gas phases of metals. For analysis of emission characteristics, incineration temperature, chlorine content and air-fuel ratio (λ_r) were chosen as major operating parameters. It was found that the distribution characteristics of heavy metals were not significantly affected by air-fuel ratio, but evaporation rate of heavy metals increased with operating temperature. Most of the heavy metals remained in solid phase of metal oxides, such as CdO, CrO₃, CrO₂, CuO and ZnO, except for lead which existed as PbSO₄ in the given operating conditions (i.e., $T_b=800^\circ\text{C}$, $\lambda_r=1.3$, and Cl/S=0). It was found that most of the heavy metals in solid phase changed to gaseous Cl compounds, which have a high volatility with regard to increasing the Cl/S molar ratio under the same conditions. However, Cr compounds were almost not affected as chlorine level increased.

Key words: Heavy Metals, Evaporation, Chlorine Content, Thermodynamic Equilibrium Model, Waste Incineration

INTRODUCTION

When wastes with high content of heavy metals are incinerated, the heavy metals are generally transformed into harmful forms, and then they are included in out-streams of residues, such as bottom and fly ashes, and flue gas streams. Therefore, the study of the transformed chemical species is very important, but reasonable verification of metal partitioning is difficult due to the diversity of chemical species transformed [Flagan and Seinfeld, 1988; Lee, 1988].

To understand the emission characteristics of heavy metals, their concentration in the ashes and flue gas streams must be measured whenever combustion conditions are changed. However, there exists a great deal of difficulty in carrying out this task, and the hazardous pollutants have been already emitted into the environment.

Besides, the partitioning characteristics of heavy metals in waste incineration process are largely affected by the chlorine content in the waste fed. Up to the present study, however, only the concentration of heavy metals which were contained in bottom and fly ashes and flue gas have been measured without considering the chlorine content in waste [Yang et al., 1994, 2001; Jakob et al., 1996; Chen and Yang, 1998; Lee et al., 2000; Wobst et al., 2000].

The chlorine in the waste is contained in very wide ranges according to the kinds of the wastes. Generally, the chlorine content in the sewage sludge is lower than that in the municipal waste, but

is higher than that in the coal. The heavy metal content in sewage sludge is also higher than that in the coal [Kawaguchi, 1985; Lee et al., 1992; Jang et al., 2001].

Consequently, in this study, a simulation calculation was carried out to predict the behavior of heavy metals during waste incineration according to the variation of chlorine content by using a thermodynamic equilibrium model. The chlorine content for input data in model simulation was varied from 0.0 to 3.0 of Cl/S molar ratio basis. To compare the predicted value with the measured value in practical incineration process, the partitioning characteristics of heavy metals with Cl/Metal molar ratio were investigated as solid, liquid, and gas phases of metals.

MODEL SIMULATION

This study was performed to predict the effect of chlorine content on the behavior of heavy metals in the waste incineration process. A simulation calculation was carried out to predict the behavior of heavy metals during waste incineration according to the variation of chlorine content using a thermodynamic equilibrium model. HSC Chemistry [Outokumpu Research, 1999] was the thermodynamic equilibrium model using the Gibbs free energy minimization method. The HSC main database with 15000 species including gas, liquid and solid phases is of course incomplete, because the number of different substances is infinite. However, it does offer a quite good thermochemical data source for many common substances.

Incineration temperature, air-fuel ratio and chlorine content are chosen as major operating parameters in this study. The air fuel ratio (λ_r) and Cl/S molar ratio were changed to 0.6-2.0 and 0.0-3.0, re-

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*This paper is dedicated to Professor Dong Sup Doh on the occasion of his retirement from Korea University.

Table 1. Compositions of a sewage sludge used in the experiment

Proximate analysis (wt%)		Ultimate analysis (wt%)	
Moisture	21.00	C	14.30
Combustibles	30.64	H	2.72
Ash	48.36	N	2.33
		S	1.45
		O	17.98
		Ash	61.22
Ash analysis (wt%)		Heavy metal analysis (mg/kg)	
SiO ₂	49.60	Cr	207.86
Al ₂ O ₃	18.37	Cu	620.56
P ₂ O ₅	14.30	Pb	493
TiO ₂	0.84	Zn	1229.30
CaO	5.43		
MgO	1.30		
Na ₂ O	1.15		
K ₂ O	2.14		

spectively. To compare the predicted value with the practical measured value, the partitioning characteristics of heavy metals with Cl/Metal molar ratio were investigated as solid, liquid, and gas phases of metal compounds. Validity of predicted model was verified by comparing the predicted data against the experimental data.

The input data of the simulation program is based on the results of proximate, ultimate, ash and heavy metal analyses. The compositions of a sewage sludge used in the simulation and the practical incineration are shown in Table 1. The volatility of heavy metals in the incineration process has been classified in many ways. It has been reported that the classification based on the boiling point of metal is the general method. However, the volatility of heavy metal species is considerably affected by other parameters, such as the chlorine content besides the operating temperature. Therefore, four metals Cr, Cu, Pb, and Zn, which differ in their volatility, were selected to investigate the fate of heavy metals as listed in Table 1.

RESULTS AND DISCUSSION

1. Effect of Air-fuel Ratio on the Emissions of Heavy Metals

In general, waste incineration is a very complex thermal process involving various reactions occurring in an incinerator. Therefore, the incinerator performance and the emission characteristics are significantly affected by the various operating and design parameters. Air-fuel ratio (AFR) is one of the operating parameters which can influence the characteristics of combustion and emissions of various pollutants in the incineration process. The parameter of air-fuel ratio serves as a function of changing the partial pressure of oxygen in a combustion chamber. To achieve perfect combustion, therefore, the combustion process is generally performed under an oxidation condition which supplies a large amount of excess air with the exception of operation for the purpose of NO_x reduction [Zhao et al., 1994; Lyngfelt and Leckner, 1993].

The combustion region is changed by the extent of the air-fuel ratio as reduction or oxidation conditions, and thus the formation properties of the pollutants can also be varied. The metal species transformed are remarkably changed with reduction or oxidation

conditions of the combustion region. Therefore, the emission characteristics of the selected heavy metals were investigated with air-fuel ratio, and the results obtained are represented in Fig. 1.

Fig. 1(a) shows the phasic variation of Cr species with air-fuel ratio under 800 °C of the operating temperature and 1.0 of Cl/S molar ratio in sewage sludge incineration. As shown in the result, most of Cr species was converted to the solid phase in the whole ranges of AFR, and a small amount of gas phase compound was formed over 1.1 of AFR. But liquid phase of Cr species did not form under the condition determined in this study. Therefore, it can be estimated that Cr compounds are not effectively vaporized in waste incineration process.

The phasic variation of Cu species with AFR is profiled in Fig. 1(b). The formation rate of the liquid phase of Cu compound can be found to be predominant in the reduction condition, but the formation rate of Cu compound is changed in the order of Solid > Gas > Liquid phase over 1.0 of AFR. From these results, the formation rate of the liquid phase of Cu compound is decreased in the oxidation condition. On the contrary, the gas phase of Cu compound is slightly increased in this condition.

Fig. 1(c) shows the phasic variation of Pb compounds. From this figure, the formation rate of the Pb compound appeared in the order of Solid > Gas > Liquid phase over 1.05 of air-fuel ratio, but the formation rate of the gas and liquid phases is much higher than that of solid phase in reduction condition. With excess air injection, the solid phase of Pb compound is rapidly formed. As shown in the partitioning of Pb species, the formation of the gas phase of Pb compound is relatively higher than those of the other metal species selected in oxidation condition. This implies that a large amount of Pb compound may be vaporized in this condition.

The profile of the solid phase zinc compound is similar to that of the Cr compound as shown in Fig. 1(d). But, the formation rate of the gas and liquid phase is also predominant in the reduction condition, and their molar fraction is of relatively high concentration.

Consequently, the partitioning of heavy metals is roughly affected by the reduction or oxidation conditions, but the effect of excess air on the partitioning of heavy metals does not significantly appear in the oxidation condition over 1.0 of AFR. The solid phase of the metal compound is always the dominant species for the all species of metal in this condition. This can be attributed to the molar fraction of solid phase metal oxides increased under the oxidation condition. The molar fraction of the gas phase metal compound can be found to be in the order of Pb > Zn > Cu > Cr compounds, and thus the vaporization rate of metals can be also estimated in this order.

2. Effect of Chlorine Content on the Partitioning of Heavy Metals

When the waste incinerator is designed and/or operated, the chlorine content in the waste deals with a very important factor. The speciation and partitioning of heavy metals are largely affected by the chlorine content. The partitioning especially of metal species which has high affinity to chlorine component is remarkably varied with the chlorine content [Chiang et al., 1997; Fernandez et al., 1992].

The metal chlorides formed in the incineration process are generally more unstable and of higher leachability than their corresponding metal oxides. Thus the potentialities of additional pollution, such as soil and underground water pollution, can be forecasted as the final disposal. Therefore, the chlorine content was involved in the

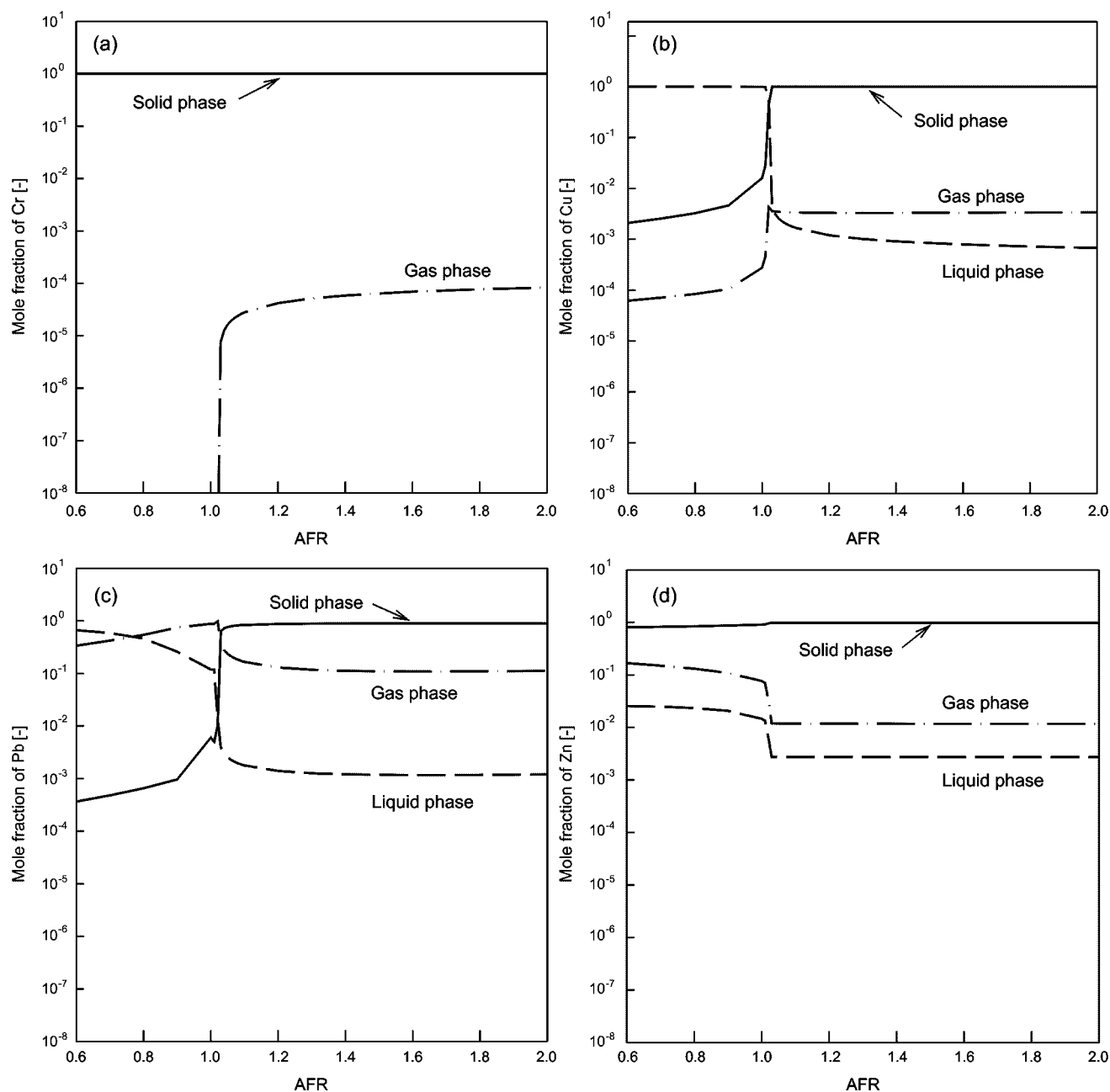


Fig. 1. Effect of AFR on the phasic variation of metal compounds at $T=800\text{ }^{\circ}\text{C}$ and $\text{Cl/S}=1.0$: (a) Cr, (b) Cu, (c) Pb and (d) Zn.

input data of the thermodynamic equilibrium model to predict the effect of the chlorine content on the partitioning of heavy metals. As mentioned above, the chlorine content in the waste was varied from 0.0 to 3.0 as Cl/S molar ratio basis, and its equivalent values of Cl/Metal ratio are listed in Table 2.

2-1. Chromium Compounds

Fig. 2 shows the behavior of the Cr compounds with the operating temperature under the conditions of $\lambda_T=1.3$ and with and without considerations of chlorine content. The solid phase of Cr_2O_3 and Cr_2O_3 is formed as dominant species in the whole temperature ranges. This implies that the affinity of oxygen to Cr component is higher than that of sulfur or chlorine. In a chlorine-free condition, considerable amount of $\text{Cr}_2(\text{SO}_4)_3$ is formed in the lower temperature, but

it is dissociated when the temperature increases. On the contrary, $\text{Cr}_2(\text{SO}_4)_3$ does not appear in the lower temperature, and a small amount of $\text{Cr}_2\text{O}_3\text{Cl}_2(\text{g})$ is formed in presence of chlorine ($\text{Cl/S}=1.0$). Note that many Cr substances will be formed by a thermodynamic equilibrium reaction, besides the Cr compounds represented in Fig. 2. However, the reaction products less than 10^{-10} moles do not appear in the figure.

Fig. 3 shows the molar fraction of Cr compounds with Cl/S molar ratio in 1.3 of AFR (λ_T), and $800\text{ }^{\circ}\text{C}$ of operating temperature conditions. The solid phase of Cr compounds is dominant as shown in the result. The gas phase of Cr compound increases with increase in Cl/S molar ratio due to the increase of $\text{Cr}_2\text{O}_3\text{Cl}_2(\text{g})$, but its level cannot bear comparison with the molar fraction of the solid phase.

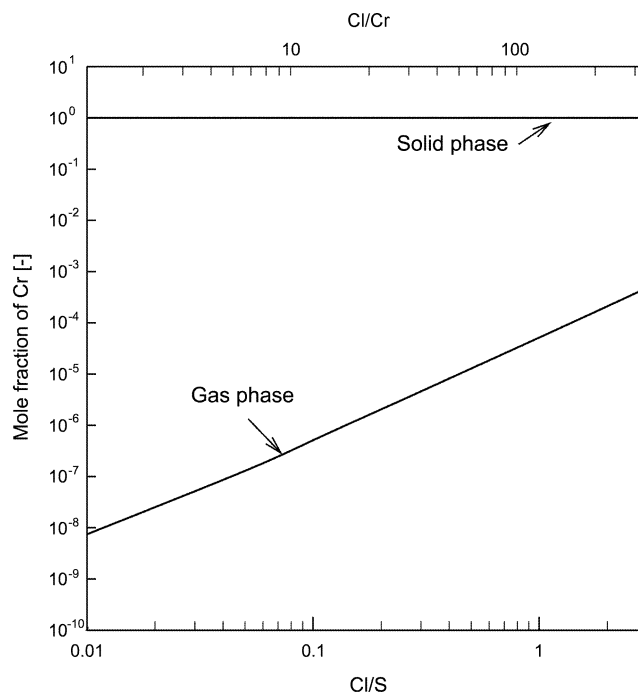
Table 2. Comparison of Cl/S and Cl/Metal molar ratios in sewage sludge

Molar ratio of Cl/S (-)	Molar ratio of Cl/Metal (-)			
	Cl/Cr	Cl/Cu	Cl/Pb	Cl/Zn
0.00	0.00	0.00	0.00	0.00
0.01	1.13	0.46	1.90	0.24
0.05	5.66	2.32	9.50	1.20
0.10	11.31	4.63	19.01	2.41
0.25	28.28	11.58	47.52	6.01
0.50	56.57	23.15	95.04	12.03
1.00	113.14	46.31	190.08	24.05
2.00	226.27	92.62	380.17	48.11
3.00	339.41	138.93	570.25	72.16

2-2. Copper Compounds

The effect of the operating temperature on the behavior characteristics of Cu compounds under the conditions of AFR=1.3 and Cl/S=1.0 is illustrated in Fig. 4. The dominant species usually consist of the solid phase of $\text{CuO} \cdot \text{Fe}_2\text{O}_3$, CuO and CuFeO_2 in the general incineration temperature. In the lower temperature region, however, the sulfate CuSO_4 is a dominant species. The sulfate CuSO_4 is decreased when the temperature is increased over 600. On the contrary, the liquid phase of Cu(l) and $\text{Cu}_2\text{O(l)}$, and gas phase of CuCl(g) , Cu(g) and CuO(g) are increased with operating temperature.

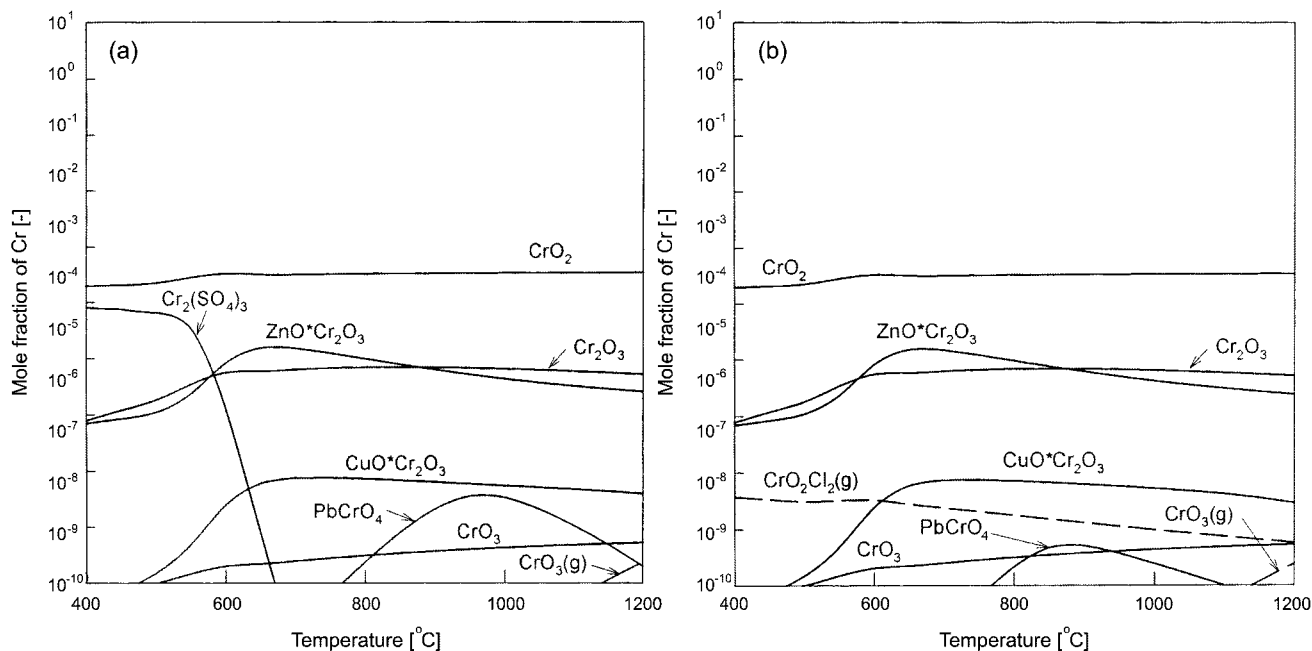
To compare the effect of the chlorine content on the partitioning of Cu compounds, the model simulation with variation of Cl/S molar ratio was carried out at temperature of 800 °C and AFR=1.3. The molar fraction of the solid phase, as illustrated in Fig. 5, indicates to be predominant in overall ranges. This means the formation rate of solid phase is higher than those of liquid and gas phase Cu compounds. Cu species of liquid phase are almost not affected by the Cl/S molar ratio, but gas phase is increased with Cl/S molar ratio

**Fig. 3. Effect of Cl/S ratio on the phasic variation of Cr compounds: $\lambda_r=1.3$, $T=800$ °C.**

due to the increase of CuCl(g) , $\text{CuCl}_2\text{(g)}$ and $\text{Cu}_2\text{Cl}_2\text{(g)}$. These tendencies remarkably appeared as the operating temperature increased.

The classification of heavy metals has been reported as groups with regard to the boiling point of metals [Fernandez et al., 1992]. According to the classification reported, most of the copper compounds were remarkably evaporated during incineration process, and a part of its compounds still remained in the ash bulk.

When the flue gas is cooled, however, their species are condensed and deposited onto the fine particles of fly ash. Rizeq et al.

**Fig. 2. Molar fraction of Cr compounds with operating temperature: $\lambda_r=1.3$, (a); Cl/S=0.0, (b); Cl/S=1.0.**

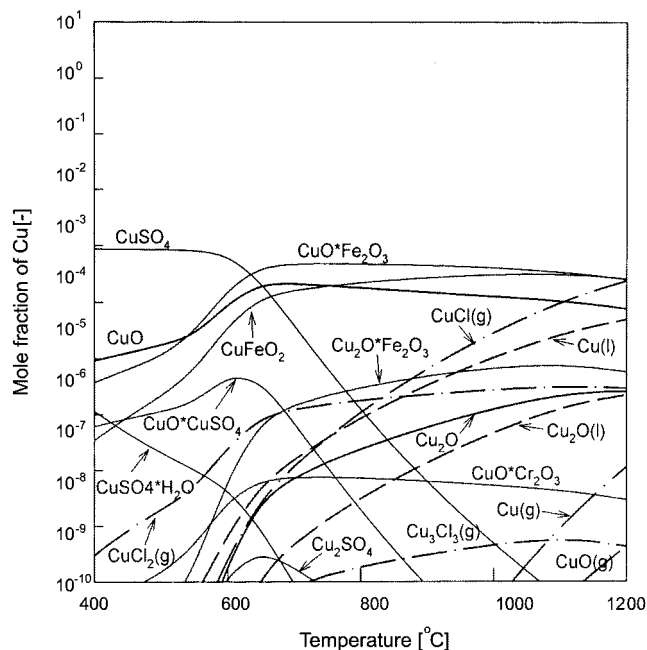


Fig. 4. Molar fraction of Cu compounds with operating temperature: $\lambda_r=1.3$, $\text{Cl/S}=1.0$.

[1992] classified that As, Cd, Pb and Hg are the high volatile species, and Cr, Be, Ba and Ni are the species of low volatility. However, Cu compound is not a vaporizing species according to the results reported by Vogg et al. [1986]. As mentioned above, there are many differences in the volatility of Cu compounds which have been reported by many researchers. This implies that the volatility of Cu compounds can be affected by the operating parameters, waste compositions or other factors. In this study, the volatility of Cu compound is not significant at low chlorine content in the waste fed, but the volatility of Cu compound is increased with Cl/S molar ratio.

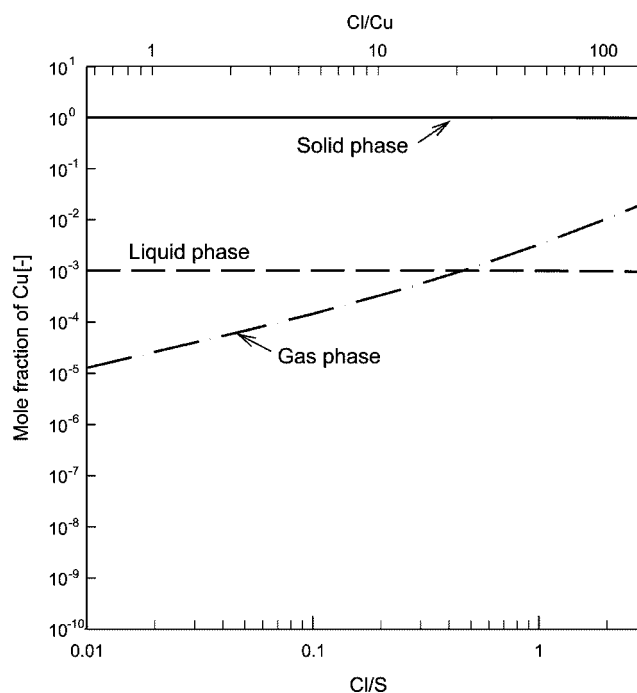


Fig. 5. Effect of Cl/S ratio on the phasic variation of Cu compounds: $\lambda_r=1.3$, $T=800\text{ }^{\circ}\text{C}$.

When the Cl/S molar ratio exceeds 0.45, the Cu compound molar ratio of the gas phase is superior to that of the liquid phase. This range of Cl/S molar ratio is equivalent to about 20 of Cl/Metal molar ratio.

2-3. Lead Compounds

As mentioned above, the lead component can be readily evaporated during the incineration process of waste due to its low boiling point. In particular, it is expected that lead compounds will be considerably affected by the operating temperature and chlorine con-

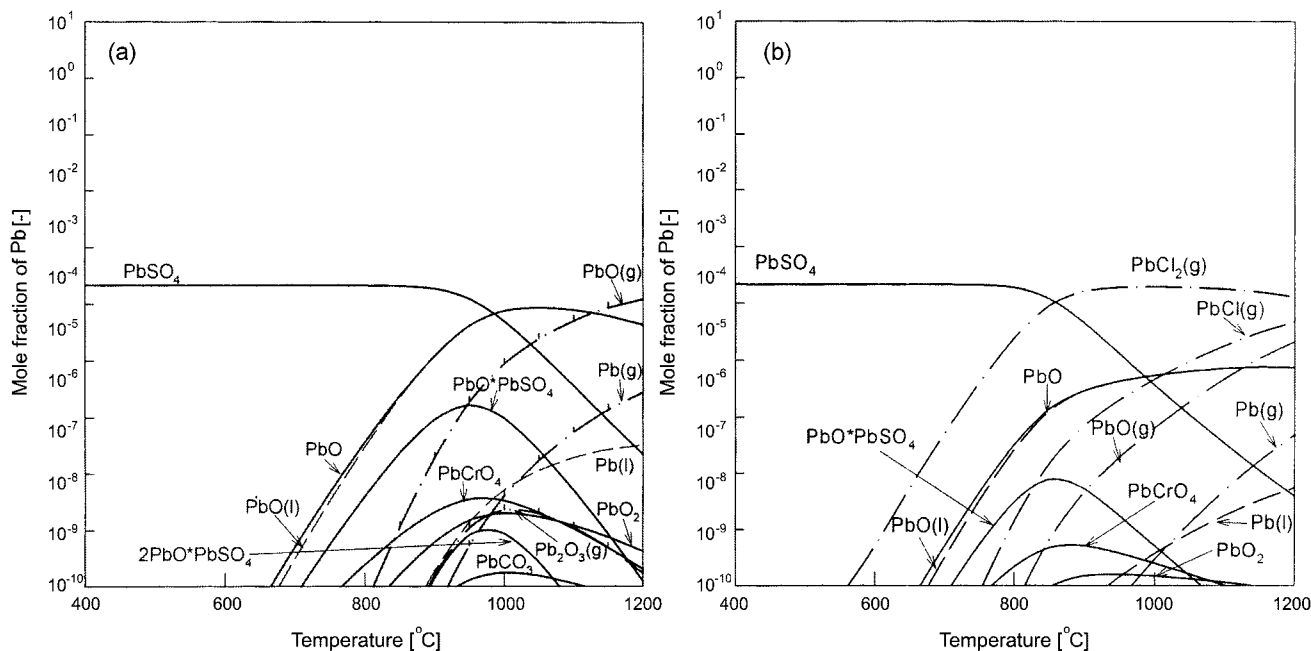


Fig. 6. Molar fraction of Pb compounds with operating temperature: $\lambda_r=1.3$, (a); $\text{Cl/S}=0.0$, (b); $\text{Cl/S}=1.0$.

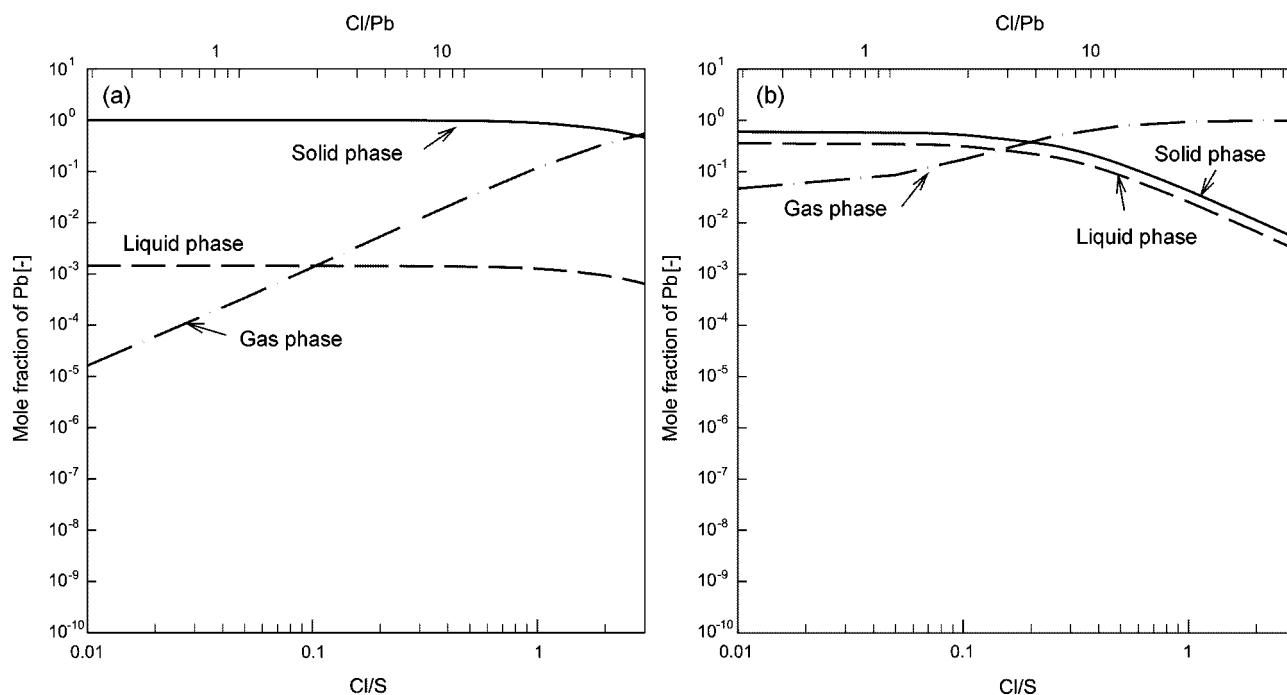


Fig. 7. Effect of Cl/S ratio on the phasic variation of Pb compounds: $\lambda_T=1.3$, (a); $T=800$ °C, (b); $T=1,000$ °C.

tent in the waste fed. Fig. 6 shows the effects of the operating temperature and chlorine content on the emission behavior of the Pb compounds. As shown in Fig. 6, the various lead compounds of gas or liquid phases are formed at high operating temperature. In absence of the chlorine, the solid phase of lead sulfate (PbSO_4) and lead oxide (PbO) is the dominant species up to 1000 of the operating temperature, and then the solid and gas phases PbO are increased with operating temperature. In existence of the chlorine, however, the solid phase of lead sulfate initiates to be dissociated over 800 °C of the operating temperature, and the formation rate of the gas phase PbCl_2 and PbCl becomes predominant in the region of high operating temperature. These tendencies are distinctly observed with increase in Cl/S molar ratio.

Fig. 7 shows the molar fraction of the phases of Pb compounds produced with regard to Cl/S molar ratio and the operating temperature. As shown in Fig. 7(a), the formation rate of the gas phase is increased with Cl/S molar ratio, and it is higher than the formation rate of the solid phase over a Cl/S molar ratio of 3. This condition is equivalent to about 570 of Cl/Metal molar ratio. In addition, the evaporation rate of Pb compounds is increased with the increase in the Cl/S molar ratio, and Pb compound of gas phase exceeds the liquid phase of compound in 0.1 of Cl/S molar ratio and 800 °C of the operating temperature. However, Cl/S molar ratio, which the molar fraction of gas phase exceeds those of the solid and liquid phases, is decreased with increase of the operating temperature, and then it becomes about 0.2 of Cl/S molar ratio which is equivalent to about 30 of Cl/Metal molar ratio at 1,000 °C of the operating temperature. In this condition, the molar fractions of the gas and liquid phases are highly increased. Therefore, the chlorine content and the operating temperature have a great influence on the evaporation rate of Pb compounds.

PbSO_4 is a typical lead compound of solid phase, and PbO and

$\text{PbO} \cdot \text{PbSO}_4$ of the solid phase are partially produced in the incineration process. Therefore, the behavior of Pb compound may be conspicuously changed with additional rate of the lime or limestone for the purpose of desulfurization.

2-4. Zinc Compounds

In absence of the chlorine content, the effect of the operating temperature on the behavior of Zn compounds can be observed in Fig. 8(a). The gas phase of zinc compounds is slightly produced over 1,000 °C of operating temperature. When chlorine is contained, however, $\text{ZnCl}_2(\text{g})$ initiates to be produced from the region of relatively low temperature, and the molar fraction of gas phase is higher than that of the liquid phase over the whole range of the operating temperature. This means the vaporization rate of zinc compound increases in existence of chlorine content, but the solid phase of Zn compound is largely dominant over the whole temperature conditions.

Fig. 9 shows the effect of the chlorine content on the behavior of the zinc compound under the conditions of an air-fuel ratio (λ_T) of 1.3, and 800 °C and 1,000 °C of the operating temperatures. In 800 °C of the operating temperature, as shown in Fig. 9(a), the order of phases formed is Solid>Liquid>Gas phase up to 0.5 of Cl/S molar ratio, but the formation rate of gas phase is largely increased over 0.5 of Cl/S molar ratio in the order of Solid>Gas>Liquid phases. In addition, the formation rate of the liquid and gas phases of zinc compound is markedly increased with increase of the operating temperature from 800 °C to 1,000 °C. The overall tendency is similar to Fig. 9(a), and the Cl/Metal molar ratio, which the molar fraction of gas phase exceeds to that of liquid phase, is about 16 at 1,000 °C of operating temperature.

Consequently, the molar ratio of Cl/Metal offers some important information on the vaporization of metal species. From simulated calculation, it is found that the gas phase of metals selected is al-

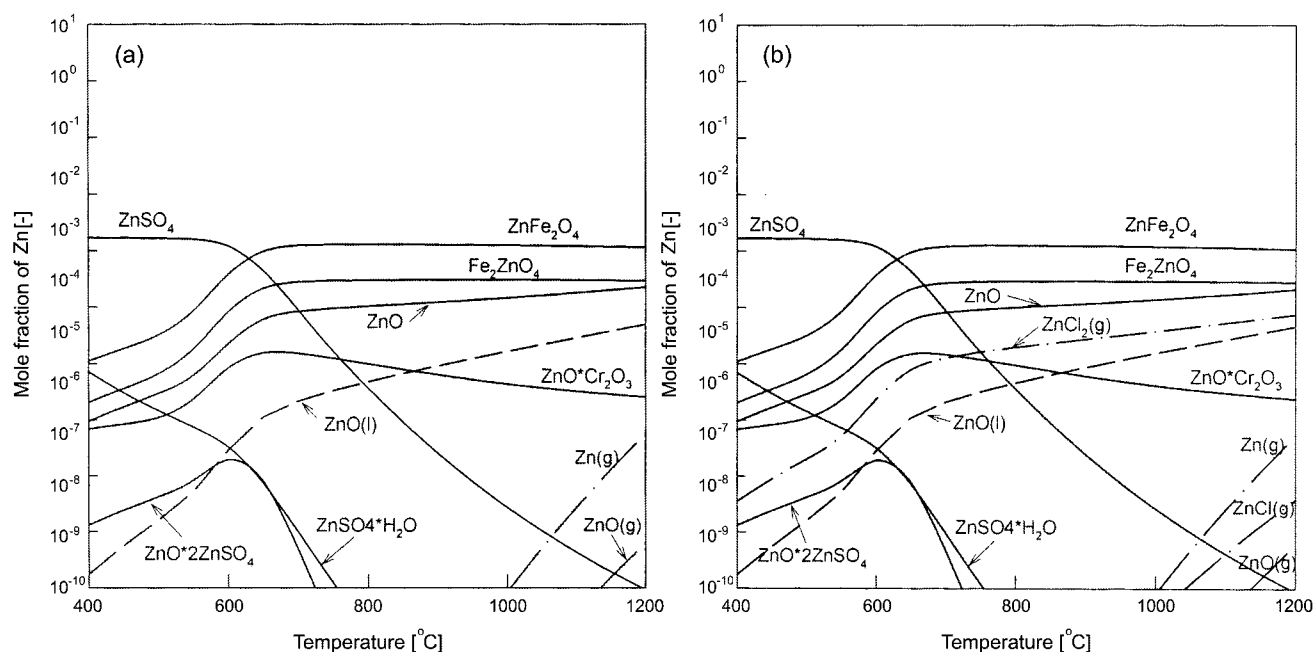


Fig. 8. Molar fraction of Zn compounds with operating temperature: $\lambda_r=1.3$ (a); Cl/S=0.0, (b); Cl/S=1.0.

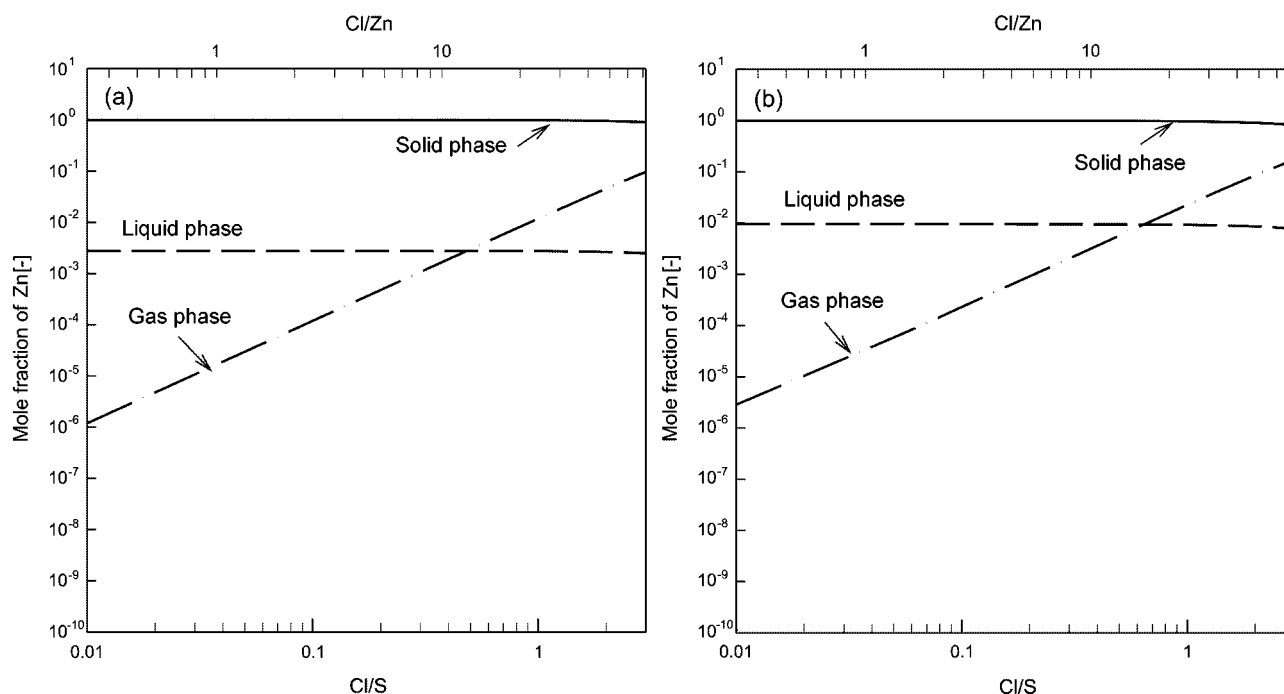


Fig. 9. Effect of Cl/S ratio on the phasic variation of Zn compounds: $\lambda_r=1.3$, (a); $T=800\text{ }^{\circ}\text{C}$, (b); $T=1,000\text{ }^{\circ}\text{C}$.

most superior to that of the liquid phase in ranges from 10 to 30 of Cl/Metal in spite of the variation of Cl/S molar ratio. This implies that the vaporization rate of metal species is considerably affected by Cl/Metal molar ratio, and it is markedly increased in this range of Cl/Metal molar ratio.

3. Comparison of Predicted and Measured Values

A model simulation was carried out using the Gibbs free energy minimization method to investigate the effect of the chlorine content on the fate of heavy metals in the waste incineration process.

There is a need to verify the predicted values to apply those to the practical incineration process. However, it can be thought that the behavior of each phase of metal compound is as follows. 1) The metal compound of solid phase may be almost involved in bottom ash stream, and very small part of that is distributed into fly ash and flue gas streams. 2) Most metal compound of gas phase is exhausted with flue gas, and a part of that may be deposited on the fly ash particle and internal surface of duct when flue gas cools. 3) Liquid phase shows various behavior which can remain and be agglomerated in

Table 3. Comparison of the predicted and measured value in incineration process of sewage sludge; (T=800 °C, $\lambda_T=1.2$)

Species		Molar fraction of metal species						
		Experimental value		Predicted value				
		Cl/S	-	Cl/S	1.0	1.5	2.0	3.0
Sewage sludge	Cr	X_g	-	G	4.20×10^{-5}	9.6×10^{-5}	1.73×10^{-4}	4.0×10^{-4}
		X_{fa}	0.18	L	-	-	-	-
		X_{ba}	1.03	S	0.99996	0.99990	0.99983	0.99960
	Cu	X_g	0.06	G	3.30×10^{-3}	6.43×10^{-3}	1.05×10^{-2}	2.16×10^{-2}
		X_{fa}	0.13	L	1.20×10^{-3}	1.18×10^{-3}	1.17×10^{-3}	1.13×10^{-3}
		X_{ba}	0.81	S	9.95×10^{-1}	9.92×10^{-1}	9.88×10^{-1}	9.77×10^{-1}
	Pb	X_g	0.01	G	1.29×10^{-1}	2.48×10^{-1}	3.69×10^{-1}	5.66×10^{-1}
		X_{fa}	0.11	L	1.39×10^{-3}	1.19×10^{-3}	9.88×10^{-4}	6.69×10^{-4}
		X_{ba}	0.88	S	8.70×10^{-1}	7.50×10^{-1}	6.30×10^{-1}	4.34×10^{-1}
	Zn	X_g	0.08	G	1.18×10^{-2}	2.61×10^{-2}	4.55×10^{-2}	9.70×10^{-2}
		X_{fa}	0.12	L	2.74×10^{-3}	2.70×10^{-3}	2.64×10^{-3}	2.48×10^{-3}
		X_{ba}	0.80	S	9.85×10^{-1}	9.71×10^{-1}	9.52×10^{-1}	9.01×10^{-1}

X_g , X_{fa} and X_{ba} are the partitioning coefficients defined as molar fraction of the metal compounds in flue gas, fly ash and bottom ash, respectively. $X_g + X_{fa} + X_{ba} = 1$.

G, L and S represent the gas, liquid and solid phases of metal compounds, respectively.

the bed, and can be deposited onto fine particles in the freeboard section and the dust collectors.

In this study, the predicted results are compared with the results obtained from fluidized bed incineration of sewage sludge [Lee, 1992], and the comparative table is presented in Table 3.

As shown in Table 3, the chlorine content in sewage sludge is not analyzed, and the partitioning of the metal compounds is represented as three parts of flue gas, fly and bottom ashes in the incineration experiment, but the predicted value is classified as three phases. For these reasons, therefore, it is difficult to compare exactly the predicted value with the actual measured value. By comparing with practical measured values, therefore, there is a need to investigate continuously the correlations of the partitioning coefficients and three phases predicted.

It is assumed that the total solid phase of metal compound remains in the bottom ash, and the liquid and gas phases are involved into fly ash and flue gas streams in this study. As shown in Table 3, with comparison of predicted and measured values, the predicted partition coefficients of metal compounds were shown to be a similar trend with the measured values in the Cl/S molar ratio range of 1.0-3.0. The deviations in a part estimated to be caused by the other factor, such as the distribution coefficient of each phase of metal compound, and ash compositions of waste [Abanades et al., 2001]. In incineration of waste which contain high ash content as in the sewage sludge, the ash compositions are also major causes of the sintering or the agglomeration phenomena in fluidized bed, and of which the emission level of the gaseous air pollutants predicted are largely differed from the measured values [Manzoori, 1993].

CONCLUSIONS

The partitioning of heavy metals is roughly affected by the reduction/oxidation condition, but the effect of excess air on the partitioning almost did not appear in oxidation condition (over 1.0 of AFR). The solid phase of metal compound is always the dominant

species for all species of metal in this condition. The molar fraction of the gas phase metal compound was found to be in the order of $Pb > Zn > Cu > Cr$ compounds, and thus the vaporization rate of metals can be also estimated in this order.

It is found that the gas phase of metals selected is almost superior to liquid phase in ranges from 10 to 30 of Cl/Metal molar ratio throughout the whole calculations. This implies that the vaporization rate of metal species is considerably increased in this range.

When assuming that the total solid phase remains in bottom ash, and the liquid and gas phases are involved into fly ash and flue gas, the predicted value shows relatively high correlation with the measured value in 1.0-3.0 of Cl/S molar ratio ranges. The deviations in a part are estimated to be caused by other factors, such as the distribution coefficient of each phase of metal compound, and ash compositions of waste.

Further study is in progress on the correlations of the partitioning coefficients and three phases predicted, and on the effect of the ash compositions.

NOMENCLATURE

- G : gas phase of metal compounds
- L : liquid phase of metal compounds
- S : solid phase of metal compounds
- X_g : partitioning coefficient of any metal component in flue gas [-]
- X_{fa} : partitioning coefficient of any metal component in fly ash [-]
- X_{ba} : partitioning coefficient of any metal component in bottom ash [-]
- λ_T : total air-fuel ratio to theoretical air flow ratio [-]

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