

Effects of operating factors in the coal gasification reaction

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Abstract—The effects of operating factors on a gasification system were reviewed by comparing a computational simulation and real operation results. Notable operation conditions include a conveying gas/coal ratio of 0.44, an oxygen/coal ratio of 0.715, a reaction temperature of 1,000 °C, and reaction pressure of 5bar in the case of Adaro coal; based on this, the cold gas efficiency was estimated as 82.19%. At the point of the reaction temperature effect, because the cold gas efficiencies are more than 80% when the reaction temperatures are higher than 900 °C, the gasifier inner temperature must remain over 900 °C. At high reaction temperature such as 1,400 °C, the reaction pressure shows little effect on the cold gas efficiency. The addition of steam into the gasifier causes an endothermic reaction, and then lowers the gasifier outlet temperature. This is regarded as a positive effect that can reduce the capacity of the syngas cooler located immediately after the gasifier. The most significant factor influencing the cold gas efficiency and the gasifier outlet temperature is the O₂/coal ratio. As the O₂/coal ratio is lower, the cold gas efficiency is improved, as long as the gasifier inner temperature remains over 1,000 °C. With respect to the calorific value (based on the lower heating value, LHV) of produced gas per unit volume, as the N₂/coal ratio is increased, the calorific value per syngas unit volume is lowered. Decreasing the amount of nitrogen for transporting coal is thus a useful route to obtain higher calorific syngas. This phenomenon was also confirmed by the operation results.

Key words: IGCC, Gasifier, O₂/Coal Ratio, N₂/Coal Ratio, Steam/Coal Ratio, Cold Gas Efficiency, Calories of Syngas Per Unit Volume

INTRODUCTION

The coal gasification process provides a means of generating a wide range of products, including power, chemicals, substitute natural gas and transport fuels. The capacity of this process is currently around 39% for chemical production parts, 38% for Fisher-Tropsch liquids production parts, 6% for gaseous fuels production parts and 16.6% for electricity production, including planned capacity [1,2]. Electricity generation has emerged as a large new market in relation to coal gasification, since gasification is seen as a means of enhancing the environmental acceptability of coal, as well as of increasing the overall efficiency of the conversion of the chemical energy in the coal into electricity [2-8].

In Korea, a 300 MW class IGCC(Integrated gasification combined cycle) power plant producing electricity is being designed and will be constructed from 2012 to 2014 with the design of the gasifier provided by Shell Global Solutions under a project funded by the Korean government and several power companies. In parallel, the design technology development of a gasification block in the IGCC demonstration plant has also been progressing since January of 2010 as a nine-year project at KEPSCO. Under this development project, we reviewed the effects of operating factors on the gasifier through a computational simulation and compared the estimation results with the real operation results from a 1 ton/day class gasification system.

OPERATING FACTORS ON THE GASIFICATION REACTION

To analyze the main operating factors on the gasification reaction, the Cycle-Tempo [9] program for the computational simulation was used for calculation of heat and mass balance. The flow diagram is as follows: a gasifier, quencher under the gasifier, scrubber, and flare stack are connected in series. Simplified flow diagrams appear in Figs. 1 and 2 and the actual system is shown in Fig. 3.

Previous to the present study, KEPRI already had a furnace for combusting residue oil at a rate of 30 kg/h. This furnace was modified into a coal gasifier by adding a quencher to the lower part of the furnace. The burner was modified into a vertical, dual type for supplying LPG and coal as fuel. For removal of ash, a quencher and a scrubber were used. After the scrubber, a valve was installed for controlling the pressure of the system and a flow meter was employed for measuring the produced gas from the gasifier. A desulfurizer was used for removal of sulfur compounds. This was accomplished by passing the produced gas through a tower containing activated carbon. Finally, the produced gas was combusted at the flare stack.

The real amount of coal was obtained from calibration of the amount of coal according to the output value of the motor inverter under varying speed of the coal screw feeder. The real amount of produced gas was measured with a flow meter located after the scrubber and the pressure control valve. The gas composition was analyzed at the position between the scrubber and the pressure control valve utilizing a mass spectrometer (Prima 600s). Cooling water

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The Design condition of Gasification

- $N_2/\text{coal} = 0.7$, $O_2/\text{coal} = 0.82$, $\text{Steam}/\text{coal} = 0.1$, $\text{coal} = 30.1407 \text{ kg/h}$, $\text{Reaction Temp} = 1000^\circ\text{C}$, $\text{heat loss} : 7.35 \text{ kW}$

Coal (Shenhwa) : C 69.52, H 4.38, N 0.91, S 0.28, O 13.35, Ash 5.46 H_2O 6.09 wt%

Steam temp. = 240°C

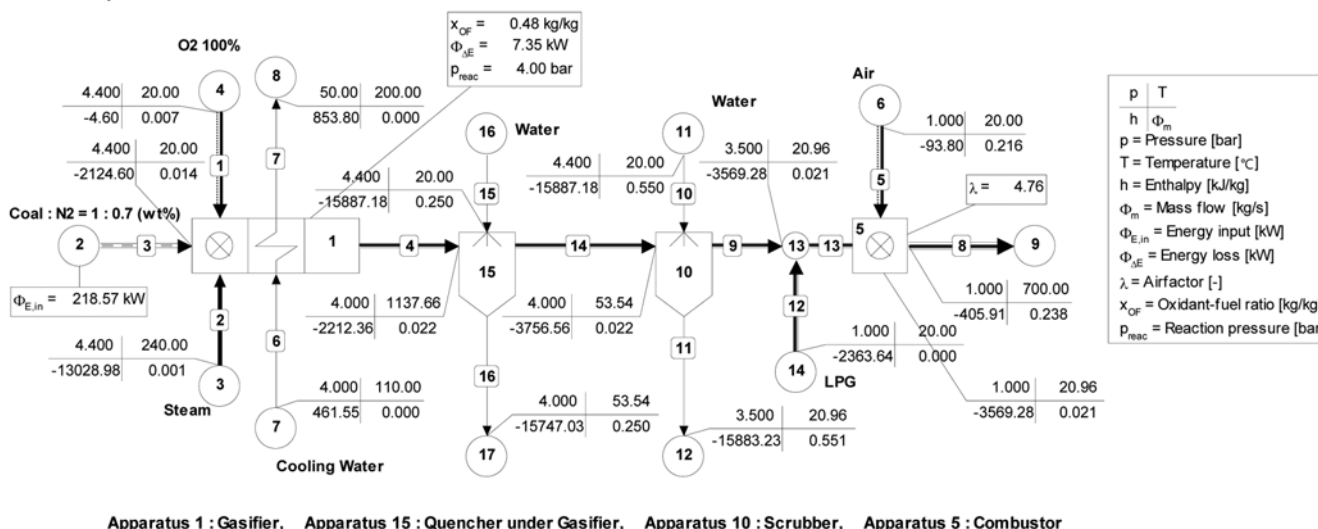


Fig. 1. Flow diagram of heat & mass balance at the operation condition of 1 ton/day coal gasification system (Shenhua coal).

The Design condition of Gasification

- $N_2/\text{coal} = 0.44$, $O_2/\text{coal} = 0.715$, $\text{Steam}/\text{coal} = 0.1$, $\text{coal} = 30.758 \text{ kg/h}$, $\text{Reaction Temp} = 1000^\circ\text{C}$, $\text{heat loss} : 7.35 \text{ kW}$

Coal (Adaro) : C 66.76, H 4.77, N 1.44, S 0.26, O 18.21, Cl 0.104, Ash 5.57, H_2O 2.89 wt%

Steam temp 240°C

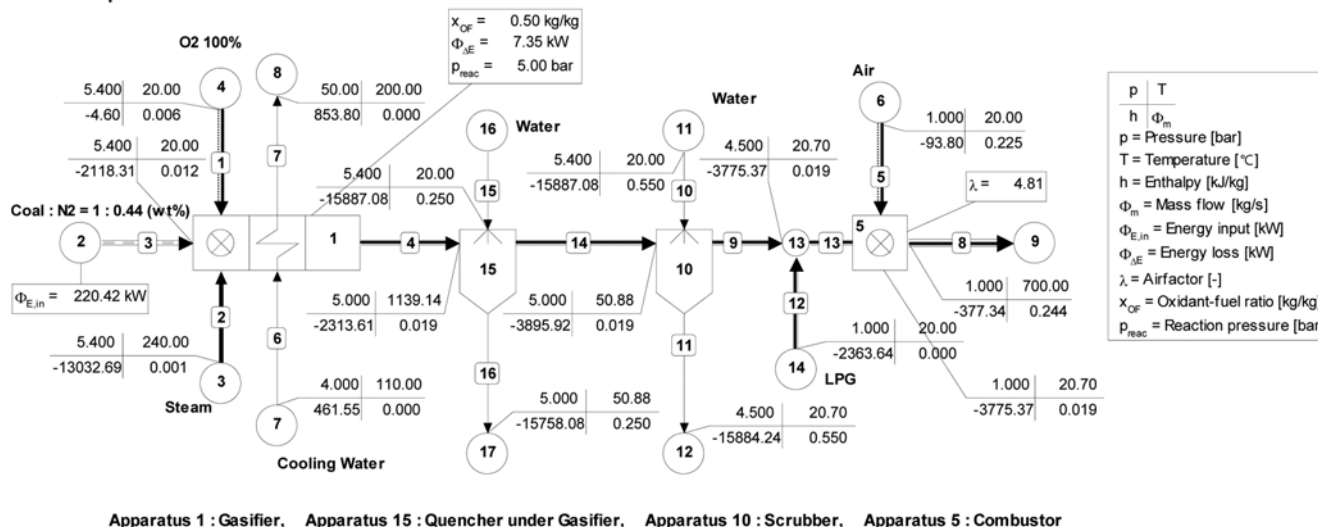


Fig. 2. Flow diagram of heat and mass balance at the operation conditions of 1 ton/day coal gasification system (Adaro coal).

for the quencher and scrubber was supplied from the cooling tower and circulated after being passed through bag filters.

The operation results from this real system were compared with the estimated results obtained through a computational simulation.

Shenhua coal from China and Adaro coal from Indonesia were used as coals for the computational simulation and real operation. The results of proximate and ultimate analyses of the two coals are shown in Table 1.

For the computational simulation, the operation conditions were as follows: (1) coal supply of 30.14 kg/h with N_2 as a conveying gas at a N_2/coal ratio of 0.7, oxygen at an O_2/coal ratio of 0.82 for

partial oxidation of coal, steam at a steam/coal ratio of 0.1 for the additional gasification reaction and operation pressure of the gasifier of 4 bar for Shenhua coal; (2) coal supply of 30.76 kg/h with N_2 as a conveying gas at a N_2/coal ratio of 0.44, oxygen at an O_2/coal ratio of 0.715, steam at a steam/coal ratio of 0.1, and operation pressure of the gasifier of 5 bar for Adaro coal. These conditions were also used in the real system for respective experiments. The heat loss from the fire production wall was applied as 7.4 kW according to the experimental results.

System diagrams for the computational simulation are presented in Fig. 1 for the case of Shenhua coal, and Fig. 2 for that of Adaro

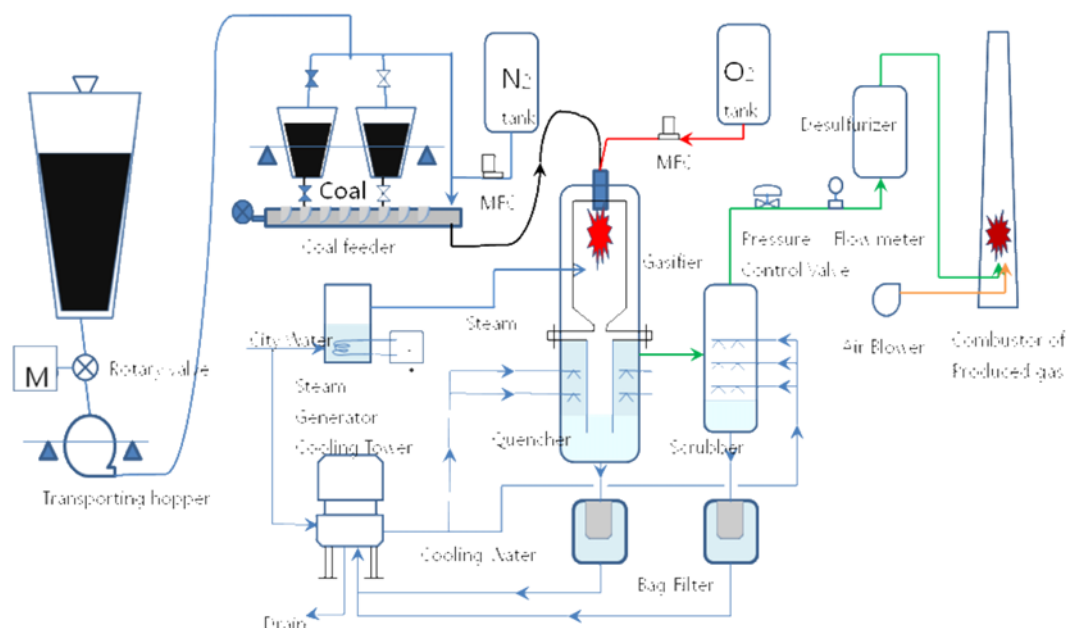


Fig. 3. Configuration of the 1 ton/day coal gasification system.

Table 1. Results of proximate and ultimate analyses of Shenhua and Adaro coal

Name of coal		Shenhua	Adaro
Proximate analysis (wt%)	Moisture	6.09	2.89
	Volatile	33.33	43.33
	Ash	5.46	5.57
	Fixed carbon	55.12	48.21
Higher heating value (kcal/kg)		6,880	6,580
Coal size		Under 200 mesh	Under 200 mesh
Ultimate analysis (wt%)	Carbon (C)	78.6	72.93
	Hydrogen (H)	4.96	5.21
	Nitrogen (N)	1.03	1.57
	Oxygen (O)	15.09	19.90
	Sulfur (S)	0.32	0.28

coal. The gas composition of each pipe was thereupon obtained, as shown in Table 2 in the case of Shenhua and Table 3 in that of Adaro.

The cold gas efficiencies [2] of the two coals were calculated as follows:

Cold gas efficiency % (LHV basis)

$$\begin{aligned}
 &= \frac{\text{Heating value in product gas (MW)}}{\text{Heating value in feedstock (MW)}} \times 100 \\
 &= \frac{\text{Heating value of CO} + \text{Heating value of H}_2 + \text{Heating value of CH}_4 \text{ (MW)}}{\text{Heating value in feedstock (MW)}} \times 100 \\
 &= \left(\frac{282.984 \text{ MJ}}{\text{kmol}} \times \frac{0.0208823 \text{ Nm}^3}{\text{s}} \div \frac{22.4 \text{ Nm}^3}{\text{kmol}} \times 0.4693 \right) \\
 &\quad + 0.0524 + 0.0001 \\
 &= \frac{230.04 \text{ MJ/kmol} \times 0.014233 \text{ kg/s} \div 14.98 \text{ kg/kmol}}{\times 100} = 80.70\% \text{ (Shenhua coal)}
 \end{aligned}$$

Cold gas efficiency % (LHV basis)

$$\begin{aligned}
 &= \left(\frac{282.984 \text{ MJ}}{\text{kmol}} \times \frac{0.019292 \text{ Nm}^3}{\text{s}} \div \frac{22.4 \text{ Nm}^3}{\text{kmol}} \times 0.5117 \right) \\
 &\quad + 0.05598 + 0.0005 \\
 &= \frac{248.68 \text{ MJ/kmol} \times 0.012303 \text{ kg/s} \div 13.88 \text{ kg/kmol}}{\times 100} = 82.19\% \text{ (Adaro coal)}
 \end{aligned}$$

Here, the lower heating value of each element was applied as follows: CO as 282.984 MJ/kmol, H₂ as 241.818 MJ/kmol, and CH₄ as 802.625 MJ/kmol [10].

The cold gas efficiency was calculated with the composition of pipe number 9 in Fig. 1 (or Fig. 2) and the obtained values were 80.70%, on the basis of taking the lower heating value in the case of Shenhua and 82.19% in that of Adaro.

1. The Effects of Reaction Temperature and Pressure

Through Cycle-Tempo, the effects of reaction temperature and pressure were estimated. Figs. 4, 5 and 6 in the case of Adaro coal show the effects at the following conditions: O₂/coal ratio of 0.715, N₂/coal ratio of 0.44, steam/coal ratio of 0.1, and coal feeding rate of 30.76 kg/h. Steam at a temperature state of 240 °C was used in the computational simulation, because steam coexists with the state of water at high pressure and any temperature under 240 °C. Fig. 4 shows that the product gas mole fraction, cold gas efficiency, and the gasifier outlet temperature were determined according to the reaction temperature input into the Cycle-Tempo program at a reaction pressure of 5 bar. Because the cold gas efficiencies are more than 80% when the reaction temperatures are higher than 900 °C, the gasifier inner temperature should remain over 900 °C. The same requirement applies for the case of Shenhua coal.

Fig. 5 shows the effect of reaction pressure in the case of Adaro coal. The gasifier outlet temperature is affected by the absolute pressure. Fig. 5 also shows the effects of reaction pressure at three different reaction temperatures. At a reaction temperature of 1,000 °C, the cold gas efficiency of the produced gas is lightly reduced with

Table 2. Gas compositions (mol/mol %) according to the pipes of Fig. 1 in the case of Shenhua coal

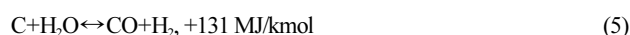
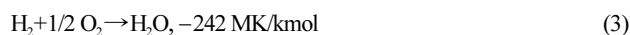
# pipe	1	2	3	4	5	8	9	12	14
N ₂			0.2230	0.2206	0.7729	0.7417	0.2286		0.2218
O ₂	1.0000		0.0367		0.2075	0.1517			
H ₂ O		1.0000	0.0298	0.0417	0.0101	0.0369	0.0070		0.0364
C (s)			0.5100	0.0000		0.0000	0.0000		0.0000
H ₂			0.1917	0.2246			0.2326		0.2258
S (s)			0.0007						
SiO ₂ (s)			0.0080	0.0079		0.0009	0.0082		0.0080
Ar					0.0092	0.0085			
CO ₂				0.0516	0.0003	0.0602	0.0531		0.0515
CH ₄				0.0002			0.0002		0.0002
C ₃ H ₈								1.0000	
H ₂ S				0.0007			0.0007		0.0007
CO				0.4529			0.4693		0.4555
SO ₂						0.0001			
M.W. (kg/kmol)	32.00	18.02	14.98	22.83	28.85	29.35	23.01	44.10	22.86
LHV (kJ/mol)	0.00	0.00	230.04	183.01	0.00	0.00	189.68	2044.22	184.06
HHV (kJ/mol)	0.00	0.00	2239.78	192.93	0.00	0.00	199.97	2220.19	194.04
Vol. Flow (m ³ /s)	0.0011885	0.00044315	6.6094e-06	0.027949	0.18262	0.65428	0.0064244	0.0000	0.0064348
N. Vol. Flow (N m ³ /s)	0.0048724	0.0010376		0.021636	0.17015	0.18357	0.0208823	0.0000	0.0215190

Table 3. Gas compositions (mol/mol %) according to the pipes of Fig. 2 in the case of Adaro coal

# pipe	1	2	3	4	5	8	9	12	14
N ₂			0.1563	0.1569	0.7729	0.7411	0.1616		0.1584
O ₂	1.0000		0.0549		0.2075	0.1540			
H ₂ O		1.0000	0.0155	0.0346	0.0101	0.0379	0.0054		0.0255
C (s)			0.5356	0.0000		0.0000	0.0000		0.0000
H ₂			0.2279	0.2609			0.2688		0.2634
S (s)			0.0008						
SiO ₂ (s)			0.0080	0.0090		0.0010	0.0092		0.0091
Ar					0.0092	0.0086			
CO ₂				0.0401	0.0003	0.0573	0.0413		0.0405
CH ₄				0.0007			0.0007		0.0007
C ₃ H ₈								1.0000	
H ₂ S				0.0007			0.0008		0.0007
CO				0.4967			0.5117		0.5013
HCl				0.0003		0.0000			0.0003
SO ₂						0.0001			
M.W. (kg/kmol)	32.00	18.02	13.88	21.81	28.85	29.30	21.92	44.10	21.84
LHV (kJ/mol)	0.00	0.00	248.68	204.62	0.00	0.00	210.77	2044.22	206.49
HHV (kJ/mol)	0.00	0.00	259.38	216.19	0.00	0.00	222.69	2220.19	218.17
Vol. Flow (m ³ /s)	0.00086167	0.00036701	5.6054e-06	0.020560	0.19029	0.67334	0.0046121	0.0000	0.0046724
N. Vol. Flow (N m ³ /s)	0.0043354	0.00105467		0.019874	0.17730	0.18892	0.019292	0.0000	0.019692

an increase of reaction pressure, while the gasifier outlet temperature increases with an increase of pressure. As the reaction temperature is decreased, the cold gas efficiency decreases, but the gasifier outlet temperature rises. At a reaction temperature of 1,400 °C, the reaction pressure shows little effect on the cold gas efficiency.

The following equations indicate the reactions in the gasifier [2].



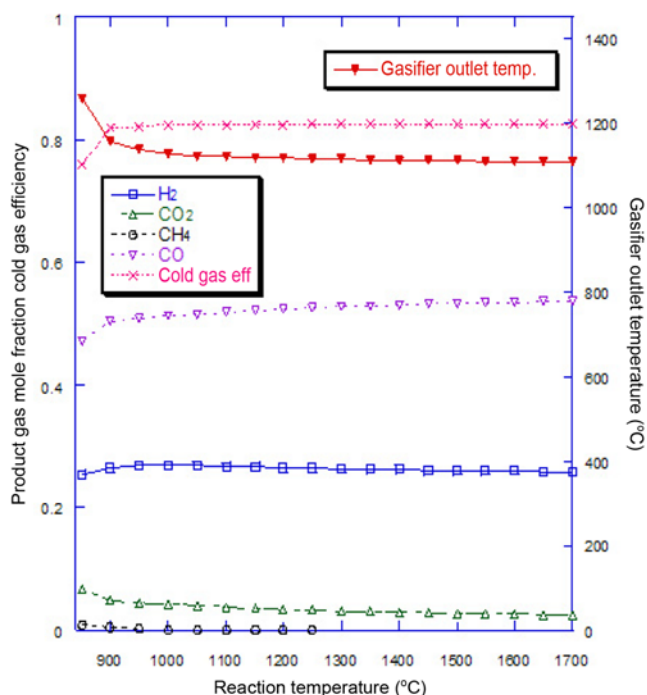


Fig. 4. Effect of reaction temperature at O₂/coal of 0.715, steam/coal of 0.1, N₂/coal of 0.44, and 5 bar (Adaro coal).

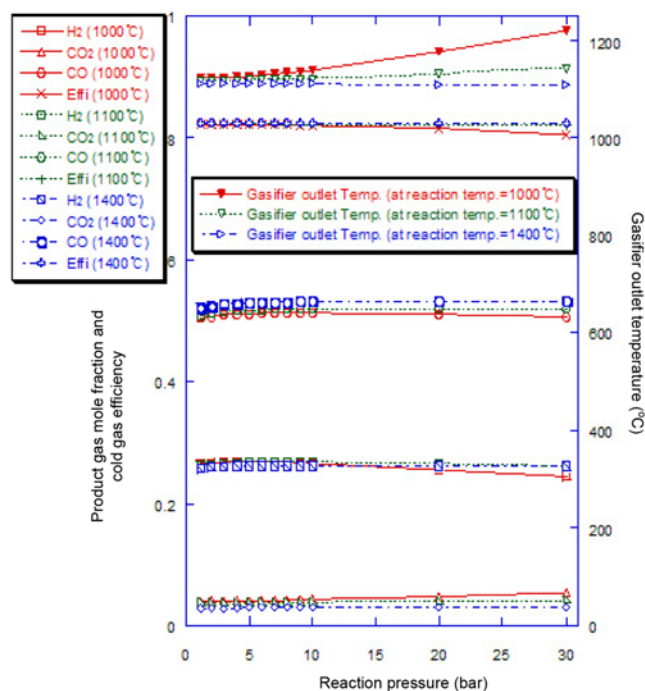
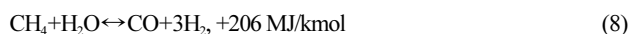
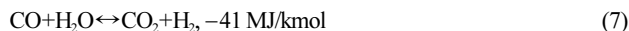


Fig. 5. Effect of reaction pressure at 3 reaction temperatures, O₂/coal of 0.715, steam/coal of 0.1 and N₂/coal of 0.44 (Adaro coal).



Eqs. (1) to (3) are related with combustion, and Eqs. (4) to (6) with gasification reactions. The forward reactions of the endothermic

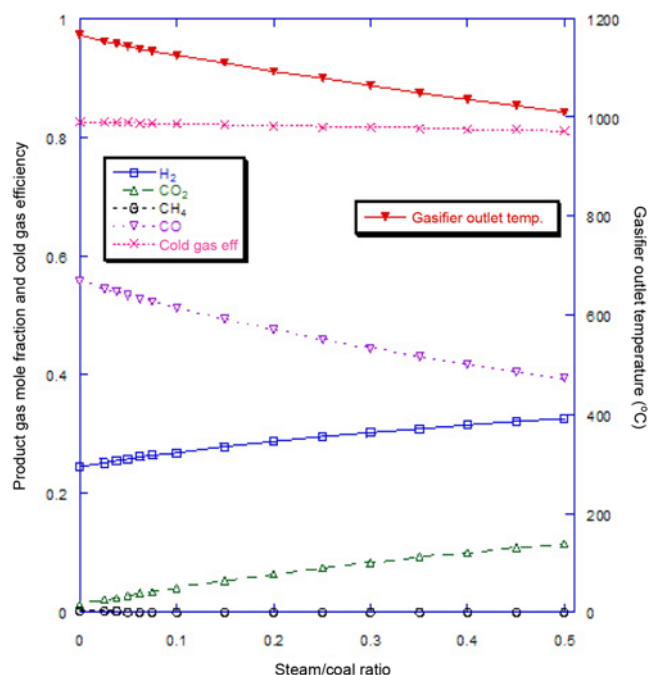


Fig. 6. Effect of steam/coal ratio at O₂/coal of 0.715, N₂/coal of 0.44, reaction temperature of 1,000 °C and 5 bar (Adaro coal).

equations of (4) and (5) are dominant at high temperature with less effect on the pressure variation. On the other hand, the reverse reactions of Eqs. (4) and (5) are subject to the effects of the reaction pressure at low reaction temperature; that is, when the reaction pressure is increased, the reverse reaction becomes more dominant. Fig. 5 shows these phenomena. The same phenomena occur in the case of Shenhua coal.

2. The Effects of Steam/Coal Ratio

Fig. 6 shows the effects of the steam/coal ratio at a reaction temperature of 1,000 °C, a reaction pressure of 5 bar, and an O₂/coal ratio of 0.715. As steam is added, the gasifier outlet temperature and the concentration of CO decreases and the concentration of hydrogen increases. When the reaction temperature is low, the forward reaction of Eq. (7) is more dominant than that of Eq. (5). It is estimated that the cold gas efficiency is the highest at a steam/coal ratio of 0 but does not decrease substantially. However, the gasifier outlet temperature decreases considerably according to the addition of steam. In the commercial IGCC plant, the syngas cooler is located immediately after the gasifier, functioning to lower the temperature of the produced gas from the gasifier. Because the addition of steam into the gasifier causes an endothermic reaction, as delineated in Eq. (5), subsequently lowering the gasifier outlet temperature, an important advantage can be derived: the capacity duty of downstream of the gasifier, that is, at the syngas cooler, can be reduced.

We also obtained the same phenomenon in the case of Shenhua coal.

3. The Effects of O₂/Coal Ratio and N₂/Coal Ratio

Fig. 7(a) shows the effects of the O₂/coal ratio on the cold gas efficiency and the gasifier outlet temperature in the case of Adaro coal. The cold gas efficiency is highest at an O₂/coal ratio of 0.63. Further, the gasifier outlet temperature is estimated to be 772.64 °C when the reaction temperature in the computational simulation is

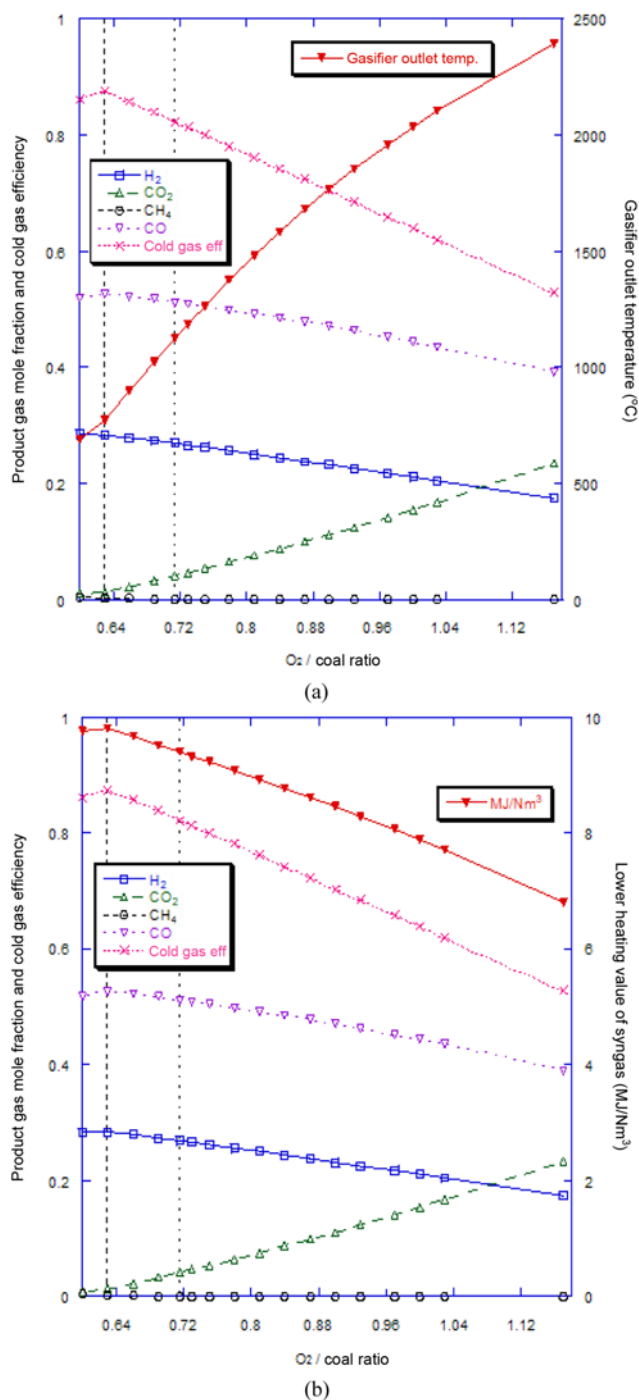


Fig. 7. (a) Effect of O_2 /coal ratio on the cold gas efficiency and gasifier outlet temperature at 5 bar, reaction temperature of 1,000 °C, steam/coal of 0.1 and N_2 /coal ratio of 0.44 (b) Effect of O_2 /coal ratio on the lower heating value (LHV) of product gas (Adaro coal).

assumed to be fixed at 1000 °C, where the endothermic gasification reactions such as reactions (4) and (5) proceed without problem. However, this estimated outlet temperature is not realistic, because the reaction temperature in the gasifier and the gasifier outlet temperature are close to each other in a real gasifier. It is regarded that the point at which the gasifier outlet temperature indicates 1,139 °C is the optimal point. This is because an ambient temperature over 1,139 °C

can sustain a reaction temperature of 1,000 °C in the gasifier despite some heat loss. At a gasifier outlet temperature of 1,139 °C, the O_2 /coal ratio is 0.715.

In the entrained-flow, slagging gasifiers, which are used in the majority of commercial-sized IGCC plants, the temperature must be sustained at a high value of at least 1,400 °C, which is above the ash melting point [2]. However, our gasifier employs a non-slugging type, because the fire protection material is only durable below 1,400 °C. Therefore, we selected a low reaction temperature of 1,000 °C.

As noted above, because an increase of the gasifier outlet temperature requires that the syngas cooler have a large capacity duty, higher gasifier outlet temperatures resulting from the cases of an O_2 /coal ratio exceeding 0.715 do not have a positive effect.

Fig. 7(b) shows the calorific value (based on the LHV) of the product gas per unit volume according to the O_2 /coal ratio in the case of Adaro coal. A calorific value (based on the LHV) of 9.4 MJ/Nm³ is obtained at an O_2 /coal ratio of 0.715. Compared to commercial gasifiers (i.e., Shell gasifier producing 10 to 12 MJ/Nm³, Texaco 9 to 10 MJ/Nm³, and BGL roughly 12 MJ/Nm³ [4]), the result is regarded as small. This is attributed to the amount of nitrogen for transporting coal. Compared to the Shell gasifier, which has an N_2 /coal ratio less than 0.1, the ratio used in our simulation and the real system is 0.44. Because the amount of nitrogen is larger in our system, calories of syngas per unit volume are lower.

The relation of N_2 /coal ratio with calories of syngas per unit volume in the case of Adaro coal is presented in Fig. 8. As the N_2 /coal ratio is increased, the calorific value (based on the LHV) of syngas per unit volume is lowered.

Shenhua coal was simulated at an N_2 /coal ratio of 0.7. The optimal O_2 /coal ratio was estimated as 0.82, showing a gasifier outlet temperature of 1,137 °C. At this point, the lower heating value was estimated as 8.44 MJ/Nm³. The calorific value (based on the LHV)

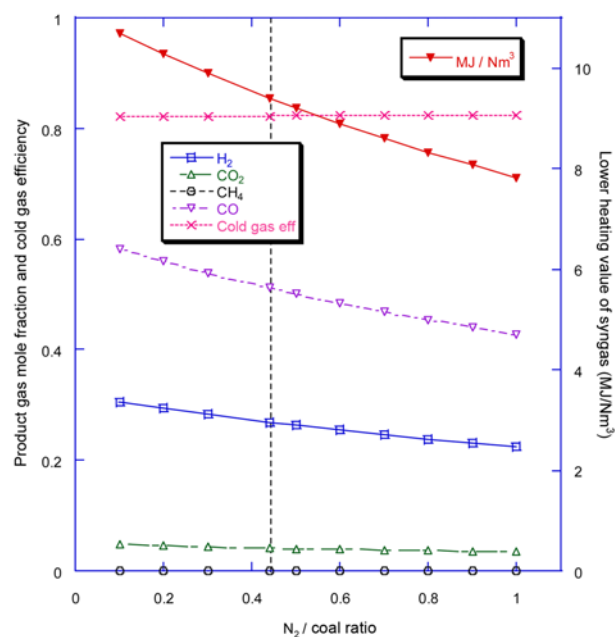


Fig. 8. Effect of N_2 /coal ratio on the cold gas efficiency and LHV value at 5 bar, reaction temperature of 1,000 °C, steam/coal of 0.1 and O_2 /coal ratio of 0.715 (Adaro coal).

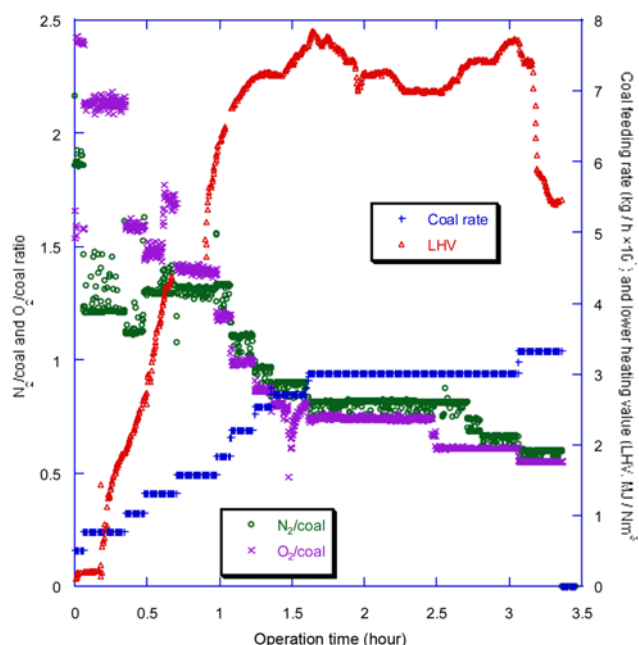


Fig. 9. Real LHV of gas produced according to the coal feeding rate, N_2/coal , and O_2/coal (Shenhua coal).

of syngas per unit volume is lower than that of Adaro coal because the amount of nitrogen for transporting coal was more than that in the case of Adaro coal. This phenomenon was also reflected in the real operation results. Fig. 9 shows that the calorific values per gas volume produced from Shenhua coal gasification are in a range of 7-7.8 MJ/Nm³ at the gasification zone 1 hour after operation. Fig. 10 shows that the calorific values of Adaro coal are in a range of 8-8.5 MJ/Nm³. Although these experimental results are approximately 1 MJ/Nm³ lower than the estimated results, the phenomenon that

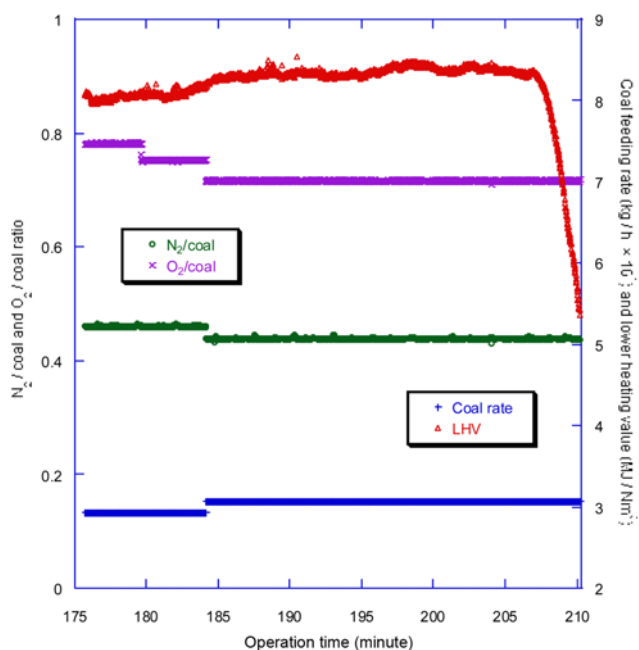


Fig. 10. Real LHV of gas produced according to the coal feeding rate, N_2/coal , and O_2/coal (Adaro coal).

larger N_2/coal ratio results in lower calorific value per unit volume is confirmed.

CONCLUSION

In Korea, the design technology of a commercial class coal-gasification system for IGCC has been under development as an R&D project of KEPCO in parallel with the construction of a 300 MW class IGCC demonstration plant through a government project. IGCC technology is considered to be highly efficient and environmentally friendly. In this paper, the effects of operating factors on the gasification system were reviewed by comparing the results of a computational simulation and real operation results. Notable operation conditions include a conveying gas/coal ratio of 0.44, an oxygen/coal ratio of 0.715, reaction temperature of 1,000 °C, and reaction pressure of 5 bar in the case of Adaro coal; based on this, the cold gas efficiency was estimated as 82.19%.

A 1 ton/day class gasifier and burner were retrofitted from an existing furnace for residue oil and operated in order to obtain results for comparison with those of the computation simulation. Ash was removed by using a water quencher attached under the gasifier and a scrubber following the quencher, and sulfur was removed by adsorption in an activated carbon tower. The gas produced from the gasifier was burned at a flare stack.

At the effect point of the reaction temperature, because the cold gas efficiencies are more than 80% when the reaction temperatures are higher than 900 °C, the gasifier inner temperature must be sustained at more than 900 °C. At a high reaction temperature such as 1,400 °C, the reaction pressure shows little effect on the cold gas efficiency. The addition of steam into the gasifier causes an endothermic reaction, and then lowers the gasifier outlet temperature. This is advantageous in that it can reduce the capacity of the syngas cooler located immediately after the gasifier. The most influential factor on the cold gas efficiency and the gasifier outlet temperature is the O_2/coal ratio. As the O_2/coal ratio is decreased, the cold gas efficiency is positively affected as long as the gasifier inner temperature remains over 1,000 °C. From the perspective of calories of produced gas per unit volume, as the N_2/coal ratio is increased, the calorific value (based on the LHV) per unit volume is accordingly reduced. Decreasing the amount of nitrogen for transporting coal is thus one route to obtain high caloric syngas. These findings were also confirmed in the operation results.

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The operation and innovation of this experimental class coal gasification system is a part of the design technology development of a commercial coal gasification system for an IGCC plant through KEPCO project. Mr. Theo Woudstra from Delft University of Technology contributed greatly to the elimination of errors in the calculation of the system efficiency. The authors gratefully acknowledge his kindness and technological support.

NOMENCLATURE

MW : power unit, $10^6 \text{ W} = 10^6 \text{ J/s}$

M.W.: molecular weight [kg/kmol]

LHV : lower heating value [MJ/kmol or kJ/mol]
 HHV : higher heating value [MJ/kmol or kJ/mol]
 LHV/ Nm³ : lower heating value per unit volume [MJ/Nm³]
 Nm³ : normal volume meter at 0 °C, 1atmosphere
 Vol. Flow : volume flow [m³/s]
 N. Vol. Flow : normal volume flow at 0 °C, 1atmosphere [Nm³/s]
 p : pressure [bar]
 T : temperature [°C]
 h : enthalpy [kJ/kg]
 Φ_m : mass flow [kg/s]
 $\Phi_{E, in}$: energy input [kW]
 Φ_{AE} : energy loss [kW]
 λ : air factor
 X_{OF} : oxidant-fuel ratio [kg/kg]
 p_{reac} : reaction pressure [bar]

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