THERMODYNAMIC ANALYSIS OF COAL GASIFIER PERFORMANCE

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ABSTRACT

Performance data of large scale fluidized bed gasifier which were operated at the temperature ranging from 1000 to 1200 °C were reviewed and the optimum steam/oxygen ratio were demonstrated.The extents of four basic reactions evaluated on the basis of mass and enthalpy balances were effectively used to explain the relation between the coal gas efficiency and the steam/oxygen ratio. A thermodynamic model was developed to analyse the effect of operating condition on the gasifier performance. The simulation model can explain not only the performance data of fluidized bed gasifier but also estimate the performance under various operating conditions.

INTRODUCTION

It is not uncommon that the temperature of fluidized bed gasifier can not be raised high enough to achieve the high conversion of coal and the excess steam has to be introduced , because of problems of hot spot and ash agglomerates. Thus the improvement of fluidized bed gasifier efficiency requires the technological development to reduce the consumption of excess steam and the understanding of the optimum operating condition.

The gasification performance is controlled by both of kinetic and thermodynamic factors. If the retention time of gases and solids as well as the temperature in the reactors are almost the same, kinetically determined factors such as carbon conversion and the gas conversion can be assumed to be the same. Thus by the selection of reactor scale and gasification temperature, the effect of kinetic parameters on the cold gas efficiency can be eliminated in the thermodynamic analysis of gasifier performance. Consequently the present authors analysed only large scale fluidized bed gasifiers which operated at the temperature ranging from 1000 to 1200°C. The simulation model was developed on the assumption that heat loss is 5% of the heat of combustion of coal, temperatures of steam and oxygen fed are 300 °C , the carbon conversion is 0.9 and product gases reach the shift equilibrium. The effect of the steam/oxygen ratio on the cold gas efficiency was simulated covering various gasification conditions.

ANALYSES OF GASIFICATION PERFORMANCE

In the present analyses, data in which gasifier scale larger than 4.5 [t/d] were selected. Considering a coal with a composition $CHaOb$, the overall equation for coal gasification is expressed as follows.

$$CHaOb + xO_2+yH_2O=pCO+qCO_2+rH_2+sCH_4+uH_2O+(1-m_c)C \quad (1)$$

This equation can be divided into four independent basic reaction equations as follows.

e1:	$C+O_2 = CO_2$	Hr_1= -94050	[kcal/kmol]	(2)
e2:	$C+H_2O = CO+H_2$	Hr_2= 31380	[kcal/kmol]	(3)
e3:	$C+2H_2 = CH_4$	Hr_3= -17880	[kcal/kmol]	(4)
e4:	$CO+H_2O= CO_2+H_2$	Hr_4= -9840	[kcal/kmol]	(5)

The extents of four reactions (e_i) can be evaluated by the mass and heat balances. Three independent equations of mass balance can be given for carbon, hydrogen and oxygen respectively.

$$C: \quad e_1+e_2+e_3 = m_c \quad (6)$$
$$H: \quad 2e_2+4e_3+2e_4 = a+2(y-u) \quad (7)$$
$$O: \quad 2e_1+e_2+e_4 = b+2x+y-u \quad (8)$$

Enthalpy balance is formulated as follows.

Summation of heat of reaction in Eqs.(2) to (5)
= (heat of combustion of coal)
-(heat of combustion of product gases) (9)

$$\sum Hr_i \cdot e_i = HHV- Hc[pCO+rH_2+sCH_4-(1-m_c)C] \quad (10)$$

SIMULATION MODEL DEVELOPMENT

A simulation model was developed to analyse the effects of various operating conditions on the cold gas efficiency. This model was formulated based on the following assumptions:

1) No external heat is supplied.
2) Heat loss is 5% of HHV.
3) Coal composition is $CH_{0.8}O_{0.1}$.
4) Temperature of coal fed is 25°C.
5) Temperatures of steam and oxygen fed are 300°C.
6) The carbon conversion is 0.9.
7) Pressure is atmospheric.
8) The gas composition of CO,CO_2,H_2,H_2O, is determined by the shift reaction of which equilibrium constant is given as follows.

$$K_s= \exp[1/8.31431(41568/T_a-2.15\ln(T_a)+0.013T_a -3.678*10^{-6}T_a^2)-4.19149] \quad (11)$$

9) The formation of CH_4 is determined by the equilibrium of hydrogasification of which equilibrium constant is given as

$$K_h= \exp[1/8.31431(56680/T_a-61.14\ln(T_a)+.03645T_a -3.678*10^{-6}T_a^2+439320/T_a^2)+37.6711] \quad (12)$$

Thus the model is composed of three mass balance equations(6)-(8), one enthalpy balance equation (13) and two equilibrium equations(14) and (15).

Summation of heat of reaction in (2) to (5)
= (enthalpy of exist gas stream)+(heat loss)
-(enthalpy of feed stock)-(enthalpy of gasifying agents) (12)

$$\sum Hr_i \cdot e_i = H_{og}+H_l-(H_{if}+H_{ig}+H_{is}) \quad (13)$$

$$K_s = (qr)/(pu) \quad (14)$$

$$e_3 = 0.5(1-1/\sqrt{(4K_hP)+1}\ (e_2+e_4) \quad (15)$$

By choosing "x" and "y" as variable parameters, T_a could be obtained by solving the above equations. Therefore the cold gas efficiency can be estimated only from steam and oxygen feed rates.

RESULTS AND DISCUSSION

The cold gas efficiency of gasification temperature 1000-1100 °C increases to the maximum where steam/oxygen ratio is around 2-4, and then decreases with the increased steam/oxygen ratio. In the cases of higher or lower temperature than this, the tendency is not clear owing to the shortage of data.

The extents of reaction could be used to explain the correlation between the cold gas efficiency and steam/oxygen ratio. As shown in Fig. 2 the extent of reaction (e_2) also increases to the maximum and then decreases with increased steam/oxygen ratio. Fig. 3 shows the extent of reaction (e_4) first increases rapidly from negative to positive value and then slowed down with the increased steam/oxygen ratio. When the value of e_4 is negative, the shift reaction proceeds reversely and endothermically to produce H_2O and CO. Thus the heat of reaction is carried out with the produced steam. While the larger steam/oxygen ratio is employed, the amount of unconverted steam is increased. As a result, the cold gas efficiency attains the maximum when steam/oxygen ratio is around 3.

The simulation model could describe the above results. The analyses of the data proved that the gasification temperature is 100-200 °C higher than the shift equilibrium temperature owing to the heat loss. The temperature indicated in Fig.4 is the shift equilibrium temperature while the temperature in Fig. 1 is that of gasification. Consequently, it is reasonable to consider that the curve of 1000-1100 °C in Fig.1 is corresponding to the curve of 800 °C in Fig.4. Also in Fig. 4 increase of temperature resulted in reducing the cold gas efficiency. In practical the coal conversion increases with increased temperature, thus the higher cold gas efficiency will be obtained.

It is demonstrated that this simulation model can also estimate the extents of reactions fairly well. The extent of reaction (e_2) significantly affects the entire efficiency but the steam/oxygen ratio of the peak in Fig. 5 does not give the maximum of the cold gas efficiency. Because of the effect of the exothermic heat of shift reaction, the steam/oxygen ratio of the peak in Fig.4 is larger than that in Fig. 5.
Further analyses of gasification performance will be given in the forth coming paper.

CONCLUSIONS

Performance data of large scale fluidized bed gasifiers were analysed. The optimum molar ratio of steam to oxygen feed proved to be around three. The extents of four basic reactions introduced were effectively used to explain the relationship between the cold gas efficiency and the steam/oxygen molar ratio. The extents of steam gasification and shift reaction significantly affect the cold efficiency. A thermodynamic model was developed to evaluate the effects of various conditions on the gasifier performance . This model can describe the performance data of fluidized bed gasifiers as well as the extents of the reactions.

NOMENCLATURE

a : atom ratio of hydrogen to carbon [-]
b : atom ratio of oxygen to carbon [-]
e_i : extent of reaction [-]
H_a : heat supply [kcal/kmol of CH_aO_b]
HHV : higher heating value of coal [kcal/kmol of CH_aO_b]
H_{if} : amount of preheat of coal feed [kcal/kmol of CH_aO_b]
H_{ig} : amount of preheat of gasifying agents [kmol/kmol of CH_aO_b]
H_{is} : amount of preheat of steam [kcal/kmol of CH_aO_b]
H_l : heat loss [kcal/kmol of CH_aO_b]
H_{og} : enthalpy of exist gas stream [kcal/kmol of CH_aO_b]
m_c : coal conversion [-]
p : molar production rate of CO [kmol/kmol of CH_aO_b]
P : pressure [atm]
q : molar production rate of CO_2 [kmol/kmol of CH_aO_b]
r : molar production rate of H_2 [kmol/kmol of CH_aO_b]
s : molar production rate of CH_4 [kmol/kmol of CH_aO_b]
T_a : shift equilibrium approaching temperature [°C]
u : molar unconverted steam [kmol/kmol of CH_aO_b]
x : molar feed of oxygen [kmol/kmol of CH_aO_b]
y : molar feed of steam [kmol/kmol of CH_aO_b]

REFERENCES

1. Patel, J.G., Energy Research 1980,4,149-165
2. Elliot, M.A. (Editor), "Chemistry of Coal Utilization", Second Supplementary Volumn, 1981, 166-1663
3. Yagi, S., D. Kunii, Nenryo-kyokai-shi, 1955, 34,426

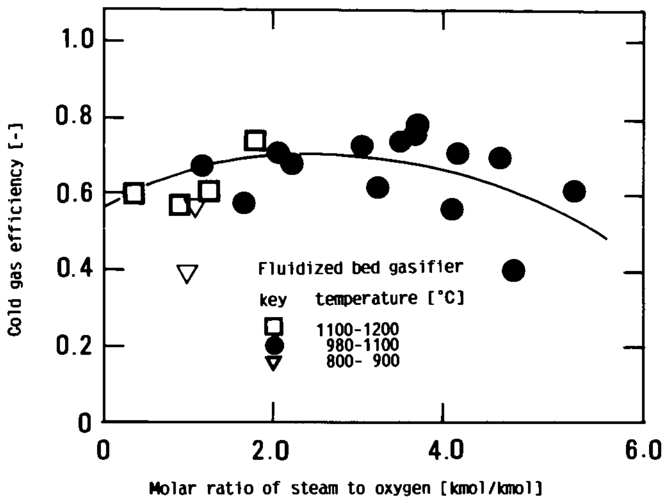

Fig. 1 The relation between the cold gas efficiency and molar ratio of steam to oxygen.

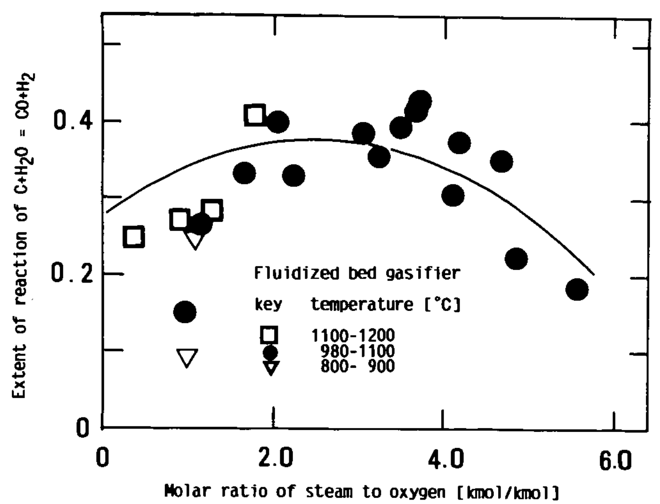

Fig. 2 The extent of steam gasification reaction vs molar ratio of steam to oxygen.

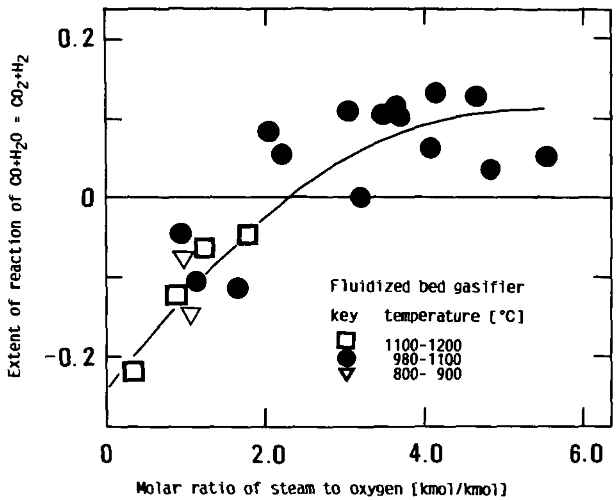

Fig. 3 The extent of shift reaction vs molar ratio of steam to oxygen.

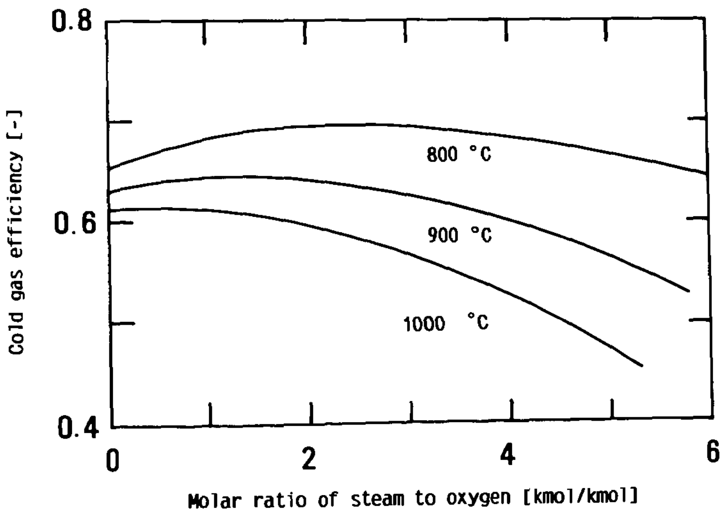

Fig. 4 The relation between the cold gas efficiency and molar ratio of steam to oxygen obtained from the simulation.

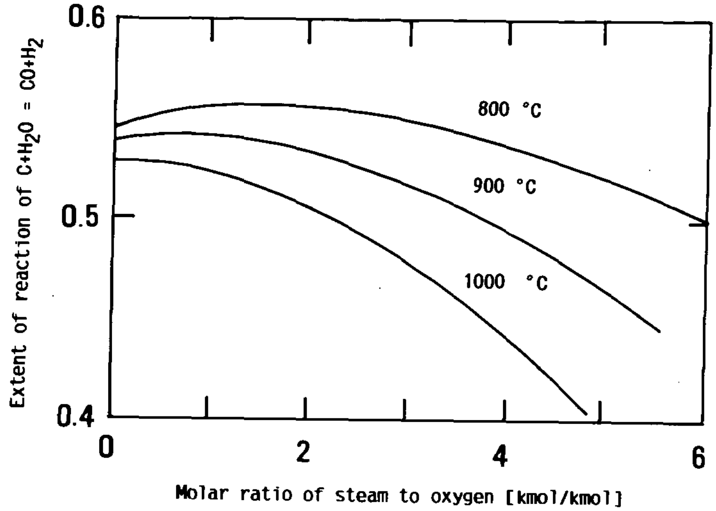

Fig. 5 The extent of steam gasification reaction vs molar ratio of steam to oxygen obtained from the simulation.

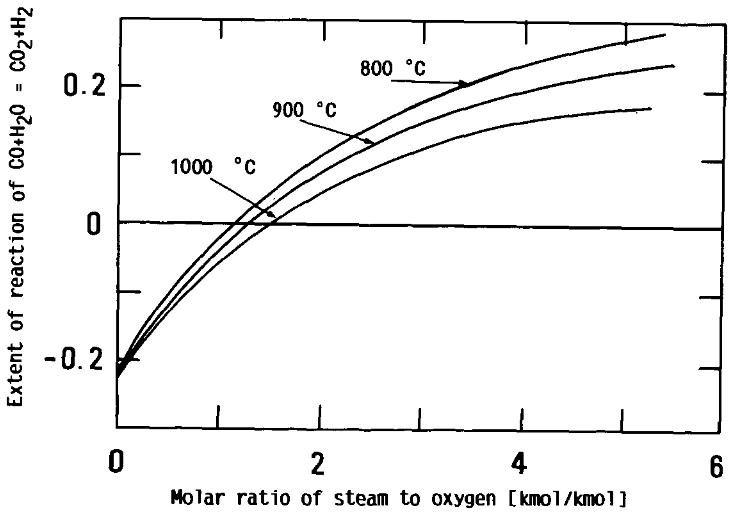

Fig. 6 The extent of shift reaction vs molar ratio of steam to oxygen obtain from the simulation.