The Impacts of Operational Conditions on Charcoal Syngas Generation using a Modeling Approach

구동 조건에 따른 숯 합성가스 생산 효과 모델링

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ABSTRACT

바이오매스 가스화는 세계적인 증가 추세에 있는 에너지 수요를 충족할 수 있는 기술 중의 하나이다. 바이오매스 가스화를 통해서 농업 폐기물 등 다양한 바이오매스 자원을 에너지로 전환할 수 있고 CO_2 배출량 또한 줄일 수 있다. 본 연구에서는 COMSOL® 3.4 소프트웨어를 이용하여 바이오매스 원료와 운전 조건에 따른 가스화 효율 및 합성가스 조성의 변화를 분석하였다. 원료와 구동조건을 최적화하기 위해 가스화 모델을 세우고 원료와 구동조건을 달리하여 합성가스의 성분을 분석 및 예측하였다. 이 모델은 물리적인 실험을 통해 알고 있는 조건을 통해서 합성가스 성분을 시간에 따라 예측할 수 있다. 모델을 이용하여 함수비 5~30 %, 공기중 산소함량 5~50 %, 공기공급 유량 5~45 L/min, 온도 973~1273 K의 조건에서 합성가스의 성분을 예측한 결과 실제 실험 결과와 일치하는 것을 알 수 있다. 모델링 결과 양질의 합성가스를 생산하려면 원료의 회분함량이 적어야 하고 수소 함량이 높은 합성가스를 생산하려면 반응 온도가 높게 유지되고 원료의 함수비가 높아야 한다. 가스화장치의 온도를 높이면 합성가스의 성분 중 CO의 함량이 많아지고, CO의 함량이 많아지면 가스의 발열량이 높아지는 것을 알 수 있다. 또한 CO의 농도가 높고 발열량이 높은 합성가스를 생산하기 위해 서는 ER값은 작아야 한다.

Keywords: charcoal gasification; syngas; modeling; COMSOL

I. INTRODUCTION

Gasification is a process that converts carbonaceous materials, such as coal, petroleum, biofuel, or biomass, fuel gas. The gas is composed of carbon monoxide and hydrogen and called synthesis gas or syngas. The process requires high temperature and limited amount of oxygen. The advantage of biomass gasification is it has low carbon dioxide emission. Syngas can be used for producing chemical materials and fuels like ethanol and hydrogen (Gaddy, 1992). Industrial-scale gasification can be used for the power generation with gas engines or turbines. Combined heat and power (CHP) application is more desirable due to its higher efficiency. Today, more interests in gasification technologies are drawn because of the increased fuel price and environmental concern. Gasification is being integrated with modern and more sophisticated technologies and it is widely applied in developing countries (Hong, S., 2005). However, considering current status of biomass to energy generation, the gasification of biomass energy generation is still fairly limited in its application. The main reason for this is probably that the technology still has not reached in full maturity. Research efforts to develop improved biomass gasification technologies are impressive during the last 15 years (FAQ, 1986).

Gasification has very complex processes. Gasification modeling enables understanding different processes and assessment of operation conditions. Different types of biomass gasification models have been developed such as kinetic model, equilibrium model, Computational Fluid Dynamics (CFD) model and so on. Kinetic model is fundamental model which is applicable to different types

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of gasifiers including fixed bed gasifier and fluidized bed gasifier. Considering different expressions of reaction rates, gas composition and temperature can be predicted along the residence time. CFD model is an advanced numerical modeling method that can solve the problems of fluid flow, heat transfer, and species transfer. The CFD model can be implemented base on the structure and geometry of the gasifier. The process of chemical reaction and heat transfer are not homogeneous inside a gasifier. Therefore, CFD model can simulate the gasification process more reasonably than other models. Wang and Kinoshita (1993) (Wang and Kinoshita, 1993) built a kinetic model based on the mechanism of surface reactions. The kinetic model is validated by comparing the prediction results with the experimental data for different equivalence ratios. The composition of syngas was affected on residence time, temperature, pressure, equivalence ratio, char particle size and moisture contents of fuel. Sharma (2008) (Sharma, 2008) proposed a full equilibrium model of global reduction reaction for a downdraft biomass gasifier in order to predict the accurate distribution of various gas species, unconverted char, and reaction temperature. This model used ther-modynamics principles based on the stoichiometry. The model describes the influences of moisture content, pressure, equivalence ratio and initial temperature input on dry gas composition, unconverted char, calorific value of gas, gasification efficiency, outlet gas temperature and endo-thermic heat released in char bed. Tinaut and Francisco (2008) (Tinaut et al., 2008) presented a one-dimensional stationary model for a downdraft gasifier. The model is based on the mass and energy conservation equations, the energy exchange between solid and gas phases, and the heat transfer by radiation from the solid particles. The model was validated for different conditions of fuel particle size and varying superficial velocity of air. It is proposed a possible sustainable auto thermal mechanism of the flame front in downdraft fixed bed gasifiers. Nguyen et al. (2009) (Nguyen et al., 2009) developed a three-dimensional turbulent reacting flow computational fluid dynamics (CFD) model for coal gasification. The governing equations are dealing with chemical species, turbulent flow, chemical reaction in the turbulent flow and the droplet phase.

In this study a simulation model was constructed based on kinetics of gasification using COMSOL. The model was validated through comparing the prediction results with the experiment at observations. The main objective of this study is to assess operational parameters influencing syngas compositions reaction temperature, and related gasification processes. The results of this study would be used in designing downdraft gasifiers for converting biomass to syngas.

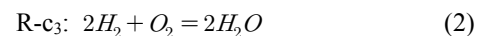## II. MATERIALS AND METHODS

1. Model using COMSOL

Biomass gasification model can be built by the software with appropriate reaction formula and parameters. The parameters considered in the model includes concentration of reactants, moisture, reaction zone's temperature, pressure and so on. Transient changes in concentrations of gas species can be illustrated in the program. The residence time is the reaction time between supplied air flow and biomass materials in the gasifier. COMSOL was used in this study for developing a gasification model based on a gasification kinetics model. Mass balance and energy balance are considered in the model. The reaction mechanism and kinetics parameters are given in the following sections.

A. Reactions Considered

Charcoal gasification is simpler than other biomass ma-terials because the main composition is char. The chemical reactions occurred in the gasifier are described as eight reaction formulas in the model as below :
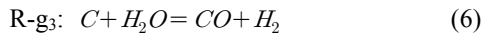
Combustion reaction:

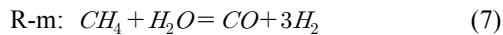$$\text{R-c}_1:\ 2CO + O_2 = 2CO_2 \tag{1}$$

$$\text{R-c}_3:\ 2H_2 + O_2 = 2H_2O \tag{2}$$

$$\text{R-c}_4:\ 2C + O_2 = 2CO \tag{3}$$

Gasification reaction:

$$\text{R-g}_1:\ C + CO_2 = 2CO \tag{4}$$

Methanating reaction:

$$\text{R-g}_2: \quad C + 2H_2 = CH_4 \tag{5}$$

Carbon-water reaction:

$$\text{R-g}_3: \quad C + H_2O = CO + H_2 \tag{6}$$

Steam methane reforming reaction:

$$\text{R-m}: \quad CH_4 + H_2O = CO + 3H_2 \tag{7}$$

Water-gas shift reaction:

$$\text{R-wg}: \quad CO + H_2O = CO_2 + H_2 \tag{8}$$
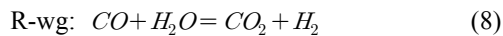
These reactions were described in the model. The important reactions in the gasification include CO and carbon combustion, CO production (gasification), steam reforming and water-gas shift reactions.

B. Mass Balance

A batch type reaction was assumed in this model. A gasification process in this model is simulated for the residence time using a constant initial temperature.

Mass conservation is expressed in the following equations,

$$\frac{d(C_i V_r)}{dt} = V_r R_i \tag{9}$$

$$\frac{dC_i}{dt} = R_i \quad \text{(constant volume)} \tag{10}$$

where C_i is the species molar concentration (mol/m³), V_r is the reactor volume (m³), R_i is the species rate expression (mol/ (m³・s)).

The equations may be re-written using concentration term as follows:

$$\frac{d(V_r c)}{dt} = V_r R \tag{11}$$

where c is concentration vector, and V_r is the volume of gasifier where reaction occurs.

$$R = S^T r, S = stoichiometric \tag{12}$$

Equations of Stoichiometry:

$$S_{ij} = V_{ij} \tag{13}$$

The pressure equation is derived from the ideal gas equation as follows:

$$P = R_g T(C_{CH_4} + C_{O_2} + C_{CO} + C_{H_2O} + C_{CO_2} + C_{H_2} + C_C) \tag{14}$$

where T is temperature. C is concentration, and R_g is the gas constant.

C. Energy Balance

COMSOL Reaction Engineering Lab User's Guide supply the equation of energy balance in the batch reactor of the model which is presented as following equation.

$$V_r \sum_i C_i C_{p,i} \frac{dT}{dt} = W_s + Q + Q_{ext} + V_r \frac{dp}{dt} \tag{15}$$

where V_r is the system volume (m³), C_i is the species concentration (mol/m³), $C_{p,i}$ is the species molar heat capacity of gas i. T is temperature (K), Q is the heat due to chemical reaction (J/s), Qext is the heat added to the system (J/s). The molar heat capacities are estimated by polynomials, The polynomials for Cp (J/ (mol・k)) as

$$\frac{C_p}{R_g} = \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \tag{16}$$

W_s is the shaft work in the system (W), which is zero since no mechanical agitation is provided. Overall reaction of the gasification is exothermic and no external heat is supplied. The reaction heat is determined as

$$Q = V_r(Q_1 + Q_2 + Q_3 + Q_4 + Q_5 + Q_6 + Q_7 + Q_8) \tag{17}$$

The heat of reaction can be also presented using enthalpy as:

$$Q = -V_r \sum_j H_j r_j \qquad (18)$$

where H_j is enthalpy of reaction j (J/mol·K), r_j is reaction rate (mol/m^3·s).

D. kinetic Properties in the Model

Arrhenius equation is used in the COMSOL reaction model. The Arrhenius equation is a simple accurate formula describing the temperature dependence of chemical reaction rates.

$$k = A \cdot T^n \cdot \exp(-\frac{E}{R_g T}) \qquad (19)$$

where k is the rate coefficient, A is frequency factor, E is the activation energy (J/mol), Rg is the universal gas constant (8.3144 J/ (mol·k)), Tn is temperature factor and T is the temperature (in Kelvin). The kinetic constants of frequency factor (A) and the activation energy (E) are summarized in Table 1.

All the reactions given in Table 1 are irreversible except water-gas shift reaction. The reaction rate k of the water-gas shift reaction can be presented as:

$$k = \frac{k^f}{k^r} \qquad (20)$$

Table 1 The kinetic constants of gasification reactions

Reaction	A	E (kJ/mol)	Reference
R-c$_1$: $2CO + O_2 = 2CO_2$	2.2e12	167	F. V. Tinaut (2008)
R-c$_2$: $2H_2 + O_2 = 2H_2O$	1e11	42	F. V. Tinaut (2008)
R-c$_3$: $2C + O_2 = 2CO$	5.67e9	160	C. Y. Wen (1979)
R-g$_1$: $C + CO_2 = 2CO$	3.616e1	77.39	Babu and Sheth (2006)
R-g$_2$: $C + 2H_2 = CH_4$	4.189e-3	19.21	Babu and Sheth (2006)
R-g$_3$: $C + H_2O = CO + H_2$	1.517e4	121.62	Babu and Sheth (2006)
R-m: $CH_4 + H_2O = CO + 3H_2$	7.031e-2	36.15	Babu and Sheth (2006)
R-wg: $CO + H_2O <=> CO_2 + H_2$	2.78	12.6	F. V. Tinaut (2008)
	0.0265	32.90	F. V. Tinaut (2008)

$$k^f = A_{fi} \cdot T^{n_{fi}} \cdot \exp(-\frac{E_{fi}}{R_g T}) \qquad (21)$$

$$k^r = A_{ri} \cdot T^{n_{ri}} \cdot \exp(-\frac{E_{ri}}{R_g T}) \qquad (22)$$

Reaction rate of water-gas reaction can be presented as:

$$r = k_{fi} \cdot C_{co} \cdot C_{H_2O} - k_{ri} \cdot C_{co_2} \cdot C_{H_2} \text{ mol/ (m}^3\cdot\text{s)} \qquad (23)$$

Reaction thermodynamic properties:
Enthalpy of reaction:

$$H = -h_{CO} - h_{H_2O} + h_{CO_2} + h_{H_2} \qquad (24)$$

Entropy of reaction:

$$S = -S_{CO} - S_{H_2O} + S_{CO_2} + S_{H_2} \qquad (25)$$

Heat source of reaction:

$$Q = -H \cdot r \qquad (26)$$

Standard specific heat formation and Standard Entropy of each gas phase species are expressed as:

$$C_{p,i} = R_g(\alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4) \qquad (27)$$

$$h_i = R_g(\alpha_1 T + \frac{\alpha_2}{2} T^2 + \frac{\alpha_3}{3} T^3 + \frac{\alpha_4}{4} T^4 + \frac{\alpha_5}{5} T^5 + \alpha_6) \qquad (28)$$

$$S_i = R_g(\alpha_1 \ln T + \alpha_2 T + \frac{\alpha_3}{2} T^2 + \frac{\alpha_4}{3} T^3 + \frac{\alpha_5}{4} T^4 + \alpha_7) \qquad (29)$$

E. Model Construction in COMSOL Software

The gasification model is constructed by assigning major parameters in model and reaction setting windows in COMSOL. The model settings panel as shown in Fig. 1 asks types of reactor and related properties. In this study, thermodynamic properties and energy balance were provided in model construction.
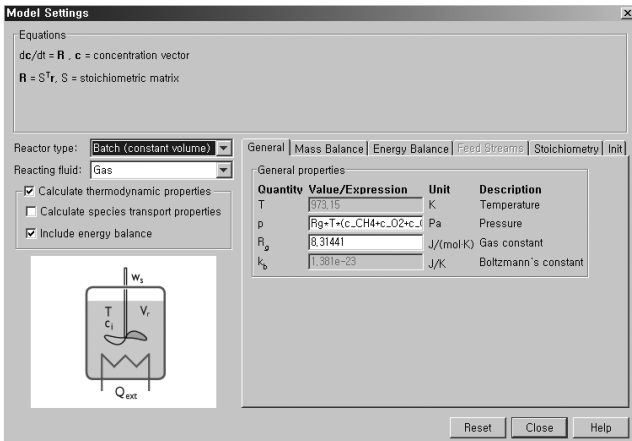
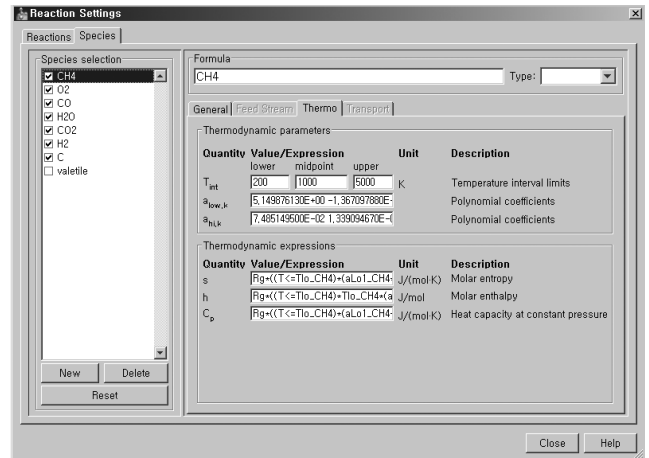Fig. 1 Model setting of COMSOL® reaction engineering lab

Fig. 2 Reaction setting of formula and kinetic parameter in COMSOL® reaction engineering lab
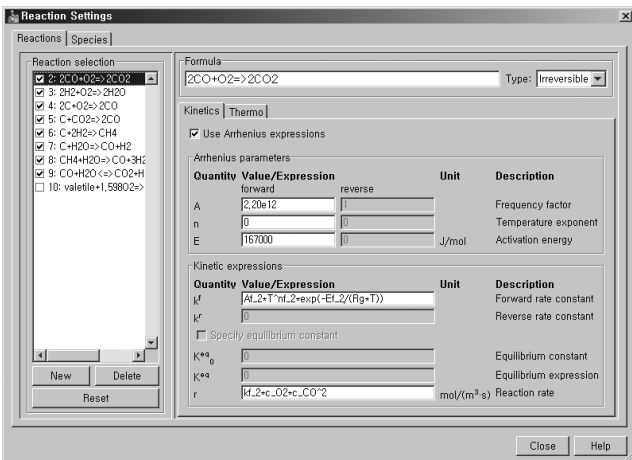

Fig. 3 Reaction setting of thermodynamic parameter in COMSOL® reaction engineering lab

in chemical reactors. Sivakumar et al. (S. Sivakuma et al.) presented an equation about gas reduction time (GRT), which is defined as the average time spent by the gas phase passing through reduction zone. The gas reduction time is about the same as residence time in the gasification model. The equation they presented is:

$$GRT = (V\epsilon/G) \cdot (273/T) \cdot 360 \text{sec} \qquad (30)$$

where V is the total volume of reactor (m³), ε is the void fraction (volume of voids in the bed/total volume of reactor), T is average temperature inside the reactor (K), G is gas flow rate (m³/hr)

2. Experiments

A small scale downdraft gasifier was assembled for experiments as in Fig. 4. The gasifier is made of steel. The length of gasifier is 1300 mm, internal diameter is 100 mm, external diameter is 120 mm, thickness is 10 mm, mesh diameter is 100 mm and hopper diameter is 66.7 mm. There are 10 nozzles (Φ 10 mm) around the neck.

Air is supplied by an air compressor and air flow mater is installed at air inlet of the gasifier. Three temperature sensors are installed at air inlet zone, reaction zone and gas outlet zone. The temperature number is read on an electronic display. The reaction temperature can be controlled by air flow rate. The producer gas passes through
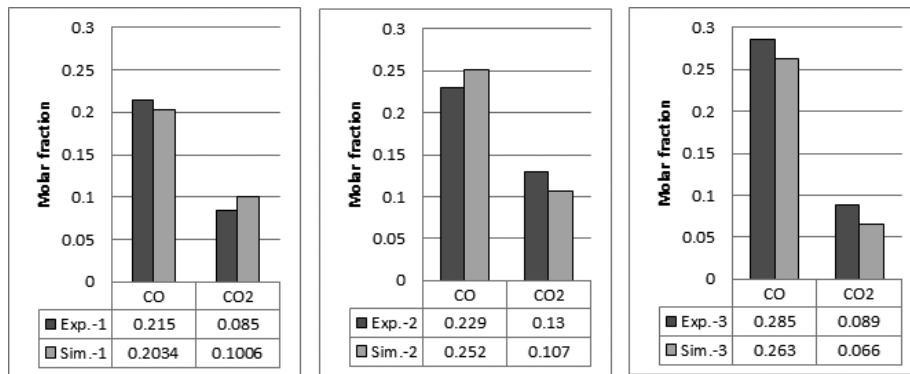
In the mass balance panel, the volume of reaction zone in the gasifier is provided. Initial temperature of 700 ℃ ～1000 ℃ is also provided.

In the reaction setting panel the reaction formulas of gasification are typed in and the option of "Use Arrhenius expression" is checked. The constants of frequency factor (A) and the activation energy (E) are also required. In the thermodynamic parameter panel, polynomial coefficients of each gas are required. The value of $a_{low,k}$ and $a_{hi,k}$ shown in Fig. 3 can be obtained from NASA polynomial data (NASA).

F. Residence Time

The residence time in a gasifier is defined as the time for which air passes through the reaction zone inside the gasifier, contacting biomass fuels. It controls the convection

Fig. 5 Validating of simulations and experiments
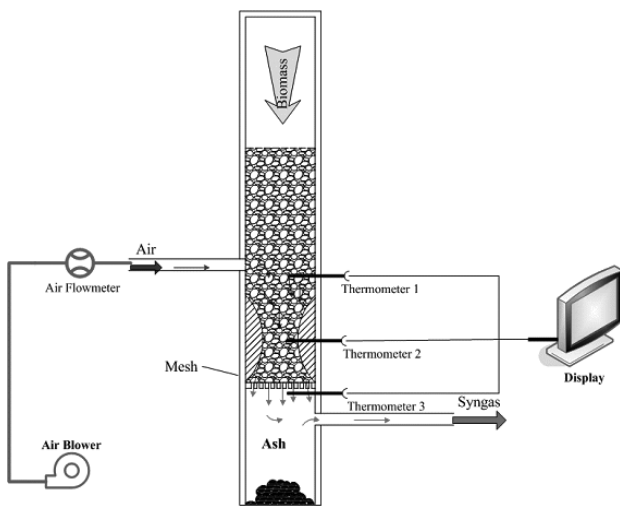
Fig. 4 Sketch of experimental gasifier

Table 2 Material and operational conditions of experiments

	Experiment 1	Experiment 2	Experiment 3
Material	charcoal	charcoal	charcoal
Moisture	0.08	0.08	0.08
Ash content	0.05	0.05	0.05
Feed rate	0.45 kg/hr	0.38 kg/hr	0.38 kg/hr
Air flow rate	20 L/min	20 L/min	20 L/min
Temperature	700 ℃	680 ℃	780 ℃
Residence time	0.15s	0.15s	0.147s

Table 3 Physical dimension of gasifier

	Downdraft Gasifier
Length of reaction zone	0.29 m
Diameter of reaction zone	0.10 m
Volume of reaction zone	0.0029 m^3
Diameter of nozzle	0.01 m

a cooling heat exchanger and then was combusted or extracted by gas syringe for gas analysis. The gas composition was determined by gas chromatography (GC, Agilent model 7890A) linked to a thermal conductivity detector (TCD). A micro-packed column (2 m×1 mm ID) was used and the carrier gas was helium. The column temperature was programmed from 50 ℃ to 250 ℃ at 15 ℃/min. The final temperature was maintained for 5 minutes.

III. RESULTS AND DISCUSSIONS

1. Experiments

The model is validated using three sets of experimental results. The experiments using the gasifier described in the previous chapter. The details of gasifier and experiments' conditions presented in Tables 2 and 3.

The ash content of charcoal is assumed as 0.05. The ash content of charcoal varies from about 0.5 % to more than 5 % depending on the species of wood.

2. Model Validation

The molar fractions of CO and CO_2 of syngas between simulations and experiments are compared in Fig. 5. The present model shows molar fractions of CO has good agreements between simulation results and experimental ones. The simulated molar fraction of CO ranged from 21.5 to 28.5 %, while experimental results showed 20.34 to 26.3 %. The molar fractions of CO_2 show some differences between simulation results and experimental ones. The molar fractions of CO_2 in simulation 1 and experiment 1 are 8.5 % and 10.06 % respectively. The error between

simulation and experiment is 5 %. And the molar fraction of CO_2 in simulation 3 and experiment 3 are 8.9 % and 6.6 % respectively. The error between simulation and experiment is 26 %. Overall the simulation validation showed good agreements in most cases. It could be seen that this model set up by COMSOL® Reaction Engineering Lab can be used to simulate biomass gasification processes reasonably.

3. Parametric Study

The effects of ash content, moisture, O_2 ratio in air and air flow rate is evaluated with the results of model applications with respect to syngas composition and calorific value of syngas.

A. Ash Content

Since ash is inorganic chemicals in biomass. it can not be combusted and mostly less than 8 %. The effect of ash content on syngas composition is assessed. For the assessment, the moisture content of charcoal is set 8 %, air flow rate is 20 L/min, material flow rate is 0.45 kg/hr. The assessment was conducted for ash contents from 1 % to 10 %, and temperatures of 973 K, 1073 K, 1173 K, and 1273 K. The simulation results are presented in Figures 6 (a) to (d). As the ash content increases from 1 % to 10 %, the molar fraction of CO decrease. The CO molar fractions are changed from 20.5 % to 16.5 % in 973 K, from 22.0 % to 19.9% in 1073 K, from 21.7 % to 21.0 % in 1173 K and from 22.5 % to 20.5 % in 1273 K. Meanwhile the molar fraction of CO_2 increased, The CO_2 molar fractions are from 7.0 % to 8.0 % in 973 K, from 6.0 % to 7.2 % in 1073 K, from 5.5 % to 6.7 % in 1173 K and from 6.0 % to 7.0 % in 1273 K. The molar fraction of H_2 change is stable when ash content increased. It remains about 3 %. The simulation data shows that the increase in ash content bring down the CO molar fraction of syngas at a constant air flow rate. More CO from carbon would be combusted to CO_2 when ash content increase. The CO_2 molar fraction is increased
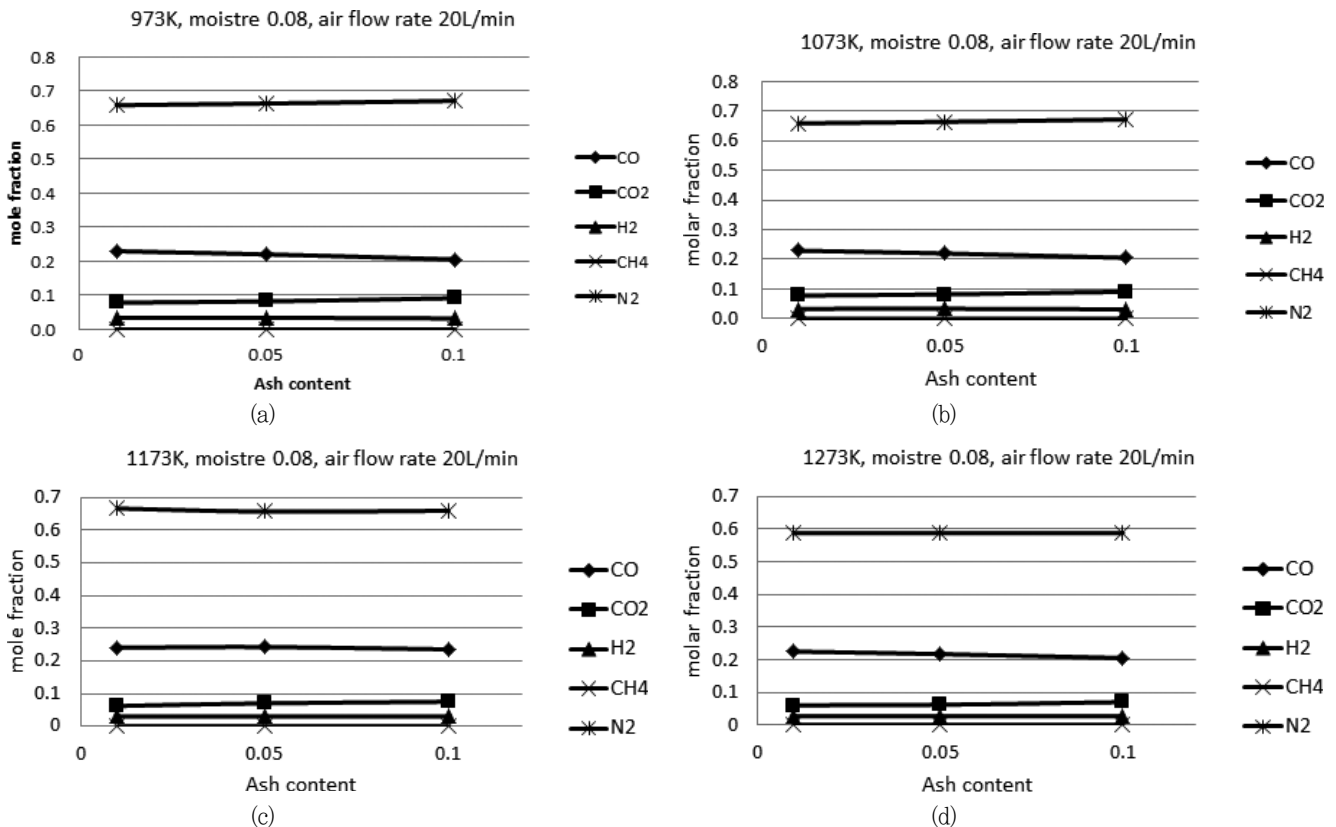

Fig. 6 Simulation result of molar fraction of syngas composition for different ash contents, temperature (a) 973 K (b) 1073 K (c) 1173 K (d) 1273 K

as shown in the simulation results. The H_2 molar fraction is not affected by ash content.

B. Moisture

The effect of moisture on syngas composition was also assessed in this study. The ash content is 5 %, air flow rate is 20 L/min, material flow rate is 0.45 kg/hr. Syngas composition is predicted for moisture contents ranging from 5 to 30 % because the moisture of biomass used for gasification usually less than 30 %, and temperatures of 973 K, 1073 K, 1173 K and 1273 K. The simulation results are presented in the figures 7 (a) to (b). When the moisture increases from 5 % to 30 %, the molar fractions of CO decreased. The CO molar fraction changed from 18.7 % to 16.3 % in 973 K, from 20.3 % to 15.4 % in 1073 K, from 21.0 % to 15.5 % in 1173 K and from 21.3 % to 15.4 % in 1273 K. The CO_2 molar fractions increased from 5.6 % to 14.2 % in 973 K, from 6.3 % to 12.8 % in 1073 K, from 6.0 % to 12.7 % in 1173 K and from 6.0 % to 12.7 % in 1273 K. The molar fraction of H_2 is increased when moisture content increased. The H_2 molar fractions in different temperature are increased from 1.8 % to 10.8 % in 973 K, from 21.8 % to 9.8 % in 1073 K, from 1.8 % to 9.8 % in 1173 K and from 1.8 % to 9.7 % in 1273 K. The simulation results show that moisture contents of charcoal affected the molar fraction of H_2 in syngas. The molar fraction of H_2 increase when moisture contents increase under the fixed reaction temperature as in this study. The water gas shift reaction seems to take place under high vapour concentration. The molar fraction of CO_2 also increased as the moisture contents increase.

C. Oxygen Concentration in Air

Air is usually used as gasification medium. Naturally it has about 79 % of N_2 and 21 % of O_2. The O_2 ratio in air is an important factor for gasification because the main constituents of syngas, CO and CO_2 are coming from oxidizing reactions occurred in the gasifer. The effect of O_2 ratio in air on syngas composition is evaluated. The assumptions for the model application is that the ash
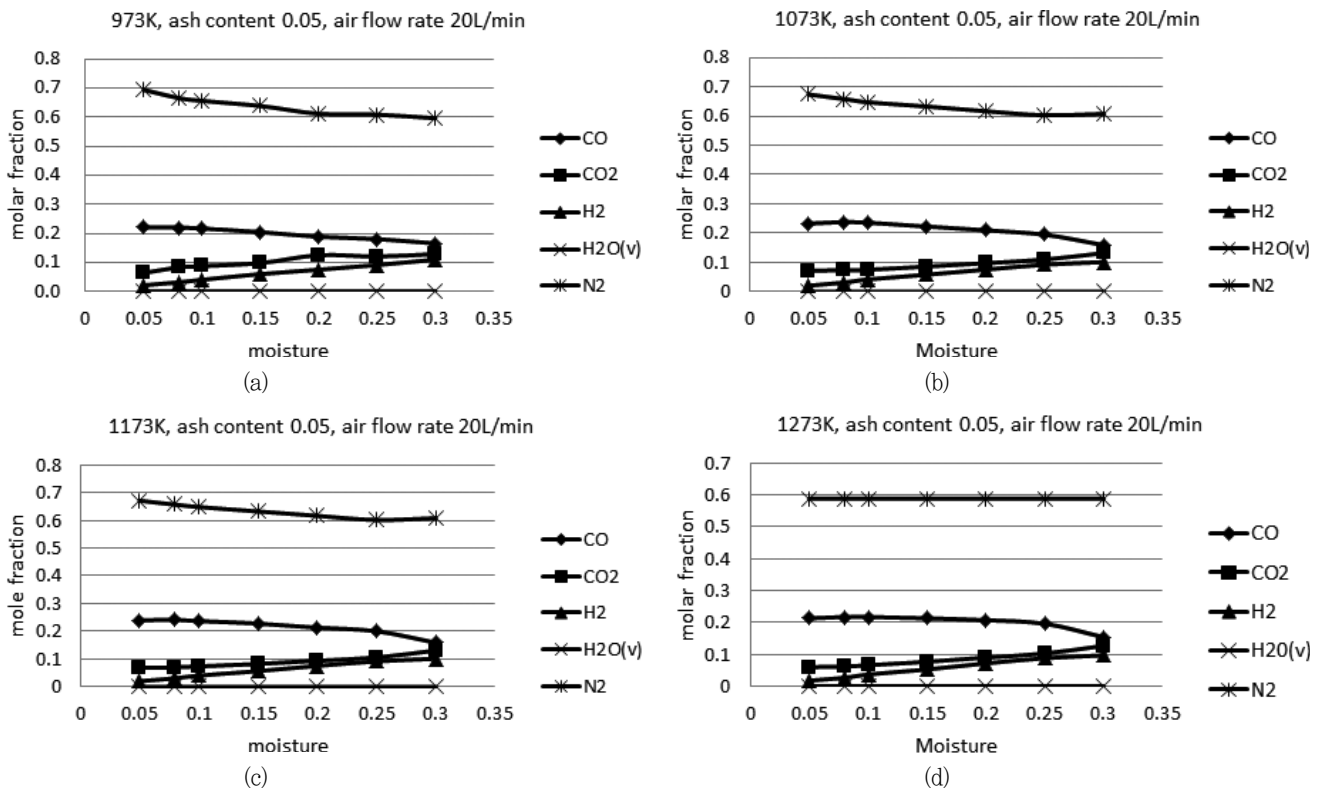

Fig. 7 Simulation result of molar fraction of syngas composition for different moisture contents, (a) 973 K (b) 1073 K (c) 1173 K (d) 1273 K
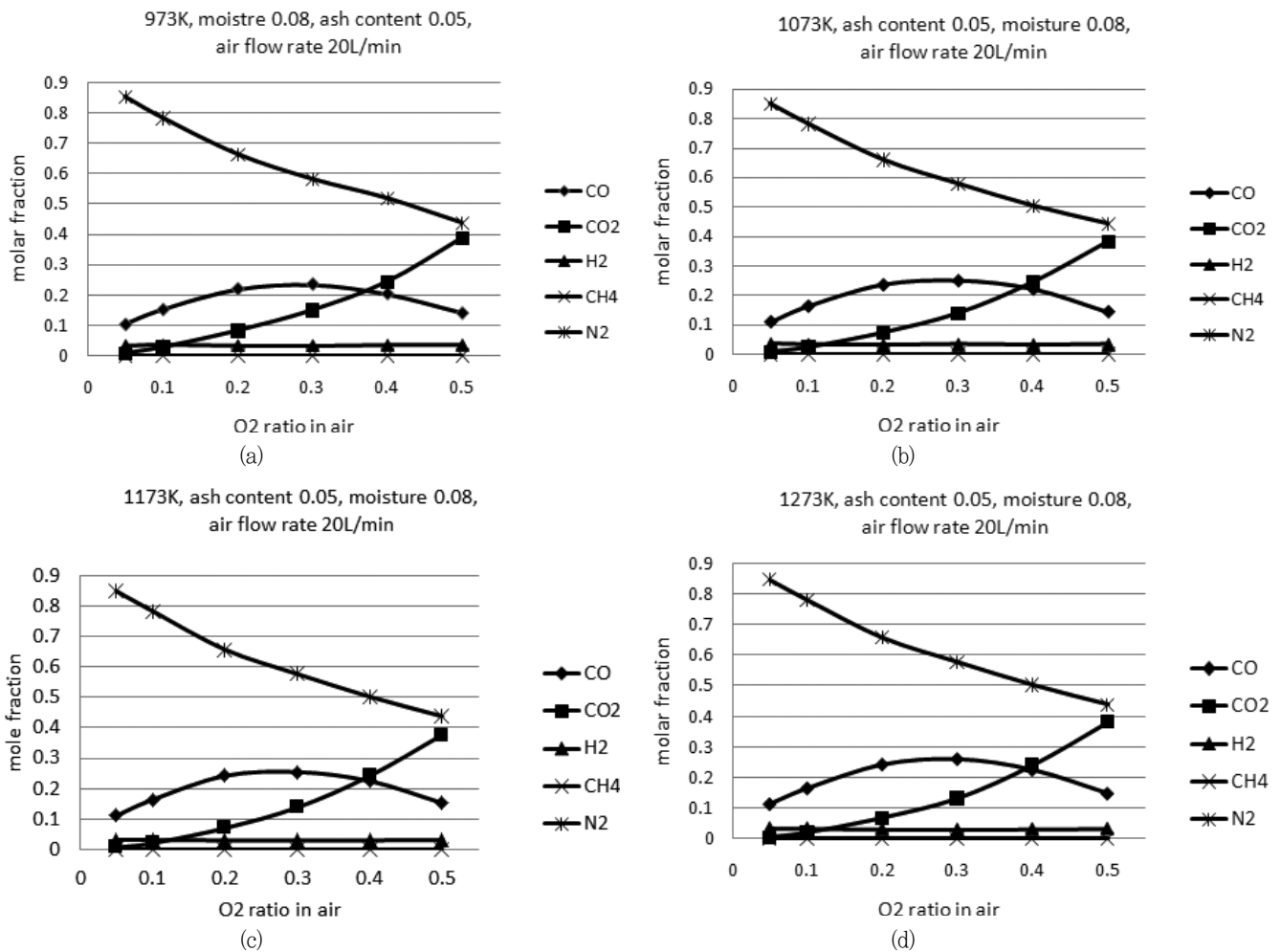
Fig. 8 Simulation result of molar fraction of syngas composition, temperature (a) 973 K (b) 1073 K (c) 1173 K (d) 1273 K

content is 5 %, moisture is 8 %, air flow rate is 20 L/min and material flow rate is 0.45 kg/hr. Different concentrations of O_2 was provided from 5 % to 50 %, and temperatures of 973 K, 1073 K, 1173 K and 1273 K. The simulation results are presented in the Fig. 8. As the figure show, when the O_2 ratio in air increases from 5 % to 30 %, the molar fraction of CO increases while decreases when the O_2 ratio in air increases from 30 % to 50 %. The CO molar fractions range from 10.4 % to 23.4 % in 973 K, from 10.8 % to 25.0 % in 1073 K, from 11.2 % to 25.5 % in 1173 K and from 11.3 % to 26.1 % in 1273 K. The CO_2 molar fractions range from 0.97 % to 38.7 % in 973 K, from 0.84 % to 38.1 % in 1073 K, from 0.72 % to 37.7 % in 1173 K and from 0.60 % to 38.3 % in 1273 K. The changes in the molar fraction of H_2 negligible is very little when

O_2 concentration in air increased. It remains about 3 %. The simulation results show that the molar fractions of CO change sensitively when O_2 concentration in air is 30 %. The molar fraction of CO is relatively low both in O_2 concentration in air is 5 % and 50 %. The molar fraction of CO_2 is increase with the increased in O_2 concentration in air.

D. Air Flow Rate

Air flow rate is an important operation parameter for gasification. If the air flow rate is too high, complete combustion is resulted. With the minimum air flow rate, the gasification reaction could be occurred very slowly since the reaction heat can not provide enough heat to keep the high temperature continuously. The effect of air
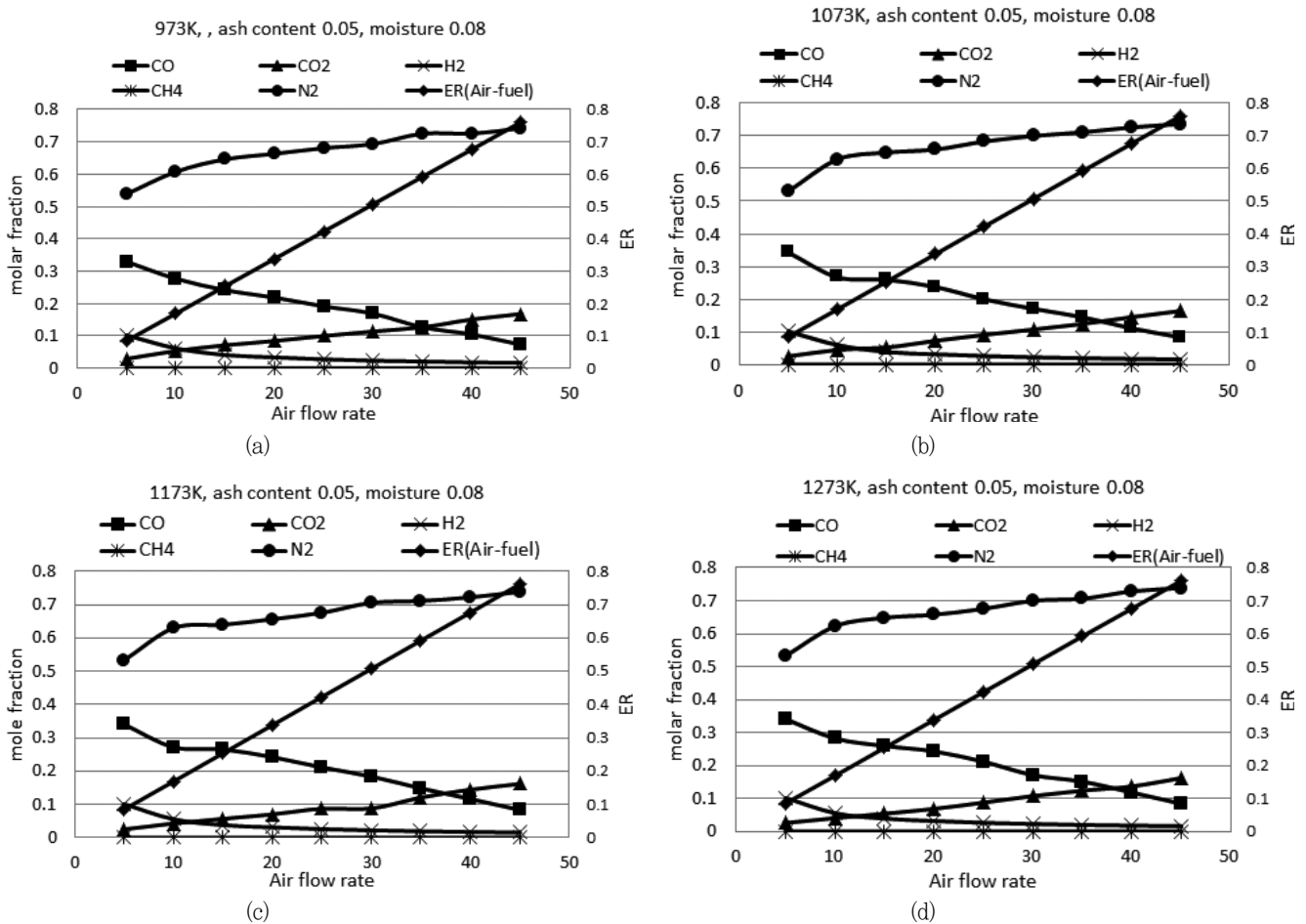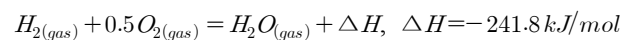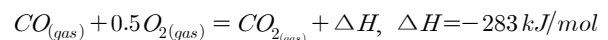
Fig. 9 Simulation result of molar fraction of syngas composition for different air flow, temperature (a) 973 K (b) 1073 K (c) 1173 K (d) 1273 K

flow rate for syngas composition is analyzed. The ash content is 5 %, moisture is 8 %, and material flow rate is kept in 0.45 kg/hr. The composition of syngas is simulated with the air flow rate ranging from 5 L/min to 45 L/min, and temperatures of 973 K, 1073 K, 1173 K and 1273 K. The simulation results are presented in the Fig. 9. As the figure presented, the molar fractions of CO decrease when the air flow rate increases from 5 L/min to 45 L/min. The CO molar fractions range from 32.9 % to 7.29 % in 973 K, from 34.3 % to 8.35 % in 1073 K, from 34.1 % to 8.38 % in 1173 K and from 34.1 % to 8.38 % in 1273 K. The CO_2 molar fraction increased from 2.93 % to 16.8 % in 973 K, from 2.53 % to 16.4 % in 1073 K, from 2.53 % to 16.2 % in 1173 K and from 2.54 % to 16.2 % in 1273 K. The molar fraction of H_2 is also decreased when air flow rate increase. The H_2 molar fractions range is from 10.3 %

to 1.1 % in 973 K, from 10.1 % to 1.56 % in 1073 K, from 10.1 % to 1.56 % in 1173 K and from 10.1 % to 1.56 % in 1273 K. The simulation results show that the increase in air flow rate oxidize more CO to CO_2. Low air flow rate results in high CO and H_2 molar fraction.

E. Calorific Value

CO and H_2 are combustible gases, and their the reaction heat are as follows:

$$CO_{(gas)} + 0.5 O_{2(gas)} = CO_{2(gas)} + \triangle H, \ \triangle H = -283 \, kJ/mol$$

$$H_{2(gas)} + 0.5 O_{2(gas)} = H_2O_{(gas)} + \triangle H, \ \triangle H = -241.8 \, kJ/mol$$

So the calorific value of syngas depend on the concentration of CO and H_2. The changes in calorific values of
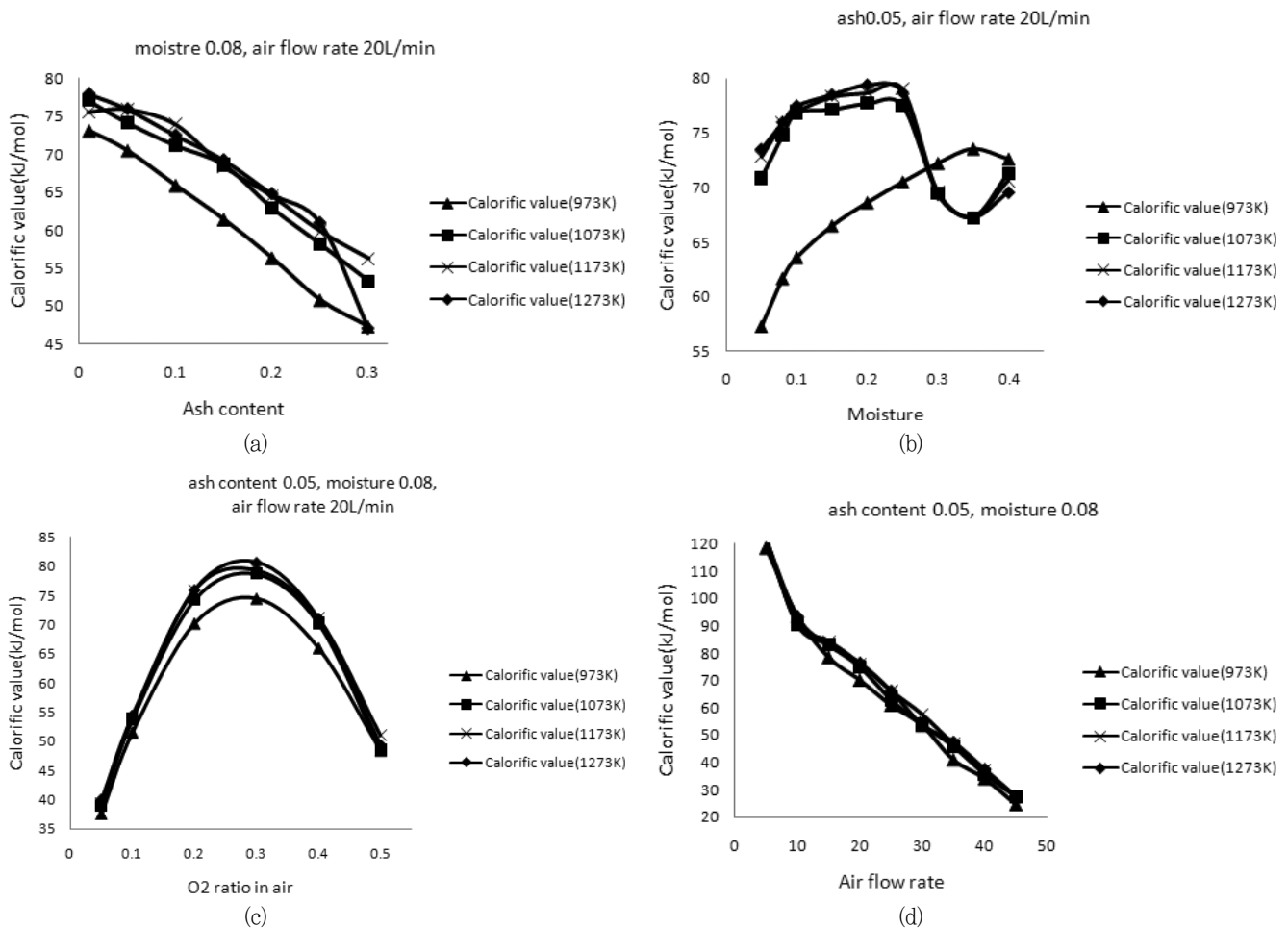
Fig. 10 Effects of ash content (a), moisture (b), O₂ ratio in air (c) and air flow rate (d) on calorific values at different temperature

syngas for different conditions are presented in Fig. 10. They decrease with increasing air flow rate as shown calorific values of syngas increase with increasing moisture from 0.05 to 0.2 and then decrease from 0.2 to 0.4. The highest of calorific value is 79.4 KJ/mol at the moisture of 0.2. It shows that the calorific value of syngas increases when O_2 flow rate increases from 5 % to 30 %, the highest calorific value of syngas is 80.7 KJ/mol when O_2 concentration in air is 0.3. And then they decrease as O_2 concentration increases from 30 % to 50 %. It is also seen that gasification temperature has effect on the calorific value of syngas. The calorific value of syngas is lower when gasification temperature is 973 K and gradually increase as gasification temperature increases from 1073 K to 1273 K.

F. Temperature

Temperature is also an important factor in gasification. Fig. 11 shows the effect of temperature on syngas composition. It is seen that molar fractions of CO increase rapidly as temperature goes up from 773 K to 873 K, and they increase slowly as temperature is raised from 873 K to 1273 K. The molar fractions of CO_2 decrease with temperature. The molar fraction of CO increases with temperature because the formation of CO from C and CO_2 is an endothermic reaction:

$$C + CO_2 = 2CO + \triangle H, \quad \triangle H = 135.6 \text{kJ/mol}.$$

More CO is produced from CO_2 when temperature increase. The effect of temperature on calorific value of syngas is

shown in Fig. 11. It shows that calorific values of syngas increase rapidly with temperature changes from 773 K to 873 K, and then increase slowly with temperature changes from 873 K and above. The reason for this seems that CO concentrations increase with higher reaction temperature. In reality, temperature is influenced by many other conditions and it can be controlled by changing air flow rate in the experiments. H_2 production was not be influenced by temperature.

G. Equivalence ratio (ER)

The equivalence ratio affected syngas compositions and calorific values as shown in Fig. 12. The molar fractions

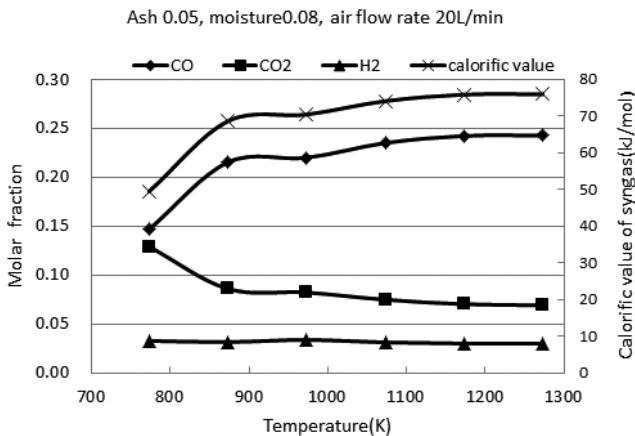

Fig. 11 Molar fraction and Calorific value of syngasof syngas with temperature, charcoal, ash content 0.05, moisture 0.08, air flow rate 20 L/min, equivalence ratio (ER) 0.338
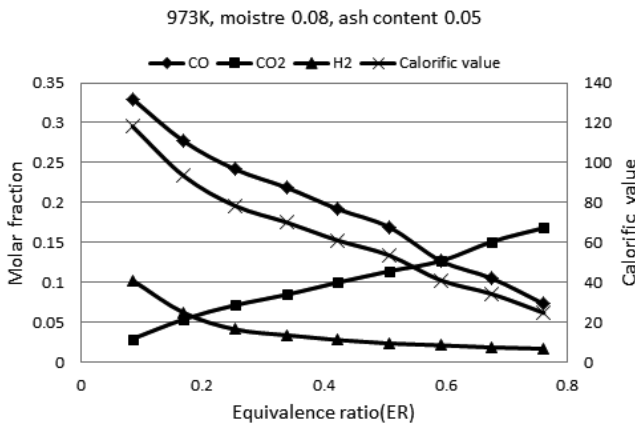

Fig. 12 Influence of equivalence ratio on compositions and calorific value of syngas, 793 K, moisture 0.08, ash 0.05

of CO and H_2 decrease as equivalence ratio increases, while molar fractions of CO_2 increase. It shows that the calorific values of syngas decrease with increasing equivalence ratio since the concentrations of CO and H_2 decrease but CO_2 concentrations increase.

IV. CONCLUSIONS

In this study a simplified gasification model was constructed using a commercial software. The model predictions show reasonable agreement with the experimental data. After validation, the model was applied to evaluate the effects of parameters including feedstock ash content, moisture, O_2 ratio in air, air flow rate, temperature and equivalence ratio (ER). The model can also be used as a design tool for the biomass gasifiers. Feedstock and operation conditions in the downdraft gasifier is summarized as below:

1. Low ash content feedstocks are required to produce high quality syngas in biomass gasification.

2. Air flow rate needs to be controlled within appropriate ER ranges.

3. Higher reaction temperature resulted in CO concentrations and calorific values of syngas.

4. For producing high concentration of CO and high calorific value syngas, lower equivalence ratio (ER) must be keep during the gasification process.

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