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Establishment and analysis of performance model of biofuel gasifier

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ABSTRACT

In order to study the performance of a biomass-fed gasifier, a gasification model was established based on chemical equilibrium. In this model, sewage sludge with different water content was used as feedstock. Air was introduced into the gasifier as a gasifying agent. The objectives of the model were (a) calculating the equilibrium temperatures in the gasifier; (b) calculating syngas compositions and heating values at corresponding equilibrium temperatures; (c) finding out the effect of moisture content in the sludge and equivalence ratio on the gasification process; and (d) using a mixed feedstock instead of single feedstock to improve syngas yield. The model was built in MATLAB and Cantera. Elements balance, chemical equilibrium, and enthalpy balance were used in the model. For 1 kg sludge, the moisture contents of sludge range from 0.1 to 0.8, and the equivalence ratios range from 0.5 to 4. The results show that (a) when moisture content = 0.1, ER = 2.47, the CO yield reaches maximum value of 17.548 mol/(kg sludge); (b) when moisture content = 0.1, ER = 2.83, the H_2 yield reaches maximum value of 20.756 mol/(kg sludge). Gasification performance can be improved by mixing sludge with lignite. For 1 kg mixture, the results show that (a) the maximum yield of CO increases from 3.04 to 12.3 mol/(kg mixture) with the increase of lignite content from 10% to 40%; (b) the maximum yield of H_2 increases from 13.75 to 21.88 mol/(kg mixture) with the increase of lignite content from 10% to 40%.

Keywords: Sewage sludge; Gasification; Element balance; Chemical equilibrium; Energy balance

1. Introduction

Sewage sludge is the residue produced in municipal wastewater treatment plants. According to ultimate analysis, sewage sludge is composed of C, H, O, N, and S elements, ash, and moisture. The waste sludge has a water content of 97%–99% and the water content should be reduced before transportation and disposal because dewatering reduces the sludge volume greatly. For instance, when the water content is reduced from 97% to 60%, the sludge volume will be reduced to less than 10% of the original sludge volume [1].

Gasification is that oxygen in the form of air, steam, or pure oxygen is reacted at high temperature with the available carbon in feedstock to produce a gas product, ash, and a tar product. In this process, combustion occurs to produce heat and the reaction proceeds exothermically to produce a low to medium calorific value fuel gas [2,3]. The operating temperatures are relatively high compared to pyrolysis, at 800°C–1,100°C with air gasification, and 1,000°C–1,400°C with oxygen. Calorific value of the product gas is low for air gasification, in the region of 4–6 MJ/m³, and medium, about 10–15 MJ/m³ for oxygen gasification. Steam gasification is endothermic for the main char-steam reaction and consequently, steam is usually added as a supplement to oxygen gasification to control the temperature. Steam gasification under pressure is, however,

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exothermic. Steam gasification at pressures up to 20 bar and temperatures of between 700°C and 900°C produces a fuel gas of medium calorific value, approximately 15–20 MJ/m³. The product calorific value can be compared with natural gas at about 37 MJ/m³ [4–6].

Gasification can be used for biomass converting to energy. The number of different uses of gas shows the flexibility of gasification and therefore allows it to be integrated with several industrial processes, as well as power generation systems. Gasification represents an attractive alternative to the well-established thermal treatment systems for the recovery of energy from waste sludge. So, the study on energy recovered from sludge gasification should be paid more attention to Ibrahim et al. [7], Belgiorno et al. [8], Klein and Themelis [9], and Edson and Rapheal [10].

2. Reactions

A typical fixed bed gasifier is shown in the Fig. 1. From this Fig. 1, we can see that there are "four zones" in the gasifier: drying, pyrolysis, gasification, and combustion.

As feedstock proceeds through a gasifier, the following physical, chemical, and thermal processes may occur sequentially or simultaneously, depending on the reactor design and the feedstock material.

2.1. Drying

As the feedstock is heated and its temperature increases, water is the first constituent to evolve:

$$\text{Moist feedstock} + \text{Heat} \rightarrow \text{Dry feedstock} + H_2O(g) \quad (1)$$

2.2. Pyrolysis or devolatilization

Pyrolysis (also called partial gasification) takes place and the feedstock is converted to char as the temperature of the dry feedstock increases.

$$\text{Dry feedstock} + \text{Heat} \rightarrow \text{Char} + \text{Gases} + \text{Liquid} \quad (2)$$

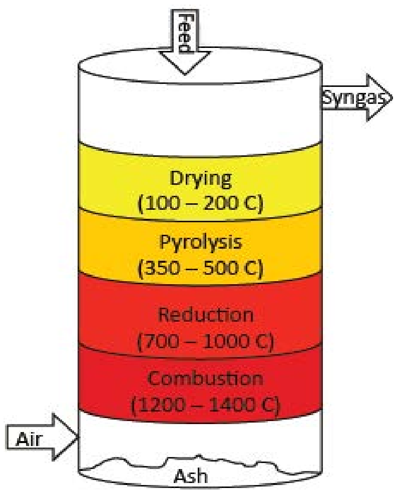


Fig. 1. "Four zones" in a typical fixed bed gasifier.

Pyrolysis generally produces the following three products:

- Light gases such as H_2, CO, CO_2, H_2O, and CH_4;
- Tar, a black, viscous, and corrosive liquid composed of heavy organic and inorganic molecules;
- Char, a solid residue mainly containing carbon.

Composition of the pyrolysis product depends on several factors including the temperature and rate of heating.

2.3. Combustion

The oxidation or combustion of char is one of the most important chemical reactions taking place inside a gasifier, providing practically all the thermal energy needed for the endothermic reactions. Oxygen supplied to the gasifier reacts with the combustible substances present, resulting in the formation of CO_2 and H_2O [5,11]:

$$C + O_2 = CO_2 \quad (3)$$

The other combustion reaction is the oxidation of hydrogen in fuel to produce steam:

$$H_2 + \frac{1}{2}O_2 = H_2O \quad (4)$$

2.4. Gasification

Gasification involves a series of endothermic reactions supported by the heat produced from the combustion reaction described above. Gasification yields combustible gases such as hydrogen, carbon monoxide, and methane through a series of reactions. The following are four major gasification reactions.

2.4.1. Water–gas reaction

Water–gas reaction is the partial oxidation of carbon by steam, which comes from different sources, such as water vapor associated with the incoming air, vapor produced from the evaporation of water, and pyrolysis of the solid fuel:

$$C + H_2O = CO + H_2 \quad (5)$$

2.4.2. Boudouard reaction

The carbon dioxide present in the gasifier reacts with char to produce CO according to the following endothermic reaction, which is known as the Boudouard reaction:

$$CO_2 + C = CO \quad (6)$$

2.4.3. Shift conversion

The heating value of hydrogen is higher than that of carbon monoxide. Therefore, the reduction of steam by carbon monoxide to produce hydrogen is a highly desirable reaction:

$$CO + H_2O = CO_2 + H_2 \quad (7)$$

This endothermic reaction, which is known as water–gas shift, results in an increase in the ratio of hydrogen to carbon monoxide in the synthesis gas.

2.4.4. Methanation

Methane can also form in the gasifier through the following overall reaction:

$$C + 2H_2 = CH_4 \tag{8}$$

This reaction can be accelerated by nickel-based catalysts at 1,100°C and 6–8 bar. Methane formation is preferred especially when the gasification products are to be used as a feedstock for other chemical process.

3. Modeling

3.1. Objectives

In this model, air is used to supply oxygen rather than steam or pure oxygen. The model is developed to find a relationship between produced gas and sludge introduced into gasifier. The objectives are as follow:

- Calculating the equilibrium temperatures in the gasifier;
- Calculating syngas compositions and heating values at corresponding equilibrium temperatures;
- Calculating the efficiencies of gasification process (CGE) at different conditions;
- Finding out the effect of moisture content in the sludge and equivalence ratio (ER) on the CGE;
- Using a mixed feedstock instead of single feedstock to improve syngas yield.

The results will be shown in 3D figures. As is shown in Fig. 2, *X*-axis represents moisture content, *Y*-axis represents ER or mass of air. For each moisture content and ER, there will be corresponding temperature, syngas composition, and heating value in the space. Thus, lots of spots will be got and a 3D figure can be drawn by means of interpolation.

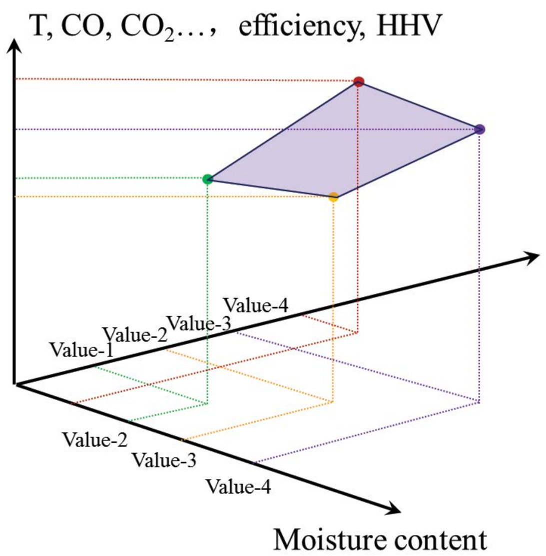


Fig. 2. 3D figure results.

3.2. Element balance

Assume all the nitrogen in sludge is converted into N_2. The global reaction in gasification process can be expressed as Eq. (9).

$$C_xH_yO_zN_mS_n + a(O_2 + 3.76N_2) + bH_2O = cCO + dCO_2 + eCH_4 + fH_2 + gH_2O + hH_2S + iN_2 \tag{9}$$

For a specific kind of sludge, *x*, *y*, *z*, *m*, and *n* are known by element analysis. Five equations can be derived from the element balances of reactants and products.

Carbon balance:

$$x = c + d + e \tag{10}$$

Hydrogen balance:

$$y + 2b = 4e + 2f + 2g + 2h \tag{11}$$

Oxygen balance:

$$z + 2a + b = c + 2d + g \tag{12}$$

Nitrogen balance:

$$m + (3.76 \times 2)a = 2i \tag{13}$$

Sulfur balance:

$$n = h \tag{14}$$

3.3. Chemical equilibrium

If the residence time within the reactor is long enough, the chemical reactions will approach equilibrium. At that condition, the direct, and inverse rates are equal. Chemical equilibrium requires that at each temperature, there will be an equilibrium constant for each reaction.

For example, in the case of the water–gas shift reaction, the equilibrium constant K_1 is written as equation (15):

$$K_1 = \frac{[CO_2][H_2]}{[CO][H_2O]} = \frac{d \cdot f}{c \cdot g} \tag{15}$$

where $[CO_2]$, $[H_2]$, $[CO]$, and $[H_2O]$ are equilibrium concentrations of CO_2, H_2, CO, and H_2O expressed in respective partial pressures.

The same, another two equations (Eqs. (16) and (17)) can be obtained for Boudouard reaction and methanation reaction.

$$K_2=\frac{[CO]^2}{[CO_2]}=\frac{c^2}{d\cdot(c+d+e+f+g+h+i)} \quad (16)$$

$$K_3=\frac{[CO]^2}{[CO_2]}=\frac{e}{f^2\cdot(c+d+e+f+g+h+i)} \quad (17)$$

The value of equilibrium constant is found out at constant temperature and pressure using the standard state Gibbs function of change ΔG_T°:

$$K_i=e^{-\frac{\Delta G_T^{\circ}}{RT}} \quad (18)$$

where ΔG_T° for shift reaction, boudouard reaction, and methanation reaction are expressed as Eqs. (19)–(21):

$$\Delta G_T^{\circ}=\Delta g_{f,CO_2}^{\circ}+\Delta g_{f,H_2}^{\circ}-\Delta g_{f,CO}^{\circ}-\Delta g_{f,H_2O}^{\circ} \quad (19)$$

$$\Delta G_T^{\circ}=2\Delta g_{f,CH_4}^{\circ}-\Delta g_{f,CO_2}^{\circ} \quad (20)$$

$$\Delta G_T^{\circ}=\Delta g_{f,CH_4}^{\circ}-2\Delta g_{f,H_2}^{\circ} \quad (21)$$

where $\Delta g_{f,\text{specie}}^{\circ}$ represents Gibbs function of the pure species at standard state pressure (P = 1 atm) at constant temperature. $\Delta g_{f,\text{specie}}^{\circ}$ can be written as Eq. (22):

$$\Delta g_f^{\circ}=h_f^{\circ}-AT\ln(T)-BT^2-\left(\frac{c}{2}\right)T^3-\left(\frac{D}{3}\right)T^4+\left(\frac{E}{2T}\right)+F+GT \quad (22)$$

3.4. Energy balance

The energy balance-also known as the first law of thermodynamics can be written as Eq. (23):

$$\frac{dE}{dt}=\sum_{i=1,\text{reactants}}^{n} m\left(h_i+\frac{u_i^2}{2}+gz_i\right)-\sum_{j=1,\text{products}}^{n} m\left(h_i+\frac{u_i^2}{2}+gz_i\right)+Q+W \quad (23)$$

For adiabatic, isobaric steady-state operation, the energy balance can be simplified by Eq. (24):

$$\sum_{i=\text{reactants}}^{n} y_i\left(h_{f,i}^{\circ}+h_{S,i}(T)\right)=\sum_{j=\text{products}}^{n} y_i\left(h_{f,j}^{\circ}+h_{S,i}(T)\right) \quad (24)$$

where $h_{f,i}^{\circ}$, $h_{f,j}^{\circ}$ are the specific enthalpies of formation of reactants and products. $h_{s,i}(T)$, $h_{s,j}(T)$ are the sensible enthalpies. Sensible enthalpy $h_s(T)$ can be expressed as Eq. (25).

$$h_s(T)=\int_{T_0}^{T} C_{p,i}\,dT \quad (25)$$

where $C_{p,i}$ is the specific heat capacity at temperature T and it can be calculate by Eq. (26):

$$C_{p,i}=A+BT+CT^2 \quad (26)$$

The enthalpy of formation of sludge $h_{f,\text{sludge}}^{0}$ can be calculated by the following method based on the Hess Law:

$$C_xH_yO_zN_mS_n+\left(x+\frac{y}{4}+m+n-\frac{z}{2}\right)O_2=xCO_2+\frac{y}{2}H_2O+mNO_2+nSO_2 \quad (27)$$

$$C+O_2=CO_2 \qquad \Delta h_r1=-393.522\ \text{kJ/mol} \quad (28)$$

$$H_2+\frac{1}{2}O_2=H_2O(l) \qquad \Delta h_r2=-285.83\ \text{kJ/mol} \quad (29)$$

$$\frac{1}{2}N_2+O_2=NO_2 \qquad \Delta h_r3=33.1\ \text{kJ/mol} \quad (30)$$

$$S+O_2=SO_2 \qquad \Delta h_r4=-296.842\ \text{kJ/mol} \quad (31)$$

$$(28)\times x+(29)\times\frac{y}{2}+(30)\times m+(31)\times n-(27)xC+\frac{y}{2}H_2+\frac{m}{2}N_2+nS+\frac{z}{2}O_2=C_xH_yO_zN_mS_n \quad (32)$$

So,

$$h_{f,\text{sludge}}^{\circ}=\Delta h_r1\times x+\Delta h_r2\times\frac{y}{2}+\Delta h_r3\times m+\Delta h_r4\times n+\text{HHV\_sludge} \quad (33)$$

4. Results

4.1. Single feedstock

4.1.1. Sludge properties and operating conditions

The properties of sludge introduced into the gasifier are shown in Table 1.

The mass flow rate of sludge is 1 kg/s, moisture content ranges from 10% to 80%, a large range of equivalence

Table 1
Ultimate analysis of sludge

Property (wt.%)	Value
C	34.00
H	4.90
O	20.01
N	4.70
S	1.30
Ash	35.00
Moisture	0.00
Total	100.00

ECN Phyllis 2 (Database for biomass and waste)-sludge-sewage sludge (#658).

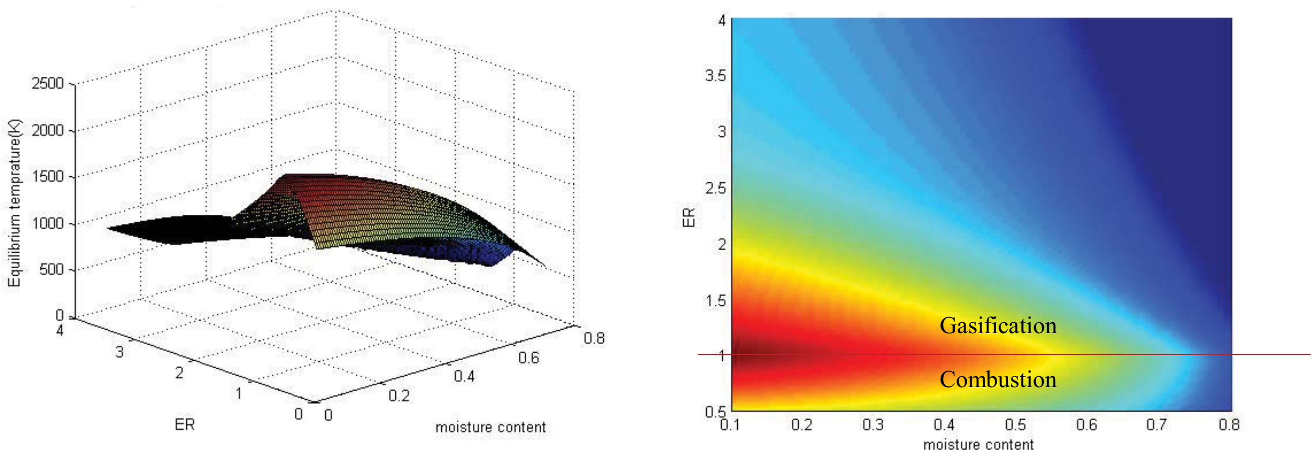
ratio (0.5–4) which covers combustion process is used in the model. The effect of ash on the process is neglected. The process is adiabatic and isobaric. The initial temperature is 298.15 K and initial pressure is 1 atm.

4.1.2. Equilibrium temperature

The equilibrium temperatures as a function of moisture content and ER are shown in Fig. 3, meanwhile, the equilibrium temperatures as a function of moisture content and air are shown in Fig. 4. In Figs. 3b and 4b, red lines are drawn to separate gasification area and combustion area. From these two figures, we can see that when moisture content = 0.1 and ER = 1.04 (which is complete combustion), the maximum temperature will be 2,108.9 K. When moisture content = 0.6 and ER = 3.91, the minimum temperature will be 300.1 K. This is a very low temperature and reactions hardly occur at this condition. Fig. 4 shows the same temperatures as that in Fig. 3, but the mass of air is used in the model rather than ER.

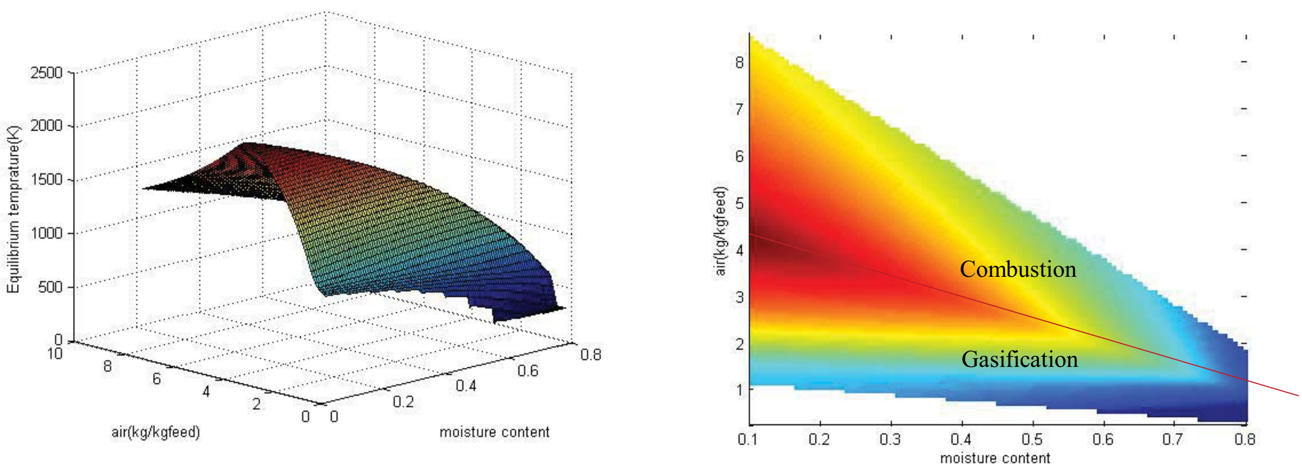
4.1.3. CO yield

Fig. 5 shows CO yield as a function of moisture content and ER. From this Fig. 5, we can see that when moisture content = 0.1 and ER = 2.47, CO will reach a maximum yield, which is 17.548 mol/(kg sludge). However, when moisture content = 0.8 and ER = 0.5, the minimum CO yield is 0 mol/(kg sludge). It shows that in lean combustion process, no CO will be obtained, all the carbon in sludge will be converted to CO_2.



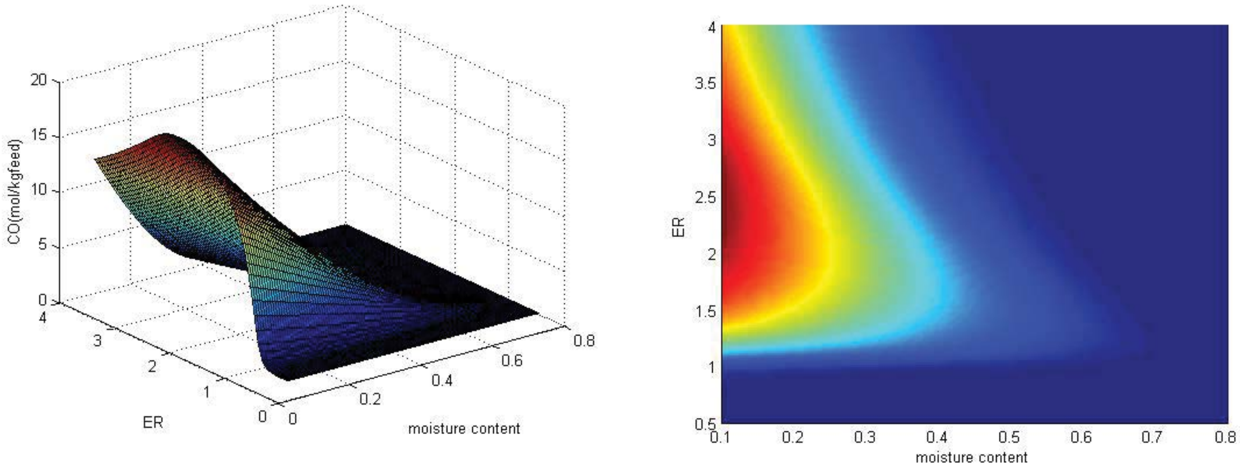
(a) (b)

Fig. 3. (a and b) Equilibrium temperature as a function of moisture content and ER.



(a) (b)

Fig. 4. (a and b) Equilibrium temperature as a function of moisture content and mass of air.



(a) (b)

Fig. 5. (a and b) CO yield as a function of moisture content and ER.

4.1.4. H_2 yield

Fig. 6 shows H_2 yield as a function of moisture content and ER. From this Fig. 6, we can see that when moisture content = 0.1 and ER = 2.83, H_2 yield will get a maximum value of 20.76 mol/(kg sludge). However, when moisture content = 0.8 and ER = 0.5, the minimum H_2 yield is 0 mol/(kg sludge). It shows that in lean combustion process, no H_2 will be obtained.

4.1.5. Gasification process

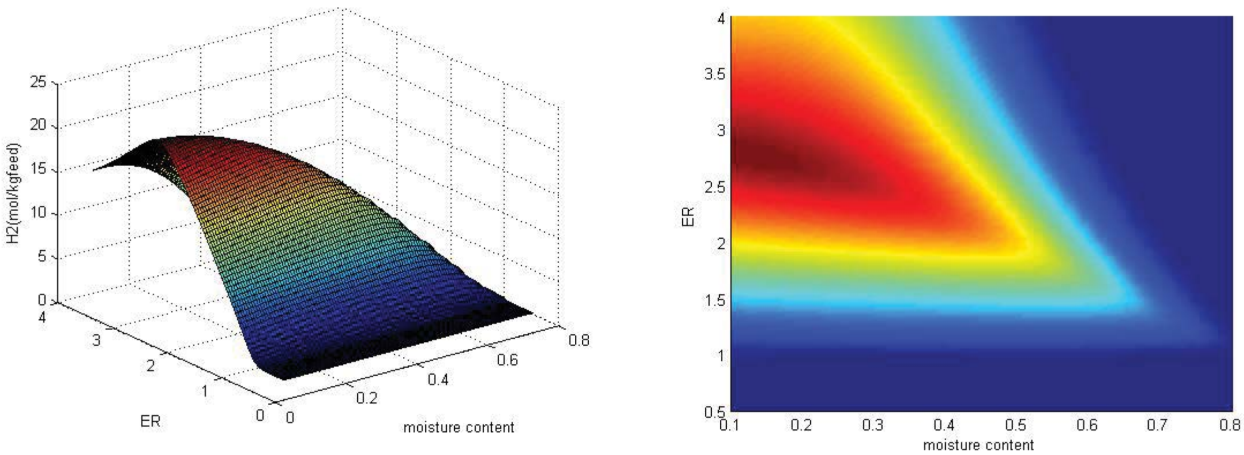
As is shown in Fig. 7, CGE has a maximum value of 0.87 when the moisture content = 0.1 and ER = 4, this process is not gasification, and CH4 will be generated in this process, so CGE gets a maximum value. When moisture content = 0.8 and ER = 0.5, CGE has a minimum value of 0, this indicates no combustible gas will be produced in combustion process.

4.1.6. HHV of syngas

As is shown in Fig. 8, HHV has a maximum value of 158.82 kJ/mol when moisture content = 0.1 and ER = 4, CH_4, CO, and H_2 contribute all the heating value of produced gas. When moisture content = 0.8 and ER = 0.5, HHV has a minimum value of 0 kJ/mol.

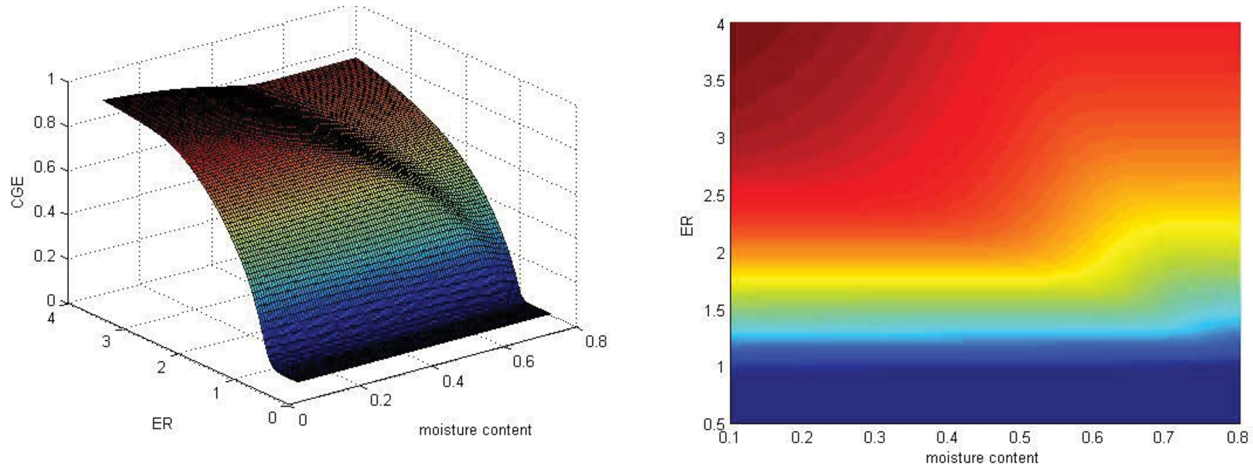
4.1.7. Comparison of sludge gasification process with different water content

Table 2 shows a comparison of sludge gasification process with water contents of 30%, 40%, 50%, and 60%. From



(a) (b)

Fig. 6. (a and b) H_2 yield as a function of moisture content and ER.



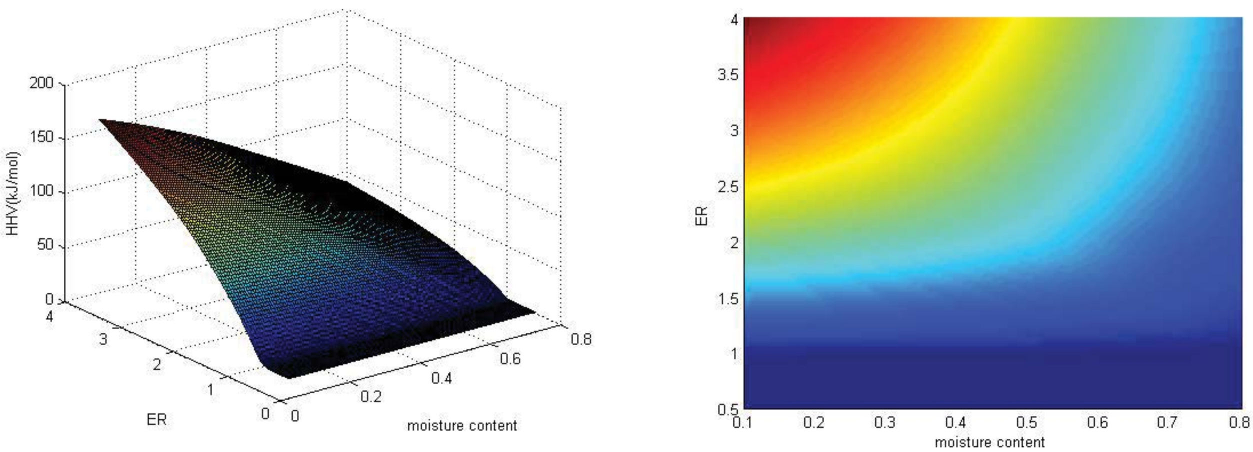
(a)

(b)

Fig. 7. (a and b) CGE as a function of moisture content and ER.

Table 2
Comparison of sludge gasification process with water contents

Moisture content	30%	40%	50%	60%
ER	1.58–3.46	1.31–3.91	1.22–2.65	1.22–1.94
T (K)	1,418.2–804.7	1,471.1–701.2	1,366–716	1,133.6–707.9
CO (vol.%)	4.92–9.09	0.66–5.81	0.6–3.16	0.73–1.21
H_2 (vol.%)	7.48–21.65	4.12–19.55	3.19–16	3.54–11.15
CH_4 (vol.%)	0–5.55	0–9.14	0–4.12	0–1.61
HHV (kJ/mol)	43–118	23–113	15–73	13–42



(a)

(b)

Fig. 8. (a and b) HHV of syngas as a function of moisture content and ER.

this table, we can see that mole fractions of CO and H_2 and heating value of syngas increase separately with the increase of water content from 30% to 60%. The dryer the sludge is introduced into gasifier, the more heating value will be recovered.

Table 3
Properties of lignite

Property (wt.%)	Value
C	55.3
H	3.91
O	25.07
N	0.61
S	0.27
Ash	3.32
Moisture	13.4
Total	100.00

*ECN Phyllis 2 (database for biomass and waste)-sludge-sewage sludge (#658).

4.2. Mixed feedstock

4.2.1. Lignite properties

The properties of lignite mixed with sludge are shown in Table 3.

The mass flow rate of mixture is 1 kg/s. Lignite contents (mass fraction) in the mixture are 10%, 20%, 30%, and 40%. Equivalence ratio is in a range of 0.5–4, which also covers combustion process. The effect of ash on the process is neglected. The process is adiabatic and isobaric. The initial temperature is 298.15 K and pressure is 1 atm which is the same as that of a single feedstock.

4.2.2. Equilibrium temperature of mixed feedstock

As shown in Fig. 9, equilibrium temperature will be increased with the increase of lignite content in mixture from 10% to 40% (mass fraction).

4.2.3. Syngas compositions of mixed feedstock

Fig. 10 shows produced gas compositions with different contents of lignite (mass fraction). When lignite content of

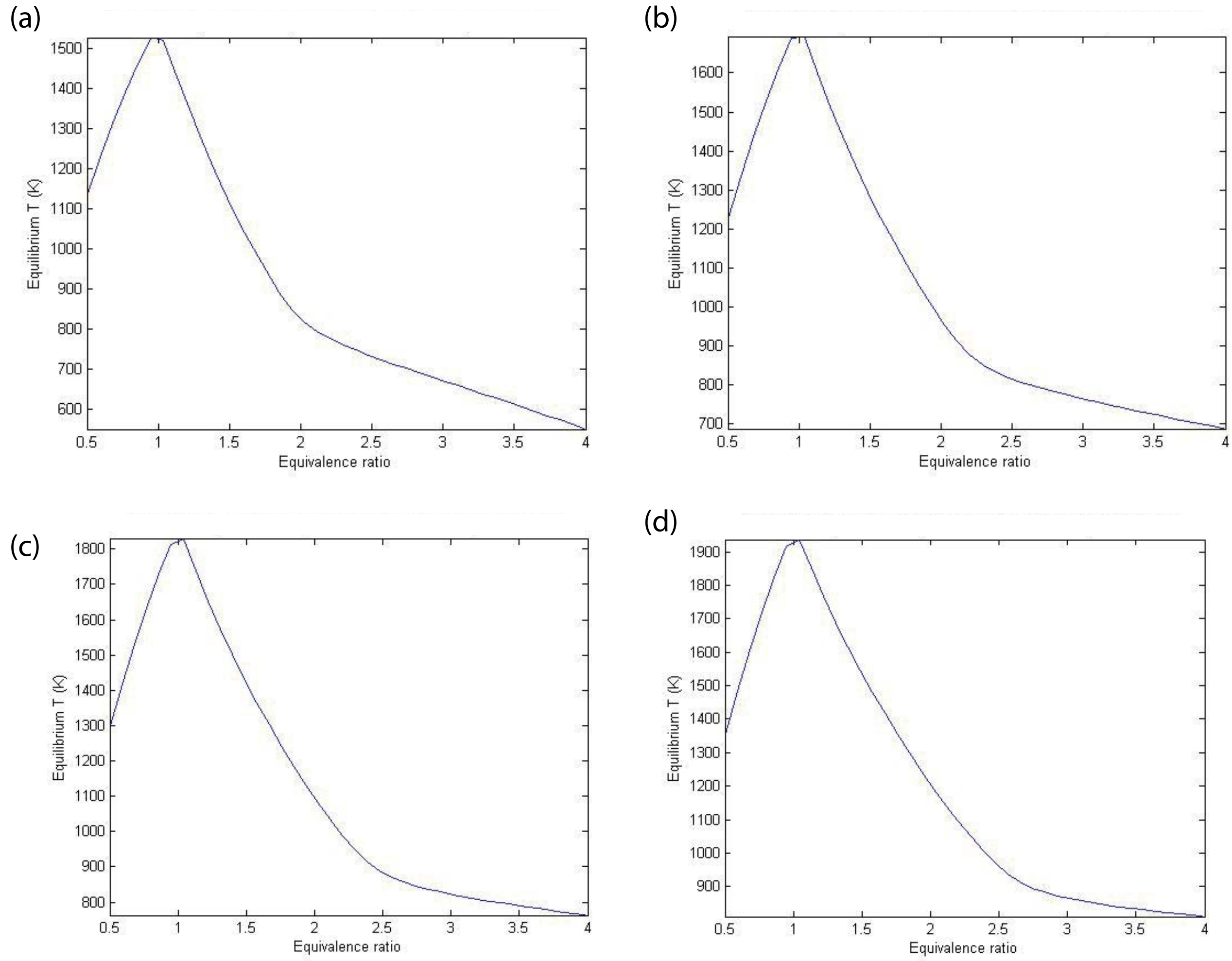


Fig. 9. Equilibrium temperatures with different contents of lignite (mass fraction): (a) 10% lignite, (b) 20% lignite, (c) 30% lignite, and (d) 40% lignite.

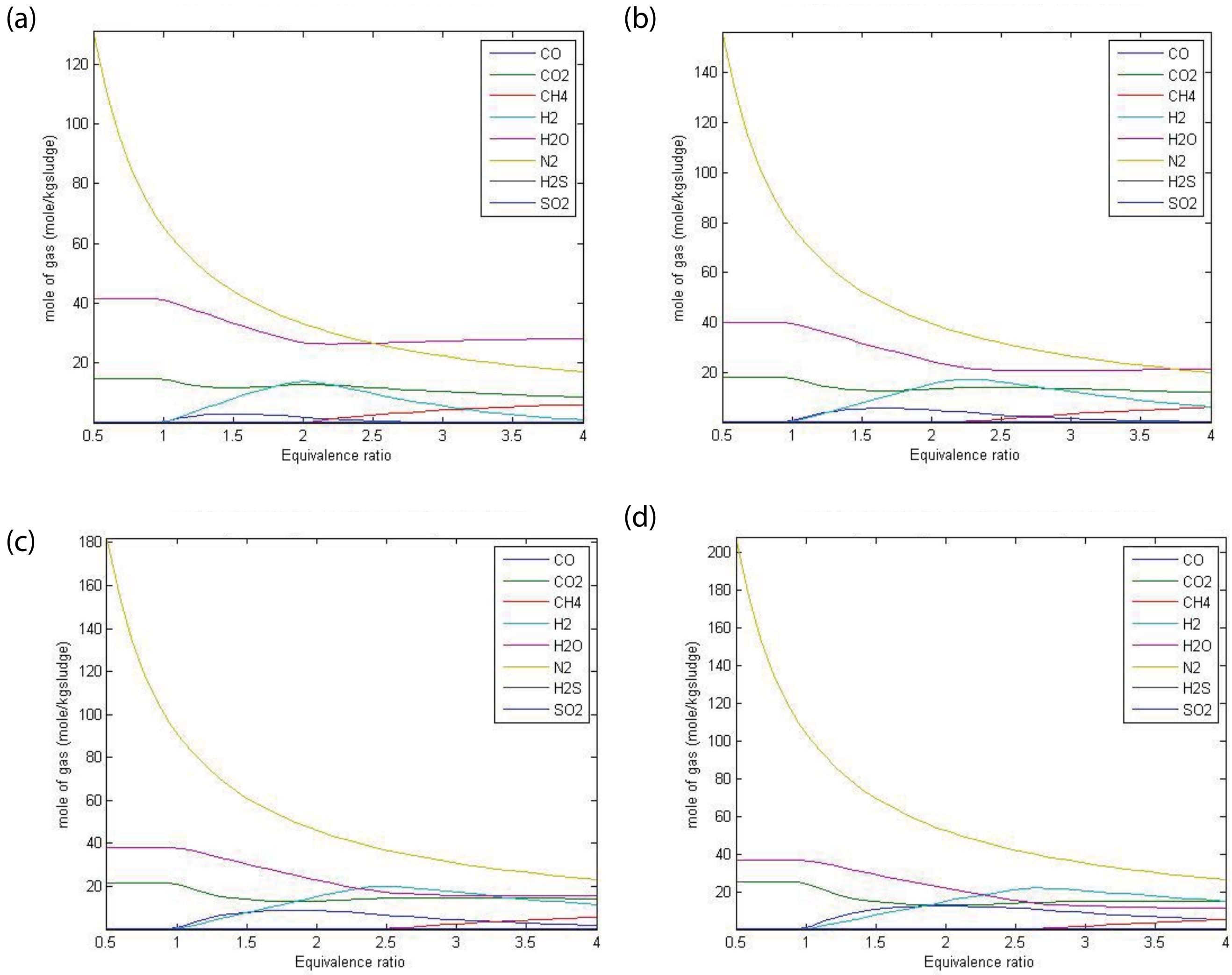


Fig. 10. Gas compositions with different contents of lignite (mass fraction): (a) 10% lignite, (b) 20% lignite, (c) 30% lignite, and (d) 40% lignite.

mixture is 10%, CO will get a maximum yield of 3.04 mol/(kg mixture) at ER = 1.49 and H_2 will get a maximum yield of 13.75 mol/(kg mixture) at ER = 1.94; When lignite content of mixture is 20%, CO will get a maximum yield of 5.65 mol/(kg mixture) at ER = 1.67, and H_2 will get a maximum yield of 17.3 mol/(kg mixture) at ER = 2.29; When lignite content of mixture is 30%, CO will get a maximum yield of 8.78 mol/(kg mixture) at ER = 1.85 and H_2 will get a maximum yield of 20.0 mol/(kg mixture) at ER = 2.47; When lignite content of mixture is 40%, CO will get a maximum yield of 12.3 mol/(kg mixture) at ER = 1.94 and H_2 will get a maximum yield of 21.88 mol/(kg mixture) at ER = 2.65.

4.2.4. Syngas compositions of mixed feedstock

Fig. 11 shows that HHV of syngas will be increased with the increase of lignite content in mixture from 10% to 40% (mass fraction).

5. Conclusions

For 1 kg sludge, the moisture contents of sludge range from 0.1 to 0.8, and the equivalence ratios range from 0.5 to 4. Conclusions can be drawn as follows:

- When moisture content = 0.1, ER = 2.47, the CO yield reaches maximum value of 17.548 mol/(kg sludge);
- When moisture content = 0.1, ER = 2.83, the H_2 yield reaches maximum value of 20.756 mol/(kg sludge).

Gasification performance can be improved by mixing sludge with lignite. For 1 kg mixture, Conclusions can be drawn as follows:

- The maximum yield of CO increases from 3.04 to 12.3 mol/(kg mixture) with the increase of lignite content from 10% to 40%;

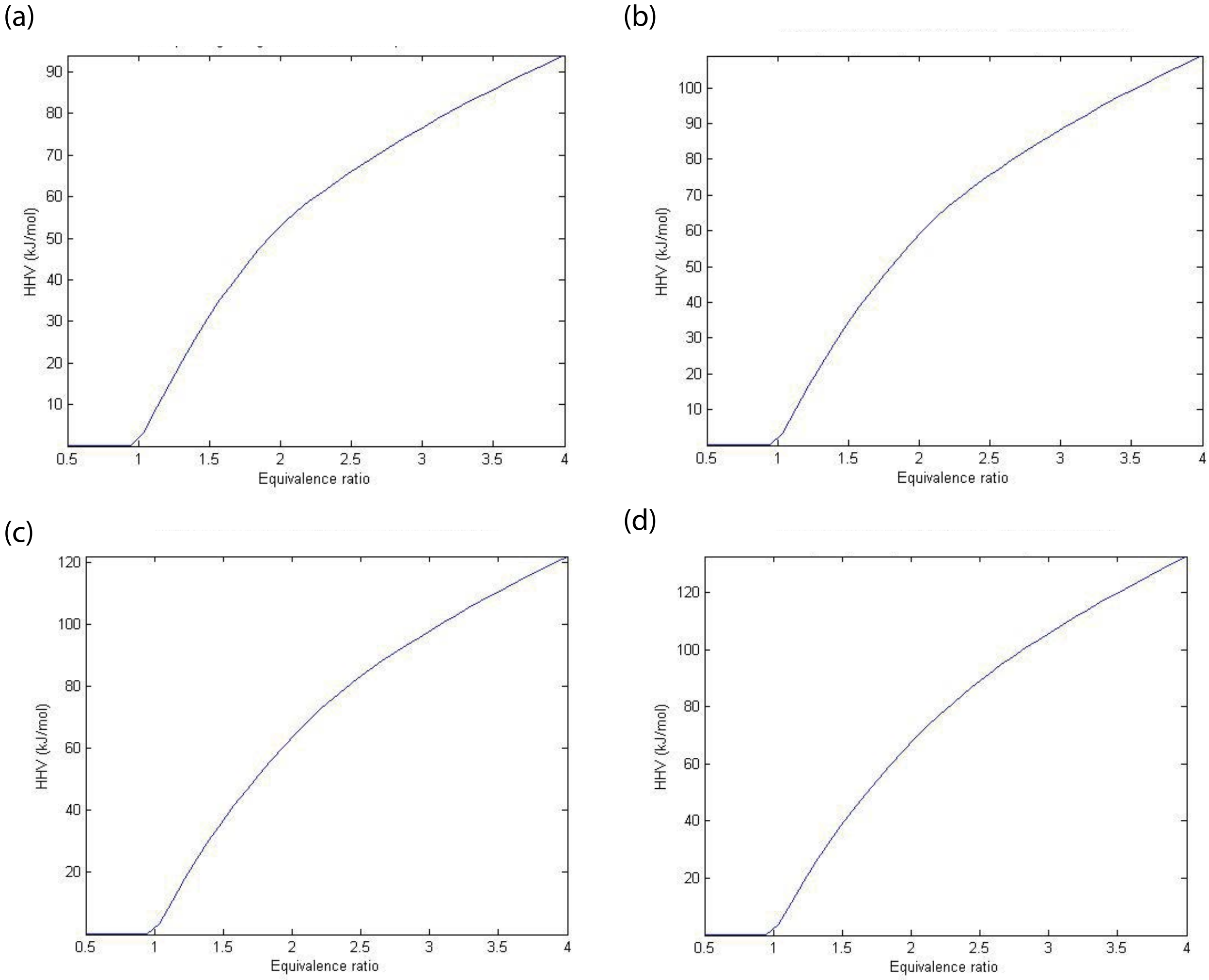


Fig. 11. HHV of syngas with different contents of lignite (mass fraction): (a) 10% lignite, (b) 20% lignite, (c) 30% lignite, and (d) 40% lignite.

- The maximum yield of H_2 increases from 13.75 to 21.88 mol/(kg mixture) with the increase of lignite content from 10% to 40%.

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