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A Simulation Study for Low Rank Coal Gasification in Coal-Water Slurry Gasifier

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Abstract: By using a 3-D CFD model, the gasification process of low-rank anthracite coal in a coal-water slurry gasifier was simulated and investigated. The effects of oxygen/coal ratio and inlet slurry temperature on the gasification furnace temperature characteristics, gas composition distribution, carbon conversion and effective gas content were investigated for different kinds of low-rank anthracites. The higher the ash content of anthracite, the lower the gasification efficiency and the lower the effective gas content. Increasing the oxygen/slurry ratio showed no significant change in the effective gas content, but a slight increase in the furnace outlet temperature and CO_2 content. Increasing the inlet temperature of CWS enhances both the effective gas yield and gasification efficiency and decreases the CO_2 content.

Keywords: Coal gasification; Coal-water slurry; Low rank coal; Simulation study; Oxygen/coal ratio

I. INTRODUCTION

Coal-water slurry (CWS) gasifier is one of the entrained flow coal gasifiers which is widely used in the world, because of the advantages of simple feedstock system, reuse of the waste water and the competence of up to 8.0 MPa high pressure. Syngas from CWS gasifier contains a large amount of vapor and no additional steam is needed for the reforming reaction of CO, so it is commonly used to produce syngas for chemical industry.

Several investigations have been carried out for the simulation of coal gasification.

Three chemical processes such as devolatilization, char gasification, and gas-phase reaction are reviewed and discussed to simulate the coal gasification [1]. For devolatilization, the high accurate network-based model will be implemented directly or indirectly with enhancing the computational resource [6]. For char gasification, it should be essential to model the pore structure formation as a series of processes throughout from the devolatilization to char gasification. For gas-phase reaction, the model taking the elementary reactions into account will be paid more attention that can be coupled with the highly accurate turbulence model [1]. Other investigation included the influence of water/coal ratio, oxygen/coal ratio, and temperature on the composition of the product gas, the yield of the product and the quench water amount [2]. Turbulent flow, heat transfer, and chemical reactions were included in the computational fluid dynamics (CFD) model to predict the internal velocity field, temperature distribution, component distribution, and carbon conversion rate of coal gasification. In this simulation, a high-quality syngas was obtained with a lower consumption of pure oxygen, and the effective-gas ratio reached 91.73% when the optimum oxygen/coal rate was 0.7 [4].

Most simulation studies predicted the temperature field, velocity field and gas component distribution according to the variation of conditions and analyzed the influence of oxygen/coal rate and vapor/coal rate on the proportion of effective composition and carbon conversion rate [2, 3].

Meanwhile, some researchers introduced a slurry preheating technology using shell-and-tube heat exchangers (STHXs) with ladder-type fold baffles to improve energy efficiency of CWS gasification. The effect of structural parameters of heat exchanger which is used for the heating of CWS on cold gas efficiency and total cost is discussed coupling system design and unit equipment optimization, so that oxygen consumption decreases by 7.6% and cold gas efficiency increases by 6.5% than that without preheating technology [5].

Generally, entrained flow coal gasification uses high rank coals with high volatile content and low ash content to enhance the gasification efficiency. However, coal in DPR Korea is low-rank anthracite with low volatile content and high ash content. There are few studies on gasification processes using these low-grade anthracites. This is probably due to the absolute acceptance of previous studies that coal gasification must use low-ash and high-volatile high-rank coals. In order to enhance the efficiency of low-grade anthracite gasification, the temperature of the reaction furnace should be increased, which requires an increase in the oxygen/coal ratio. However, this may lead the complete combustion reaction of coal, which contrarily reduces the gasification efficiency and increases CO_2 content in the syngas. Therefore, we considered it necessary to research the gasification process of the low-rank anthracite coal in DPR Korea and to determine the influences of some factors on the gasification efficiency.

In this paper, the CWS gasification process using low rank anthracite with low volatile and high ash has been simulated to determine the gasification efficiencies according to the coals with different content of volatile and ash. The reasonable operating factors of low rank anthracite gasification were also determined based on the calculation of the temperature distribution, cold gas efficiency, syngas composition and carbon conversion rate according to the oxygen/coal ratio.

II. COMPUTATIONAL MODEL

The 3-D numerical model was proposed for present study. The global coal gasification process can be characterized by several chemical reactions which are presented in Table 1.

Table 1. Chemical reactions and constants

	Reactions	Ap	E, J/Kmol
Homogeneous reactions	$Vol+0.8942O_2=0.11465CO_2+2.72467H_2O+0.04497N_2+0.05029SO_2$	2.119×10^{11}/s	2.027×10^{8}
	$H_2+0.5O_2=H_2O$	5.69×10^{11}/s	1.47×10^{8}
	$CO+H_2O=CO_2+H_2$	2.75×10^{9}/s	8.36×10^{9}
	$CO+0.5O_2=CO_2$	1.93×10^{13}/s	1.26×10^{8}
Heterogeneous reactions	$C(s)+0.5O_2=CO$	425.04/s	1.55×10^{8}
	$C(s)+H_2O=CO+H_2$	100.285/s	2.38×10^{8}
	$C(s)+CO_2=2CO$	6.325/s	2.14×10^{8}

This process can be described using Navier-Stokes equation considering mass and energy conservation.

The turbulence was characterized with the utilization of realizable k-□ equation with enhanced wall treatment model.

$$\frac{\partial}{\partial x}(\rho u\varphi)+\frac{\partial}{\partial y}(\rho v\varphi)+\frac{\partial}{\partial z}(\rho w\varphi)\varphi=\frac{\partial}{\partial x}\left(\Gamma_\varphi\frac{\partial\varphi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\Gamma_\varphi\frac{\partial\varphi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\Gamma_\varphi\frac{\partial\varphi}{\partial z}\right)+S_\varphi+S_{p\varphi} \quad (1)$$

Where □ is three momentum components, Γ□□□is diffusion coefficient of the transported variable □, S□ is source term of the mass from the gas phase, S*p*□ is source term for the mass of the coal particles.

Turbulent gas phase reactions were assumed that they are governed by turbulent mixing. Gas phase absorption was described by using weight-sum-of-gray-gases model (WSGGM), which is useful to determine gas phase absorption coefficient. [8, 9] As the gasification process is accompanied by radiation under high temperature conditions, considering radiation is crucial. Decision operator (DO), which is expressed as Eq. (2), was used to describe the radiation as its results showed good argument for alternative methods. [9-11]

$$\nabla(I(\vec{r},\vec{s})s) + (a+\sigma_s)I(\vec{r},\vec{s}) = an^2\frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi}\int_0^{4\pi} I(\vec{r},\vec{s})\Phi(\vec{s},\vec{s}')d\Omega' \quad (2)$$

Where $\vec{r}$is position vector, $\vec{s}$is direction vector, $\vec{s}'$is scattering direction vector, *a* is absorption coefficient, n is refractive index, □s is scattering coefficient, □ is Stefan-Boltzmann constant, I is radiation intensity, T is local temperature, □ is phase function. Reactions for coal gasification can be represented with the species transport model, which are described in table 1. And the solution includes all of the species involved in the reaction.

The oxygen, which is oxidant, is considered as the Euler form within the continuous phase and the trajectories of each particle are individually tracked with Laglangian method as they are treated as dispersed phase. In order to describe the effects of interaction with continuous and dispersed phase, virtual mass force is employed. The slurry consisted of water and low rank coal particles, is introduced using liquid droplet and combustion particle injection. [12]

$$m_p\frac{du_{ip}}{dt} = C_D\rho_g\frac{A_p}{2}\left(\bar{u}_{ip}+u'_{ig}+u_{ip}\right)\left|\bar{u}_{ip}+u'_{ig}+u_{ip}\right| + m_p g_k \quad (3)$$

Where, u_{ip} is the particle velocity component, $\bar{u}_{ig}$ is average velocity u'_{ig} is pulsating velocity of the gas phase in a certain direction, m_p is particle mass, $□_g$ is density of gas, A_p is particle surface area, g_k is gravity, and C_D is resistance coefficient.

Heterogenous and homogeneous reactions are employed to implement the eddy dissipation model. And the methanation reactions are ignored as their influence to overall process are not notable under operating conditions. Reaction rates are assessed with both finite-rate and eddy dissipation models. Reaction constants are introduced in the following table. In order to reflect the devolatilization, single rate model introduced below was employed.

$$\frac{dm}{dt} = Aexp\left(\frac{-E}{RT_p}\right)(m_0 - m) \quad (4)$$

Where m_0 is initial volatile fraction mass, m is postreaction volatile fraction, R is universal gas constant, T_p is particle temperature, $A=312000s^{-1}$, $E=7.4\times10^7 J\ kmol^{-1}$

Depletion rate of solid particle along with the reaction is expressed as the function of kinetic rate.

III. METHOD AND BOUNDARY AND INLET CONDITIONS

A. Method

We simulated the gasification process of three different kinds of low-rank anthracites, and the characteristics of the coal used in the simulation are given in Table 2.

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The simulation calculations of the gasification process for each species are represented by Case 1, Case 2 and Case 3, respectively. Also, for the model validation, the Case 0 was performed separately. The characteristics of the coal for Case 0 is after [5].

Table 2. Coal analysis

Case	Proximate analysis				Ultimate analysis					HHV, kJ/kg
	Vol	FC	Ash	Moi	C	H	O	N	S	
Case 0	32.24	57.95	7.49	2.32	71.58	4.63	16.46	1.04	0.54	29 000.1
Case 1	5.95	68.49	22.84	2.72	68.76	1.09	4.02	0.25	0.32	22 175.2
Case 2	5.58	60.62	23.42	8.38	60.49	1.38	3.36	0.67	0.3	20 506.4
Case 3	5.64	65.03	24.46	4.87	65.34	1.24	3.37	0.41	0.31	21 962.1

The oxygen-slurry ratio was varied from 0.62 to 0.72 by 0.02, and the inlet temperature of slurry was increased by 50 K from 373 K to 525 K, and the gasification characteristics were analyzed, respectively.

B. Boundary Condition

The amount of inlet CWS is 49 786 kg/h, and the ratio of water to coal is 1:2. As a gasification agent, the oxygen inlet of 99.4% purity is 31 243 kg/h. The gasifier pressure is 4.0 MPa and the coal particle size is 76 ㎛.

IV. RESULT AND DISCUSSION

A. Model validation

In order to validate the accuracy of computational model and the simulation, simulation results are compared with the experimental data from Ref. [5]. The deviation of outlet temperature is 3.5%-4.9%, and the deviations of CO, H_2, and CO_2 content among syngas are 2.1%-2.5%, 3.2%-3.6%, 1.8%-2.2%, respectively. The deviations may be regarded as the neglect of CH_4 formation, simplification of boundary conditions, or measurement errors in experiments. As seen above, the furnace temperature as well as syngas compositions are good agreement with acceptable accuracy, as a consequence, our computational method is reliable.

B. Gasification performance according to coals with different ash content.

Coal ash is one of the main factors affecting the normal operation of gasification process, and the higher the ash content, the more negative the effect on gasification process. Thus, during gasification, the surface of carbon is covered with ash, which leads to poor contact of the gasification agent with the carbon surface and low gasification efficiency. Also, as the ash content increases, the ash yield inevitably increases and the amount of carbon discharged along the ash from the furnace increases together. And the presence of inert components in the ash reduces the gasification efficiency, resulting in a high consumption of oxygen and slurry.

In this study, the CFD model used in the simulation was validated and, as described in Section 3.1, the analysis of the coal-water slurry gasification process was carried out for three kinds of coal, and the comparison was carried out with the results of the validated calculations of the model using coal with 7.49% ash content and 29000 kJ/kg calorific value.

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Fig. 1 and Fig. 2 show the temperature and velocity distributions inside the reaction furnace obtained in Case 1, 2 and 3, and Table 3 shows the temperature at the reaction furnace outlet and the molar ratio of the obtained syngas.

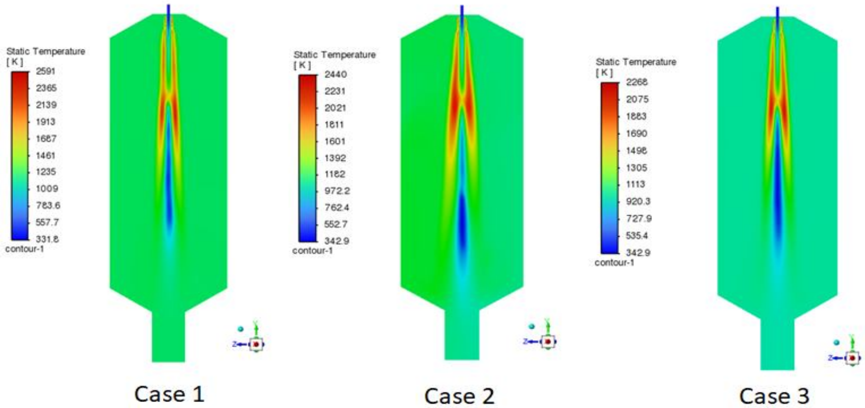

Fig 1. Temperature distributions for different coals

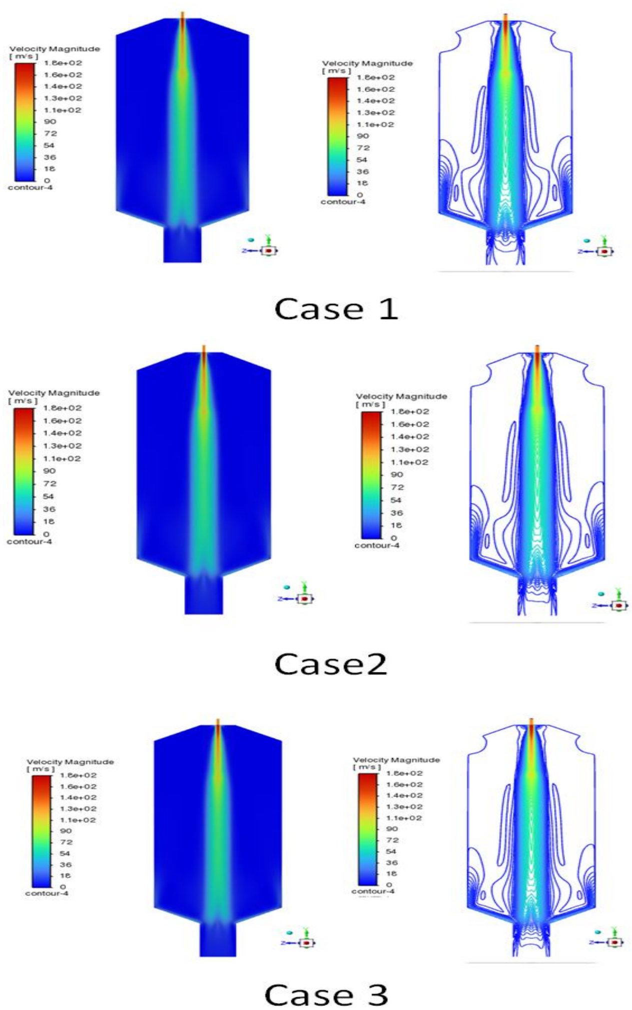

Fig 2. Velocity distributions for different coals

Table 3. Outlet temperature and proportion of effective composition

	Outlet temperature, °C	CO, %	H_2, %	CO+H_2, %
Case 0	1480	43.66	38.14	81.8
Case 1	1312	47.73	25.04	72.77
Case 2	1297	47.56	24.13	71.69
Case 3	1294	45.39	24.32	69.71

As shown in Fig. 1, Fig. 2 and Table 3, the highest outlet temperature was found in Case 1 (1312 °C) and the lowest temperature was 1294 °C in Case 3. This is probably due to the highest ash content of the coal used in Case 3, which is 24.46%. However, the relative error of the furnace outlet temperature values obtained in Case 1, 2 and 3 is less than 1.2 %. This is because the difference in the properties of the three kinds of coal is not very significant. On the other hand, comparing the simulation results obtained in Case 3 with those obtained in the model verification (Case 0), the outlet temperature in Case 0 are about 185 °C higher than that in Case 3 and the proportion of effective gas composition is about 12% higher. The reason is that the ash content of coal used in Case 0 is 7.5% and the calorific value is 29 000 kJ/kg, while the ash content of coal used in Case 3 is 24.46%, and the calorific value is 21962 kJ/kg, which is significantly different. Thus, if gasification is carried out using low-rank anthracite with high ash content, the temperature of the reaction furnace is about 1300 °C, which is 170 °C lower than the fluid temperature of coal ash, which means that the flux must be added for liquid ash treatment.

Meanwhile, as shown in Table 3, the hydrogen contents in the syngas obtained in Case 1, 2 and 3 is 24-25%, which is much lower than 38.14% in Case 0. The higher hydrogen content in the syngas produced in Case 0 could be attributed to the enhanced endothermic reaction of steam with carbon to produce hydrogen due to the high temperature of the reaction system. The proportion of effective gas composition in the syngas during the CWS gasification using high-rank coals was 81.8%, while it was only 71-72% for low-rank anthracites. From the simulation results, it is obvious that the gasification using low-rank coal has less gasification efficiency and effective gas content.

C. *Effect of the Oxygen/Slurry Ratio*

Oxygen/coal ratio is also an important factor that directly affects gas yield, gasification efficiency, proportion of effective gas, gas composition. Since the structural dimensions, gasification temperature and pressure, and coal used as raw materials are different, the optimum oxygen/coal ratio is not constant according to the literatures.

Many studies have investigated the effect of oxygen/coal ratio on the temperature of the reaction furnace, gasification efficiency, carbon conversion, composition of syngas, etc. [2,3,5]. Increasing the oxygen content means the high oxygen inlet rate, which leads to the higher oxygen concentration in the recirculation zone of the reaction furnace, and thus the gasification reaction rate also increases [3]. With the increasing oxygen content, the high temperature region expands and more CO is used to produce CO_2. [2] Since the reaction between CO and water is exothermic, increasing the temperature leads to a lower conversion of CO and a higher CO content in the produced syngas.

In this study, the gasification process was simulated by varying the oxygen/slurry ratio from 0.62 to 0.72, and the results are shown in Fig. 3 and Fig. 4.

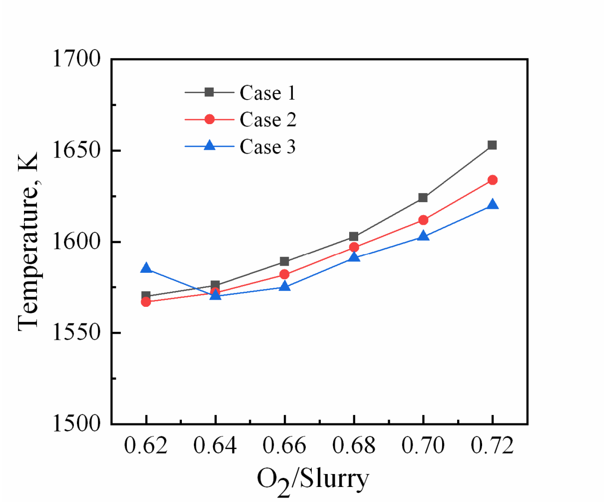

Fig 3. Gas composition according to the oxygen/slurry ratio

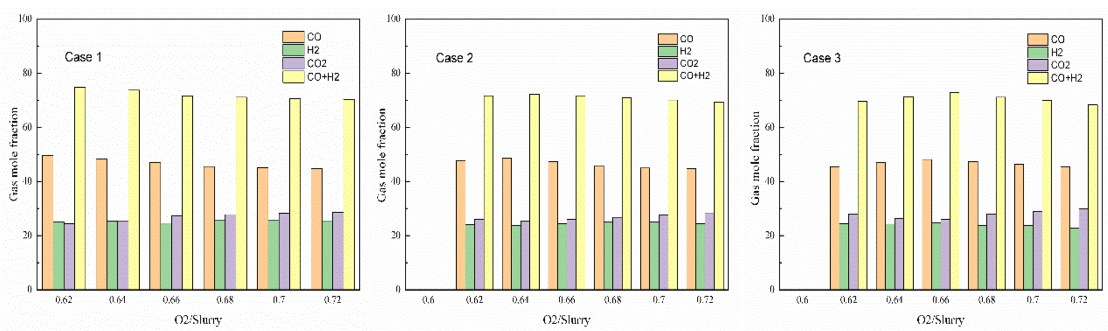

Fig. 4. Outlet temperature according to the oxygen/slurry ratio

As shown in the Fig. 3, with the increase of oxygen /slurry ratio, Case 1 shows a decreasing trend of CO content and an increasing trend of CO_2 content, while H_2 shows a slight increase and then a decreasing trend. This is because the higher the oxygen /slurry ratio, the higher the O_2 amount and the more the CO_2 conversion. And also, the reason for the increase in H_2 content is that the temperature increases with increasing oxygen /slurry ratio, which favors the synthesis of the endothermic aqueous gas, and, to a certain extent, the amount of inlet water in the slurry is reduced, so that conditions are not given to generate H_2. In Case 2, the CO content increased and then decreased again with increasing oxygen /slurry ratio, and with this, the CO_2 also decreased and then increased again, while H_2 tended to oscillate around a certain value. This is because the ash content of coal in Case 2 is higher than that in Case 1, as shown in Table 1, the temperature of the reaction furnace is not enough high to happen the gasification reaction. At this time, the increasing of the O_2 content results in the combustion of CO to produce CO_2, which leads to higher furnace temperature and favorable conditions for the synthesis of water gas. Meanwhile, hydrogen content oscillated in a certain amount, which is related to the production condition of hydrogen described above. In Case 3, there was a similar varying tendency for CO, CO_2, and H_2 content as Case 2, which can be regarded to the above analysis.

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Finally, in Case 1 - Case 3, when the oxygen/slurry ratio increased from 0.62 to 0.72, the temperature of the furnace outlet increased, but there was no significant difference in the effective gas content. This indicates that the equilibrium of the reaction moves towards the more production of carbon dioxide with the increasing of oxygen concentration.

D. Effect of the Inlet Temperature

Some studies have reported that the preheating of slurry increases the gasification efficiency. The preheating of slurry can save energy for the increase of the reaction temperature and the heat required for this can be recovered from the waste heat of the gasifier, thus it is effective in terms of gasification efficiency.

As explained in Section 3.1, the gasification processes are simulated by varying the inlet slurry temperature from 20 °C to 250 °C, and the results are shown in Fig. 5 and Fig. 6. The coal of Case 3 with the highest ash content of the above three samples is used for gasification simulation.

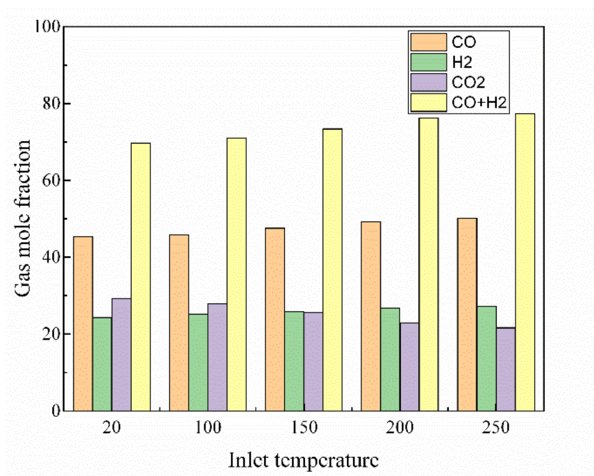

Fig. 5. Gas mole fraction with the change of inlet temperature

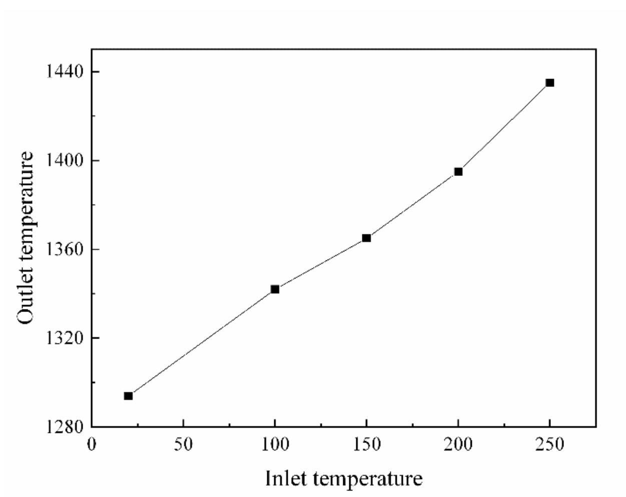

Fig. 6. Outlet temperature with the change of inlet temperature

As shown in Fig. 5 and Fig. 6, the CO content increased a lot while the hydrogen content increased slightly, and the effective gas content increased by 7.6% during the increase of the inlet temperature from 20 °C to 250 °C. And also, the temperature of the furnace outlet increased from 1294 °C to 1435 °C by 140 °C and the content of carbon dioxide decreased from 29.3% to 21.8% by 7.5%. When the temperature of the inlet material increases, the temperature of reactant also rapidly increases, creating a favorable temperature condition for the syngas reaction, which may result in the enhancement of reaction temperature and effective gas content. This calculation is in good agreement with the results of the Ref. [5and it can be confirmed that increasing the temperature of CWS entering the gasifier is a good way to increase the gasification efficiency and the effective gas content. The initial temperature of slurry was increased to 250 °C, but the reactor outlet temperature was around 1435 °C, which did not reach the fluid temperature of the ash, indicating that flux must be added for normal operation of the gasifier.

V. CONCLUSIONS

The higher the ash content of anthracite, the lower the gasification efficiency and the lower the effective gas content. Increasing the oxygen/slurry ratio showed no significant change in the effective gas content, but a trend of increasing the reactor outlet temperature and carbon dioxide content. Also, increasing the inlet temperature of low-rank CWS increases both the gasification temperature, the effective gas yield and the gasification efficiency, and decreases the carbon dioxide content.

Credit authorship contribution statement

Ri Kwang Jin: Methodology, Investigation. Hong Chol: Conceptualization, Writing original draft. Jon Chol Jin: Data curation

Conflict of Interest:

The authors declare that they have no conflict of interest.

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