Since January 2020 Elsevier has created a COVID-19 resource centre with free information in English and Mandarin on the novel coronavirus COVID-19. The COVID-19 resource centre is hosted on Elsevier Connect, the company's public news and information website.

Elsevier hereby grants permission to make all its COVID-19-related research that is available on the COVID-19 resource centre - including this research content - immediately available in PubMed Central and other publicly funded repositories, such as the WHO COVID database with rights for unrestricted research re-use and analyses in any form or by any means with acknowledgement of the original source. These permissions are granted for free by Elsevier for as long as the COVID-19 resource centre remains active.
Optimization of gasification process parameters for COVID-19 medical masks using response surface methodology

Benjapon Chalermsinsuwana, Yueh-Heng Lib, Kanit Manaturac,∗

a Department of Chemical Technology, Faculty of Science, Chulalongkorn University, Bangkok, Thailand
b Department of Aeronautics and Astronautics, National Cheng Kung University, Tainan, Taiwan, ROC
c Department of Mechanical Engineering, Faculty of Engineering at Kamphaeng Saen, Kasetsart University, Kamphaeng Saen campus, Nakhonpatom, Thailand

Received 2 May 2022; revised 30 June 2022; accepted 22 July 2022
Available online 26 July 2022

KEYWORDS
COVID-19; Medical waste; Gasification; Optimization; Response surface methodology

Abstract Due to the COVID-19 pandemic, large amounts of medical wastes have been produced and their disposal has resulted in environmental and human health problems. This medical waste may include face masks, gloves, face shields, goggles, coverall suits, and other related wastes, such as hand sanitizer and disinfectant containers. To address this issue, the effect was investigated of gasification process parameters (type of COVID-19 medical mask based on the polypropylene ratio, pressure, steam ratio, and temperature) on hydrogen syngas and cold gas efficiency. The gasification model was developed using process modeling based on the Aspen Plus software. Response surface methodology with a 3k statistical factorial design was used to optimize the process aiming for the highest hydrogen yield and cold gas efficiency. Analysis of variance showed that both the steam ratio and temperature were significant parameters regarding the hydrogen yield and cold gas efficiency. Proposed models were constructed with very high accuracy based on their coefficient of determination (R²) values being greater than 0.97. The optimum conditions were: 65 % polypropylene in the mixture, a pressure of 1 bar, a steam ratio of 0.38, and a temperature of 900 °C, producing a maximum hydrogen yield of 40.61 % and cold gas efficiency of 81.43 %. These results supported the efficacy of the primary design for steam gasification using a mixture of plastic wastes as feedstock. The hydrogen could be utilized in chemical applications, whereas the efficiency could be used as a basis for further development of the process.

© 2022 THE AUTHORS. Published by Elsevier BV on behalf of Faculty of Engineering, Alexandria University. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

1. Introduction

The COVID-19 epidemic has impacted humans globally from many aspects, including lifestyle, work conditions, and especially health. SARS-CoV-2 or the COVID-19 virus can be...
conveyed by droplet transmission (coughing and sneezing) and contact transmission (oral, nasal, and eye mucous membrane) [1]. To protect against the virus, personal protective equipment (PPE) has been widely utilized including face masks, gloves, face shields, goggles, coverall suits, and other related items, such as hand sanitizer and disinfectant containers. It was reported that the PPE decreased aerosol transmission of the infectious influenza virus by 94–99% [2]. The used products have been termed ‘COVID-19 municipal waste’ (CMW) [3].

Face masks have been extensively used by most people and their use has been enforced by many governments around the world [4]. The mask is usually made from polymeric materials, commonly polypropylene (PP), polyethylene (PE), and polyesters (PES). The fraction of PP constitutes the greatest portion of the mask, followed by PEs and PE [5]. The global use of PPE has resulted in large amounts of plastic waste and pollution in the environment, including in landfills, rivers, and oceans [6]. In addition, the waste has a direct impact on human health, especially food safety [7], when some of its components enter the human body by ingestion and inhalation causing likely respiratory symptoms and lung cancer [8]. Thus, optimal waste treatment technology is a mandatory requirement in waste management for the safe treatment of the daily accumulation of CMW.

Thermal treatment technology is a promising method to deal with municipal waste and contaminated materials [9,10], especially CMW (fluffy material), because it is easier to dry and co-treat with other solid fuel or waste [3]. It not only eliminates the waste but also provides energy and material recovery. A temperature greater than 800 °C for 1 min is required to nullify infection from CMW [11]. Four technologies of thermal treatment (combustion, carbonization, pyrolysis, and gasification) are commonly used to handle CMW. Among these four, combustion in an incinerator is generally applied. A temperature greater than 800 °C can treat CMW and destroy the virus [12]. However, the resultant environmental impact, including high CO2 emission and fuel consumption, are negative outcomes. Furthermore, there is a high cost associated with cleaning the flue gas system to meet the air pollution emission regulations. Carbonization and pyrolysis are possible choices to adapt waste treatment [3]. However, the high risk of inadequate conditions in waste degradation can be a problem when a large number of harmful volatile gases are released.

Gasification is an effective method for energy production and chemical applications [13]. Synthetic gas (syngas) including hydrogen, carbon monoxide, carbon dioxide, methane, and longer chains of hydrocarbon gases, is transformed from solid carbon under the high temperature of gasifying agents (air, steam, and CO2 or their mixture) in a controlled atmosphere [14]. A great advantage of gasification is its flexibility to accommodate mixtures of plastics and other feedstock with no significant effect on the syngas quality [13]. Thus, it has been considered a good choice for the treatment of plastic wastes, especially CMW [15]. Syngas quality relies on the applied gasifying agent such as air, steam, oxygen, or their mixture. Gasification of plastic wastes with air can produce an average syngas heating value of 6–8 MJ/Nm3 [16]. Gasification using steam can produce a higher syngas heating value (above 15 MJ/Nm3) [17].

Studies involving optimization of process parameters in plastic gasification are mostly conducted using the one-factor-at-a time method a full or fractional factorial design, Taguchi design, response surface methodology (RSM), and design of experiments (DOE) [18]. However, many factors are involved in the gasification process that may influence each other simultaneously during syngas production. Thus, the main and interaction effects of the parameters must be studied to understand the process and this normally involves using statistical methods. One of the most promising methodologies to examine process parameters and their interactive effects is response surface methodology (RSM) [19]. RSM can be applied in situations involving multiple variables or measures, allowing mathematical modeling to be created to obtain the system with the best efficiency [20].

To date, numerous studies involving the gasification process have been conducted, including biomass, coal, biomass-coal blending, waste plastic, and more recently biomass-plastic as feedstocks in steam gasification. For example, Wilk and Hofbauer [21] reported on a plastic mixture in 100 kW dual fluidized bed steam gasification. They operated their gasification reactor using olivine as an in situ primary catalyst at 850 °C with a steam/plastic (S/P) ratio of 2. The effects were investigated of the gasification temperature and the plastic blending ratio on gasification performance based on product distributions and the lower heating value (LHV) of the syngas. They found the H2 concentration reached 40 % for gasification of PE and PP. Erkiaga et al. [22] carried out steam gasification of High Density Poly Ethylene (HDPE) in continuous mode in a conical spouted bed reactor. They found at 850–900 °C, the hydrogen yield in the syngas was above 60% and the carbon conversion efficiency was as high as 91%. They recommended this range as suitable for gasification to achieve a high yield of H2 and a low yield of tar. Both Wilk and Hofbauer [21] and Erkiaga et al. [17] concluded that the produced syngas was attractive for the synthesis of dimethyl ether [22]. They also concluded that the temperature was the most significant factor because it boosted the endothermic cracking reactions relating to hydrocarbons and tar, which increased the syngas and hydrogen production in plastic steam gasification. Dou et al. [23] conducted a continuous fluidized bed gasifier combined with steam reforming/CO2 adsorption in a moving bed reactor. The effect of steam reforming on the Ni-Al2O3 catalyst and CO2 retention on CaO resulted in a high yield of H2. An operating temperature below 700 °C was necessary for active CO2 adsorption. Mojaver et al. [24] applied Taguchi analysis to study the hydrogen-rich syngas yield and exergy destruction rate of steam gasification for polyethylene, polypropylene, polycarbonate, and polyethylene terephthalate. The maximum hydrogen production and minimum exergy destruction rates were used for optimization in that study. They found the optimum conditions were polyethylene waste with a 1.75 steam-to-plastic ratio and at 1,300 K, 10 % moisture, and 400 kPa pressure. The hydrogen content was 66.71% and the exergy destruction rate was 54.86 kW for the optimum conditions.

To the best of our knowledge, there has only one work (Mojaver et al. [24]) using an optimization technique on the operating parameters for plastic in the steam gasification process. Steam gasification is suitable for operating with mixtures of polypropylene (PP) and polyethylene (PE) that are main components of COVID-19 medical waste [3]. This process also produces a high hydrogen yield and a high syngas heating value. Details for distinguishing between steam and hydrother-
mal gasification are listed in Appendix (Table A1). Thus, the aim of the current study was to optimize the steam gasification of the waste plastic mixture (PP and PE) using RSM via full fractional design based on process modeling using the Aspen Plus software by simulating the syngas composition from gasification modeling. It was expected this would lead to identifying the optimal conditions for maximizing the hydrogen yield and cold gas efficiency of gasification. The hydrogen could be used in chemical applications, whereas the efficiency could be used as a benchmark for improving the process [21]. The effects of the input variables (polypropylene ratio in the mixture and the pressure, steam ratio, and gasification temperature) on these two responses were investigated and optimized using RSM.

2. Materials and methods

2.1. Feedstock selection

COVID-19 medical masks mainly consist of two types of plastics (PP and PE) [25]. They were selected as the feedstock and for optimization in this study. Different PP contents (in weight %) of 65 % (PP65), 75 % (PP75), and 80 % (PP85) were investigated in the plastic mixture with (PP + PE) levels of 65 %, 75 %, and 85 % by weight%, respectively, as shown in Table 1. Table 2 presents the proximate and ultimate analyses, heating values, and chemical formulas of the plastic mixtures. It was noticed that the properties of PP and PE were very similar. Thus, it might be expected that similar amounts of syngas would be produced.

2.2. Gasification process simulation

The gasification process was modeled using the Aspen Plus software to predict the amount of syngas produced from the process. The general steam gasification process flow chart is shown in Fig. 1 and consists of three steps. First, the selected feedstock is decomposed in DECOMP where non-conventional feedstock is converted to conventional feedstock. Then, it is sent for gasification in GASIFIER where steam is injected to generate raw producer gas under thermodynamic equilibrium conditions. In this state, the heat requirement is the residence time of the reactants is longer enough to reach chemical equilibrium. The gasifier performs at the thermodynamic equilibrium; the heat capacity and density of the mixture, and chemical formulas of the plastic mixtures, was considered as a non-conventional element based on their proximate and ultimate analyses. The MCINCPSD stream class includes three sub streams (MIXED, CIPSD, and NCPSD) that were used in this model. The HCOALGEN and DC0ALIGT models were chosen to determine the heat of formation, and the heat capacity and density of the mixture, respectively.

The process diagram of the plastic waste gasification simulation using Aspen Plus is shown in Fig. 2. Brief explanations of the unit operations of the blocks are provided in Table 4. The stream PP was fed into the system and was heated with N2 by block DRY-REAC (RStoic model). In the block, some parts of the PP reacted to form water that was expelled by DRYFLASH with EXHAUST stream, leaving DRYPP. Next, DRYPP passed to the devolatilization stage operated in the block DECOMP for which the Ryield reactor was used. The PP was converted from non-conventional solid into volatiles and char in DECOMP. The volatiles from ultimate analysis include carbon, hydrogen, oxygen, and nitrogen, while the char was transformed into ash and carbon [28]. The yield was the same as the volatile content based on the proximate analysis. In DECOMP, the real yield distributions were also calculated using a calculator block which was modeled by the FORTRAN statements corresponding to the feedstock components. A GASIFIER block represents gasification of the PP which minimized the Gibbs free energy to obtain the chemical equilibrium. Heat requirement (Qin in Fig. 1) was applied to maintain the equilibrium state. Conventional water (H2O) was heated by the block HEATER to form steam (STEAM) and injected into the gasifier to generate syngas. Finally, the produced syngas was separated into two streams (SYNGAS and ASH) in the block SEPARATE using a cyclone separator. Values of SYNGAS were then used in the analysis of gasification performance and to obtain other statistics. Detailed information on the modeling is provided in Appendix B (Table B1 and Fig. B1).

2.3. Gasification reaction

Gasification is a complex process that involves many heterogeneous reactions [30].

Drying zone.

\[ \text{Moist plastic} + \text{Heat} \rightarrow \text{Dry plastic} + \text{H}_2\text{O} \]  
\hspace{1cm} (1)

Pyrolysis zone.

\[ \text{Dry plastic} + \text{Heat} \rightarrow \text{Char} + \text{Volatiles} \]  
\hspace{1cm} (2)
Partial oxidation zone.

Char partial oxidation.

\[ C + 0.5O_2 \rightarrow CO, \Delta H^0 = -111kJ/mol \] (3)

CO partial oxidation.

\[ CO + 0.5O_2 \rightarrow CO_2, \Delta H^0 = -283kJ/mol \] (4)

\[ H_2 + 0.5O_2 \rightarrow H_2O, \Delta H^0 = -242kJ/mol \] (5)

\[ C + CO_2 \leftrightarrow 2CO, \Delta H^0 = +172kJ/mol \] (6)

\[ C + H_2O \leftrightarrow CO + H_2, \Delta H^0 = +131kJ/mol \] (7)

\[ CO + H_2O \leftrightarrow CO_2 + H_2, \Delta H^0 = -41kJ/mol \] (8)

\[ C + 2H_2 \leftrightarrow CH_4, \Delta H^0 = -75kJ/mol \] (9)

\[ CH_4 + H_2O \leftrightarrow CO + 3H_2, \Delta H^0 = +206kJ/mol \] (10)

Gasification performance can be determined based on an important index of the system, namely the cold gas efficiency (CGE) [28], which is the ratio of the energy in syngas as a product of the syngas volume flow rate and its associated LHV and the mixture higher heating value. The LHV of syngas can be presented as Eq.(11) [31]:

\[ LHV_{syngas}(kJ/Nm^3) = (30.0y_{CO} + 25.7y_{H_2} + 85.4y_{CH_4}) \times 4.2 \] (11)
where \( y \) represents the mole fraction of the syngas species (dry basis) obtained from the model developed in Aspen Plus. In addition, the CGE is expressed as:

\[
\text{CGE} \% = \left( \frac{\text{SG}}{\text{HHV}_{\text{syngas}}/C_2} \right) \times 100
\]

where \( \text{SG} \) is the volume of syngas per unit weight of fuel \((\text{Nm}^3/\text{kg}_{\text{fuel}})\) obtained from the developed model and \( \text{HHV}_{\text{fuel}} \) is the higher heating value of the plastic waste \((\text{MJ/kg}_{\text{fuel}})\) obtained from Table 2.

\( \text{H}_2 \) yield can be obtained from the Aspen Plus results and can be presented as the mole fraction of the dry syngas as determined from Eq. (13):

\[
\text{H}_2 \text{ yield} = \frac{y_{\text{H}_2}}{y_{\text{H}_2} + y_{\text{CO}} + y_{\text{CH}_4} + y_{\text{CO}_2} + y_{\text{N}_2}} \times 100
\]

### 2.4. Model validation

The developed model of steam gasification was validated by comparing the predicted results to the simulated results of Mojaver et al. [24]. In the literature, polyethylene, polypropylene, polycarbonate, and polyethylene terephthalate wastes were used as the feedstock in steam gasification. The steam-to-plastic waste ratio, temperature, moisture content, and pressure were used to determine the hydrogen yield and exergy destruction rate. The Taguchi method was employed to evaluate and optimize the process. The results from the validation between this study and the literature are shown in section 3.1.

### 2.5. Experimental design

A three-level, three-factor \((3^3)\) factorial design was applied to determine the key effects, interaction effects, and quadratic effects of the gasification conditions (polypropylene ratio, pressure, steam ratio, and temperature) because they are the main parameters of steam gasification [21,32]. The response was based on the \( \text{H}_2 \) yield in syngas and the CGE. Coding of the independent factor consisted of three levels \((+1, 0, -1)\) representing the minimum, intermediate, and maximum levels, respectively. The gasification ranges were selected from Zaman et al. [33] as presented in Table 1, based on the temperature and S/B ratio being in the ranges 650–900 °C and 0.6–1.5, respectively, in a study of the optimization of rice husk and almond shell steam gasification. Thus, our selected values were 0.1–1 and 700–900 °C for SR and T, respectively. In the statistical analysis and interpretation, the polypropylene ratio (PP), pressure (P), steam ratio (SR), and temperature (T) were denoted as A, B, C and D, respectively. The parameters and codes are summarized in Table 5.

### 2.6. Statistical analysis

The results were evaluated using analysis of variance (ANOVA) and regression analysis. A confidence level of 95 % \((P = 0.05)\) was selected to evaluate the statistical significance of the model. Descriptive statistics analyses consisted of ANOVA including the p-value, F-value, and degrees of freedom.
dom (DF), whereas the regression analysis was presented using
the coefficient of determination ($R^2$), the adjusted coefficient of
determination ($R^2_{adj}$), and the predicted coefficient of determi-
nation ($R^2_{pred}$) to compare developed models [34]. Their defini-
tions are presented in section 3.3. Finally, the regression model
was constructed as a two-dimensional response surface plot
and a three-dimensional response surface plot. These could
be used to optimize the response parameters.

3. Results and discussion

3.1. Model validation

The hydrogen content of the steam gasification for the five dif-
ferent conditions from Mojaver et al. [24] was used to validate
the developed model. They conducted steam gasification per-
formance of various plastic wastes (polyethylene (PE),
polypropylene (PP), polycarbonate (PC) and polyethylene
terephthalate (PET)). Four main parameters (steam-to-plastic
waste ratio, temperature, moisture content, and pressure) were
studied for their hydrogen-rich syngas and exergy destruction
rate. The comparisons are shown in Table 6. Errors in the
dry $H_2$ yield were in the range 0.49–2.60\%. The error may
have been due to differences in some of the selected properties
in the Aspen plus package. These results confirmed that the
predicted results agreed with the literature.

3.2. Effect of process parameters on gasification performance

A set of process variables (PP, P, SR, and T) were used to
model the response variables ($H_2$ and CGE) based on process
modeling using Aspen Plus. In total, there were 81 (34) runs, as
shown in Appendix A (Table A2). The $H_2$ and CGE varied
(1.62–68.11 vol% and 64.29–100.14 %, respectively) for PP
(65–85 %), P(1–7 bar), SR(0.1–1), and T(700–900 °C). The maximum and minimum $H_2$ yields were produced at 85 %,
1 bar, 0.1, 700 °C, and at 85 %, 7 bar, 1, and 900 °C for PP,
P, SR and T, respectively. The maximum and minimum values
for CGE were 85 %, 1 bar, 1, and 900 °C and 64 %, 1 bar, 0.1,
and 700 °C, respectively. These results indicated that the max-
imum values of $H_2$ and CGE were with the largest portion of
PP (85 %) and normal atmospheric pressure (1 bar). However,
main parameters studies and optimum conditions for steam
gasification must be investigated further.

3.3. Statistical analysis

ANOVA was performed to evaluate the contribution of
the main and interaction parameters to the model based on the
sum of squares (SS), F-value, p-value, and $R^2$, as presented
in Table 7. The four independent variables were denoted as
A for the polypropylene ratio (PP), B for the pressure (P), C
for the steam ratio (SR), and D for the temperature (T). Accord-
ing to Table 7, the obtained model of $H_2$ and CGE accounted for 99.94 % and 97.38 %, respectively, of the obtained data, based on the SS and displayed as %contribution, respectively. Fisher’s statistical test ($F_{test}$) was applied
to evaluate the effect of each factor on the model. Higher F-
value and lower p-values indicate the models are statistically
significant [34]. Fisher’s F-values for $H_2$ and CGE were
7320.11 and 175.16, respectively, whereas the associated p-
values were mostly lower than 0.05 (< 0.0001). These results
confirmed that the models were statistically significant, as
noted in Table 7. The accuracy of the model was also verified
based on the $R^2$ value with an $R^2$ value greater than 0.95 indic-
ating that more than 95 % of the data could be represented by
the model [35]. The $R^2$ values of the $H_2$ and CGE models were
0.9994 and 0.9738, respectively, indicating the accuracy of the
adopted models. The adjusted coefficient of determination ($R^2_{adj}$) is also a useful parameter to appraise model correction,
as it adjusts the $R^2$ value of the model based on the number of
terms. [36]. The $R^2_{adj}$ values were greater than 0.95, verifying
that the adopted models were highly accurate for the responses
according to the given conditions. In addition, the predicted
$R^2$ ($R^2_{pred}$) and $R^2_{adj}$ values were very similar (~0.2 in differ-
ence) for the models [37]. Thus, the variables chosen were suit-
able in the developed regression model. Table 7 shows the
significance of the main and interaction effects on the
responses by contribution based on the SS. The influence on
$H_2$ was C > D > CD > B > D2 > BC > C2 > BD. C was the most influential factor with a contribution of
87.27 %, followed by D with 10.27 %. The interaction factor
CD had a minor contribution (1.86 %), while the remaining
factors (B, D2, C2, and BD) contributed <1 %. Similarly, the
effect of CGE was D > C > CD > D2. Based on contribu-
tion, the most important factor was D (48.99 %) followed by
C (34.56 %), interaction CD (11.52 %), and D2 (1.32 %). Based
on the results in Table 7, the two mainly influences on
$H_2$ and CGE were the steam ratio (C) and temperature (D),
respectively. This finding was similar to Mojaver et al. [24]’s
who studied the optimum performance of steam gasification
on polyethylene, polypropylene, polycarbonate, and polyethy-
lene terephthalate waste. They found the gasification of
polypropylene waste produced highest the highest hydrogen
yield and the ratio of steam was the most important parameter,
followed by temperature for $H_2$, Zaman et al. [33] also
reported similar results, with the steam ratio and gasification
temperature being the main influences on steam gasification
using rice husks from optimization via RSM for the CGE.
In summary, the steam ratio and temperature were main influ-
encers for steam gasification.

| Plastic | SR | T (K) | MC (%) | P (kPa) | Mojaver et al. (vol%) | This study (vol%) | %Error |
|---------|----|------|--------|--------|----------------------|-----------------|-------|
| PE      | 1  | 1000 | 0      | 100    | 54.01                | 53.44           | 0.64  |
| PE      | 1.75 | 1100 | 10     | 400    | 63.62               | 64.33           | 1.75  |
| PE      | 1.75 | 1300 | 10     | 400    | 66.71               | 67.03           | 0.49  |
| PP      | 1  | 1100 | 20     | 1000   | 47.45               | 46.22           | 2.60  |
| PP      | 3  | 1200 | 10     | 100    | 69.72               | 68.37           | 1.94  |
3.4. Effect of process parameters on steam gasification performance

The average values of the responses and the variables were plotted as straight lines to identify the main and interaction effects. The lines represent the average of the responses at 3 levels (-1, 0 and +1), as shown in Figs. 3 and 4. The significance and whether the effect is positive or negative of each variable on the responses can be determined from the slope [38]. In Fig. 3, the most important effect on the H₂ yield was the steam ratio followed by the temperature. These results were consistent with the statistical analysis in Table 7. The polypropylene ratio (PP) and pressure (P) were less important in this response, as indicated by their steady trend lines. Increasing the PP contents in the mixture may not increase the H₂ yield due to the composition of PP and PE being very similar. Wilk and Hofbauer [21] found H₂ was in range 33–38 vol% compared to the current simulation result of 37 vol%. Increased pressure reduced the H₂ yield from 39.48 % to 36.62 vol%. This finding agreed with Kitzler et al. [39] where higher pressure led to reduced H₂ and CO while the yield of CO₂ and CH₄ increased. They recommended operating the gasifier under low pressure (<4 bar). It is known that steam gasification can increase the amount of hydrogen from water gas (Eq.(7)) and water gas shifts the reaction (Eq.(8)). If more steam is injected, more hydrogen will be produced [40]. However, this finding showed the opposite trend, which was consistent with Dong et al. [41]. This phenomenon probably occurred because at a higher steam ratio, the amount of steam was sufficient inside the reactor and so this was no longer the rate-limiting step. Then, any further increase in the steam ratio would not facilitate the reaction; on the contrary, this would result in less available heat in the reactor by the absorption of the excess steam.

![Fig. 3 Effects of variables on H₂ yield.](image1)

![Fig. 4 Effects of variables on CGE.](image2)

Table 7 ANOVA for quadratic model of H₂ and CGE.

| Source | Sum of Squares (SS) | % contribution | DF | F-value | p-value |
|--------|--------------------|----------------|----|---------|---------|
| H₂     |                    |                |    |         |         |
| Model  | 33534.74           | 99.94          | 14 | 7320.11 | < 0.0001|
| B-B    | 109.95             | 0.33           | 1  | 336.02  | < 0.0001|
| C-C    | 29284.47           | 87.27          | 1  | 89492.88| < 0.0001|
| D-D    | 3446.32            | 10.27          | 1  | 10531.91| < 0.0001|
| BC     | 17.31              | 0.05           | 1  | 52.90   | < 0.0001|
| BD     | 7.69               | 0.02           | 1  | 25.3    | < 0.0001|
| CD     | 622.79             | 1.86           | 1  | 1903.23 | < 0.0001|
| C²     | 14.14              | 0.04           | 1  | 43.20   | < 0.0001|
| D²     | 26.93              | 0.08           | 1  | 82.30   | < 0.0001|
| Residual | 21.68             | 6.52          |    |         |         |
| Total  | 33556.34           |                |    |         |         |

R² = 0.9994, R²_adj = 0.9992, R²_pred = 0.9990

| CGE    |                    |                |    |         |         |
|--------|--------------------|----------------|----|---------|---------|
| Model  | 7626               | 97.38          | 14 | 175.16  | < 0.0001|
| C-C    | 2706.72            | 34.56          | 1  | 870.38  | < 0.0001|
| D-D    | 3836.16            | 48.99          | 1  | 1233.57 | < 0.0001|
| CD     | 902.3              | 11.52          | 1  | 290.15  | < 0.0001|
| D²     | 103.75             | 1.32           | 1  | 33.36   | < 0.0001|
| Residual | 205.25            |                |    |         |         |
| Total  | 7831.25            |                |    |         |         |

R² = 0.9738, R²_adj = 0.9682, R²_pred = 0.9603
on the CGE, with similar slope trends. The polyethylene ratio and pressure did not have insignificant effects on the CGE, similar to the finding for the H₂ yield. The main reason for the steady trend in the polyethylene ratio was the similar components of the mixture. Increased pressure produced less H₂ and CO that was compensated by producing more CO₂ and CH₄. This compensation affected the CGE (Eq. (11)) which led to the steady trend in the pressure [42]. Increasing the temperature and steam ratio resulted in increasing the CGE. The water gas shift and methanation in Eq. (8) and (9), respectively, were the main contributors to the higher CH₄ production that improved the LHV of the syngas and increased the CGE. It seems that the temperature was more sensitive than the steam ratio because steam gasification favors temperature [21]. It can be concluded that the steam ratio and the temperature had the most significant effects on the H₂ yield and CGE. To predict the response variables (H₂ and CGE), the relationship between the input variables and responses was developed using second order polynomial equations with interaction terms. The proposed models are presented in coded factors in which PP, P, SR, and T are represented as A, B, C, and D, respectively, in Eq. (14) and (15):

\[
H₂ = 37.77 + 0.0311A - 1.43B - 23.29C - 7.99D - 0.0095AB - 0.039AC + 0.000804AD + 0.6934BC + 0.4622BD - 4.16CD - 0.0386A² + 0.5267B² + 0.8863C² - 1.22D²
\]

(14)

\[
CGE = 74.8 - 0.1226A + 0.2138B + 7.08C + 8.43D - 0.0099AB - 0.0004AC + 0.00064AD - 1.15BC - 0.6007BD + 5.01CD + 0.1541A² - 0.0112B² + 0.845C² + 2.4D²
\]

(15)

3.5. Optimum conditions

The current study investigated the optimum conditions of gasification to maximize both H₂ and CGE. Based on the second order polynomial equations, RSM was used to optimize the four input variables (PP, P, SR, and T). RSM is commonly utilized for optimizing, designing, and developing existing or new systems using statistical and mathematical techniques [43]. The optimal plots of the two main factors (SR and T) are presented in Fig. 5 and Fig. 6 for the H₂ yield and CGE, respectively. The values of SR and T were in the range from -1 (minimum) to 1 (maximum) while the H₂ and CGE were in the ranges 0–70 vol% and 60–100 %, respectively. H₂ was more sensitive to SR than T, based on its slope in Fig. 3 and its coefficient in Eq. (14). The CGE was affected by SR and T at similar levels, based on its slope in Fig. 4 and its coefficient in Eq. (15). Notably, H₂ and CGE showed opposite trends regarding the steam ratio and temperature. The maximum H₂ yield was achieved with lower SR (0.1) and T (700 °C) values, while the minimum yield was at higher SR (1) and T (900 °C) values. In contrast, the maximum CGE was achieved at higher SR (1) and T (900 °C) values, whereas the minimum CGE was at lower SR (0.1) and T (700 °C) values.

In this study, the H₂ yield and CGE were proposed to have equal importance (0.5 and 0.5, respectively) because both responses influence gasification performance. As shown in Table 8, the optimal conditions were at a polypropylene ratio of 65 %, pressure of 1 bar, a steam ratio of 0.38, and a gasification temperature of 900 °C to produce an H₂ yield of 40.61 % and a CGE of 81.44 %. Mojaver et al. [24] reported a steam-to-plastic waste ratio of 1.75, 1,300 K, 10 % moisture, and 400 kPa pressure to achieve hydrogen production of 66.71 %. Our findings produced a lower H₂ yield than this; however, our range was different and may be useful for gasification due to lower temperature and pressure. Similar results for CGE were observed by Zaman et al. [33]. They reported a CGE of 87.1 % at an operational temperature and S/B ratio of 800.3 °C and 0.8, respectively. These results confirmed that our results could be applied to the optimization of steam gasification using a lower steam flow rate at atmospheric pressure and would be more realistic by covering many gasification parameters.
4. Conclusions

This study applied a variable analysis based on a $3^k$ factorial experimental design and optimization using response surface methodology of steam gasification for COVID-19 medical wastes mainly composed of polypropylene and polyethylene. Steam gasification was simulated using the Aspen Plus software based on equilibrium conditions. The simulated results were validated using the related literature with the error of syngas production in the range 2.5–8.6 %. The four operating parameters (polypropylene ratio, pressure, steam ratio, and gasification temperature) were investigated as the main and interaction variables affecting the hydrogen yield and cold gas efficiency. ANOVA indicated that the most significant factors influencing the $H_2$ yield and CGE were the steam ratio and temperature, respectively. The polypropylene ratio and pressure were not significant factors. The optimization conditions were: 65 % polypropylene in the mixture, a pressure of 1 bar, a steam ratio of 0.38, and a temperature of 900 °C to generate 40.61 % $H_2$ and a cold gas efficiency of 81.43 %. These findings should be useful for the optimization of steam gasification of plastic mixtures from COVID-19 medical masks on a broad scale, such as chemical and thermal applications. However, the actual components of CMW should be used for modeling and validation based on experimental work for accuracy and reliability.

Table 8  Optimum conditions of gasification process.

| Item                 | Range        | Value |
|----------------------|--------------|-------|
| Feedstock            | PP (65–85 %) | 65    |
| Pressure (bar)       | 1–7          | 1     |
| Steam ratio (-)      | 0.1–1        | 0.38  |
| Temperature (°C)     | 700–900      | 900   |
| Maximum $H_2$ (vol%) | –            | 40.61 |
| Maximum CGE (vol%)   | –            | 81.43 |

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.

Acknowledgements

This research was supported by a grant from the Kasetsart University Research and Development Institute (KURDI), Bangkok Thailand (R-M 21.61) and the Faculty of Engineering at Kamphaeng Saen, Kasetsart University, Thailand.

Appendix A. Table A1 and Table A2

Table A1  Distinguishing between steam and hydrothermal gasification [1].

| Factor                  | Conventional gasification  | Hydrothermal gasification          |
|-------------------------|----------------------------|-----------------------------------|
| Moisture contents of the feedstock | Required drying with moisture greater than 35 wt% | Fit for very high moist feedstock (up to 99 wt%) |
| Gasifying agents        | May be $O_2$, steam, air, or $CO_2$ | Supercritical water               |
| Temperature and pressure| 500 and 1400 °C Often conducted at atmospheric pressure Less common at higher pressure | Above critical point of water (P greater than 22.1 MPa, T > 374 °C) |
| Residence time          | 30–60 min for bench-scale | 15–60 min for batch reactors 30–90 s for continuous reactors |
Table A2  Responses from $3^k$ experimental design.

| Run no. | PP (%) | P (bar) | SR (-) | $T$ ($^\circ$C) | $H_2$ (vol%) | CGE (%) |
|---------|--------|---------|-------|-----------------|-------------|--------|
| 1       | 85     | 7       | 1     | 900             | 1.62        | 98.92  |
| 2       | 85     | 7       | 1     | 800             | 15.71       | 79.70  |
| 3       | 85     | 7       | 1     | 700             | 25.59       | 71.79  |
| 4       | 85     | 7       | 0.55  | 900             | 28.69       | 83.14  |
| 5       | 85     | 7       | 0.55  | 800             | 36.58       | 76.20  |
| 6       | 85     | 7       | 0.55  | 700             | 42.43       | 71.10  |
| 7       | 85     | 7       | 0.1   | 900             | 55.63       | 75.62  |
| 8       | 85     | 7       | 0.1   | 800             | 60.03       | 71.00  |
| 9       | 85     | 7       | 0.1   | 700             | 63.44       | 67.33  |
| 10      | 85     | 4       | 1     | 900             | 1.65        | 100.14 |
| 11      | 85     | 4       | 1     | 800             | 16.09       | 80.12  |
| 12      | 85     | 4       | 1     | 700             | 26.35       | 71.79  |
| 13      | 85     | 4       | 0.55  | 900             | 29.37       | 83.16  |
| 14      | 85     | 4       | 0.55  | 800             | 37.61       | 78.81  |
| 15      | 85     | 4       | 0.55  | 700             | 43.76       | 70.39  |
| 16      | 85     | 4       | 0.1   | 900             | 56.79       | 74.97  |
| 17      | 85     | 4       | 0.1   | 800             | 61.34       | 70.17  |
| 18      | 85     | 4       | 0.1   | 700             | 64.89       | 66.42  |
| 19      | 85     | 1       | 1     | 900             | 1.79        | 103.06 |
| 20      | 85     | 1       | 1     | 800             | 17.00       | 81.60  |
| 21      | 85     | 1       | 1     | 700             | 28.05       | 72.10  |
| 22      | 85     | 1       | 0.55  | 900             | 30.79       | 83.52  |
| 23      | 85     | 1       | 0.55  | 800             | 39.80       | 75.28  |
| 24      | 85     | 1       | 0.55  | 700             | 46.65       | 69.08  |
| 25      | 85     | 1       | 0.1   | 900             | 59.12       | 73.58  |
| 26      | 85     | 1       | 0.1   | 800             | 64.18       | 68.41  |
| 27      | 85     | 1       | 0.1   | 700             | 68.11       | 64.33  |
| 28      | 75     | 7       | 1     | 900             | 1.64        | 98.79  |
| 29      | 75     | 7       | 1     | 800             | 15.72       | 79.73  |
| 30      | 75     | 7       | 1     | 700             | 25.59       | 71.76  |
| 31      | 75     | 7       | 0.55  | 900             | 28.72       | 83.14  |
| 32      | 75     | 7       | 0.55  | 800             | 36.59       | 76.19  |
| 33      | 75     | 7       | 0.55  | 700             | 42.43       | 71.09  |
| 34      | 75     | 7       | 0.1   | 900             | 55.60       | 75.49  |
| 35      | 75     | 7       | 0.1   | 800             | 60.04       | 71.02  |
| 36      | 75     | 7       | 0.1   | 700             | 63.45       | 67.15  |
| 37      | 75     | 4       | 1     | 900             | 1.67        | 100.04 |
| 38      | 75     | 4       | 1     | 800             | 16.09       | 80.14  |
| 39      | 75     | 4       | 1     | 700             | 26.35       | 71.75  |
| 40      | 75     | 4       | 0.55  | 900             | 29.40       | 83.13  |
| 41      | 75     | 4       | 0.55  | 800             | 37.63       | 75.82  |
| 42      | 75     | 4       | 0.55  | 700             | 43.76       | 70.36  |
| 43      | 75     | 4       | 0.1   | 900             | 56.78       | 74.91  |
| 44      | 75     | 4       | 0.1   | 800             | 61.35       | 70.16  |
| 45      | 75     | 4       | 0.1   | 700             | 64.89       | 66.39  |
| 46      | 75     | 1       | 1     | 900             | 1.82        | 102.96 |
| 47      | 75     | 1       | 1     | 800             | 17.02       | 81.62  |
| 48      | 75     | 1       | 1     | 700             | 28.06       | 72.07  |
| 49      | 75     | 1       | 0.55  | 900             | 30.82       | 83.52  |
| 50      | 75     | 1       | 0.55  | 800             | 39.82       | 75.29  |
| 51      | 75     | 1       | 0.55  | 700             | 46.66       | 69.09  |
| 52      | 75     | 1       | 0.1   | 900             | 59.13       | 73.58  |
| 53      | 75     | 1       | 0.1   | 800             | 64.20       | 68.41  |
| 54      | 75     | 1       | 0.1   | 700             | 68.09       | 64.29  |
| 55      | 65     | 7       | 1     | 900             | 1.64        | 99.11  |
| 56      | 65     | 7       | 1     | 800             | 15.72       | 80.06  |
| 57      | 65     | 7       | 1     | 700             | 25.60       | 72.07  |
| 58      | 65     | 7       | 0.55  | 900             | 28.64       | 83.43  |
| 59      | 65     | 7       | 0.55  | 800             | 36.53       | 76.46  |
| 60      | 65     | 7       | 0.55  | 700             | 42.40       | 71.38  |
| 61      | 65     | 7       | 0.1   | 900             | 55.49       | 75.82  |
| 62      | 65     | 7       | 0.1   | 800             | 59.93       | 71.25  |
| 63      | 65     | 7       | 0.1   | 700             | 63.37       | 67.58  |
Appendix B.

FORTRAN subroutine code for the DECOMP (ryield reactor) calculation.

Table B1 Component yields of DECOMP (ryield reactor) on mass basis.

| Component | Basis yield |
|-----------|-------------|
| H2O       | 0           |
| C         | 0.85        |
| H2        | 0.14        |
| N2        | 0.0002      |
| O2        | 0.004       |
| S         | 0           |
| ASH       | 0           |

C FACT IS THE FACTOR TO CONVERT THE ULTIMATE ANALYSIS TO.
C A WET BASIS.

FACT = (100 - WATER) / 100.
H2O = WATER / 100.
ASH = ULT(1) / 100 * FACT.
CARB = ULT(2) / 100 * FACT.
H2 = ULT(3) / 100 * FACT.
N2 = ULT(4) / 100 * FACT.
CL2 = ULT(5) / 100 * FACT.
SULF = ULT(6) / 100 * FACT.
O2 = ULT(7) / 100 * FACT.

Table A2 (continued)

| Run no. | PP (%) | P (bar) | SR (-) | T (°C) | H2 (vol%) | CGE (%) |
|---------|--------|---------|--------|--------|-----------|---------|
| 64      | 65     | 4       | 1      | 900    | 1.73      | 100.38  |
| 65      | 65     | 4       | 1      | 800    | 16.09     | 80.44   |
| 66      | 65     | 4       | 1      | 700    | 26.34     | 71.97   |
| 67      | 65     | 4       | 0.55   | 900    | 29.31     | 83.46   |
| 68      | 65     | 4       | 0.55   | 800    | 37.56     | 76.07   |
| 69      | 65     | 4       | 0.55   | 700    | 43.72     | 70.66   |
| 70      | 65     | 4       | 0.1    | 900    | 56.62     | 75.20   |
| 71      | 65     | 4       | 0.1    | 800    | 61.22     | 70.40   |
| 72      | 65     | 4       | 0.1    | 700    | 64.76     | 66.59   |
| 73      | 65     | 1       | 1      | 900    | 1.83      | 103.04  |
| 74      | 65     | 1       | 1      | 800    | 17.01     | 81.87   |
| 75      | 65     | 1       | 1      | 700    | 28.04     | 72.36   |
| 76      | 65     | 1       | 0.55   | 900    | 30.69     | 83.81   |
| 77      | 65     | 1       | 0.55   | 800    | 39.71     | 75.44   |
| 78      | 65     | 1       | 0.55   | 700    | 46.59     | 69.33   |
| 79      | 65     | 1       | 0.1    | 900    | 58.94     | 73.90   |
| 80      | 65     | 1       | 0.1    | 800    | 64.03     | 68.68   |
| 81      | 65     | 1       | 0.1    | 700    | 67.92     | 64.47   |

Fig. B1 Steam gasification flowsheet with calculator block.
[38] T. Chuenphan, T. Yurata, T. Sema, B. Chalermsinsuwan, Sensitivity Analysis by the 2k Factorial Experimental Design of CO2 Capture with Amine Gas Treating Process Using Aspen Plus, Engineering Journal 25 (4) (2021) 95–104.

[39] H. Kitzler, C. Pfeifer, H. Hofbauer, Pressurized gasification of woody biomass—variation of parameter, Fuel Processing Technology 92 (5) (2011) 908–914.

[40] R. Tavares, E. Monteiro, F. Tabet, A. Rouboa, Numerical investigation of optimum operating conditions for syngas and hydrogen production from biomass gasification using Aspen Plus, Renewable Energy 146 (2020) 1309–1314.

[41] J. Dong, A. Nzihou, Y. Chi, E. Weiss-Hortalá, M. Ni, N. Lyczko, Y. Tang, M. Ducouso, Hydrogen-rich gas production from steam gasification of bio-char in the presence of CaO, Waste Biomass Valorization 8 (8) (2017) 2735–2746.

[42] C. Berrueco, J. Recari, B.M. Güell, G.D. Alamo, Pressurized gasification of torrefied woody biomass in a lab scale fluidized bed, Energy 70 (2014) 68–78.

[43] A. Secer, A. Hasanoğlu, Evaluation of the effects of process parameters on co-gasification of Çan lignite and sorghum biomass with response surface methodology: An optimization study for high yield hydrogen production, Fuel 259 (2020) 116230.