Numerical Analysis on the Reaction and Performance of Korean Test-Bed Coal Gasifier

Na Yeon Lee[1], Chan Lee[1], Seung Jong Lee[2] and Jin Wook Lee[3]

Abstract**—** Computational modeling and simulation are conducted on an entrained-bed coal gasifier of Korean test-bed facility by CFD method. The CFD modeling is made by combining Reynolds-stress averaged Navier-Stokes equation solvers, turbulence, discrete phase and gasification reaction models. By changing oxidizer feed conditions, the present CFD simulation method calculates gas flow path, coal particle track, temperature, CO and H_2 distributions inside the gasifier. Furthermore, based on the calculation results, the present study also investigates how gasifier performances such as carbon conversion and cold gas efficiency are changed due to oxidizer feed condition.

Keywords**—** CFD, Carbon conversion, Coal gasification, Cold gas efficiency, Carbon conversion.

I. Introduction

COAL gasification is an emerging clean coal technology with superior energy and environmental efficiencies compared with conventional coal utilization system[1], so worldwide R&D efforts on coal gasification have been being performed in USA, Europe, China, Japan and also in Korea. In the present study, computational analyses are conducted on an entrained-bed coal gasifier by CFD method. The CFD modeling is made by combining Reynolds-stress averaged Navier-Stokes equation solvers, turbulence, discrete phase and gasification reaction models. The present CFD simulation method calculates the gas flow path, the coal particle track, the temperature, the CO and H_2 distributions inside gasifier and their calculation results are used to compare and investigate the gasifier performances such as cold gas efficiency and carbon conversion.

II. Modeling And Simulation Methods

A. Design concept and feedstock condition of coal gasifier

For the application of coal gasification process in Korean test-bed facility, in the present study, an entrained-bed coal gasifier is designed with the bituminous coal of proximate analysis results(6% moisture, 51% fixed carbon, 28% volatile, 15% ash). The design operating conditions of the gasifier are set to 20 atm(g) and 1400°C.

1. Na Yeon Lee, Chan Lee are with the University of Suwon, Hwaseong, Gyeonggi 445-743 South Korea (corresponding author, phone: 001-82-31-220-2219 Fax: 001-82-31-220-2527; e-mail: clee@suwon.ac.kr).
2,3. Seung Jong Lee, Jin Wook Lee are with the Institute for Advanced Engineering, Yongin, Gyeonggi, South Korea (e-mail: sjlee@iae.re.kr)

The feedstock conditions of gasifier are 20 ton/day of coal, 15 ton/day of oxygen, 2 ton/day of steam and 3 ton/day of nitrogen. It is noted that oxygen/steam mixture is fed as the oxidizer of coal through primary and secondary nozzles while nitrogen being used as coal-conveying gas and fed trough coal burner. As shown in Fig. 1, the present coal gasifier is designed as entrained-bed type with the aspect ratio(L/D) of 6, and co-axial coal burner, primary and secondary oxidizer nozzles are equipped on the top plane of gasifier. One coal burner is equipped at the center of the top plane, and four primary and eight secondary nozzles are located around the inner and outer peripherals of coal burner. In order to investigate the effect of oxidizer feeding condition on coal gasification, the present study considers the secondary injection ratio(SIR) as a design variable, which is defined as the oxidizer feed rate through secondary nozzles divided by the total oxidizer one.

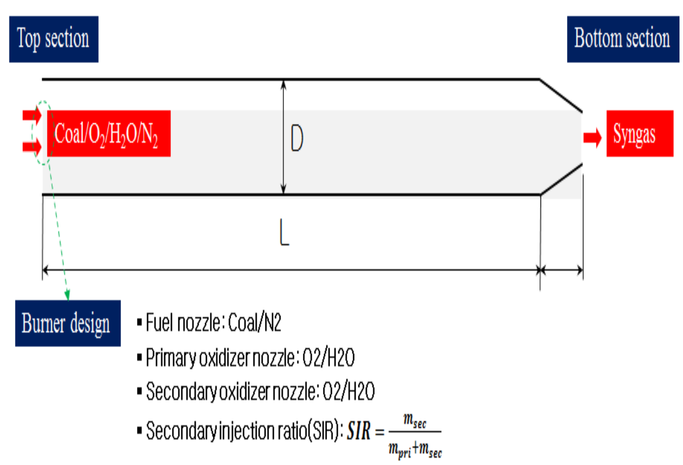


Fig. 1 Coal gasifer design concept

B. CFD models and analysis methods

The present CFD model is based on the RANS (Reynolds-stress Averaged Navier Stokes equations) solvers coupled with realizable k-ε turbulence, discrete-phase models and chemical kinetics models for gas phase and char surface gasification reactions. Discrete phase model are based on the iterative computations for the Eulerian and the Lagrangian approaches for gas and coal-solid flows, and employs the Random walk model for considering the coal particle dispersion by turbulent flow[2]. The CFD models used in the present study are summarized in Table 1.

In the present study, coal is assumed to be decomposed into volatile and char, and the devolatilization of coal is calculated by using two competing-rate model by Kobayashi[3]. Gas phase reactions are modeled by equations (1)-(7) as follows:

$$\text{Volatile} \rightarrow 0.56CO + 0.625H_2 + 0.8CH_4 \quad (1)$$

$$\text{Volatile} + 2.192\ O_2 \rightarrow 1.35\ CO_2 + 2.25\ H_2O \quad (2)$$

$$CH_4 + 0.5O_2 \rightarrow CO + 2H_2 \quad (3)$$

$$H_2 + 0.5O_2 \rightarrow H_2O \quad (4)$$

$$CO + 0.5O_2 \rightarrow CO_2 \quad (5)$$

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \quad (6)$$

$$CO + H_2O \leftrightarrow CO + H_2 \quad (7)$$

Char surface reactions are analyzed by the apparent rate /diffusion rate model for three kinds of reactions as follows:

$$C(s) + 0.5O_2 \rightarrow CO \quad (8)$$

$$C(s) + CO_2 \rightarrow 2CO \quad (9)$$

$$C(s) + H_2O \rightarrow CO + H_2 \quad (10)$$

Here all the kinetic data of equations (1)-(10) such as pre-exponential factor and activation energy are referred to Watanabe and Otaka[4].

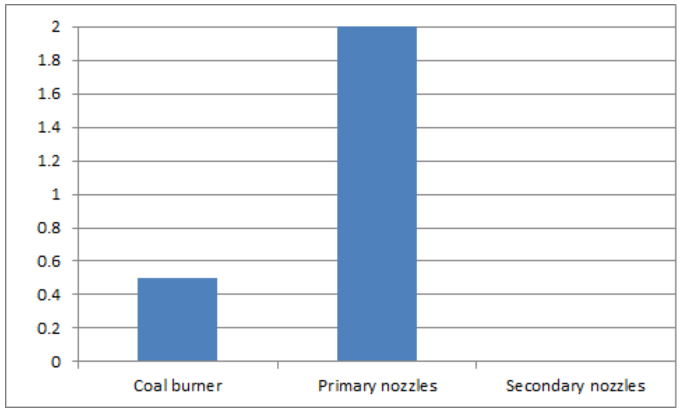
TABLE I
CFD MODELS FOR COAL GASIFICATION SIMULATION

Physical/ Chemical Phenomena	CFD models
3-D flow/energy transport	Reynolds-stress Averaged Navier-Stokes(RANS) equation solver
Turbulence	Realizable k-ε turbulence model with standard wall function
Gasification reactions	- Gas-phase(homogeneous) and Char(heterogeneous) reaction kinetics models
Coal particle track	Discrete phase trajectory model with turbulence-solid particle interaction(random walk model)
Thermal radiation	P_1 thermal radiation model for gas and solid media

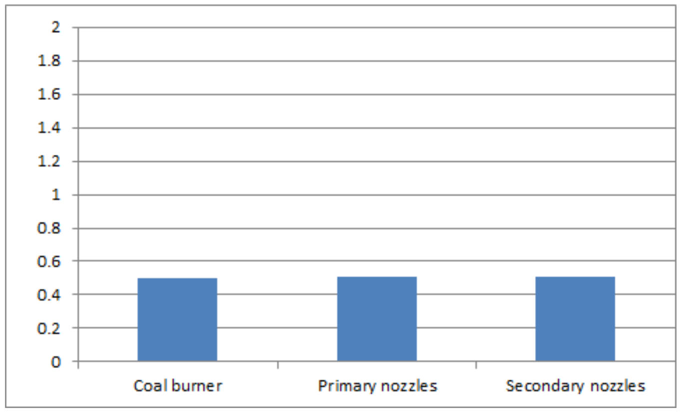
III. RESULTS AND DISCUSSIONS

A. Momentum design of coal burner and oxidizer nozzles

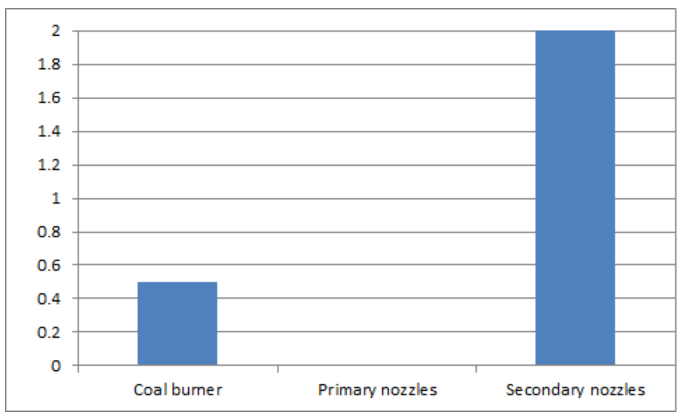
Fig. 2 shows the three different design cases for coal and oxidizer feedings and their gas momenta through coal burner, primary and secondary nozzles at different SIR conditions. As shown in Fig.2(a), in the case of SIR=0%, the gas momentum through primary nozzle is four times larger than that through coal burner. The case of SIR=100%, as depicted in Fig.2(c), also shows the big gas momentum difference between the coal burner and the secondary nozzle.



(a) SIR=0 %



(b) SIR= 50%



(c) SIR= 100%

Fig. 2 Gas momenta of coal burner and oxidizer nozzles.

In the view point of fluid mechanics, these gas momentum differences between coal burner and primary/secondary nozzle may result in the rapid mixing of coal and oxidizer in the top region of gasifier. However, as shown in Fig.2(b), when SIR set to 50%, the gas momenta of coal burner, primary and secondary nozzle are equally distributed. This gas momentum design concept may give the slow mixing of coal and oxidizer along gasifier length unlike the cases when SIR is set to 0 or 100%.

A. Simulation results by CFD method

Fig. 3 shows the gas streamlines and velocity vector of gasifier for three SIR cases, which illustrate the gas recirculation region below the top plane due to the mixing of coal and oxidizer. Comparing the lengths of the gas recirculation regions of the three cases, the recirculation region of the case at SIR= 50% is shorter than the other cases.

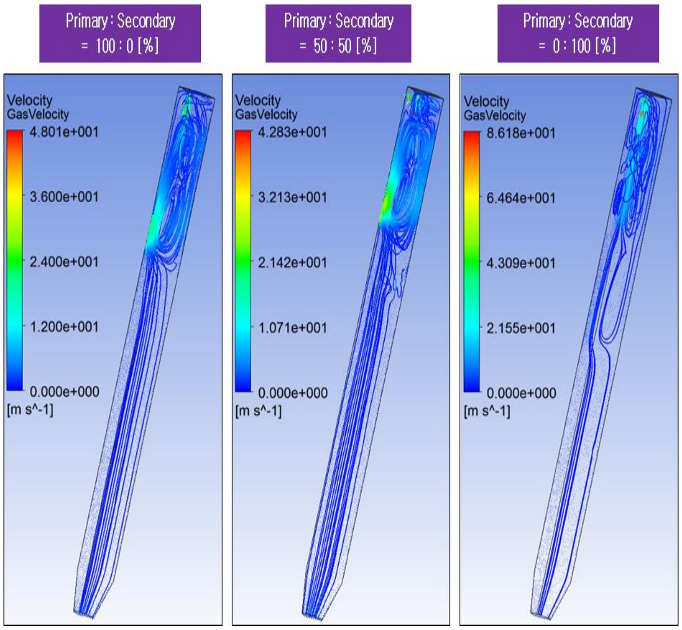


Fig. 3 Streamlines and velocity vector of coal gasifier

Fig. 4 shows the temperature distributions inside gasifier with changing SIR, and more uniform temperature distribution at SIR=50 % than those at SIR=0 and 100%. From these temperature computation results, it is know that the slow mixing between coal and oxidizer in the case of SIR=50% is more preferable for maintaining proper gasification temperature uniformly over total gasifier region than the rapid mixing at other SIR conditions. Furthermore, the wider region of high temperature in the cases of SIR=0 and 100% may trigger the combustion mode of coal , producing more CO_2 and less CO.

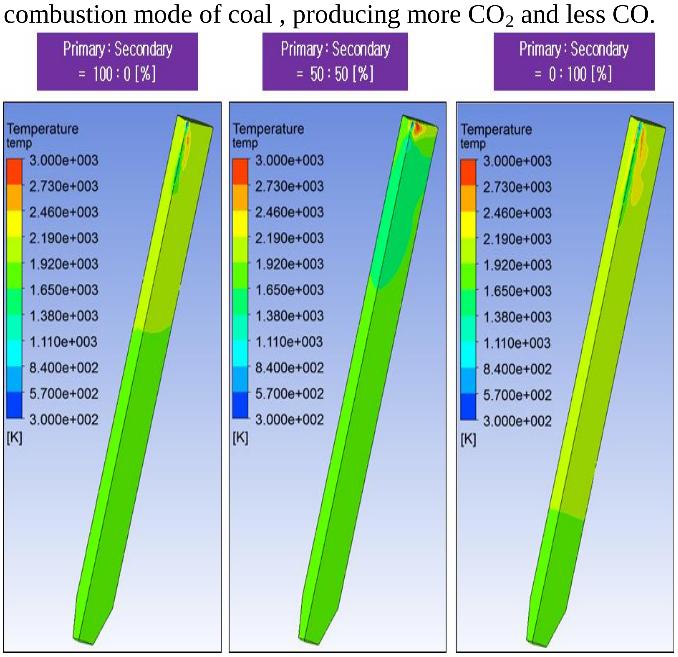


Fig.4 Temperature distributions of coal gasifier

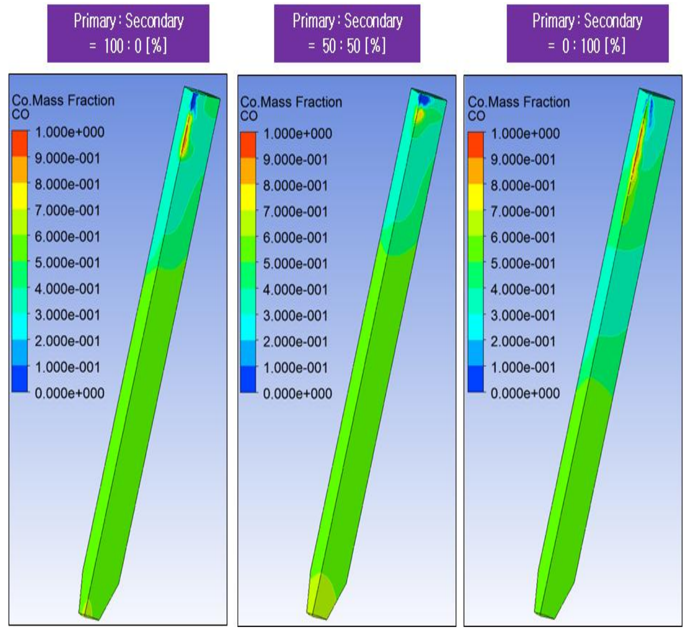


Fig. 5 CO mass fraction distributions of coal gasifier

Figs. 5 and 6 depict the distributions of CO and H_2 mass fractions inside gasifier. Fig.5 shows the case of SIR=50% results in more enhanced CO production around coal burner than other cases because of the uniform temperature distribution suitable for gasification process. However, Fig. 6 shows the similar tendency for all the SIR conditions that H_2 production is dispersed along gasifier length. Because H_2 production should be obtained through the series of reactions of coal and volatile decompositions(refer to equations (1) and (2)), so it generally takes more time and longer distance to produce H_2 than the CO.

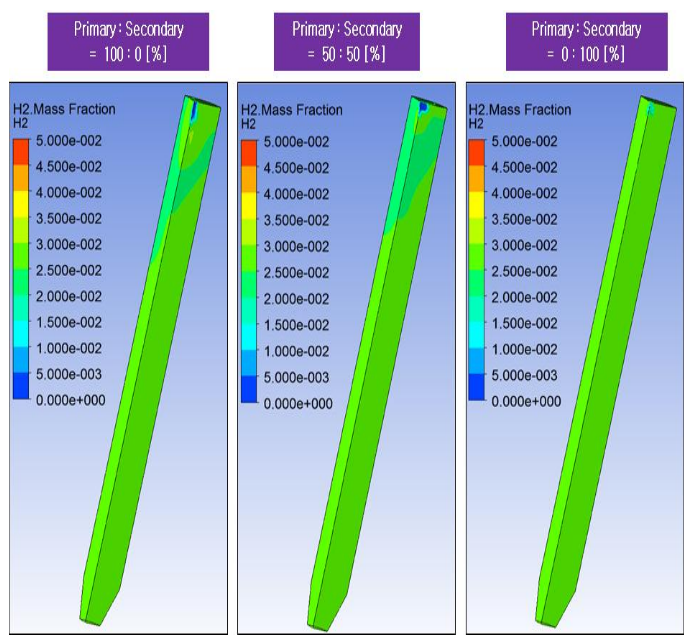


Fig. 6 H_2 mass fraction distribution of coal gasifier

Fig. 7 shows the gas compositions at gasifier exit. As shown in Fig. 7, when SIR is increased from 0 to 100%, CO composition is increased up to maximum 47% and reduced down to 44%. However, the composition of H_2 is remained as almost constant value of 30%.

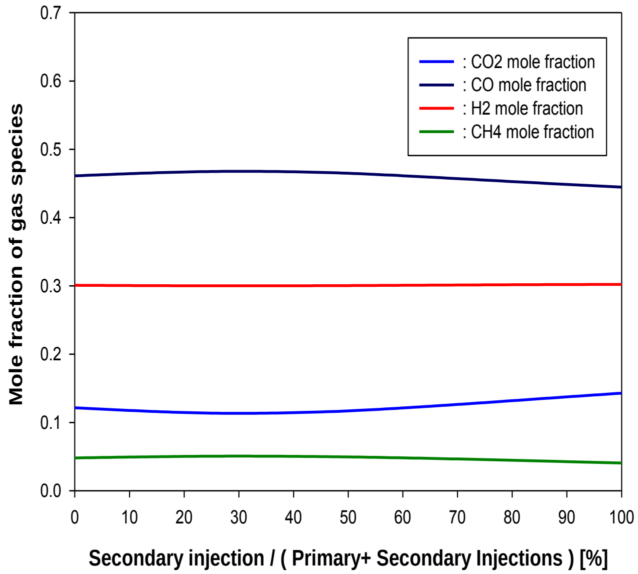


Fig. 7 Syngas composition of coal gasifier

Syngas temperature at gasifier exit is shown in Fig. 8. The syngas temperature is remarkably increased due to the transition from gasification to combustion mode in gasifier reactor when SIR is larger than 50%. However, the case of SIR=50% shows that gasifier temperature is maintained as design value, 1400^{o}C. Fig. 8 also represent the cold gas efficiency and the carbon conversion of gasifier, which are the highest, 82.2% and 97.3%, at SIR=50% and abruptly decreasing down to 76.0% and 94.7% when SIR is larger than 50%.

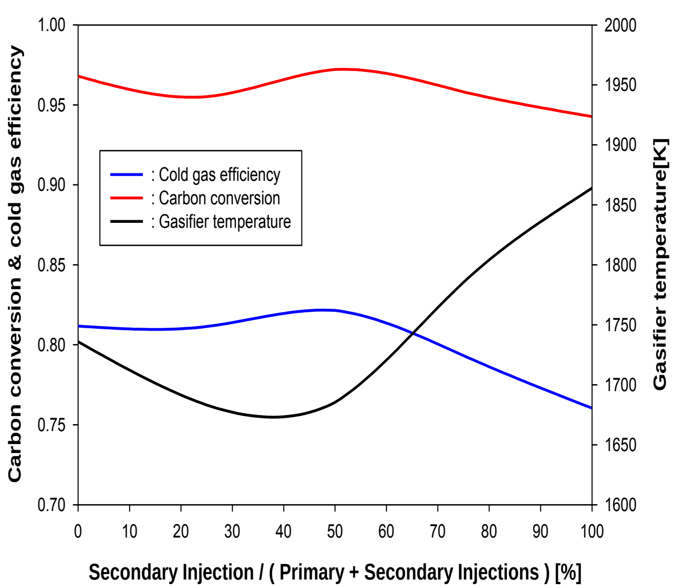


Fig. 8 Syngas temperature, carbon conversion and cold gas efficiency of coal gasifier

IV. Conclusions

Computational analyses by CFD method are conducted on an entrained-bed coal gasifier with co-axial coal burner, primary and secondary oxidizer nozzles. With the design feedstock of bituminous coal, the present CFD simulations on the reacting flow filed in gasifier are made by changing secondary injection ratio(SIR). The simulation results show that the slow mixing between coal and oxidizer at SIR=50% is the most preferable for efficient coal gasification process, and the best coal conversion and cold gas efficiency of the present gasifier can be achieved as 97 % and 82%.

Acknowledgment

This work was supported by the New & Renewable Energy Core Technology Program of the Korea Institute of Energy Technology Evaluation and Planning(KETEP) granted financial resource from the Ministry of Trade, Industry & Energy, Republic of Korea(*No. 2011951010001C*).

References

[1] A. J. Minchener (2005), "Coal gasification for advanced power generation", Fuel, Vol. 84, pp.2222-2235
[2] Fluent 6.3 User Guide(2006) , Fluent Inc.
[3] J. Song, M. Kang, D. Seo, S. Lim, M. Paek and J. Hwang (2010), "CFD Modeling for 300MW Shell-Type One-Stage Entrained Flow Coal Gasifier : Effect of O2/Steam/Coal Ratios, Particle Sizes, and Inlet Angles on the Gasifier Performance" Trans. of the Korean Hydrogen and New Energy Society, Vol. 21, No. 3, pp. 227-240
[4] H. Watanabe and M. Otaka (2006), "Numerical simulation of coal gasification in entrained flow coal gasifier", Fuel, Vol. 85, pp. 1935-1943