DETERMINATION OF AIR/FUEL AND STEAM/FUEL RATIO FOR COAL GASIFICATION PROCESS TO PRODUCE SYNTHESIS GAS

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Abstract

In this study, a coal gasification model is developed based on nine simultaneous reactions. For given gasification temperature and pressure, the air/fuel and water vapor/fuel ratio are optimized for maximum H_2/CO ratio by parametric study. Furthermore, the cold gas efficiency and higher heating value of the synthesis gas produced are computed for each case. Optimum locations of investigated parameters are also searched for maximizing cold gas efficiency and higher heating value of the synthesis gas.

Keywords: Coal gasification, production of synthesis gas, parametric study, optimization

1. Introduction

The design and operation of a gasifier requires understanding of the influence of fuel and operating parameters on the performance of the gasification process. There are numerous contemporary studies related to the syngas production for power generation in the literature. A review of the basic technology of coal gasification, with particular application to the production of synthesis gas for power generation is presented in the study of Casleton et al. [1]. There are useful and considerably large amount of references in the study. The numerical simulation of coal gasifiers is an important tool in the prediction of its gasification behavior. The main goal of the modeling of coal gasifiers is to constitute a system that maximizes gasification efficiency, and minimizes operating and investment costs and air pollutant emissions.

Steam gasification has become an area of growing interest because it produces a gaseous fuel with a relatively higher H_2 content. Furthermore, steam gasification has other advantages [2]; it is capable of maximizing the gas product with higher heating rates involved, advantageous residence time characteristics, and the efficient tar and char reduction brought about by steam reforming.

It is also important to determine the effects of operational parameters in coal gasifiers via simulation study instead of expensive and time-consuming experimental studies. From this point of view, the objective of this study is to investigate the effects of operational parameters on gasification products, synthesis gas.

2. Modeling

Achieving the best synthesis gas composition for power generation and production of coal chemicals is a challenging problem. Accurate understanding of the gasification phenomena is needed for a reliable performance prediction through modeling and can greatly avoid expensive upsets. From this point of view, in this study, a coal gasification model is developed based on eight simultaneous reactions. Table 1 show the reactions used in the model. The equilibrium constants of Boudouard, heterogeneous water-gas-shift (WGS) and hydrogenating gasification reactions are given in Table 2

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Table 1. Reactions used in the model.

$C + \frac{1}{2}O_2 \leftrightarrow CO$	(1)
$C + O_2 \leftrightarrow CO_2$	(2)
$CO + \frac{1}{2}O_2 \leftrightarrow CO_2$	(3)
$H_2 + \frac{1}{2}O_2 \leftrightarrow H_2O$	(4)
Heterogeneous WGS reaction $C + H_2O \leftrightarrow CO + H_2$	(5)
Boudouard equilibrium $C + CO_2 \leftrightarrow 2CO$	(6)
Hydrogenating gasification $C + 2H_2 \leftrightarrow CH_4$	(7)
Methane decomposition $CH_4 + H_2O \leftrightarrow CO + 3H_2$	(8)

Table 2. Equilibrium constants.

Temperature (K)	Kp,w Eq. (5)	$K_{p,b}$ Eq. (6)	$K_{p,m}$ Eq. (7)
400	7.7×10^{-11}	5.2×10^{-14}	2.99×10^{5}
600	5.1×10^{-5}	1.9×10^{-6}	9.24×10^{1}
800	4.4×10^{-2}	1.1×10^{-2}	1.34×10^{0}
1000	2.62×10^{0}	1.90×10^{0}	9.6×10^{-2}
1500	6.08×10^{2}	1.62×10^{3}	2.5×10^{-3}

Table 3. Coal properties.

C (%)	41.81
H (%)	4.28
O (%)	8.09
N (%)	2.16
S (%)	1.47
Ash (%)	28.68
Moisture (%)	13.51
LHV (kcal/kg)	5424.00
HHV (kcal/kg)	5728.00

The model results are obtained by using a combined Relaxation Newton-Raphson method with a computer code developed in FORTRAN language. The following equation is used in the solution of matrix with three bands,

$$X^{B+1} = X^{B} - \left(\frac{\partial F}{\partial X}\right)^{-1} F^{B} \qquad (9)$$

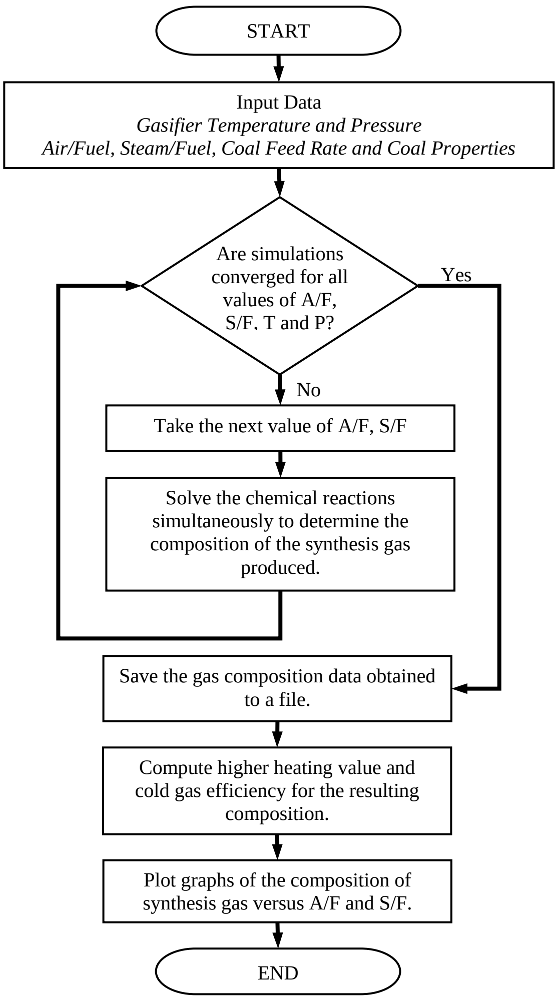

Figure 1. Flowchart of the gasification model

Where X and F represents variable and function vectors, respectively. The elements of matrix with three bands are calculated using Jacobian term, $\partial F / \partial X$. The flowchart of the computations in the model is presented in Figure 1.

The performance of a gasifier is often expressed in terms of cold gas efficiency. The term "cold gas" stands for the case when the gas is cooled down to the ambient temperature and tar vapors are removed. In this study the cold gas efficiency, η_c of the product synthesis gas is defined as follows:

$$\eta_c = \frac{\dot{V}_{syngas} HHV_{syngas}}{\dot{m}_{fuel} HHV_{fuel}} \qquad (10)$$

Where, $\dot{V}_{syngas}$ represents the volumetric flow rate of produced synthesis gas in [m^3/s], $\dot{m}_{fuel}$ is used for mass flow rate of fuel.

The higher heating value of the synthesis gas, HHV_{syngas} [kJ/m^3] is computed from the sum of heating values of individual combustible constituents, which are H_2, CO, CO_2, H_2S and CH_4. The data for the heating values and enthalpies of these gases at various temperatures are readily available in many references [3]. For this case the amount of H_2S and CH_4 are negligible and therefore have not been included in the calculations of heating value.

Input parameters for the model are coal feed rate, coal properties, gasification temperature and pressure, air/fuel ratio, and steam/fuel ratio. Simulation model calculates synthesis gas composition for air-fuel ratio and steam-fuel ratio at the given operating conditions. Simulation model also calculates the cold gas efficiency of the gasifier and higher heating value of the synthesis gas.

3. Results and Discussion

There are many parameters effecting the composition of synthesis gas which makes the problem more complex. In this study, the effects of operational parameters on gasification products in coal gasifiers such as air/fuel and steam/fuel ratio are investigated via developed numerical coal gasification model for aimed H_2/CO ratio. The fuel for the gasification is low grade coal and its composition is given in Table 3.

Parametric study is performed for the air-fuel ratio and steam-fuel ratio taking the coal feed of 1000 kg, the gasification pressure of 1 atm. and the temperature of 1400 K. The effect of the air/fuel ratio and steam/fuel ratio on synthesis gas composition is shown in Figures 2 and 3, respectively. Figure 2 shows the variation of synthesis gas composition with respect to air-fuel ratio keeping steam-fuel ratio of 0.1. In Figure 3, it is also presented that the variation of synthesis gas composition with steam-fuel ratio taking air-fuel ratio of 1 and varying steam-fuel ratio between 0.0 and 0.4 under the same conditions as in Figure 2. The distribution of components of synthesis gas is shown as volumetric percentage in Figures 2 and 3. Three components, H_2, CO and CH_4 are only viewed on the graphs to serve our purpose. As seen from Figure 2, the composition has %20 carbon monoxide, %14 hydrogen and %6 methane species at the air-fuel ratio of 0.2. Increasing air-fuel ratio to the value of 1.2 resulted with a composition of hydrogen at 0.31, carbon monoxide at 0.33 and methane at nearly zero. It is seen a steady increase in hydrogen and decreasing increase in carbon monoxide, and linear decrease in methane from Figure 2. The overall effect is that it is hard to increase the level of hydrogen above the carbon monoxide even if all of the methane were consumed at the air-fuel ratio of 1.2. Analyzing Figure 3 under the condition in which the steam is not fed, one can observe that volumetric percentages of carbon monoxide, hydrogen and methane are obtained at %25, %10 and %9, respectively. Hydrogen content reaches carbon monoxide level at which steam-fuel ratio is about 0.13 and air-fuel ratio of 1.0. Increasing steam-fuel ratio to 0.4, hydrogen content reaches %77 while holding the content of carbon monoxide at %48 and methane at zero. As shown from Figure 3, H_2 and CO compositions increase as the air/fuel ratio increases and CH_4 content of synthesis gas decreases monotonically. One can see that the slope of carbon monoxide keeps approximately the same trend while hydrogen's increases going from Figure 2 to 3. This means there is more sensible increase in hydrogen as compared to carbon monoxide when the steam-fuel ratio is increased. But, it seems there must be a limiting point in steam-fuel ratio due to economic reasons and also a limitation in H_2/CO ratio due to the nature of reactions included.

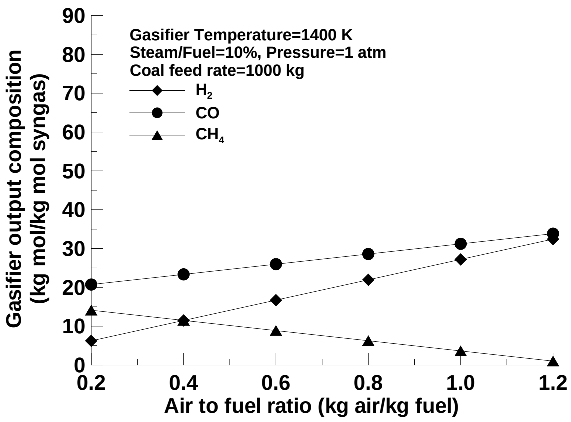

Figure 2. Effect of air/fuel ratio on synthesis gas composition.

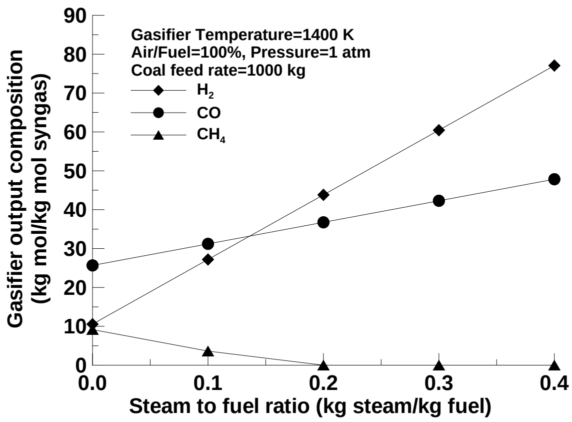

Figure 3. Effect of steam/fuel ratio on synthesis gas composition.

In Figure 4 and 5, the variation of H_2/CO ratio is presented versus air-fuel ratio and steam-fuel ratio, respectively. In Figure 4, air-fuel ratio is increased from 0.2 to 1.2 by 0.2 steps for the values of steam-fuel ratio of 0.0, 0.1, 0.2, 0.3 and 0.4. It is observed that air-fuel ratio must be kept higher than the value of 0.6 to produce H_2 when operating without steam injection. Steam injection removes this limitation on the air-fuel ratio and increases the H_2/CO ratio to 0.62 abruptly. This is why most of the gasification processes include steam injection. Further increase in steam-fuel ratio by 0.1 step result an increase of %70 in the H_2/CO ratio and the ratio elevates to 1.02. Successive increase in steam-fuel ratio results a decreasing increase in H_2/CO ratio and this trend is more clearly seen in Figure 5 in which the steam-fuel ratio is increased from 0.0 to 0.4 by 0.1 steps for the six values of air-fuel ratio between 0.2 and 1.2. Analyzing Figure 5, it is observed that H_2/CO ratio reaches unity at the following combination of steam-fuel and air-fuel ratios; (0.11, 1.2), (0.13, 1.0), (0.16, 0.8), (0.18, 0.6), (0.21, 0.4) and (0.23, 0.2). There is a reverse relationship between the steam-fuel and air-fuel ratio, i.e., an increase in steam-fuel ratio requires a decrease in air-fuel ratio to achieve fixed H_2/CO ratio in the synthesis gas.

Air-fuel mass ratio can be calculated as 1.32 by extrapolation using the data in Figure 4 where the H_2/CO ratio approaches unity. At this limiting point, methane volumetric content diminishes. One can observe that the H_2/CO ratio may be increased further by varying the steam-fuel ratio as shown in Figure 4. The value of H_2/CO ratio reaches 1.6 as steam-fuel mass ratio increased to the value of 0.4 at the air-fuel ratio of 1.0. Extending the curve to the point where H_2/CO ratio reaches 2.0, the condition is obtained at the value of steam-fuel ratio of 0.8 for air-fuel ratio of 1.2.

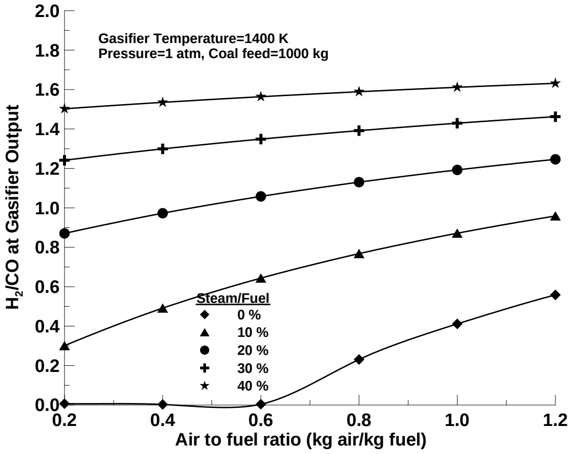

Figure 4. Effect of air/fuel ratio on synthesis gas composition.

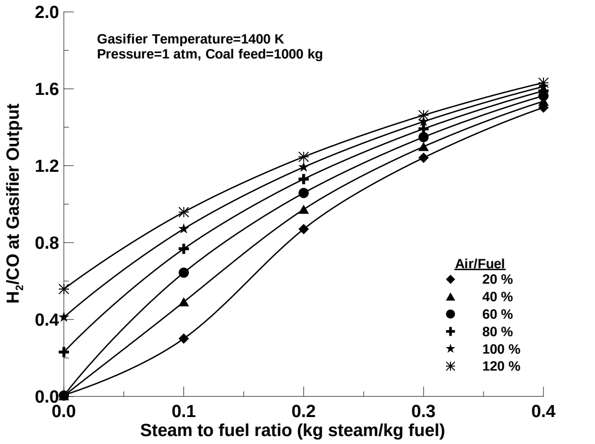

Figure 5. Effect of steam/fuel ratio on synthesis gas composition.

The cold gas efficiency for air/fuel ratio and steam/fuel ratio is presented in Figs. 6 and 7, respectively. As a result of product gas dilution, the cold gas efficiency decreases when the air/fuel ratio increases as shown in Figure 6. The carbon conversion increased due to decreased char formation as the air/fuel ratio is increased. On the other hand, this study clearly shows that dilution has more dominant effect on the cold gas efficiency. Carbon conversion of coal in the gasifier increased linearly with the increase of the steam/fuel ratio, as shown in Fig. 7. It is observed that cold gas efficiency reached the maximum for a steam/fuel ratio of 40%.

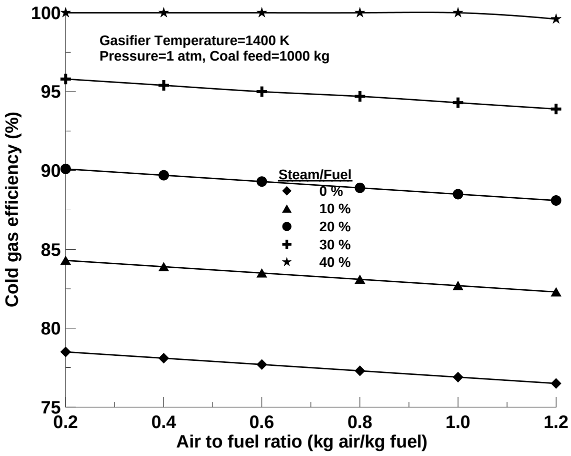

Figure 6. Effect of air/fuel ratio on cold gas efficiency.

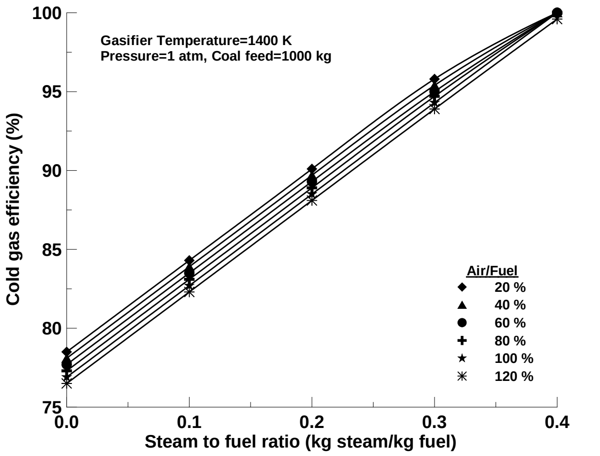

Figure 7. Effect of steam/fuel ratio on cold gas efficiency.

The effect of air/fuel ratio and steam/fuel ratio on higher heating value of synthesis gas is shown in Figures 8 and 9, respectively. Increasing the air/fuel ratio resulted in a decrease of the higher heating value of the gas due to decreases in the concentrations of methane and other light hydrocarbons which have relatively large heating values. Also, the higher concentration of nitrogen observed at higher air/fuel ratios contributed to low gas higher heating values. Nitrogen has a diluting effect on the product gas and, thus, lowers its energy content as shown in Figure 8. On the other hand, increasing the steam-fuel ratio from 0.0 to 0.40 increased the higher heating value of the synthesis gas. This increase is caused by the gas shift reaction as well as the low amount of N_2 being introduced to the system as shown in Figure 9.

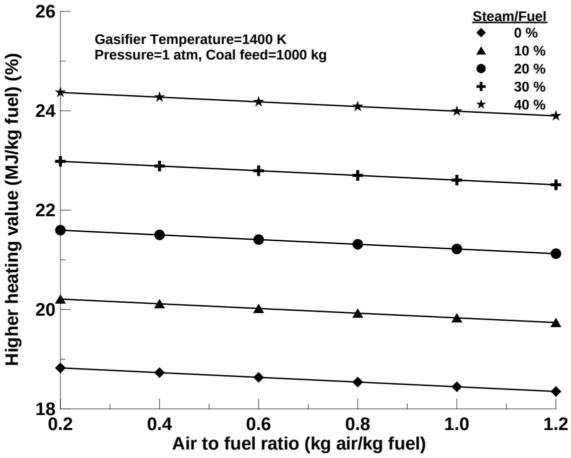

Figure 8. Effect of air/fuel ratio on HHV of synthesis gas.

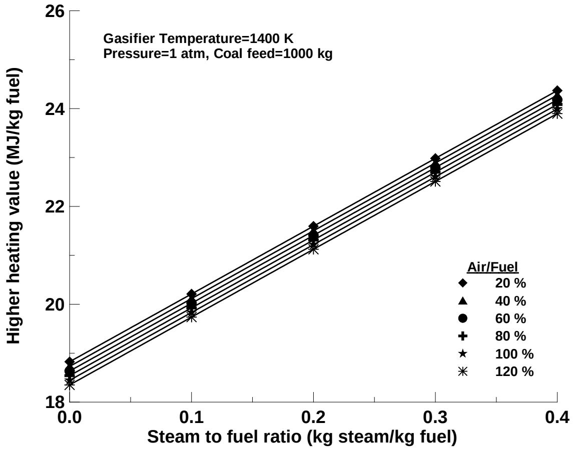

Figure 9. Effect of steam/fuel ratio on HHV of synthesis gas.

4. Conclusion

There may be an optimum value for the air-fuel ratio by searching the Figures 4 and 5. It is more appropriate to analyze the results under the combined effects of air-fuel and steam-fuel ratio. Looking at the situation from this point of view, whether an optimum present or not, it may be more appropriate to shift the optimum point for the air-fuel ratio to the point where hydrogen content reaches the carbon monoxide level. The shifted optimum occurs at the air-fuel ratio of 1.2 for steam-fuel ratio of 0.4. After determining the proper value for air-fuel ratio, the second step is to select the optimum value for steam-fuel ratio. There should be a maximum value of H_2/CO ratio corresponding to steam-fuel and air-fuel ratios. It may be appropriate to use Figure 5 to obtain optimum values of steam-fuel ratio for air-fuel ratio by extending the curves. It seems there is no optimum condition for the steam-fuel ratio even though the curves were extended to a few steps further.

Acknowledgements

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