

# TRACE ELEMENT EVAPORATION DURING COAL GASIFICATION BASED ON A THERMODYNAMIC EQUILIBRIUM CALCULATION APPROACH

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## ABSTRACT

Thermodynamic equilibrium calculations using the HSC-Chemistry program were performed to determine the distribution and mode of occurrence of potentially toxic and corrosive trace elements in gases from coal gasification processes. The influence of temperature, pressure and gas atmospheres on equilibrium composition was evaluated. In these reducing conditions, the behaviour of the trace elements is complex, but some form of organization can be attempted. Elements were classified into three groups. Group A includes those elements that, according to thermodynamic data at equilibrium, could probably be condensed in coal gasification. Mn is classified in this group. Group B contains those elements that could be totally or partially in gas phase in gas cleaning conditions, and can be divided into two subgroups, depending on whether the cleaning conditions are hot or cold. Co, Be, Sb, As, Cd, Pb, Zn, Ni, V, Cr are elements in this group. Group C contains those elements that could be totally in gas phase in all the possible conditions, including flue gas emissions. Se, Hg and B are the elements that make up this group.

**Key words:** Trace elements in coal. Coal gasification.

## INTRODUCTION

Potentially hazardous air polluting elements such as Be, Cr, Mn, Co, Ni, As, Se, Cd, Sb, Hg and Pb, and potentially corrosive elements such as V, Zn or Pb are present in coal in concentrations lower than 0.1% (trace elements), but nevertheless they may give rise to various environmental or technological problems during coal utilisation for energy production. In order to be able to address these problems and to develop suitable systems to their reduction, it is necessary to understand trace element behaviour during the coal combustion and gasification processes. Although trace element behaviour in conventional coal combustion systems is reasonably well known [1-8], there is a lack of similar knowledge in coal gasification, especially in the case of Integrated Gasification Combined Cycles (IGCC) for which gases reaching the gas turbine need to be as clean as possible.

The behaviour of volatile species in the reducing conditions of coal gasification may be different to that which occurs during combustion. For instance, trace elements, which are able to form hydrides such as  $B_2H_4$ ,  $SeH_2$ ,  $AsH_3$ , can be expected to increase volatility in reducing conditions [9]. In order to ascertain precisely how this behaviour differs, trace element partitioning among ashes, particles and gases in different coal gasification processes has been evaluated [1,7-13], the distribution of elements depending on the gasification conditions and the mode of occurrence of trace elements in coal. It has been observed that during the atmospheric pressure entrained flow gasification of a bituminous coal, a significant mass fraction of As, Se, Sb, Pb and Hg vaporized, whereas Cd, Cr, Co, Mn, Ni, U and Th remained relatively non-volatile [12]. Although Ag, As, B, Cd, Hg, Pb, Se and Zn have been identified in the raw gases from coal gasification processes [1,11], emissions of trace elements were predominantly associated with the particulate phase rather than with the vapour phase, the smallest

particles being enriched in some of these elements (As, B, Cd, Cu, Pb, Sb and Zn) [1]. It was also observed that As, Cd, Se and Pb showed increased volatility as the C:O ratio diminished and the gasification temperature rose [10], and that the concentrations of As, Cd, Hg and Sb in flue gases increased in gasifiers with particulate recycling [13]. It should be noted that the studies on trace element behaviour were mainly focused to evaluate the emission of trace elements into the environment via flue gases. However, the technological problems that some of these elements may produce, mainly in IGCC, and the interactions in gas cleaning systems at low and high temperatures, also need to be considered. It is important to be able to predict the trace element composition in gases from coal gasification at temperatures higher than those of the flue gases emitted into the atmosphere.

Thermodynamic equilibrium studies using different computer programmes have been carried out to compensate for the lack of experimental data in gasification [8, 12, 14-17]. Using different programs it has been estimated that As, Se, Hg, and Pb are present in gas phase between 200 and 1600°C at 1 atm of pressure [12], and that much greater proportions of Cd, Pb, Hg and Zn are volatilised under atmospheric fluidised-bed gasification conditions than under fluidised bed combustion [8]. It has also been inferred that Hg, Sb and Se form gaseous species between 25 and 1700°C, whereas As, B, Be, Cd, Co, Cr, Ga, Ge, Ni, P, Pb, Sn, Ti, V and Zn may form both condensed and gaseous compounds depending on the temperature [14]. In a similar way, a theoretical method based on thermodynamic data in equilibrium was used in this work to evaluate the composition of the trace element species formed during coal gasification processes at different temperatures and pressure, and to assess the influence of sulphur and chlorine compounds present in gas phase on the equilibrium composition. On the basis of these data it may be possible to estimate the trace element composition in the gasifier

and in the gases at high and low temperatures, and to establish suitable conditions for retaining trace elements in gas cleaning systems.

## **METHOD AND CALCULATION PROCEDURE**

Thermodynamics provides a powerful method of calculation for studying the effects of different process variables on a chemical system in equilibrium state. However, the calculations do not give the reaction time, which is necessary for this theoretical equilibrium state to be reached. There is no complete general theory or basic data available, which would successfully combine thermodynamics, non-ideality and kinetics for all chemical processes. For the equilibrium calculation, HSC-Chemistry 4.0 software was used in this work. HSC software was employed to make conventional thermodynamic calculations based on the minimisation of the free Gibbs energy in order to simulate chemical reaction equilibrium and processes.

Thermodynamic equilibrium calculations were used to identify the possible forms of vapour-phase trace elements produced in the gasification processes at a number of points within an IGCC system. The elements studied were As, Be, Cr, Mn, Co, Ni, Se, Cd, Sb, Hg, Pb, Zn, V and B. The calculations were performed in typical coal gasification atmospheres, at a range of pressure between 1 and 40 atm, and a temperature interval between 1600-0°C. This range of temperatures includes gasifier operation temperatures (1600-1200°C for conventional gasifiers and 900-800°C for fluidised bed gasifiers) hot (800-600°C) and low (500-200°C) temperatures in gas cleaning systems and flue gas emission temperatures (<200°C). For input conditions, the coal gasification atmosphere and the different trace elements concentrations are given in Tables 1-2. The coal gasification atmospheres used, differ in their H<sub>2</sub>S and HCl content (Table 1). The trace element compounds were similar to those most frequently found in

Table 1. Synthetic coal gasification atmospheres used for equilibrium calculations.

Atmosphere	CO	CO <sub>2</sub>	H <sub>2</sub>	H <sub>2</sub> O	HCl	H <sub>2</sub> S	N <sub>2</sub>
Mixture I	4.16E-05	2.55E-06	1.51E-05	6.24E-06	—	—	6.66E-06
Mixture II	4.16E-05	2.55E-06	1.51E-05	6.24E-06	6.67E-08	—	6.59E-06
Mixture III	4.16E-05	2.55E-06	1.51E-05	6.24E-06	—	7.27E-07	5.93E-06
Mixture IV	4.16E-05	2.55E-06	1.51E-05	6.24E-06	6.67E-08	7.27E-07	5.87E-06

coal, their concentrations being close to that expected for a coal (Table 2). Equilibrium composition was determined for each element individually whereas interactions between elements or the condensation of species on fly ash particles were not considered. This is one possible approach to the problem as heterogeneous reactions may take place in the system. In the discussion of the results the species evaluated were those that contribute by more than 1% to the total number of compounds of the element at equilibrium.

Table 2. Trace element concentrations and solid compounds used for equilibrium calculations.

Element	Compound	kmol g <sup>-1</sup> coal	Element	Compound	kmol g <sup>-1</sup> coal
As	FeAsS	1.47 E -10	Cd	CdS	4.45 E -12
Be	Be	2.22 E -10	Sb	Sb <sub>2</sub> S <sub>3</sub>	1.89 E -11
Cr	Cr <sub>2</sub> O <sub>3</sub>	3.85 E -10	Hg	HgS	4.99 E -13
Mn	Mn	1.09 E -09	Pb	PbS	2.61 E -10
Co	Co <sub>3</sub> S <sub>4</sub>	1.02 E -10	Zn	ZnS	1.71 E -09
Ni	NiS	2.98 E -10	V	V	1.28 E -09
Se	Se	1.39 E -11	B	B	4.16 E -09

## RESULTS

Equilibrium composition profiles calculated for the different trace elements, at different gas composition, pressure and temperature are shown in Figures 1-12. If the variables did not influence the composition of the element at equilibrium, and the composition were similar that in Figures 1-12, the graphs were not provided.

## Arsenic

Equilibrium composition for arsenic depends on temperature, gas atmosphere and pressure. As can be observed in Figure 1 at temperatures higher than 1000°C, all the arsenic is present as  $\text{AsO(g)}$  and at these temperatures variations in pressure and gas

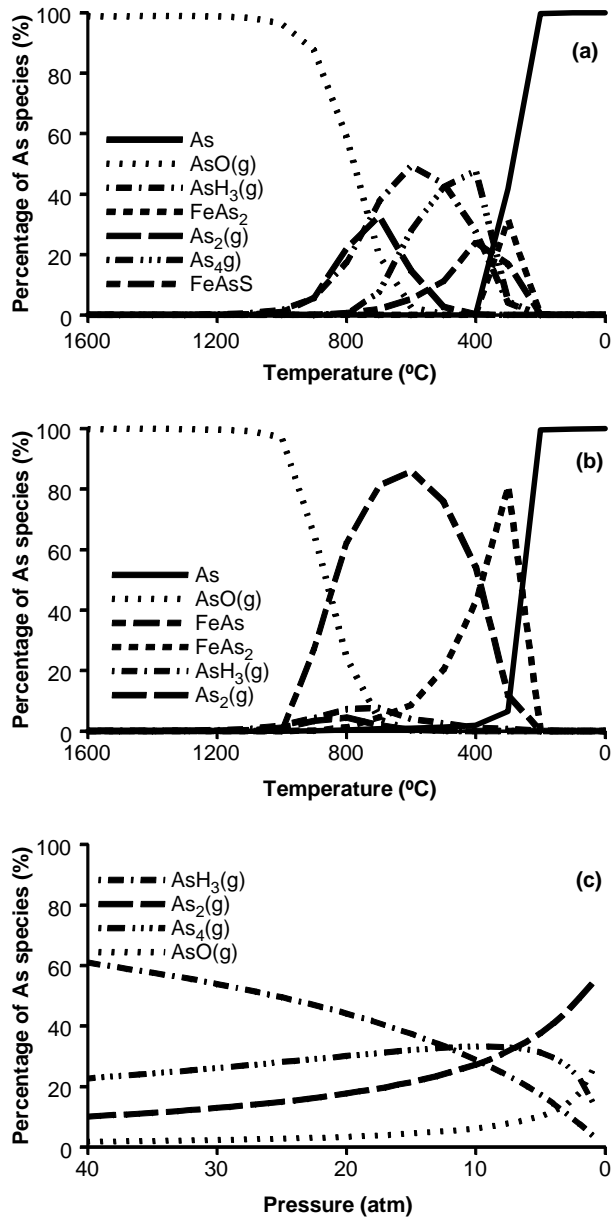


Figure 1.- Equilibrium compositions for arsenic in (a) mixture III at 25 atm; (b) mixture II at 25 atm and (c) different pressures at 600°C.

atmosphere do not modify the equilibrium composition. When temperature decreases, that is to say, at those temperatures at which gas cleaning could be carried out, different condensed and gas phase compounds may be present. Between 500 and 800°C  $\text{AsO(g)}$ ,  $\text{AsH}_3\text{(g)}$ ,  $\text{As}_4\text{(g)}$  and  $\text{As}_2\text{(g)}$  are the species formed in gas phase. These are the dominant species in a gas atmosphere containing  $\text{H}_2\text{S(g)}$  (Figure 1a), but if the gas atmospheres do not contain  $\text{H}_2\text{S(g)}$  (Figure 1b) the dominant species are the condensed  $\text{FeAs}$  and  $\text{FeAs}_2$ . Between 300-500°C,  $\text{As}_2\text{(g)}$ ,  $\text{As}_4\text{(g)}$ ,  $\text{AsH}_3\text{(g)}$ ,  $\text{FeAsS}$ ,  $\text{FeAs}$  and  $\text{FeAs}_2$  are the most stable species. When pressure increases, the concentration of  $\text{AsH}_3\text{(g)}$  increases significantly while  $\text{AsO(g)}$ ,  $\text{As}_2\text{(g)}$  and  $\text{As}_4\text{(g)}$  decrease slightly (Figure 1c). In an atmosphere free of  $\text{H}_2\text{S(g)}$ ,  $\text{As}_4\text{(g)}$  is not formed and the  $\text{FeAsS}$  is reduced to  $\text{FeAs}$  and  $\text{FeAs}_2$ . In this case, at atmospheric pressure, the condensed species are the most stable between 200 and 700°C, whereas only  $\text{AsO(g)}$  is present at temperatures higher than 700°C. At temperatures lower than 200°C at atmospheric pressure, only condensed As is formed. From these theoretical results all the arsenic present in the coal can be expected to evaporate in the gasifier at temperatures higher than 1000°C and also partially evaporate in gas phase in gas cleaning conditions. However at the low temperatures at which gases are emitted only condensed phases may be expected.

### **Beryllium**

The equilibrium composition of the beryllium species does not change at pressures between 40 and 1 atm and in the different gas atmospheres studied, but it changes with temperature (Figure 2). It should be noted that, only at temperatures higher than 1000°C, is the gaseous  $\text{Be(OH)}_2\text{(g)}$  present at equilibrium. This is the dominant species at temperatures over 1300°C. At lower temperatures only the condensed allotropic forms  $\text{BeO}$  and  $\text{BeO(B)}$  are present in significant amounts. Consequently the fraction of

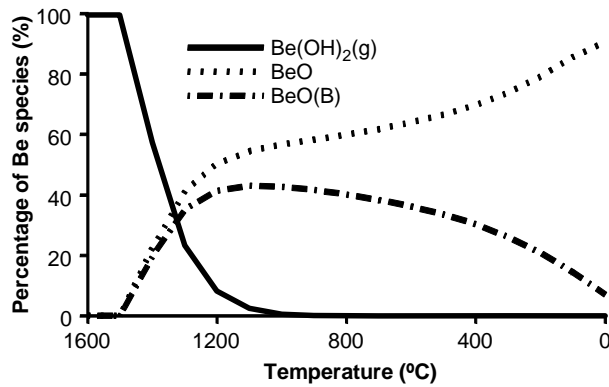


Figure 2.- Equilibrium compositions for beryllium in all the conditions considered in this work.

beryllium evaporated in the gasifier can be expected to condense before gas cleaning systems and the flue gas emissions cease to have beryllium in gas phase.

### Mercury

Mercury species at equilibrium are all in gas phase (Figure 3a). Above 400°C the dominant species is Hg(g) but at lower temperatures Hg(CH<sub>3</sub>)<sub>2</sub>(g) may also be formed, their relative proportions depending on pressure (Figure 3b). This composition does not vary when the gas atmosphere contains HCl(g) and H<sub>2</sub>S(g). Mercury is present in gas phase and is mostly emitted in flue gases.

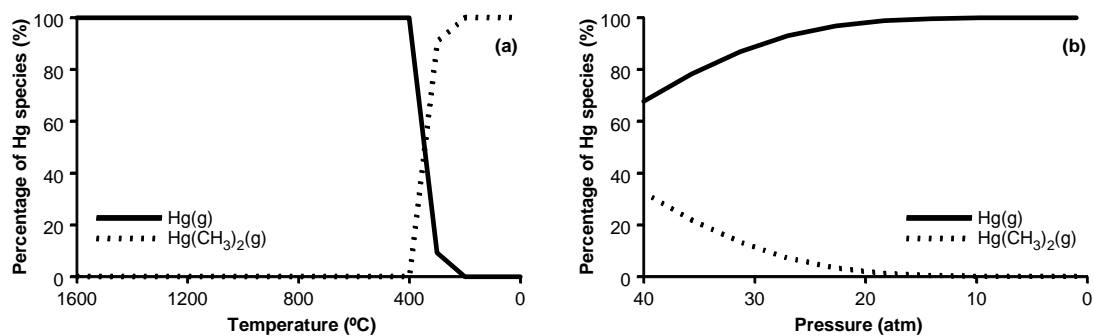


Figure 3.- Equilibrium compositions for mercury (a) in the different atmospheres and temperatures and (b) at different pressures and at 350°C.



## Chromium

Minimal variations in chromium species at equilibrium were observed with temperature and pressure. In all the conditions studied, at temperatures between 1400 and 300°C, chromium remains in the form of condensed  $\text{Cr}_2\text{O}_3$  (Figures 4a-b). At temperatures higher than 1500°C, at pressures ranging between 1-5 atm the formation of  $\text{Cr}(\text{g})$  takes place, its concentration depending on gas the atmosphere. At temperatures lower than 60°C and 1 atm some  $\text{Cr}(\text{CO})_6(\text{g})$  may form in the absence of  $\text{HCl}(\text{g})$ . In short; chromium species in gas phase may form in the gasifier, but they cannot be expected to do so in gas cleaning systems. However, a minor proportion of chromium may be emitted into the atmosphere in some particular cases.

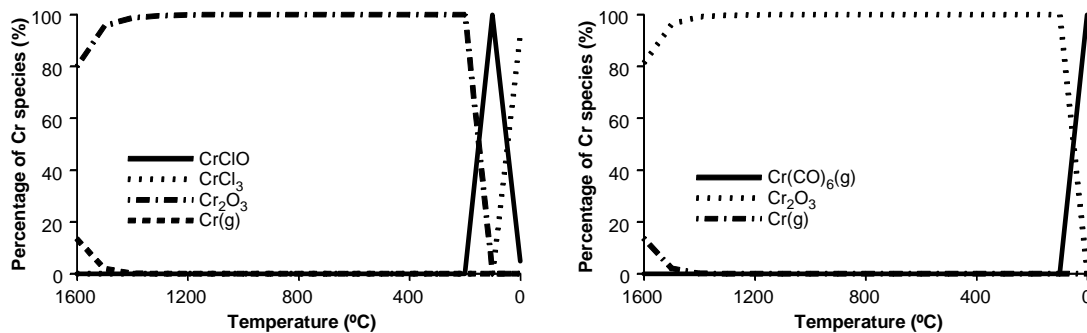


Figure 4.- Equilibrium compositions for chromium between 1 and 25 atm in (a) a gasification atmosphere containing HCl (mixtures II and IV) and (b) in a gasification atmosphere without HCl (mixtures I and III).

## Manganese

Manganese is a low volatile element, which according to thermodynamic equilibrium data, in the gasification atmospheres studied, only forms  $\text{MnC}_2$ , whose equilibrium composition is not modified by variations in pressure, temperature and gas composition.

## Boron

Boron is a highly volatile element which, theoretically, forms species in gas phase over the whole range of temperatures  $\text{HBO}(\text{g})$  being the most stable. Equilibrium composition does not depend on temperature, gas composition or pressure, and boron in gas phase may be present in all the situations relevant to this study.

## Vanadium

Vanadium is a low volatile element. The equilibrium composition for vanadium depends on temperature and pressure but not on gas atmosphere. The condensed species are stable at the different conditions studied (Figure 5a). At temperatures higher than 1400°C and low pressures (<10 atm)  $\text{VO}_2(\text{g})$  may be formed (Figure 5b).  $\text{V}_2\text{O}_3$  is the most stable at temperatures higher than 500°C. At lower temperatures the dominant species is VC. Vanadium species in gas phase cannot be expected in the gasifiers at high temperature, or in gas cleaning systems and gaseous emissions.

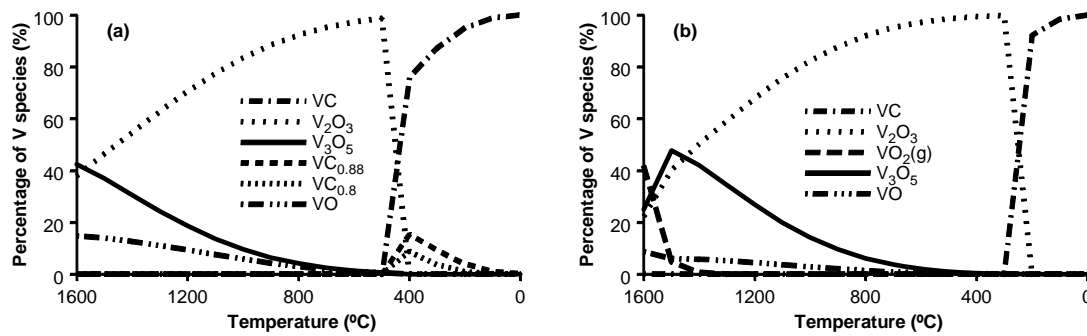


Figure 5.- Equilibrium compositions for vanadium for the different gas atmospheres at (a) 25 atm and (b) at 1 atm.

## Selenium

Selenium is present in gas phase over the whole range of temperatures (Figure 6a-b). The composition at equilibrium is not affected by variation in the gas atmosphere. However, temperature and pressure may modify the relative proportions of selenium compounds, though mainly at low pressure and high temperature. Consequently these factors do not significantly affect the gas composition in the gasifier, gas cleaning systems or flue gas emissions.  $\text{H}_2\text{Se}(\text{g})$  is the main species present in these conditions.  $\text{Se}(\text{g})$  may form at high temperatures, its concentration depending on pressure.

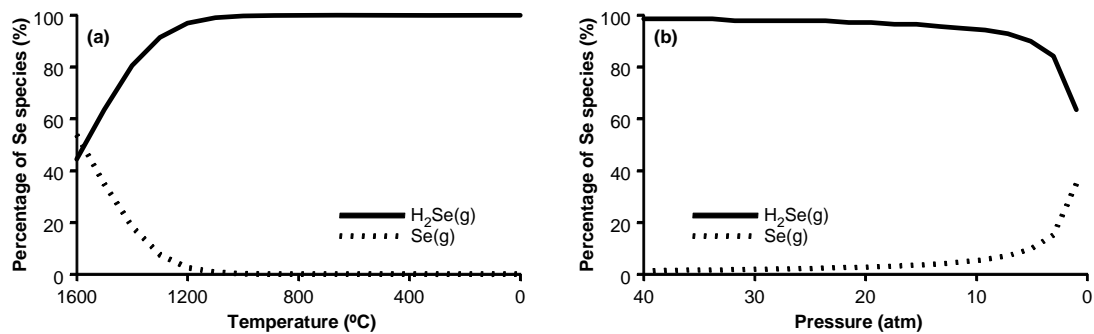


Figure 6.- Equilibrium compositions for selenium in the different gas atmospheres (a) at 1 atm and (b) at different pressures and at 1500°C.

## Nickel

Nickel composition depends on temperature, pressure and the gas atmosphere (Figure 7). The range of temperatures at which nickel species in gas phase may be formed depends on the atmosphere and pressure. In general nickel may occur in gas phase at temperatures higher than 1400°C ( $\text{Ni}(\text{g})$ ,  $\text{NiS}(\text{g})$ ,  $\text{NiCl}(\text{g})$ ) and at temperatures lower than 400°C at high pressure ( $\text{NiCO}_4(\text{g})$ ). The gaseous species always coexist with condensed species, their concentrations depending on pressure. In general the gaseous species are found in minor concentrations except at temperatures below 300°C and at high pressure (25 atm), in which case  $\text{Ni}(\text{CO})_4(\text{g})$  is the dominant species. Other nickel species that may be present in gas phase at high temperature are  $\text{Ni}(\text{g})$  (in all atmospheres),  $\text{NiS}(\text{g})$  (when  $\text{H}_2\text{S}(\text{g})$  is present in the gas atmosphere) (Figure 7a) and  $\text{NiCl}(\text{g})$  (when the gas atmosphere contains  $\text{HCl}(\text{g})$ ) (Figure 7b). Between 400 and 1200°C only the condensed species are stable according to thermodynamic data. In a gasification atmosphere free of  $\text{H}_2\text{S}(\text{g})$ , different allotropic forms of nickel ( $\text{Ni}$ ,  $\text{Ni}(\text{FCC})$ ) are dominant whereas, when the atmosphere contains  $\text{H}_2\text{S}(\text{g})$ ,  $\text{Ni}_3\text{S}_2$  is the dominant species and  $\text{NiS}_{0.84}$  and  $\text{NiS}$  also form in minor proportions. From these results it can be concluded that in gasification conditions the nickel content in the coal

may be partially in gas phase. However, in gas cleaning systems it is condensed. At temperatures lower than 150°C and 1 atm in the absence of H<sub>2</sub>S(g), a gaseous species may be present.

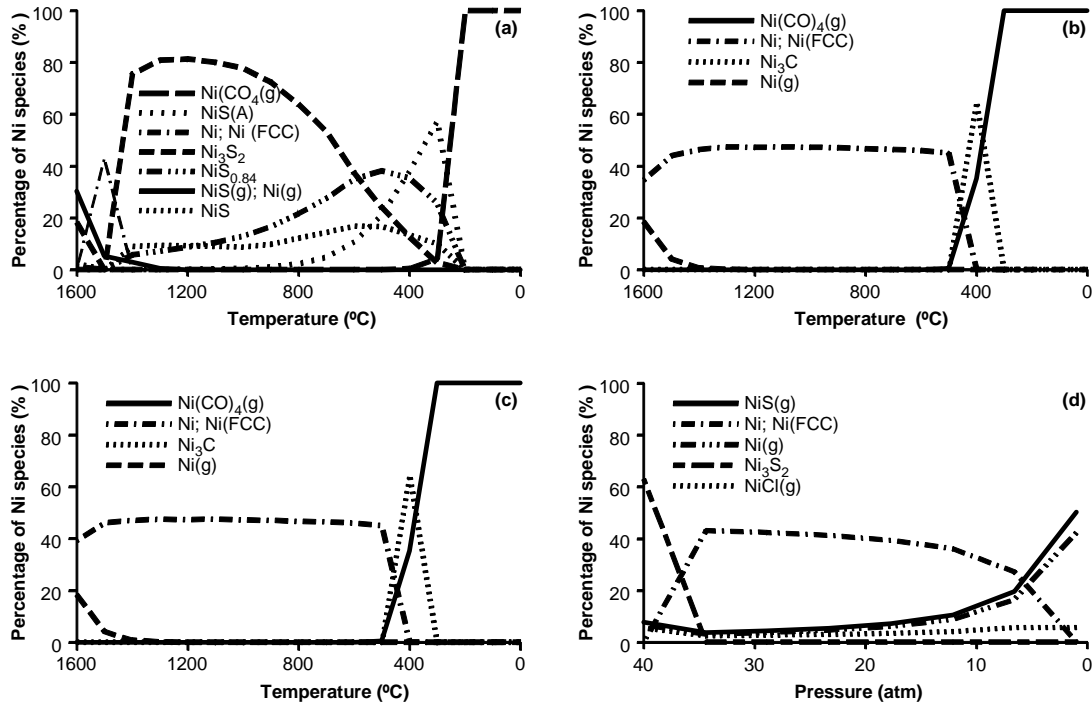


Figure 7.- Equilibrium compositions for nickel in (a) mixtures III and IV at 25 atm; (b) mixture II at 25 atm; (c) mixture I at 25 atm and (d) at different pressures at 1500°C.

## Cobalt

The equilibrium composition of cobalt is clearly influenced by temperature, pressure and the atmosphere (Figure 8). The formation of Co(g) occurs at temperatures higher than 1200°C in a gas atmosphere free of H<sub>2</sub>S(g) (Figure 8a), its concentration decreasing with pressure (Figure 8b). In a gas atmosphere containing H<sub>2</sub>S(g), Co(g) is formed at temperatures higher than 1400°C and at low pressures. The presence of HCl(g) in the gas atmosphere (Figure 8c) favours the formation of species such as CoCl<sub>2</sub>(g), and CoCl(g). CoCl<sub>2</sub>(g) is formed at temperatures higher than 800°C, its concentration increasing with pressure. CoCl(g) is formed at temperatures higher than 1200°C but its concentration is not influenced by any variation in pressure. Regarding the condensed

species, in a gas atmosphere containing  $\text{H}_2\text{S}(\text{g})$  (Figure 8d),  $\text{Co}_3\text{S}_4$  forms over the whole range of temperatures and pressures studied. In a gas atmosphere free of  $\text{H}_2\text{S}(\text{g})$  at temperatures between 500 and 1200°C the main species is Co. It should be noted that in all the atmospheres studied, at temperatures close to 200°C the cobalt species occur in condensed phase. In coal gasification conditions, and also in hot gas cleaning conditions, some of the cobalt may be in gas phase. However, in flue gas emission conditions, only condensed species may be expected.

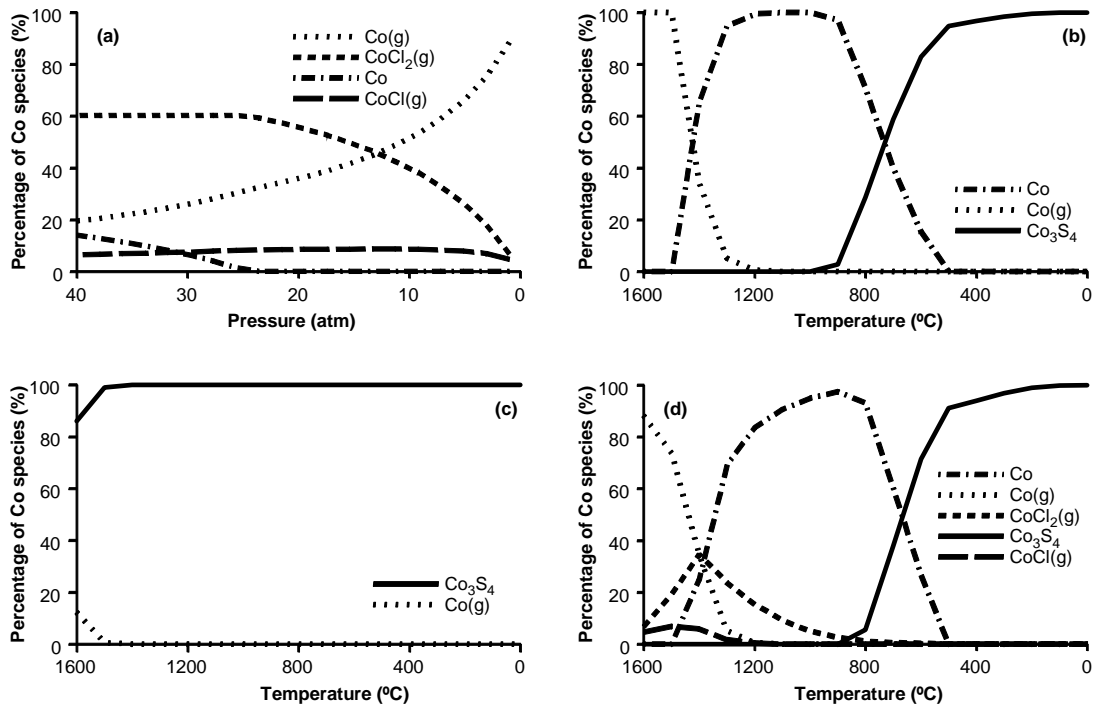


Figure 8.- Equilibrium compositions for cobalt in (a) mixture III at 1 atm; (b) mixture II at 1 atm; (c) mixture I at 1 atm and (d) at different pressures at 1500°C in mixture II.

## Antimony

Antimony equilibrium composition depends on the temperature and gas atmosphere. Minor variations are observed with pressure. At temperatures higher than 300°C this element is mainly present in gas phase,  $\text{SbO}(\text{g})$  being the dominant species (Figure 9). Between 200 and 500°C other gaseous antimony species might be present. The presence of  $\text{HCl}(\text{g})$  or  $\text{H}_2\text{S}(\text{g})$  in the atmosphere favours the formation of  $\text{SbCl}(\text{g})$ ,  $\text{SbCl}_3(\text{g})$  and

$\text{Sb}_3\text{S}_2$  (g),  $\text{Sb}_4\text{S}_3$ (g) (Figures 9a-c). However in the absence of  $\text{H}_2\text{S}$  in the gas atmosphere, condensed Sb forms between 400 and 500°C depending on the pressure. This condensed Sb is the dominant species in an atmosphere free of  $\text{HCl}$ (g) and  $\text{H}_2\text{S}$ (g) and at temperatures lower than 400°C (Figure 9d). Pressure variations at high and medium temperatures do not produce equilibrium modifications, while at low temperatures some modifications may be observed when  $\text{HCl}$ (g) is in the gas atmosphere. According to these data antimony species in gas phase may occur in the gasifier, gas cleaning systems and flue gases in different proportions depending on the conditions and gas composition. If the gas atmosphere did not contain  $\text{HCl}$ (g) and  $\text{H}_2\text{S}$ (g), gaseous antimony would not be emitted into the environment.

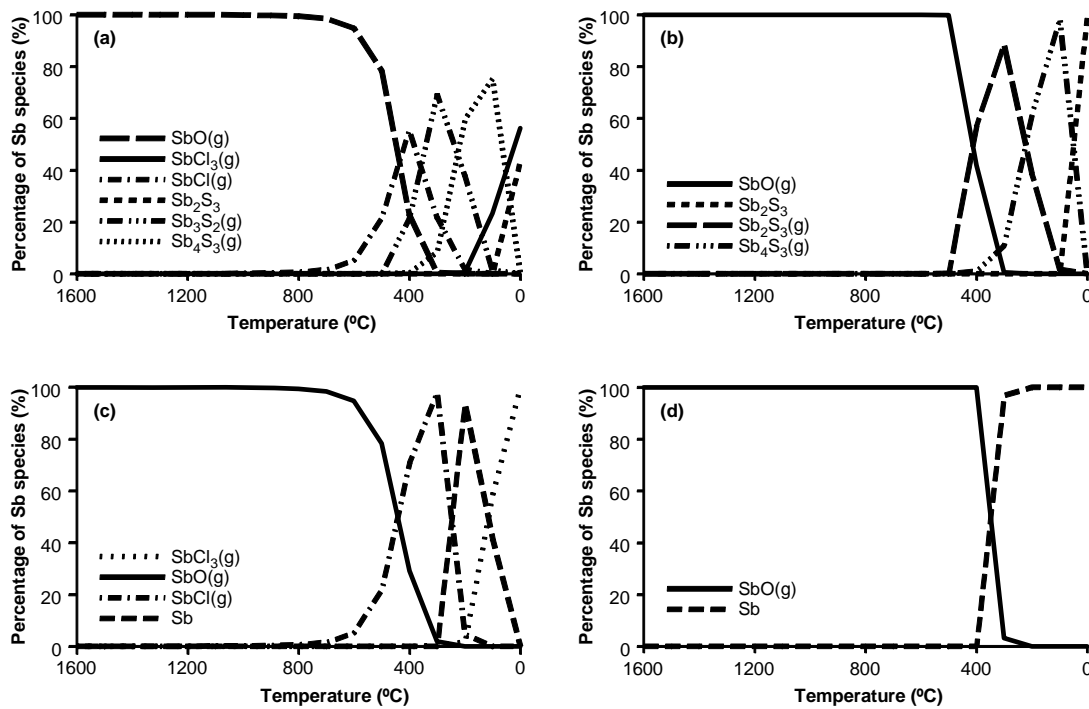


Figure 9.- Equilibrium compositions for antimony at 1 atm in (a) mixture IV; (b) mixture III; (c) mixture II and (d) mixture I.

## Cadmium

The theoretical calculations for this compound show that its composition in equilibrium depends on the temperature and the gas atmosphere (Figure 10). Minor modifications were observed with pressure variations. In all cases Cd(g) is the dominant species at temperatures higher than 500°C while at lower temperatures this depends on the gas atmosphere. When H<sub>2</sub>S(g) is present, the condensed CdS could be the dominant species at temperatures lower than 300°C. Between 300 and 500°C Cd(g) and CdS coexist (Figure 10a). However, if HCl(g) is in the gas atmosphere (Figure 10b) the formation of CdCl<sub>2</sub>(g) takes place between 300 and 600°C at high pressure and between 200 and 500°C at atmospheric pressure. From these data it may be concluded that the emission of cadmium compounds in flue gases is not probable. However, some gas compounds of cadmium may be formed in gas cleaning conditions.

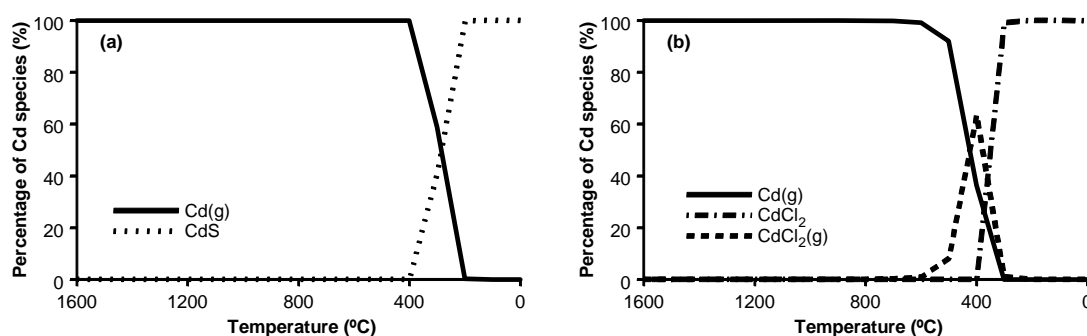


Figure 10.- Equilibrium compositions for cadmium at 25 atm in (a) mixture I and (b) mixture II.

## Lead

Lead equilibrium composition depends on temperature but the gas atmosphere modifies lead species at equilibrium considerably (Figure 11a-b). Pressure variations only produce modifications in the concentration of the species. In a gas atmosphere free of H<sub>2</sub>S(g) and HCl(g), at temperatures higher than 900°C lead occur totally as Pb(g), and at

temperatures lower than 500°C it is found in totally condensed form as Pb, PbS or a mixture of both. When the atmosphere contains H<sub>2</sub>S(g), the PbS(g) coexists with Pb(g) at temperatures higher than 700 and with PbS between 500-600°C. In the presence of HCl(g), (Figure 7d) PbCl(g) and PbCl<sub>2</sub>(g) may be formed, these being the dominant species at medium temperatures (500-800°C). At temperatures higher than 700°C all theoretical stable species for lead are in gas phase. Lead therefore can be expected to occur totally in gas phase in gasifier conditions while in gas cleaning conditions, it will be only partially in gas phase. At temperatures lower than 200°C and atmospheric pressure only the condensed species are stable.

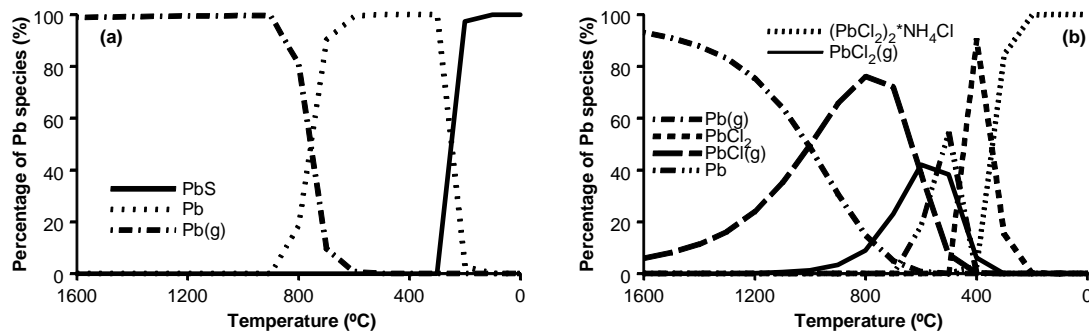


Figure 11.- Equilibrium compositions for lead at 25 atm in (a) mixture I and (b) mixture II.

## Zinc

The equilibrium composition for zinc depends on the temperature and gas atmosphere (Figure 12). Minor modifications were observed with pressure. The only stable species in gas phase in an atmosphere free of HCl(g) is Zn(g) (Figure 12a). Its formation begins between 500 and 800°C depending on the gas atmosphere. Zn(g) is the only species present in equilibrium at temperatures higher than 1000°C. At temperatures between 200-600°C only condensed species are stable, ZnS(B), ZnS(W) and ZnS coexisting. The presence of HCl(g) in the atmosphere (Figure 12b) favours the formation of ZnCl<sub>2</sub>(g)



between 300 and 1000°C, while the presence of H<sub>2</sub>S(g) in the gas mixture does not modify the equilibrium composition. Pressure modifications produce variations in the concentration of the different species at equilibrium. These results suggest that that the zinc present in coal occurs totally in gas phase in gasifier conditions and in gas cleaning conditions. However, zinc would not be emitted into the environment in gas phase.

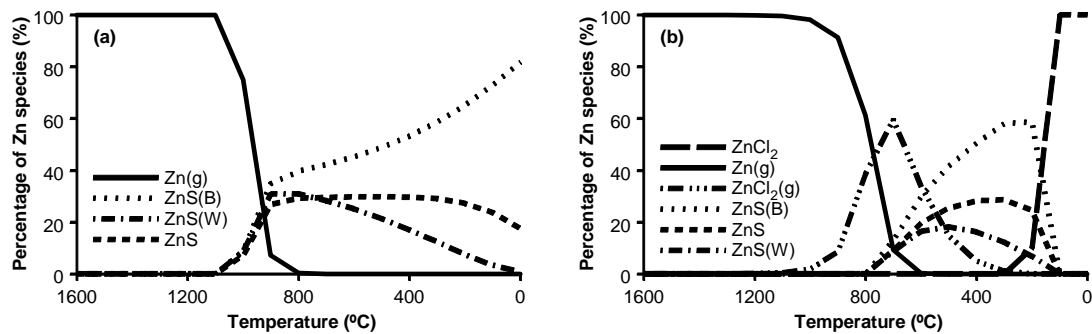


Figure 12.- Equilibrium compositions for zinc at 25 atm in (a) mixture III and (b) mixture II.

## CONCLUSIONS

From thermodynamic equilibrium calculations, trace elements may be classified, according to their volatile behaviour expected during coal gasification, such as is generally done using available experimental data as the basis [1]. This classification, which does not take into account heterogeneous reactions, would consist of three main groups. The trace elements in the first group (Group A), would include those that may be totally condensed in gasification gas cleaning and emission conditions. This is the case of Mn. This group would be similar to that defined as Group 1 for experimental coal combustion conditions [1]. The elements mainly present in gas phase in most conditions (Se, Hg and B) would be classified in Group C. This group is similar to Group 3 for combustion processes. The rest of the elements would form an intermediate

group (Group B). If the goal of assessing the elements in this group is to ascertain the possible elements in gas phase in gas cleaning conditions, two subgroups need to be considered; Group B1 which would include those elements that are totally or partially in gas phase at the temperature of hot gas cleaning systems (500-800°C), as is the case of Co and Be, and subgroup B2 which would contain the elements totally or partially in gas phase at low temperature gas cleaning conditions (<500°C), i.e. Sb, As, Cd, Pb, Zn, Ni, Cr and V.

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