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Numerical modeling of plasma gasification process of polychlorinated biphenyl wastes

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Abstract

The plasma gasification process is one of the most innovative and efficient methods for the disposal of various wastes and energy production. But it is still an extremely complicated process; therefore, to optimize it, modeling could be used as an invaluable asset. The aim of this study is to develop a computational model to evaluate the plasma gasification process of polychlorinated biphenyl wastes. The model was created in Aspen Plus[®] commercial software. It is based on the principle of Gibbs free energy minimization. The results acquired in this research were validated by the data in the literature. It has to be noted that satisfactory results have been obtained. Also, air, steam, and carbon dioxide were considered as oxidizers and the effects of various parameters such as temperature, equivalence ratio (ER), steam-to-waste (S/W) ratio, and carbon dioxide-to-waste (CO₂/W) ratio on the production of syngas components were investigated. The results show that processing this hazardous waste leads to the production of a large percentage of acidic gases, which demands a gas cleaning unit in such treatment facilities. The results also show that PCBs with lower chlorine atoms are favorable to the production of higher-quality syngas. The increase of the gasifier temperature turns the waste into purer syngas. However, after the temperature of 1200 °C the results showed that the major constituents of syngas reach almost a constant molar fraction. A steam-to-waste ratio of 0.5 can be used to produce syngas with greater percentage of hydrogen and fewer pollutants. The use of CO₂ as gasifying agent led to the production of large amounts of CO. Conclusion could be drawn that this process can be considered safe and very effective while processing the aforementioned hazardous wastes and in the production of high-quality syngas.

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1. Introduction

The energy demand is increasing daily. In addition to the fact that fossil fuels are one of the causes of environmental pollution and countless other problems, their sources are being depleted [27]. Nowadays, the use of renewable energy sources as an alternative form of energy is on the rise and these sources will play a key role in the future [9,36]. Among these, one of the results of population growth in recent years is an increase in waste production which can be used as a renewable resource in response to the ever-rising energy demand [24]. Polychlorinated biphenyl (PCB) is one of these wastes; PCB has been used in industry for many years due to its special electrical and thermal properties. However, later they became known as one of the most hazardous pollutants. Even though this material is prohibited, there are still many devices that make use of it. The methods of disposal of these wastes can be chemical, thermal or a combination of both. The chemical method is not widely used in industrial applications on the grounds that its process rate is rather low [24]. Currently, the primary method of this waste's disposal is combustion. The temperature resistance of this material makes it very difficult to process, especially since a method such as incineration causes large amounts of dioxins and furans. The high temperature of the plasma gasification process can minimize these pollutants [1]. Therefore, it would be an excellent alternative to conventional methods [22]. Suppose this waste is used for energy production. In that case, it can reduce the harmful effects of this waste on the environment and help industries that are required to get rid of it safely and adequately due to strict environmental regulations. Usually, it costs industries a fortune to treat these wastes [2,6]; they can also use their wastes to generate energy and reducing costs tending towards the circular economy concept [12].

One of the problems in conventional methods, such as incineration, is gaseous pollutants such as dioxins and furans in the outlet. According to reports, the rate of dioxins production reaches its maximum for temperatures between 300 to 400 °C. To minimize these contaminants, the reactor temperature must be above 1000 °C [9].

Plasma gasification is one of the processes that has unique features that can be used as a safe and optimal method for PCB waste processing because it works at a temperature of thousands of degrees. Plasma, referred to as the fourth state of matter, is composed of positive and negative particles formed by the ionization of gas particles that can achieve very high temperatures, essential in waste processing. Moreover, charged particles further helps to eliminate and decontaminate hazardous wastes [14,41].

The plasma gasification process is an allothermal process in which plasma is used to heat and stabilize the process temperature so that it will be easier to control the heat and temperature in comparison to the conventional processes. The higher temperatures achieved in this method allow to break off the bonds and decompose the material, resulting in a nearly pure synthesis gas (syngas) comprising mostly H₂, CO, and CH₄ [5,10]. In the PCB treatment process, a large amount of HCl is produced. However, the HCl in the gaseous phase can be easily dissolved in water to produce an aqueous solution of hydrochloric acid, hence obtaining purer syngas [48]. However, not always is it possible to perform the process, or at times, it might be time-consuming, expensive, and dangerous giving room to the use of modeling and simulation.

There are many methods for modeling the gasification process, including the use of Aspen Plus[®], computational fluid dynamics (CFD), thermodynamic equilibrium, artificial neural networks, and kinetic models [13,38]. On the other hand, due to the extensive database in Aspen Plus[®], modeling, and optimization of complex chemical processes have been facilitated. Consequently, this method was chosen to model the plasma gasification process in this paper [15,28,47].

Modeling the gasification process using Aspen Plus[®] software has been studied extensively [3,4,11,35,37,44]. Researchers have also studied the plasma gasification process [14,29–31]. Most of these models have been used to study how to process biomass and municipal wastes and only a few conducted experiments on specific wastes and hazardous wastes like PCBs [39].

Galeno et al. [14] evaluated the performance of an integrated plasma gasification/fuel cell system of refuse derived fuel on Aspen Plus[®]. They calculated the net power per kilogram of refuse derived fuel and the electric efficiency of the fuel cell in 33%. Kuo et al. [25] conducted a thermodynamic analysis of plasma gasification of raw and torrefied, non-woody, and algal biomass using different gasifying agents (air, steam, and carbon dioxide). They reported that pine wood has the best performance for producing high-quality syngas among the investigated biomasses. Ismail et al. [19] developed a 2D mathematical model of plasma gasification of forest residues and conducted a parametric study (gasifier temperature, equivalence ratio, and steam-to-biomass ratio) to understand their influence on the process. They concluded that the gasifier temperature and the equivalence ratio have contradictory influences on the quality of the syngas, while the steam-to-biomass ratio has a positive effect on the production of

hydrogen. The same authors used their model to understand the influence of some parameters (equivalence ratio, steam-to-biomass ratio, and plasma power) on the production of hydrogen when simulating the plasma gasification of municipal solid wastes. They conclude that an equivalence ratio of 0.3 seems to be the most favorable condition for greater yields of CO and H₂. A steam-to-biomass ratio of 0.5 seems to be the most favorable condition to obtain high-quality syngas. Higher plasma power is favorable to high-quality syngas increasing the amounts of CO and H₂ Ismail et al. [20]. Tavares et al. [45] studied the combination of the appropriate amount of polyethylene terephthalate and biomass to generate the highest amount of H₂ or the highest heating value in the gasification process. They have also considered the use of air, steam, and oxygen as oxidizers.

In this paper, we made an attempt to develop a model for the study of such specific hazardous wastes and to examine the important parameters affecting this process. To that end, the effect of parameters such as temperature, equivalence ratio, and oxidizing agent on the syngas components was taken into account.

2. Model description

Irrespective of the fact that much research has been done on the process of solid wastes gasification, it is a challenge to find cases that have gasified hazardous wastes [17]. Since the reactions of the gasification process are very complex and little information is available about the reactions, particularly for special wastes like PCB, the model is based on thermodynamic equilibrium and the principle of Gibbs free energy minimization is used to predict the composition of the produced syngas. This method does not require kinetic information of the reactions; thus, it is suitable for this type of waste [13]. Equations related to this method are calculated in Aspen Plus[®] engineering software. The next section provides more details of these calculations.

Modeling the plasma gasification process is similar to the conventional gasification process. Janajreh et al. [21] have divided this modeling into two parts. They examined each part separately and many others have explored it as an integrated model. The major reactions that occur in the gasification process can be seen in Table 1 [3,40,43].

Table 1. Major reactions of the gasification process.

Reaction	Chemical reaction	Process	ΔH_{298}^0 (MJ/kmol)
R1	$C + 0.5O_2 \rightarrow CO$	Partial oxidation	-111
R2	$C + CO_2 \leftrightarrow 2CO$	Boudouard reaction	+172
R3	$C + H_2O \leftrightarrow CO + H_2$	Steam reforming	+131
R4	$C + 2H_2 \leftrightarrow CH_4$	Methane formation	-74
R5	$H_2 + 0.5O_2 \rightarrow H_2O$	Hydrogen combustion	-484
R6	$CO + 0.5O_2 \rightarrow CO_2$	CO combustion	-284
R7	$CO + H_2O \leftrightarrow CO_2 + H_2$	Water-Gas Shift reaction	-42

2.1. Thermodynamics

This model is based on the assumption that the reactions in thermodynamic equilibrium possess the minimum Gibbs free energy. So, firstly, the system's Gibbs free energy (G^t) must be obtained from the following formula [40,42]:

$$G^t = \sum_{i=1}^N n_i \mu_i \quad (1)$$

where N is the total number of species, n_i the number of moles of the species, and μ_i the chemical potential of the species i . Assuming that the produced gases are ideal, the chemical potential is defined as follows:

$$\mu_i = G_i^0 + RT \ln(f_i/f_i^0) \quad (2)$$

R and T are the universal gas constant and temperature, respectively. f_i is species fugacity, G_i^0 is the standard Gibbs free energy and f_i^0 is the standard species fugacity. If the pressure is equal to 1 atm, then:

$$\mu_i = \Delta G_{f,i}^0 + RT \ln\left(\frac{n_i}{n_{tot}}\right) \quad (3)$$

in which y_i is the molar fraction of gas species and $G_{f,i}^0$ is the free energy of Gibbs formed for the species i . Introducing Eq. (3) into Eq. (1) the following is obtained:

$$G^t = \sum_{i=1}^N n_i \Delta G_{f,i}^0 + \sum_{i=1}^N n_i RT \ln \left(\frac{n_i}{n_{tot}} \right) \quad (4)$$

The workout is to discovery the set of n_i that minimizes the total Gibbs free energy objective function G^t , subjected to the elemental balance constraint given by:

$$\sum_{i=1}^N a_{ij} n_i - A_j = 0 \quad (j = 1, 2, \dots, k) \quad (5)$$

where a_{ij} represents the number of atoms of the j_{th} element in a mole of i_{th} species and A_j represents the total number of atoms of the j_{th} element in the gaseous mixture. The Lagrangian function (L) is formed through the Lagrange multipliers $\lambda_j = \lambda_1, \dots, \lambda_k$, defined as:

$$L = G^t - \sum_{j=1}^K \lambda_j \left(\sum_{i=1}^N a_{ij} n_i - A_j \right) \quad (6)$$

this function is minimized when all its partial derivatives are equal to zero.

$$\frac{\delta L}{\delta n_i} = 0 \quad (7)$$

Replacing the value of G^t from Eq. (4) in Eq. (6) and taking its partial derivatives of Eq. (7), the Gibbs free energy can be expressed as follows:

$$\frac{\delta L}{\delta n_i} = \frac{\Delta G_{f,i}^0}{RT} \sum_{i=1}^N \ln \left(\frac{n_i}{n_{tot}} \right) + \frac{1}{RT} \sum_{j=1}^K \lambda_j \left(\sum_{i=1}^N a_{ij} n_i \right) = 0 \quad (8)$$

Eq. (8) can be formed in terms of a matrix with i rows and can be solved simultaneously by iteration techniques. The Gibbs free energy of species formation can be calculated as follows:

$$\Delta G_{f,i}^0 = \Delta H_{f,i}^0 - T \Delta S_{f,i}^0 \quad (9)$$

$\Delta H_{f,i}^0$ is standard enthalpy and $\Delta S_{f,i}^0$ is standard entropy, both of which can be obtained as a function of temperature:

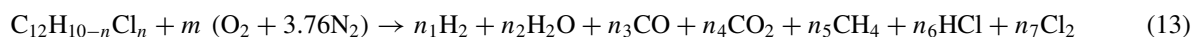
$$\frac{H_i^0}{RT} = a_1 + a_2 \frac{T}{2} + a_3 \frac{T^2}{3} + a_4 \frac{T^3}{4} + a_5 \frac{T^4}{5} + \frac{b_1}{T} \quad (10)$$

$$\frac{S_i^0}{R} = a_1 \ln(T) + a_2 T + a_3 \frac{T^2}{2} + a_4 \frac{T^3}{3} + a_5 \frac{T^4}{4} + b_2 \quad (11)$$

where a_1, \dots, a_5 , and b_1, b_2 are coefficients available in the software database for several species. The reaction temperature (T) is the temperature which fulfills the energy balance equation. Assuming the ideal gas behavior, enthalpies of products H_P and reactants H_R are temperature dependent and can be calculated by means of each species enthalpy at given temperature.

$$H_{R,P} = \sum_{n=1}^N n_i \bar{h}_f + \sum_{n=1}^N n_i \int_{298}^{T_i} C_{pi} dT \quad (12)$$

Where C_{pi} and \bar{h}_f represent the specific heat and enthalpy of formation of the species i . Using Eq. (8) together with Eqs. (5) and (12), a system of equations is obtained through which the syngas composition is found [32]. In the present model, the species considered as representative of the plasma gasification process of a mole of PCB is represented by the following global reaction:



where n_1 to n_7 are the stoichiometric coefficients and m represents the molar fraction of the gasifying agent used, here represented by the air.

2.2. Model assumptions

The following assumptions are made in the developed model [4,32]:

- The model is zero-dimensional and the temperature and pressure are assumed to be stable and uniform.
- All gases are considered ideal.
- Air is composed of nitrogen and oxygen in a ratio of 79/21.
- There is no heat loss.
- The process is at atmospheric pressure with no pressure drop.
- Tar formation is neglected.

2.3. Aspen plus model

The model diagram created in Aspen Plus® can be seen in Fig. 1. Waste enters the system through the WASTE stream. Since PCB is not defined in the software database, the decomposed PCB in the form of elements C, H, and Cl is processed and modeled as a pyrolysis process. It then enters the RGibbs (GASIFI) block in which the plasma gasification process is simulated on the basis of Gibbs free energy minimization method. Oxidizers (carbon dioxide, air, and steam) first enter the heat exchanger (TORCH) through CO₂, STEAM, and AIR streams raising their temperature up to the plasma temperature, and then enters the RGibbs block. The products of the gasification process enter the SSPLIT block (SEP) by the PRODUCT flow, where solids (slag) are separated from syngas and flow into the mixer block (SCRUBBER) by the SYNGAS stream. This block simulates the scrubber, which uses NaOH solution and removes acid gases in syngas. Pure syngas enters the separator block (SEP1) via MIXED, where gases are separated from salts and liquids formed in the previous part.

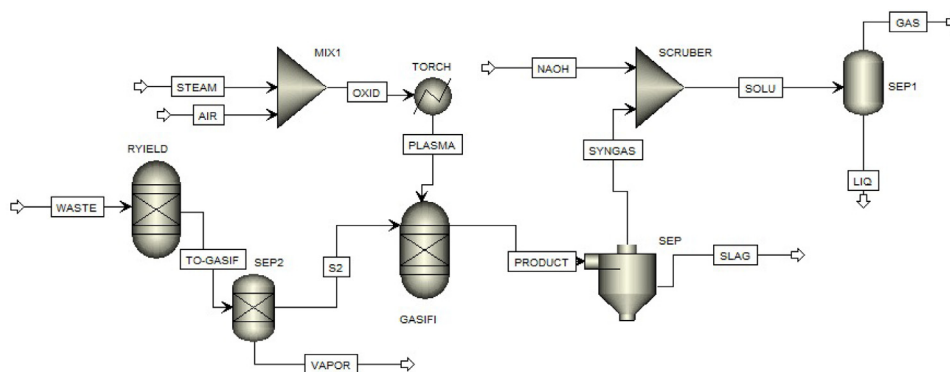


Fig. 1. Aspen Plus model diagram.

3. Materials and methods

3.1. Fuel

PCBs are a large range of anthropogenic organic chemicals consisting of chlorinated hydrocarbons. There are many forms of PCBs in nature. They vary in consistency from thin, light-colored liquids to yellow or black waxy solids. Due to their nonflammability, chemical stability, high boiling point, and electrical insulating properties, PCBs were used in a large range of industrial and commercial applications including electrical, heat transfer, and hydraulic equipment; as plasticizers in paints, plastics, and rubber products; in pigments, dyes, and carbonless copy paper; and many other industrial applications. They are often referred to by their commercial trade names, including Aroclor and Kanechlor. PCBs are a group of related chemicals, actually consisting of 209 individual chemicals with different amounts of chlorine. Therefore, the PCB wastes used as fuel in this study are known by the global chemical formula $C_{12}H_{10-n}Cl_n$, with n varying between 1 and 9. According to the literature, the global chemical formula more adopted for PCBs is $C_{12}H_6Cl_4$ corresponding to tetrachlorobiphenyl used mainly as transformer oil [23]. Therefore, this global chemical formula will be taken into account in the following sections to perform a sensitivity analysis.

PCB does not exist in the Aspen Plus[®] database, which makes it challenging to define this material in the software. The method used in our model is based on complete waste decomposition or complete waste pyrolysis.

3.2. Model validation

The research of Tavares et al. [46] was used to provide the data needed for the validation of the present model. Table 2 shows the characteristics of the waste including the proximate and approximate analysis used for verification. In this comparison, municipal solid waste (MSW) is processed at a temperature of 2500 °C. The waste flow rate is 1 kg/s and the air flow rate is 0.36 kg/s.

Table 2. Ultimate and proximate analysis of MSW used in model validation.

Ultimate analysis (%)		Proximate analysis (%)	
C	71.3	Volatiles	71.5
H	6.0	Fixed carbon	7.7
O	26.5	Moisture	27.3
N	0.8	Ash	20.8
S	0.3	LHV (MJ/kg)	25.1

Fig. 2 presents a comparison between model results and data from scientific sources. Due to the fact that scrubbers were not used in the work of Tavares et al. [46], Fig. 2 shows the syngas composition obtained by our model before the scrubber.

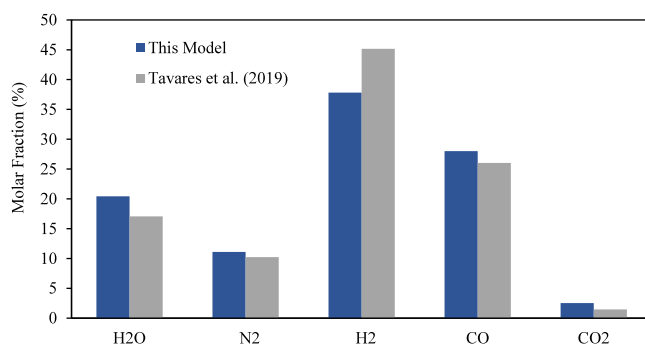


Fig. 2. Aspen Plus model simulated values compared to literature data.

Fig. 2 shows that the molar fraction of the various syngas constituents is in good agreement with the numerical data of Tavares et al. [46]. The results deviation can be quantified by using the relative error. The relative error percentage obtained for the main gaseous components of the syngas is 16.5% for H₂O, 8.0% for N₂, 19.4% for H₂, 7.1% for CO, and 42% for CH₄. The greatest deviation is seen for CH₄, which is predictable since smaller fractions tend to produce higher relative errors. Moreover, all hydrocarbons in the syngas can lump into CH₄ due to assumptions made in our model, which can further explain the higher errors obtained and generally encountered in the literature [7].

4. Analysis of results

4.1. Equivalence ratio effect

Equivalence ratio (ER) is a crucial parameter in a gasification scenario. It is defined as the ratio of air/waste mass flow divided by the stoichiometric air/waste ratio. The equivalence ratio equation can be expressed as follows [10,16]:

$$ER = \frac{\text{Air/Fuel Mass}}{\text{Stoichiometric Air/Fuel Mass}} \quad (14)$$

The ER plays a decisive role in determining the composition of syngas. To investigate the effect of this parameter on the plasma gasification process, its range was varied from 0.1 to 1.0, while keeping the gasification temperature at 1500 °C. The PCB flow rate is assumed to be 10 kg/h. The effect of this parameter on the syngas composition can be seen in Figs. 3 and 4 for the oxidizers air and O₂, respectively.

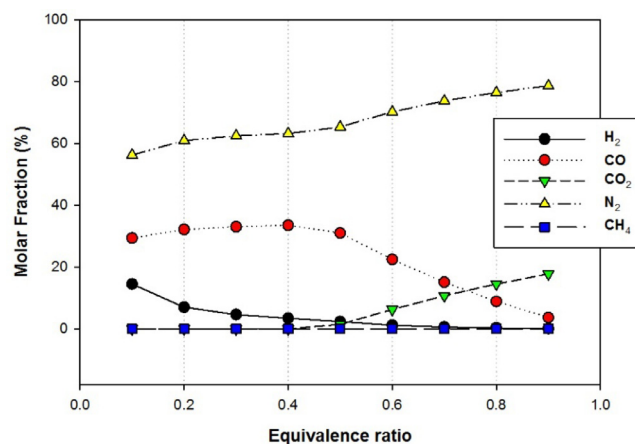


Fig. 3. Influence of ER in syngas molar fraction using air as gasifying agent.

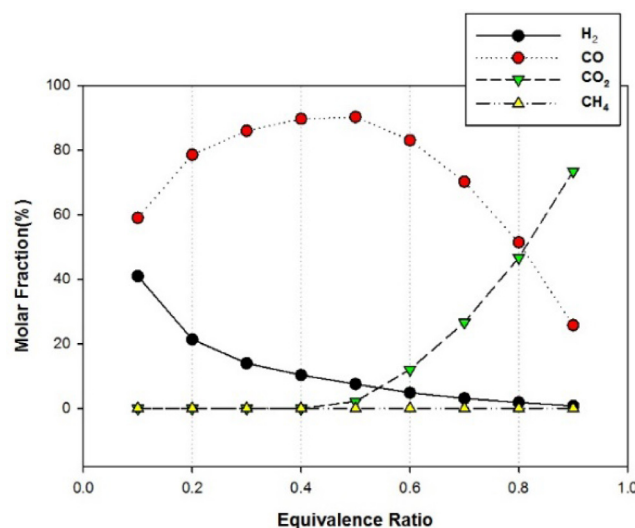


Fig. 4. Influence of ER in syngas molar fraction using oxygen as gasifying agent.

The same trend can be seen in the percentage of the molar fraction of the syngas components for both gasifying agents. As it can be seen in Fig. 3 the amount of H₂ decreases as ER increases. The amount of CO firstly increases up to an ER of 0.4 decreasing afterwards. The amount of CO₂ starts increasing precisely at an ER of 0.4. These trends find an explanation in the progress of reactions R5 and R6 due to a greater presence of oxygen.

In Fig. 4, which uses O₂ as a gasifying agent, a similar trend can be seen. As ER increases, the molar fraction of H₂ decreases from 58% to 6%. The greater presence of oxygen promotes the hydrogen combustion reducing its amount. It can be seen that the amount of CO has a maximum at an ER of 0.5, which could be explained by the Boudouard reaction (R2) and CO combustion reaction (R6). The amount of CO₂ increases as ER rises. The reason can be the enhancement of the oxidation reactions (R5 and R6) due to the presence of more oxygen [3,10].

4.2. Gasifier temperature effect

The gasifier temperature is one of the parameters that play a significant role in the gasification process [33]. Increasing the temperature will also lead to higher conversion rates of wastes into syngas [18]. Many researchers have reported that higher temperatures in the plasma gasification process would be more suitable for tars, dioxins, and furans removal. To analyze this parameter, the temperature is varied from 800 to 2000 °C while keeping ER at 0.3. Fig. 5 shows the effect of this parameter on syngas composition before scrubbing using air as oxidizer. It is noticed that the change rate in the molar fraction of CO, H₂, and HCl for temperatures above 1200 °C is negligible. On the other hand, the molar fraction of CO₂ is highly dependent upon temperature and its value is significantly reduced as temperature increases. This behavior can be explained mainly by the water-gas shift reaction (R7) [26].

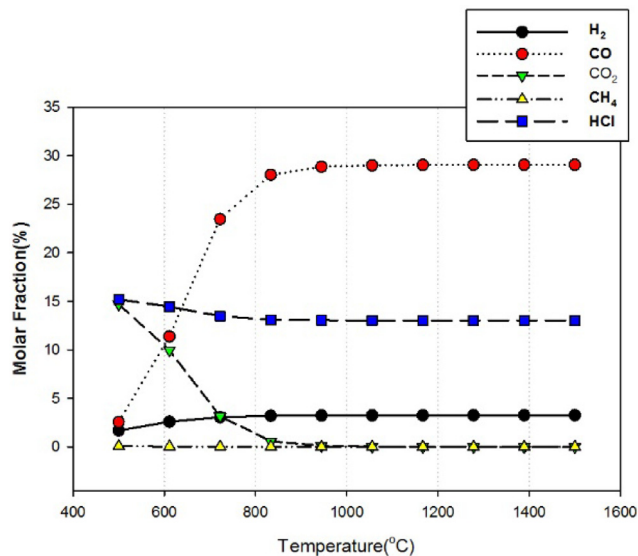


Fig. 5. Influence of temperature on syngas molar fraction before scrubbing using air as gasifying agent.

Fig. 6 presents information about the effect of temperature on the syngas composition after scrubbing. It can be seen that the HCl gas is effectively removed by the scrubber. Fig. 7 shows the effect of the temperature parameter on the molar fraction of syngas components after scrubbing using oxygen as the oxidizer.

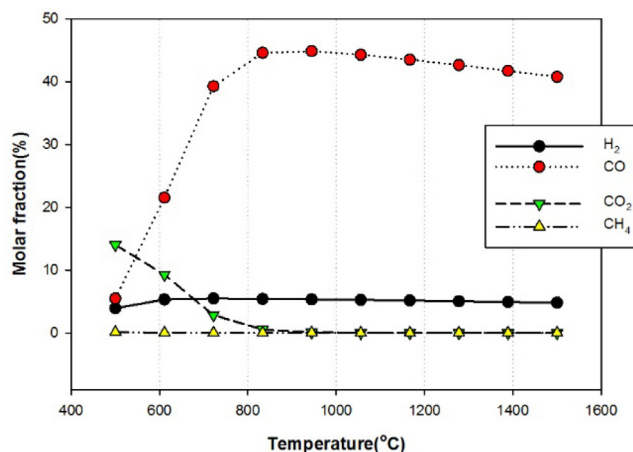


Fig. 6. Influence of temperature on syngas molar fraction after scrubbing using air as gasifying agent.

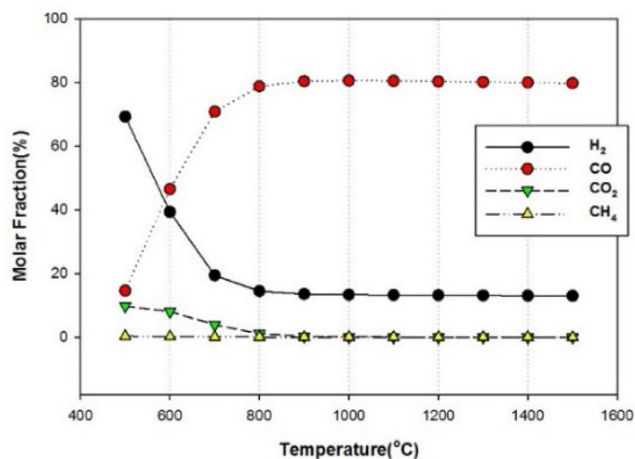


Fig. 7. Influence of temperature on syngas molar fraction using oxygen as gasifying agent.

A similar trend is formed in this process, where the amounts of H₂ and CO increase, and the amount of CO₂ decreases. The molar fractions of H₂ and CO are higher when oxygen is used as the oxidizer indicating that the quality of the produced syngas is higher [40].

4.3. Steam/waste ratio and CO₂/waste ratio

Steam is extensively used in gasification processes due to the promotion of hydrogen production [34]. Carbon dioxide is known to increase the gasification efficiency and decreasing the levels of CO₂ produced in the process [8]. However, it requires an external source of energy due to the highly endothermic nature of CO₂ gasification, which is granted by the plasma torch. To investigate the effect of steam and CO₂ on the plasma gasification process, the steam-to-waste ratio and the CO₂-to-waste ratio are defined as follows [25,45]:

$$S/W = \frac{\text{Steam Flow}}{\text{Waste Flow}} \quad (15)$$

$$\text{CO}_2/W = \frac{\text{CO}_2 \text{ Flow}}{\text{Waste Flow}} \quad (16)$$

The waste flow is fixed at 10 kg/h and the temperature is assumed to be 1500 °C. The S/W ratio varies between 0.5 and 2.0, and the CO₂/W ratio varies between 1.0 and 5.0. Figs. 8 and 9 show the influence of these parameters on the syngas components' molar fraction.

As it can be seen from Fig. 8, the amount of H₂ increases from 55% to 59%, and the amount of CO decreases from 44% to 27%. The molar fraction of CO₂ experiences an upward trend when the S/W ratio increases. The amount of H₂ and CO produced when using steam as the oxidizer is much higher than in other oxidants mainly due to the enhancement of the steam reforming reaction (R3). Fig. 9 shows the effect of CO₂/W ratio on the syngas composition. As this ratio increases, the molar fraction of CO firstly increases up to 95% for CO₂/W ratio up to 2.0 and then decreases. In opposite, the amount of CO₂ is nearly zero to CO₂/W ratios up to 2.0, increasing rapidly afterwards.

These behaviors can be explained by the Boudouard reaction (R2), in which solid carbon (C) reacts with CO₂ forming CO [8]. This behavior also means that the CO₂/W ratio should be lower than 2.0 due to the saturation of the Boudouard reaction for higher CO₂/W ratios.

4.4. PCBs empirical chemical formula

In this section, possible empirical formulas for PCBs are adopted and the structure of the produced syngas studied for each of them. The general formula of PCB is considered to be C₁₂H_{10-n}Cl_n, where *n* can vary between 1 and 9. Fig. 10 presents the results of this study.

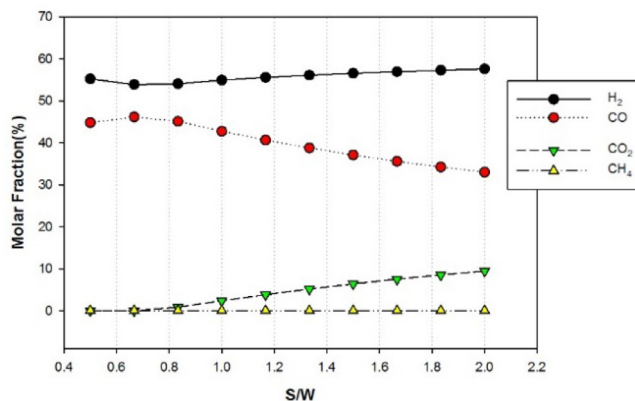


Fig. 8. Influence of the steam/waste ratio on syngas molar fraction.

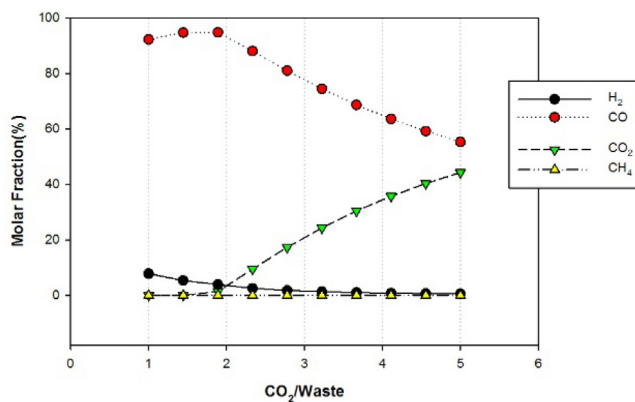


Fig. 9. Influence of the CO₂/waste ratio on syngas molar fraction.

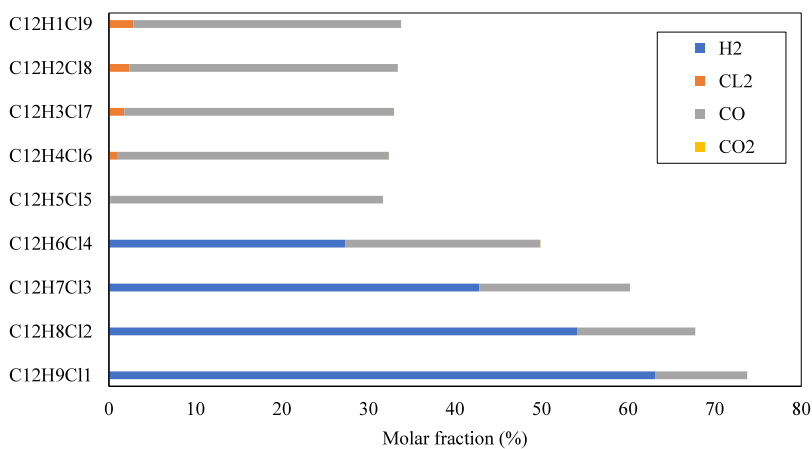


Fig. 10. Effect of the empirical formula of PCBs on syngas molar fraction.

From Fig. 10, it can be seen that by increasing n , the amount of hydrogen decreases considerably and the amount of chlorine in syngas increases. The rates of gases' production are directly related to their amounts in the empirical chemical formula. Therefore, the empirical formula C₁₂H₉Cl₁ has the highest amount of hydrogen and the and

lowest amount of chlorine. Thus, PCBs with lower n are favorable to the production of higher-quality syngas. As said before, all the parametric study performed assumes a global chemical formula for the PCB as $C_{12}H_6Cl_4$.

4.5. Hydrogen production

The presence of hydrogen in the syngas is very important for energy generation. To investigate the amount of hydrogen in syngas, several parameters such as ER and temperature were combined for air and oxygen as the oxidizing agent and the results can be seen in Fig. 11. ER varies from 0.1 to 1.0 and temperature from 800 to 2000 °C.

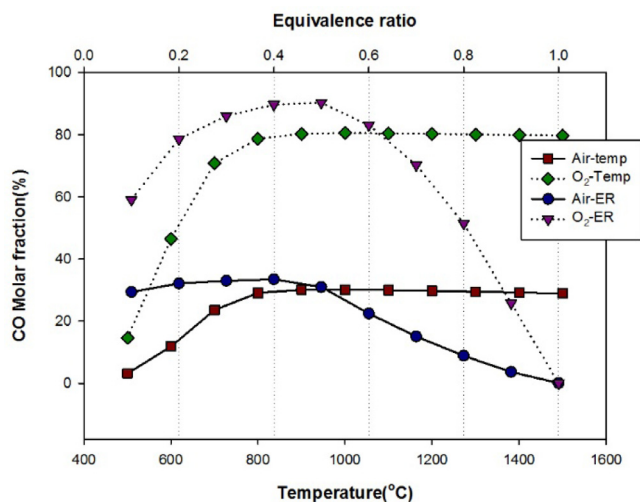


Fig. 11. Molar fraction of H₂ as a function of the gasifier temperature and ER for air and O₂ gasification.

Fig. 11 shows that the maximum value of H₂ for air as oxidizer is obtained at 0.1 ER; consequently, the falling trend of H₂ molar percentage is the same for both air and oxygen as oxidizers, but the amount of H₂ in the syngas is higher for air as oxidizer. This may have occurred because more oxygen consumes H₂ and converts it into CO and CO₂ in accordance to reactions R4 and R7. Also, in case of steam oxidation and temperature change, two parameters of temperature and steam to waste ratio were considered whose results can be seen in Fig. 12.

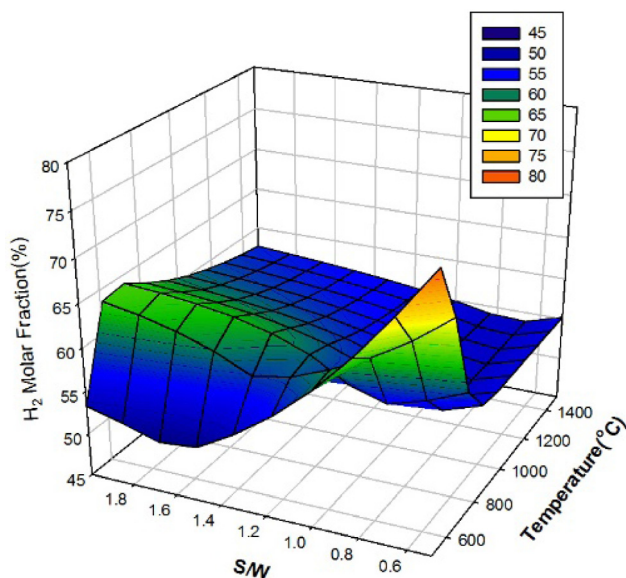


Fig. 12. Molar fraction of H₂ as a function of the gasifier temperature and S/W ratio for air and O₂ gasification.

From Fig. 12 is possible to determine the condition that maximizes the hydrogen molar fraction. As it is shown, the amount of hydrogen for low temperatures around 600 °C and S/W ratio of 0.5 reaches its maximum value which corresponds to around 75%. The S/W ratio increase enhances steam reforming (R3) and water gas shift (R7) reactions leading to the increase of H₂ molar fraction. On the other hand, temperature increase favors the products of endothermic reactions according to Le Chatelier's principle leading to the increase of the CO molar fraction rather than the H₂ molar fraction.

4.6. CO production

The combined effect of the gasification parameters ER and temperature on CO molar fraction for air and oxygen oxidants can be seen in Fig. 13. A temperature of 1500 °C was set for the ER evaluation and an ER value of 0.3 was set for the temperature evaluation. The highest amount of CO can be observed with oxidant O₂ for ER equal to 0.5, which can be explained by the progress of combustion reactions (R1).

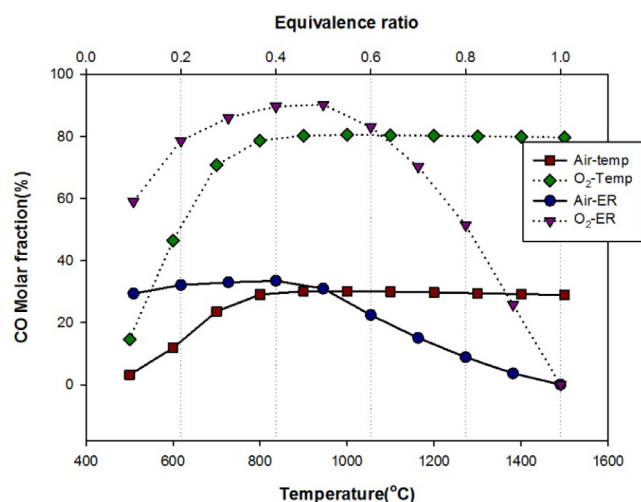


Fig. 13. Molar fraction of CO as a function of the gasifier temperature and ER using air and O₂ as gasifying agents.

Fig. 14 illustrates the effect of S/W ratio along with the effect of temperature on the molar fraction of CO. In this evaluation, the S/W ratio varies from 0.5 to 2.0, and the temperature from 500 to 1500 °C. The highest amount of CO was obtained for the S/W ratio of 0.7 and the temperature of 1500 °C. It can be observed that temperature slightly favors the increase of CO molar fraction. This is due to the progress of the water gas shift reaction (R7). The lowest CO value is obtained for the S/W ratio of 2.0, which occurs at temperatures close to 500 °C.

4.7. Lower heating value

To study the effect of ER and gasifier temperature on the lower heating value (LHV) using two oxidizing agents (air and oxygen), ER varies from 0.1 to 1.0 and the gasification temperature from 500 to 1500 °C. Fig. 15 shows the effect of these parameters on the LHV when air is used as the oxidizer. It can be seen that with increasing ER, the amount of LHV decreases from about 7 to 4 MJ/kg, which is mainly due to the dilution of the syngas with N₂.

As temperature increases, the LHV increases to around 4.0 MJ/kg using air as the gasifying agent. This is the direct result of the rise experienced in the CO molar fraction in syngas with increasing temperature. For the oxygen oxidizer, the results can be seen in Fig. 16. It is seen that the LHV value is much greater (12 MJ/kg) when oxygen replaces air as the gasifying agent (4 MJ/kg). It is obvious that by increasing ER, the LHV value decreases, which could be explained by the development of combustion reactions (R5, R6). It is also seen that the temperature has little effect on the LHV value using oxygen as the gasifying agent.

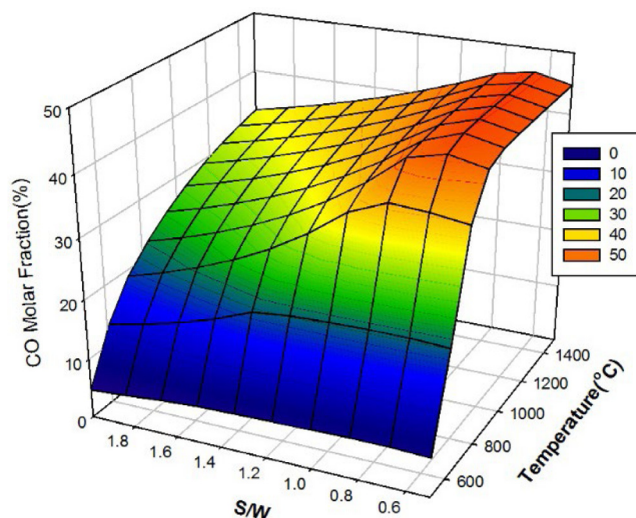


Fig. 14. Molar fraction of CO as a function of the gasifier temperature and S/W ratio using steam as gasifying agent.

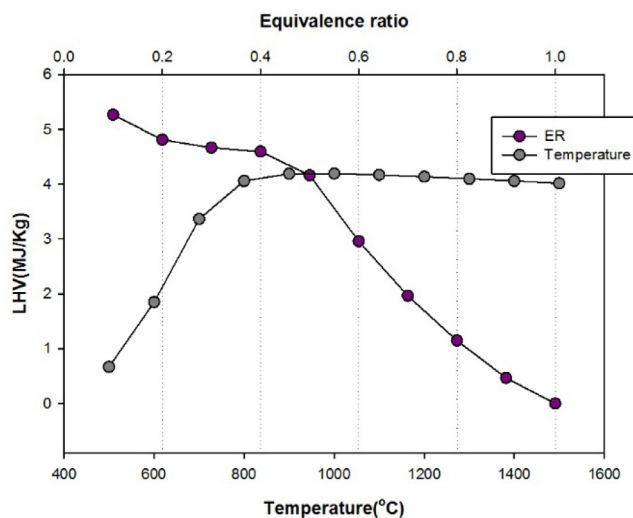


Fig. 15. Influence of ER and gasifier temperature on the lower heating value of the syngas using air as gasifying agent.

5. Conclusion

Conventional waste treatment methods have failed in dealing with hazardous wastes. Meanwhile, plasma gasification has been able to process these wastes and produce valuable energy at the same time. By studying and modeling this complicated process, many potential costs and risks can be avoided. For example, compounds such as polychlorinated biphenyl can produce hazardous pollutants when processed by incineration. Bearing that in mind, plasma gasification can be an excellent way to process this waste. However, there are limited scientific sources in the literature dealing with the plasma gasification of PCBs. Here, one offers a model based on Aspen Plus[®] software developed to evaluate this process. It is based on Gibbs free energy minimization and validated with scientific sources. Air, steam, and carbon dioxide gases were considered as the oxidizers and the effect of parameters such as temperature, equivalence ratio, steam-to-waste ratio, and carbon dioxide-to-waste ratio on the syngas composition were studied. The results show that processing this hazardous waste leads to the production of a large percentage of acidic gases. This calls for a gas cleaning unit in such treatment facilities. The results also show that PCBs with lower chlorine atoms are favorable to the production of higher-quality syngas. An increase in the

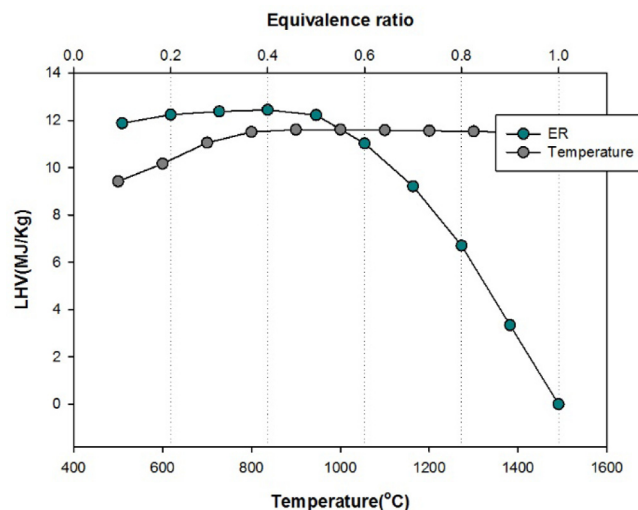


Fig. 16. Influence of ER and gasifier temperature on the lower heating value of the syngas using oxygen as gasifying agent.

gasifier temperature turns the waste into purer syngas. However, after the temperature of 1200 °C the results showed that the major constituents of syngas reach almost a constant level. A steam-to-waste ratio of 0.5 can be used to produce syngas with more hydrogen and fewer pollutants. The use of CO₂ as gasifying agent led to the production of large amounts of CO. Knowing that the safe and efficient disposal of PCBs is of paramount importance, the results of the present research are even more relevant demonstrating that it is possible to produce syngas with high heating value capable to be used to generate energy or valuable products.

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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