한국에너지공학회(2001년도)
추계 학술발표회 논문집 P69~76

Numerical and experimental study for Datong coal gasification in entrained flow coal gasifier

Y.C. Choi, T.J. Park, J.H. Kim and J.G. Lee

Energy Environment Research Department,

Korea Institute of Energy Research (KIER),

P. O. Box 103, Yusong-gu, Taejon 305-343, Korea

Abstract - The coal gasification process of a slurry feed type, entrained-flow coal gasifier was numerically predicted in this paper. By dividing the complicated coal gasification process into several simplified stages such as slurry evaporation, coal devolitilisation and two-phase reactions coupled with turbulent flow and two-phase heat transfer, a comprehensive numerical model was constructed to simulate the coal gasification process. The k-ε turbulence model was used for the gas phase flow while the Random-Trajectory model was applied to describe the behavior of the coal slurry particles. The unreacted-core shrinking model and modified Eddy Break-Up (EBU) model were used to simulate the heterogeneous and homogeneous reactions, respectively. The simulation results obtained the detailed informations about the flow field, temperature inside the gasifier. Meanwhile, the simulation results were compared with the experimental data as function of O_2/coal ratio. It illustrated that the calculated carbon conversions agreed with the measured ones and that the measured quality of the syngas was better than the calculated one when the O_2/coal ratio increases. This result was related with the total heat loss through the gasifier and uncertain kinetics for the heterogeneous reactions.

Keywords : coal gasification, entrained-flow gasifier, numerical simulation

1. Introduction

Coal gasification is a key process for Integrated-coal Gasification Combined Cycles (IGCC) power plant. Being one of the most competitive and promising coal gasification technologies, the slurry feed type entrained-flow coal gasification process has been extensively studied in the Korea Institute of Energy Research (KIER)[1, 2, 3, 4] and some important achievements have been gained by investigating the complicated nature of coal characteristics using the bench-scale, entrained-flow coal gasifier. In an entrained-flow slagging coal gasifier using coal water slurry, it should be necessary to uniformly mix the coal-water slurry with oxygen to obtain the higher carbon conversion in short residence time(0.4 5s). In the experiments, oxygen and slurry are introduced simultaneously from the burner located at the top of the reactor into the reactor. As the slurry-coal droplets traveling along the gasifier, they are evaporated, devolatilised, burned and gasified. In the meantime, a series of fuel gas combustions and reactions are occurring in gaseous phase. Therefore, the gasifier can be conceptually divided into three zones : (1) pyrolysis and volatile combustion zone, (2) combustion and gasification zone, and (3) gasification zone.

The purpose of this paper is to develop two-dimensional comprehensive mathematic model including two-phase turbulent flow, heat transfer and chemical reactions in order to predict the optimal operating conditions and coal gasification performance of entrained-flow coal gasifier. Simulation results are compared with the experimental one[5] obtained by entrained-flow coal gasifier in KIER.

2. Physical model

The overview and schematic diagram of the oxygen-blown, entrained flow coal gasifier in KIER is presented in *Figure 1*. And *Figure 2* indicates the schematic of gasifier and detailed structure of the burner. As shown in *Figure 2*, the coal-water-slurry (CWS) is injected into the gasifier through the center hole of the burner, while the oxygen is blown in through eight surrounding holes during gasification.

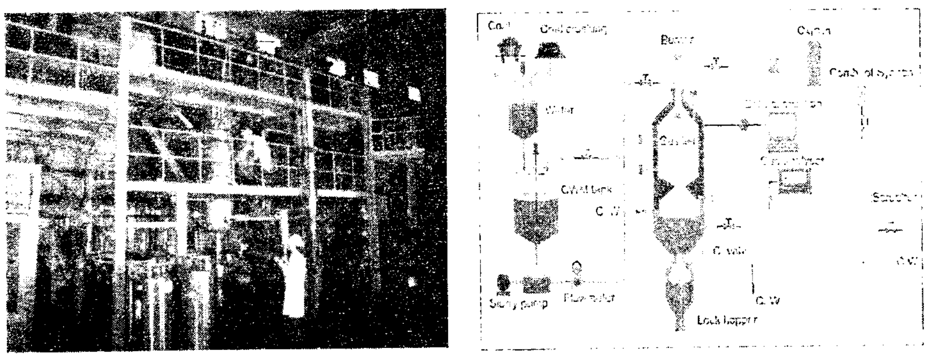

Figure 1 Overview and schematic diagram of the oxygen-blown, entrained flow coal gasifier in KIER

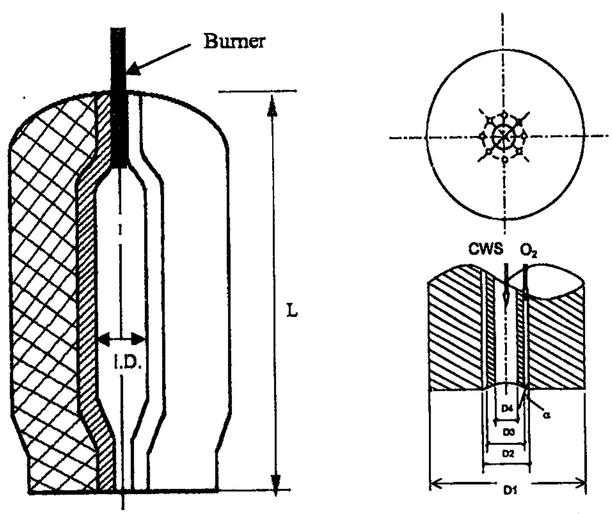

Figure 2 Schematic of the gasifier and detailed structure of the burner in KIER

The burner is designed so that there is an injection angle (α: 15°) for the secondary oxygen flow. Therefore, as soon as the slurry is fed into the gasifier, it is impacted by the high speed secondary oxygen flow and divided into droplets of different sizes. The main geometric parameters of the gasifier and burner are listed in *Table 1*.

Table 1 Some geometry parameters of gasifier and burner (mm)

Gasifier		Burner			
I.D	Length	D1	D2	D3	D4
200	1,000	60	13.28	12	3

For simplicity, the oxygen nozzle is assumed to be an annular one with the same diameter and the same flow rate as that of the eight surrounding holes during the simulation. Therefore, this three-dimensional geometry can be reduced to a two-dimensional axial-symmetric case.

3. Model description

Coal gasification is a rather complicated process coupled with two-phase turbulent flow, heat transfer, combustion and gasification. When coal slurry is injected into high-temperature gasifier, a series of physical and chemical processes will be occurred in the coal gasifier. The particle is quickly heated and the moisture is evaporated. And then the volatile material is devolatilised and the char is burned or gasified. At the same time, the gaseous products from coal particles will be fired or react with other species according to the surrounding environment and their intrinsic kinetics mechanism. A complete description of these processes and reactions is not possible due to the complexity and heterogeneity of coal. However, based on experiments and simplified mechanisms, this process can be divided into several simple sub-models. More detailed informations of these sub-models are described in our previous published work [6].

4. Experimental apparatus

The coal gasifier consists of three sections : the main burner and auxiliary LPG preheating burner at the top, the reaction zone in the center and the slag quenching part at the bottom. The reactor consists of one 30cm section and one 70 cm section, each with a 20 cm i.d and is designed to sustain up to 25 kg/cm^2 pressure. A cooling coil is inserted between the castable and the reactor vessel to prevent the reactor shell from over-heating. For the coal feeding system, coal slurry (58 - 65%, w./w.) is fed into a high pressure reaction vessel lined with high density alumina castable to maintain its high temperature. The temperature of the reaction gas is controlled by variation of the oxygen/carbon ratio and the steam evaporated from the coal slurry and is maintained at a sufficiently high level to melt the minerals in the coal into a slag.

The temperatures of the reaction gas and the reactor wall are monitored using a R-type thermocouple and 12 K-type thermocouples placed in the reactor wall, respectively. In the gasifier, coal reacts with oxygen and steam evaporated from the coal slurry and partially oxidizes at high temperature, and is converted to multi-component gas, such as CO, H_2, CO_2 and CH_4. Coal ash melts and makes slag, which flows down along the gasifier inside wall. The syngas and molten slag are cooled by quenching water at the bottom of the reactor before leaving the gasifier.

5. Numerical solution

Detailed informations of governing equations for gas and solid phase are described in our previous published work [6].

6. Results and discussion

Conditions used in experiments and simulations

The coal used in the experiments and simulation is Datong coal from China. The analysis of Datong coal and operating conditions are shown in *Table 2*. Before the injection of coal slurry into the gasifier, the gasifier is preheated to the reaction temperature (1,200 - 1,300恸恮) by using an LPG preheating burner.

Table 2 Analysis of Datong coal from China and operating conditions

Proximate analysis: (dry basis, wt %)	
Ash	8.57
VM	29.09
FC	56.46
Ultimate analysis (daf, wt %)	
C	70.80
H	4.60
N	1.08
S	0.70
O	22.82
Operating conditions	
CWS concentration	65 % (wt. %)
Slurry feed rate	60 (*l*/hr)
O_2 feed rate	24.5 (Nm^3/hr)

Flow field distribution

Figure 3 shows the calculated velocity vectors under cold and hot conditions. In cold condition, the primary flow is air instead of slurry and the momentum of the air is assumed to be equal to that of the slurry. The calculated velocity vectors indicate that there exists an obvious external recirculation zone which is caused by the high injecting oxygen gas flow. The velocity distribution of hot condition is a little different compared to that of the cold condition. In hot condition, the recirculation zone of the flow becomes smaller and it also appears that the stiffness of the injecting flow decreases. This is due to the high temperatures in the gasifier. As soon as two flows are discharged into the gasifier at a high temperature, they are rapidly heated and become hot gases immediately, especial for the secondary flow. In addition, the turbulence in the gasifier are intensified, the effect of diffusion becomes stronger and the stiffness of the injecting flow reduces.

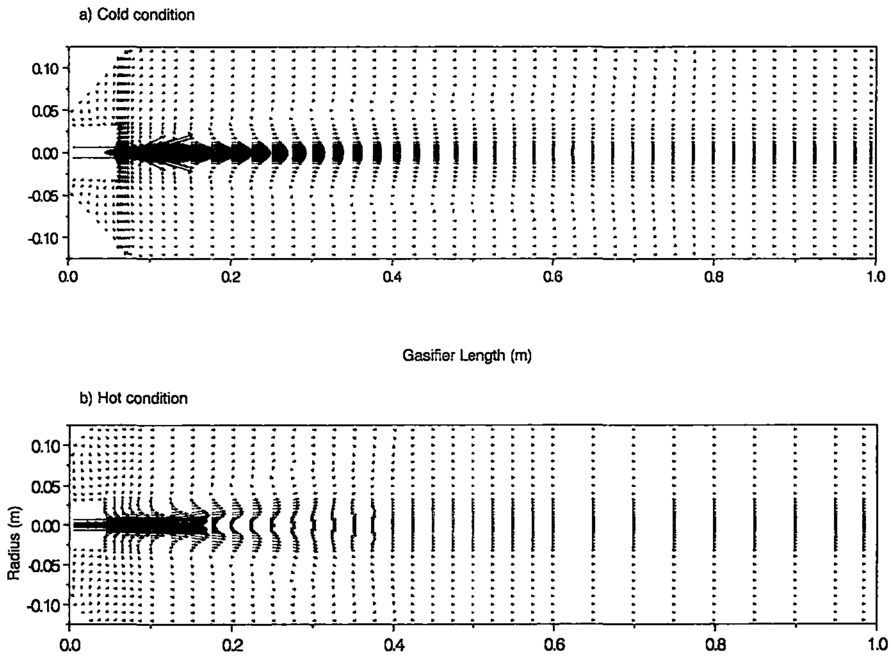

Figure 3 Velocity vectors of the flow field in cold and hot conditions.

Temperature distribution

Figure 4 is the simulated temperature distribution inside the gasifier. It can be seen that the highest temperature region is located at the center of the gasifier (0.3~0.5m) with a range of 1600°C~1800°C, which is mainly caused by the coal and gaseous fuel gas combustion. But at the inlet part (0.0~0.3m), the temperature of the inner region is lower than that of the outer region. The reason is that most of the coal slurry particles are concentrated at the inner region where the particles are heated, evaporated and devolatilisated, all these processes need to absorb heat from gas phase. After the combustion zone (0.5~1.0m), the temperature becomes lower along the gasifier due to the gasification process which need heat supply. The simulated overall temperature contour is like flame shape.

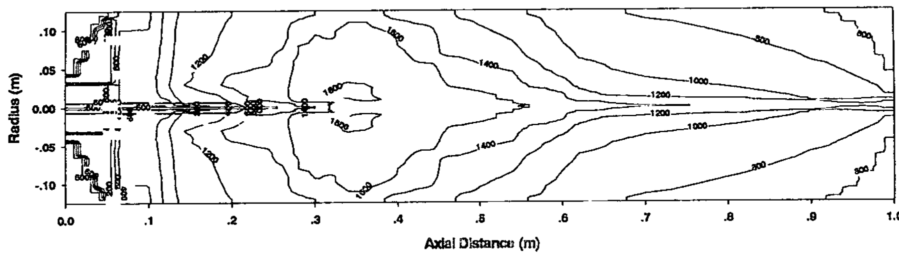

Figure 4 Temperature profile inside the gasifier with O_2/coal ratio of 0.9

Comparisons with experimental data

To verify the validity of developed model, the simulation results are compared with the experimental data as function of O_2/coal ratio. The species concentration distributions inside gasifier are described in our previous work [6]. For this study, the coal feed rate is fixed, while the oxygen feed rate is varied. *Figure 5a* shows the effect of the O_2/coal ratio on the calculated and measured carbon conversions. As we know, the calculated and measured carbon conversion increases when the O_2/coal ratio increases. It illustrates also that the calculated carbon conversions agree with the measured ones. According to the species distributions inside gasifier, the calculation results can also predict the composition changes of the product gas with respect to the O_2/coal ratio. *Figure 5b-d* shows the comparison of the product gas composition (CO_2, CO and H_2) between predictions and measurements. In general, when the coal slurry feeding rate is constant, if the O_2/coal ratio increases and then the reaction temperature is high, *Char-CO_2 Reaction* becomes active and consumes CO_2 from *Char-O_2 Reaction ($C + O_2 \rightarrow CO_2$)*. This causes CO_2 concentration in the product gas to decrease. However, if O_2/coal ratio is very high and O_2 supply is in excess, CO_2 concentration increases very rapidly and the reaction is mostly under combustion. The measured CO_2 concentration of Datong coal in *Figure 5b* is at a minimum at a O_2/coal ratio of 0.9. However, the syngas (CO and H_2) concentration in *Figure 5c-d* decreases gradually as the O_2/coal ratio increases. This comparison indicates also that the measured quality of the syngas is better than the calculated one when the O_2/coal ratio increases. This result is related with two following principal reasons. The first one is the total heat loss through the gasifier wall due to the insufficient refractory thickness, which result a low reaction temperature in the reaction zone. This low gasifier temperature restrains the char-steam reaction to produce CO and H_2. Therefore, the gasifier must be redesigned to enlarge the insulation thickness of the gasifier. The second one is the uncertain kinetics for the heterogeneous reactions used in the simulation. The kinetics used in this study were Utah bituminous coal's one extracted from the previous simulation works [6,11]. The proximate and ultimate analyses of Utah bituminous coal are similar to Datong coal, but the volatile matter is higher than that of Datong coal. This causes the reactivity of coal to be high and leads to a higher gasifier temperature in the reaction zone, which results a good quality of syngas. Actually, the authors are studing the reactivity of Datong coal to determine the proper kinetics for the heterogeneous reactions in a drop tube furnace and thermogravimetric analyzer (TGA).

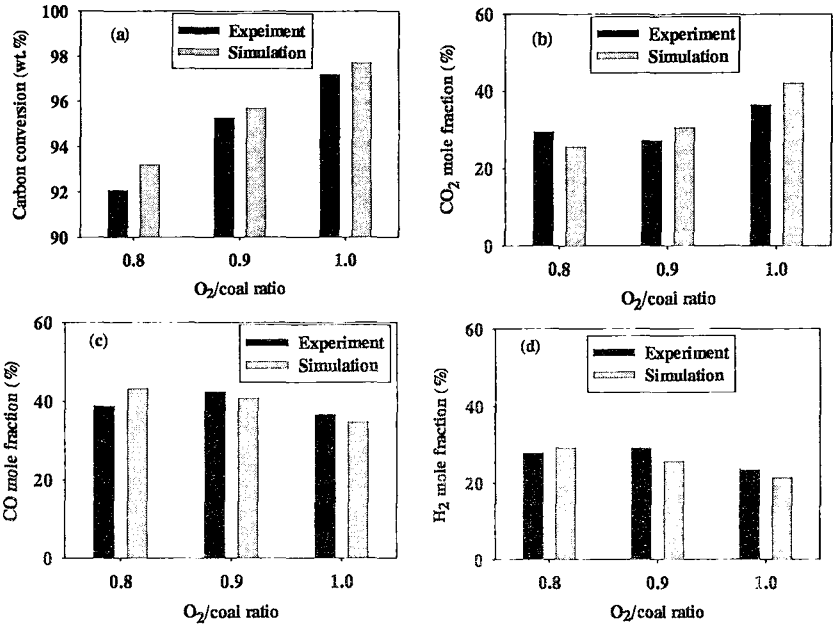

Figure 9 Comparisons between simulations and experiments with Datong coal (dry-basis)
(a) Carbon conversion, (b) CO_2 mole fraction, (c) CO mole fraction and (d) H_2 mole fraction

7. Conclusions

From the above simulation results on the coal gasification process for the slurry feed type entrained-flow coal gasifier, the following main conclusions can be drawn:

1. In the gasifier, the velocity distribution of hot condition is a little different from that of the cold flow field. The recirculation of the flow becomes weakly due to the high gas temperature at hot condition.
2. The highest temperature is located at the center of the gasifier in the combustion zone (0.3~0.5m). At the inlet part (0.0~0.3m), the temperature of the inner region is lower than that of the outer region. The reason is that most of the coal-slurry particles are concentrated at the inner region where the particles are heated, evaporated and devolatilisated,. After the combustion zone (0.5~1.0m), the temperature becomes lower along the gasifier due to the gasification process which need heat.
3. The simulation results are compared with the experimental data as function of O_2/coal ratio. It illustrates that the calculated carbon conversions agree with the measured ones. And it indicates also that the measured quality of the syngas is better than the calculated one when the O_2/coal ratio increases. This result is related with the total heat loss through the gasifier and uncertain kinetics for the heterogeneous reactions.

4. To improve the prediction performance in the near future, the refractory thickness of gasifier should be modified and the proper kinetics for the homogeneous and heterogeneous reactions included in the simulation should be determined.

8. References

1. T. J. Park, J. H. Kim, H. J. Lee, J. G. Lee., Development of entrained-flow coal gasifier, The Latin-American congress : Electricity generation and transmission, Brazil , Nov. 9-13, 1999.
2. J. G. Lee, J. H. Kim, H. J. Lee, T. J. Park, S. D. Kim, J. J. Kim, Drop Tube Reactor Studies for the Entrained Flow Coal Gasification, Korean J. of Chem. Eng., 1996, **34**, 496.
3. Y. C. Choi, X. Y. Li, T. J. Park, J. H. Kim, J. G. Lee, Numerical Analysis of the Flow Field inside an Entrained-Flow Gasifier, Korean Int. J. of Chem. Eng., 2001, **18**.
4. J. G. Lee, J. H. Kim, H. J. Lee, T. J. Park, S. D. Kim, Characteristics of Entrained Flow Coal Gasification in a Drop Tube Reactor, Fuel, 1996, **77**.
5. T. J. Park, J. H. Kim, J. G. Lee and Y. C. Choi, Experimental study on the characteristics of coal gasification by 1Ton/Day BSU gasifier (III), Annual technical report, KIER, 2000.
6. Y.C Choi, X.Y Lee, T.J. Park, J.H Kim, J.G. Lee, Numerical Study on the coal Gasification characteristics in an Entranied-Flow coal Gasifier, Fuel, Vol. 80/15, pp. 2193 - 2201, 2001
7. L. D. Smoot, Fundamentals of coal combustion, Elsevier, 1993.
8. R. Govin, J. Shah, Modeling and simulation of an entrained flow coal gasifier, AIChE Journal, 1984, **30**, 79.
9. G. S. Liu, H. R. Rezaei, J. A. Lucas, D. J. Harris, T. F. Wall, Modelling of a pressurised entrained flow coal hgasifier, Fuel, 2000, **79**, 1767.
10. X .J. Liu, Numerical simulation of coal gasification, Post-doc report, KIER, 1999.
11. C. Y. Wen, T. Z. Chaung, Entrained coal gasification modeling, Ind. Eng. Chem Proc. Des., 1979, **18**.
12. B. W. Brown, L.D. Smoot, P. J. Smith, P. O. Hedman, Measurment and prediction of entrained-flow gasification processes, AIChE Journal, 1988, **34**, 435.
13. D. B. Spalding, Numerical prediction of flow, heat transfer, turbulence and combustion, Pergamon press, 1983.