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Numerical analysis of plasma gasification of hazardous waste using Aspen Plus

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Abstract

The COVID-19 pandemic raised the problem of dealing with the hazardous wastes generated. The World Health Organization (OMS) recommends the treatment of these wastes at high temperatures in order to neutralize their negative impact. For this reason, the main objective of this work is the development and analysis of a sustainable way to treat hazardous wastes generated by the COVID-19 pandemic. Thus, to achieve that goal, this paper presents an improved computational model that replicates a high-temperature thermal treatment system for COVID-19 wastes using plasma gasification in Aspen Plus V12.2. The distinctive aspect of the present plasma gasification model is the inclusion of an extra Gibbs reactor in order to enhance the calorific value of the syngas. The model validation results show an increase in the CO and CH₄ molar fractions and a decrease of the H₂ and CO₂ molar fractions, which allows to increase the calorific value of the syngas from 4.97 to 5.19 MJ/m³. The most common types of hazardous waste generated during the pandemic were determined to be masks and syringes. COVID-19 waste from Turkey, discarded masks from Indonesia, Korea, and Lithuania, and Chinese syringes were used as feedstock into the computational model. The results suggest that the hazardous waste that allows for higher hydrogen molar fractions is Korean masks. On the other hand, the highest carbon monoxide molar fractions are obtained with medical waste from Turkey, while the highest molar fractions of methane are obtained with medical waste from Lithuania. A conclusion could be drawn that the lowest syngas calorific value is obtained with medical wastes from Turkey, while the highest syngas calorific value is obtained with medical wastes from Korea.

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1. Introduction

Hazardous waste is produced mainly in industry and the health sector [1]. This is even more evident after the COVID-19 pandemic. According to the OMS and the European Council, waste produced to carry out infection

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prevention measures is classified as hazardous waste. There was an estimated increase of 280 tonnes per day of hazardous waste, which overcharged the treatment facilities and storage [2]. This type of waste requires more careful treatment because of its danger to public health. They should be stored separately in specific areas that should have a controlled environment. Subsequently, suitable means of transport should collect this waste and take it to appropriate treatment centers, which causes high costs. Given the fact that the SARS-CoV-2 virus remains on a surface for up to 72 h, appropriate means should be used to transport hazardous waste to the high temperature treatment center [3], since the OMS recommended the treatment of this type of waste at high temperatures in order to neutralize its negative impact. Since there are few high-temperature treatment centers, most countries have to export this type of waste. This process is extremely expensive, and therefore inadequate management practices are often used in an attempt to save economic resources. For this reason, often these wastes are deposited as conventional waste, which results in waste being dumped into the environment improperly. This phenomenon may pose serious risks to public health with the accumulation of hazardous waste in landfills. That poses a serious threat to the entire ecosystem. Fortunately, nowadays, the governments of developed countries have increasingly defined their policies in order to promote the right destination for waste. Government policies have clearly targeted thermal waste treatments due to safety, environmental risks, and high volume and weight reduction.

Within the thermal treatment processes, plasma gasification is already considered one of the most promising, since it complies with the emissions imposed by the requirements of European Council 2000/76/EC and is capable of neutralizing the harmful components through thermal destruction [4]. Therefore, since the environmental performance of a heat treatment system is extremely important to evaluate its effectiveness, application potential, and acceptance by the population, the plasma gasification will be modeled for the treatment of hazardous waste.

There are numerous methods for modeling a gasification process, including computational fluid dynamics (CFD), kinetic, thermodynamic equilibrium, and artificial neural networks [5]. Due to the fact that Aspen Plus has an extensive database for modeling and optimizing a complex chemical process, this software has been used to evaluate the potential of plasma gasification plants as well as the result of the final composition of syngas [6,7].

A sample of medical waste (MW) can contain paper, plastic, food, and other types of materials [8]. Erdogan and Yilmazoglu [2] claim that this type of material can be composed of up to 54% paper, 20% textile, 10% metal, 50% plastic, and 26% organic. When these characteristics are compared to municipal solid waste (MSW), many similarities are discovered [2]. According to various experimental and numerical studies in the literature, it is evident that MSW can be used to generate energy. An example of that is the work on performance assessment of the co-gasification for sustainable management of municipal solid waste in Morocco [9] or the work on modeling and simulation of a fixed bed gasification process for the thermal treatment of municipal solid waste and agricultural residues [10].

The plasma gasification process comprises three phases: drying, pyrolysis, and combustion. Thus, the model used must guarantee each of these phases [11]. In order to maximize the lower heating value (LHV) of syngas, that is, the energy that it releases when burned and that can be used to produce energy, an additional reactor was implemented to enhance the reactions of water-gas-shift and methanation which mainly promote the increase of CO and CH₄.

The main objective of this work is the development and analysis of a sustainable way to treat wastes generated by the COVID-19 pandemic. As SARS-CoV-2 has spread all over the world, it is particularly relevant to analyze MW from different countries. For this purpose, several bibliographies were consulted in order to identify the proximate and ultimate analyses. As already mentioned, the Aspen Plus V12.2 software was used for modeling and simulating the plasma gasification process. Its functionalities will allow the possibility of understanding what happens to the LHV of the syngas when additional reactors promoting the water-gas-shift and methanation chemical reactions are introduced. The introduction of an additional reactor to the basic plasma gasification process constitutes an innovation in relation to the typical Aspen Plus plasma gasification models such as those of Favas et al. [12] or Zhang et al. [13].

The methodology followed in this work starts with first analyzing which types of MW were most frequently discarded during the pandemic (e.g., masks and syringes). Then, we analyze in which locations of the world the generation of this waste was more pronounced in order to select them as the feedstock for the plasma gasification process. The next step is the development of the simulation model in Aspen Plus V12.2. To make this model reliable, is necessary to validate it by comparing it with works carried out by other authors using the same raw material (MW) and also materials of similar composition (MSW), always respecting the operating conditions. Once the model is validated, it is used to simulate the syngas composition obtained from the different MW in order to understand whether a particular type of waste is more promising for future studies.

2. Materials and methods

2.1. Aspen plus model

This study aims to validate the computational model illustrated in Fig. 1, carried out in Aspen Plus V12.2. It is necessary to obtain credible results, so these results have to be compared with the values of other authors.

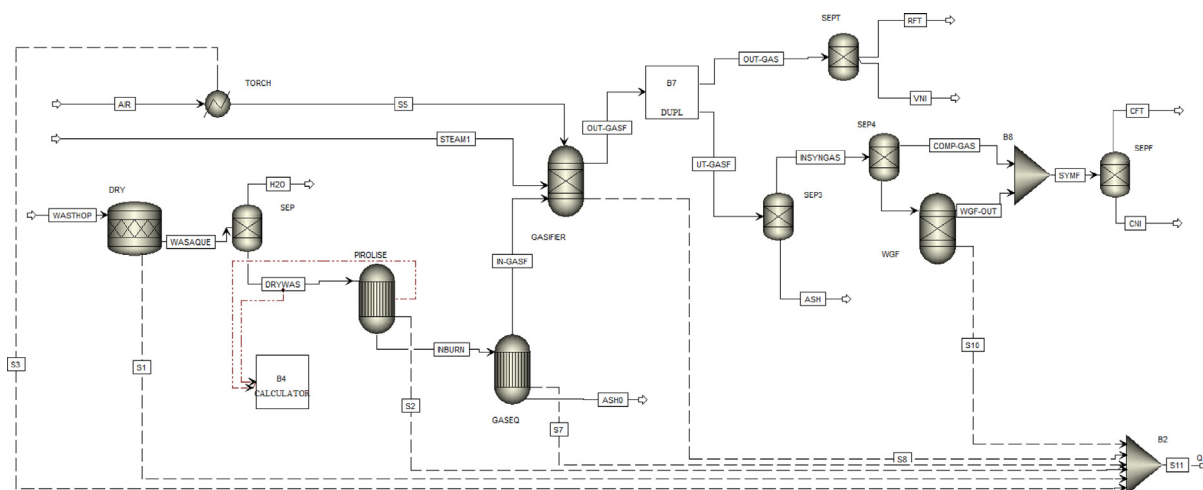


Fig. 1. Plasma gasification model developed in Aspen Plus for medical waste treatment.

However, before demonstrating this process of convergence of values, it is important to explain the arrangement of blocks present in Fig. 1. The model starts with the entry of MW (WASTHOP) into the heat exchanger (DRY). The function of the heat exchanger (DRY) is to remove moisture from the sample, which results in a dry MW (DRYWAS), which will undergo the pyrolysis process. The block that simulates this process and allows the MW to decompose into its constituent elements is a “RYIELD” reactor. There is also, as can be seen in Fig. 1, another “B4 CALCULATOR” block that determines the quantities of each of these constituent elements by a FORTRAN calculation method.

After that, the flow into the incinerator goes to the first gasification stage. Here, a “requil reactor” is used, since this device allows placing the reactions that occurred during the gasification process.

This first gasification stage increases the temperature of the waste in order to accelerate combustion, increasing the probability of complete combustion in the second combustion stage. It is also possible to carry out a first ash cleaning.

In this way, the first gasifier is equivalent to a first combustion chamber, while the second gasifier can be seen as a second chamber, represented by an “RGibbs reactor”. It uses the Gibbs free energy minimization method to calculate the resulting composition of the gasification process using the state of phase and chemical equilibrium.

Analyzing Fig. 1, two flows are injected into this gasifier: a flow of steam and another of air that will be ionized by the torch. Using the same conditions as those imposed in our model, it is possible to compare the results of the final composition of the syngas produced.

After this second gasification stage, a “Manipulator Dupl” block was placed. This feature allows you to duplicate the properties of the gasifier’s output flow, “OUT-GASF”, in two other flows that have the same properties as the latter: “OUT-GAS” and “UT-GASF”.

This breakdown was carried out to evaluate the effects of subjecting the flow out of the second gasifier to another reactor, “WGF”, which characterized the water-gas-shift and methanation reactions. Later, the UT-GASF flow with properties equal to OUT-GASF is taken to a new separator, “SEP3”, so that ash is removed from this flow. Subsequently, another separator is added to the model in order to isolate the elements that participate in the water-gas-shift and methanation reactions, which are supplied to an extra Gibbs reactor (WGF). The resulting products are mixed again with the elements that do not participate in these reactions and were found in the flow

resulting from the action of “SEP3”. After this mixture, “SYMF” flow is created, being directed to a new separator: “SEPF”, which separates the flow into “CFT” and “CNI”.

2.2. Model validation

The developed model was validated against literature-based data from Erdogan and Yilmazoglu [2]. The proximate and ultimate analyses of MW, considered for model validation purposes, are shown in Table 1.

Table 1. Proximate and ultimate analyses of the medical waste sample [2].

Proximate analysis		Ultimate analysis	
Moisture	0.32%	C	81.81%
Ash	0.00%	H	12.17%
Volatiles	99.13%	O	5.76%
Fixed carbon	0.55%	N	0.15%
		S	0.11%

Taking into account the plasma gasification model in Fig. 1, the results of the syngas are in Table 2.

Table 2. Comparison between model results and literature data.

Parameter	This study	Erdogan and Yilmazoglu [2]	Relative error %
Temperature	1990 °C	1990 °C	–
H ₂	25.39%	27.96%	9.19
CO	17.66%	20.77%	14.97
CO ₂	7.48%	9.04%	17.26
CH ₄	0.00%	0.00%	0.00
H ₂ O	0.00%	0.00%	0.00
N ₂	49.47%	42.22%	17.17
O ₂	0.00%	0.00%	0.00
LHV	4.97 MJ/m ³	5.64 MJ/m ³	11.83

Considering that in a CFD model the fluid mechanics are treated in detail, this is the crucial distinction when CFD is compared with other kinds of models. On the other hand, equilibrium models, such as the one used in this work, predict the thermodynamic limits of the chemical reaction process. Therefore, the CFD model is far more precise than equilibrium models, especially considering such a complex process as gasification. However, equilibrium models continue to be very important for the prediction of syngas compositions in relation to variations in the operating parameters, providing an irreplaceable instrument for process design and development purposes before attempting experimental investigations.

Analyzing Table 2, it is concluded that the values simulated are very comparable to the values presented by Erdogan and Yilmazoglu [2]. The maximum relative error found is 17.26%, which can be explained by the different models used. In the case of this study, an equilibrium model was used, while in the study of Erdogan and Yilmazoglu [2], a CFD model was used. Relative errors below 20% are generally considered a good performance for the equilibrium model given the complex nature of the biomass gasification process [14]. This degree of divergence can be attributed to the model's nature and assumptions, suggesting that it is reasonable to continue the study with the developed model.

2.3. Hazardous waste characterization

The recovery of energy contained in MW is a sustainable and ecological way to eliminate them. Given the fact that preventive safety measures for human health involved the use of masks as well as mass vaccination to transmit antibodies against the SARS-CoV-2 virus, masks will be analyzed and discarded in different regions: Indonesia, Lithuania, and Korea. Syringes from the preventive vaccination against the pandemic from China will also be used as another material. In addition, the MW with which the model was validated was also evaluated. In Table 4 are the approximate and ultimate analyses of these residues.

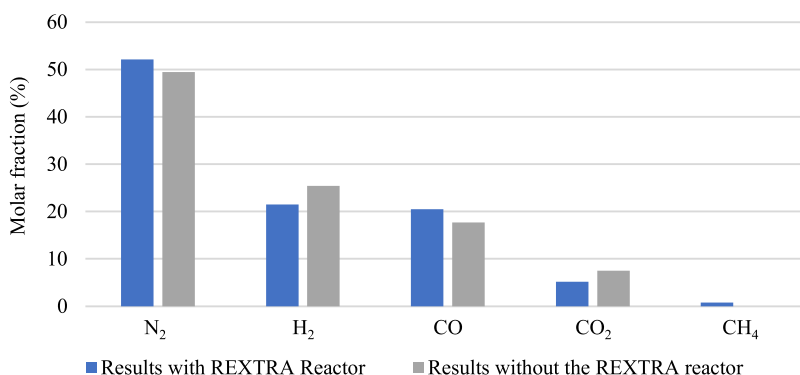
Table 4. Main reactions [20].

Reaction type	Reactions
Water Gas Shift:	$\text{CO}_2 + \text{H}_2 \leftrightarrow \text{CO} + \text{H}_2\text{O} - 41.2 \text{ kJ/kmol}$
Methanation reactions:	$2\text{CO} + 2\text{H}_2 \leftrightarrow \text{CH}_4 + \text{CO}_2 - 247 \text{ kJ/kmol}$
	$\text{CO} + 3\text{H}_2 \leftrightarrow \text{CH}_4 + \text{H}_2\text{O} - 206 \text{ kJ/kmol}$
	$\text{CO}_2 + 4\text{H}_2 \leftrightarrow \text{CH}_4 + 2\text{H}_2\text{O} - 165 \text{ kJ/kmol}$

The system in Fig. 3, compared to the system at the top of Fig. 1, has one additional reactor, “REXTRA”. This addition aimed to optimize the system so that the highest possible amounts of CH_4 , CO , and H_2 were produced, and consequently LHV too. It is known that the higher the LHV, the greater the amount of heat released by syngas during its combustion, thus making syngas richer and more capable of producing energy.

To accomplish this, a separator, “SEP2”, was installed at the exit of the “GASIF1” to separate the ashes from the “OUT-GASF” gas stream. Once this is accomplished, the stream “SYNGASIN” is imposed on “SEP3”, which separates the components O_2 , H_2 , CO , and CO_2 so that they enter the reactor “REXTRA”, where water-gas-shift and methanation reactions occur (Table 4).

Fig. 4 shows a comparison between the molar fractions of the main syngas species before and after the water-gas-shift and methanation reactor (REXTRA). The high composition of H_2 , CO , and CH_4 in terms of percentage is due to the fact that only the intended components are isolated in this gas flow, making it necessary to mix the flow again in the “B8” mixer.

**Fig. 4.** Comparison of Syngas elemental composition results with and without the REXTRA reactor.

Carrying out the LHV calculations only for this fraction of the syngas flow part, it can be seen that “REX-IN” presents a value of 9.82 MJ/m^3 , while “REX-OUT” presents 10.04 MJ/m^3 . Given that the process taking place in “REXTRA” is exothermic, the addition of this reactor allows for a more profitable final energy balance. The LHV of the syngas after the B8 mixer increases from 4.97 to 5.19 MJ/m^3 . Therefore, it can be concluded that the addition of the REXTRA reactor is beneficial.

3. Results and discussions

The results will include a comparison of the syngas produced by various MWs. These aim to understand which material is the most valuable, and they also intend to demonstrate that although most of the waste is of the same type (masks), they come from different locations in the world.

In this analysis, the operational conditions used were the same as those that allowed the validation of the model; however, as operational parameters are modified, the influence of the torch temperature and the modification of the flow of gasification agents can be evaluated: air flow and steam flow.

The purpose of using a certain material may be to obtain the maximum production of LHV for syngas or the maximum production of H_2 , CH_4 , or CO . The purpose of using a certain material may be to obtain the maximum production of LHV for syngas or the maximum production of H_2 , CH_4 , or CO .

It is important to individually analyze the results of the sensitivity analyses for each material since the heat treatment of each of them can dictate that different optimal operating conditions are used so that the maximum production of LHV, CO, H₂, or CH₄ is achieved.

Given the large number of analyses that must be performed, such as the effect of torch temperature and air and steam flow on the final composition of syngas in terms of CO, CH₄, H₂, and LHV. In this way, as a result of this work, the thermal treatment of the different wastes originated by the COVID-19 pandemic will be discussed through the plasma gasification system shown in Fig. 3, which already presents the benefit of using the extra reactor.

The raw materials to be analyzed are those shown in Table 3. Under normal operating conditions, the model has an injected air flow of 0.04362 kg/s, an injected steam flow of 0.0029 kg/s at 400 °C, a waste flow rate of 0.029 kg/s, and a torch temperature of 1500 °C. The results of the syngas composition are shown in Fig. 5.

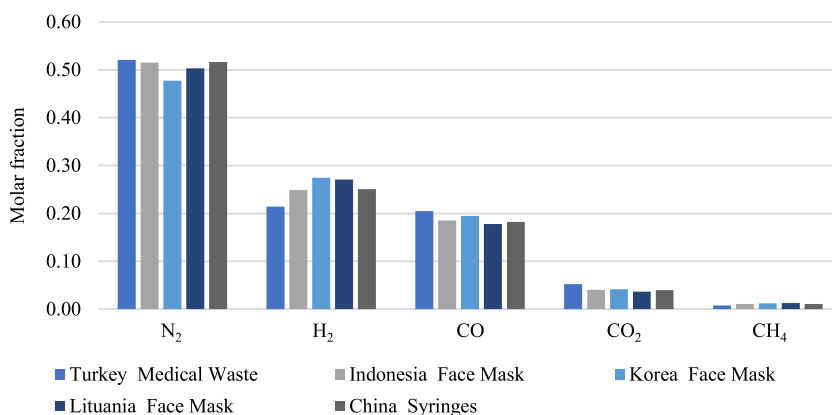


Fig. 5. Comparison of the final composition of syngas obtained from the plasma gasification of different medical wastes.

It can be concluded from Fig. 5 that the results are similar for all medical wastes. Identifying the composition of the three most significant elements, which are hydrogen, carbon monoxide, and methane, it is clear that the medical waste that allows a higher molar fraction of hydrogen is the Korean masks. On the other hand, the medical waste that allows the highest CO molar fractions is the medical waste from Turkey, while the highest composition of methane is obtained for the medical wastes from Lithuania.

The rationale for these results is based on the feedstock characteristics and the inclusion of the extra Gibbs reactor. From Table 3, it is possible to verify the similar composition of the various MW, with the distinctive aspect of the lower percentage of volatiles and carbon in Korean masks and their higher hydrogen and oxygen contents. The volatiles are released in the pyrolysis step, generating CO, H₂, and hydrocarbons (mostly CH₄) as gas products [21–23]. The highest amount of hydrogen in the feedstock is reflected in the syngas hydrogen content. The highest oxygen content enhances the carbon incomplete combustion reaction, which together with the Boudouard reaction generates higher amounts of CO. Moreover, the extra Gibbs reactor enhances the water-gas-shift and methanation reactions expressed in Table 4, magnifying the CO and CH₄ contents and reducing the hydrogen and carbon dioxide contents in the syngas.

Fig. 6 shows that the syngas produced through the syringes has practically the same LHV as the syngas produced from Indonesian face masks. It is also noted that the syngas with less LHV was from Turkey (MW), while the syngas with greater LHV was from Korea.

Another interesting detail to analyze is the difference in lower heating value for the disposable masks. Depending on its origin, syngas produced under the same operating conditions and in the same heat treatment system has a higher LHV if the masks come from Korea and a lower value from this entity if the masks come from Indonesia. Given that the objective of this study is to maximize the energy use of the syngas produced, it can be considered that the most advantageous medical waste to employ in a plasma gasification treatment plant is the ones coming from Korea.

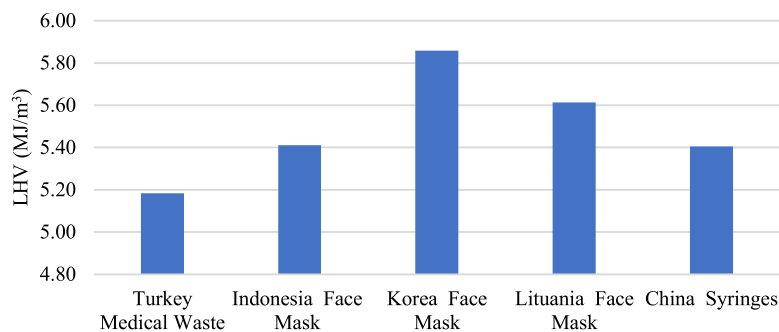


Fig. 6. Effect of SFR on syngas composition.

4. Conclusions

This work presents an improved plasma gasification model developed in Aspen Plus V12.2 as a thermal treatment method for COVID-19 wastes from different parts of the world. An extra Gibbs reactor was included in the model to enhance the water-gas-shift and methanation reactions based on the hypothesis of increasing the calorific value of the syngas. COVID-19 waste from Turkey, discarded masks from Indonesia, Korea, and Lithuania, and Chinese syringes were used as feedstock into the improved model. The results suggested that:

- The inclusion of an extra Gibbs reactor allows for an increase in the calorific value of the syngas from 4.97 to 5.19 MJ/m³ by increasing the CO and CH₄ and decreasing the H₂ molar fractions.
- The hazardous waste that allows for higher hydrogen molar fractions is Korean masks.
- The highest carbon monoxide molar fractions are obtained with medical waste from Turkey, while the highest molar fractions of methane are obtained with medical waste from Lithuania.
- The lowest syngas calorific value is obtained with medical wastes from Turkey, while the highest syngas calorific value is obtained with medical wastes from Korea.

A general conclusion could be drawn pointing to the facemask wastes from Korea as the most promising for further studies since a higher calorific value and higher hydrogen yields can be achieved.

Declaration of competing interest

I (we) certify that there is no conflict of interest with any financial organization regarding the material discussed in the manuscript.

Data availability

No data was used for the research described in the article.

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