EFFECT OF OPERATION PARAMETERS ON GASIFICATION FOR THE PRODUCTION OF SYNTHESIS GAS

Atilla Bıyıkoğlu, Department of Mechanical Engineering, Faculty of Engineering, Gazi University, Ankara, Turkey abiyik@gazi.edu.tr

Afşin Güngör, Department of Mechanical Engineering, Faculty of Engineering and Architecture, Niğde University, Niğde, Turkey
Coşku Kasnakoğlu, Department of Electrical Engineering, TOBB University of Economics and Technology, Ankara, Turkey
Murat Özbayoğlu, Department of Computer Engineering, TOBB University of Economics and Technology, Ankara, Turkey
Bekir Zühtü Uysal, Department of Chemical Engineering, Faculty of Engineering, Gazi University, Ankara, Turkey

Abstract

The sensitivity of operating parameters on the gasification of different Turkish coals was investigated for the production of synthesis gas. The coal properties were determined by detailed analysis in Turkish Coal Enterprises. The calculations and the analysis were carried out assuming the kinetic equilibrium model for gasification. The higher heating value of the synthesis gas produced was calculated for the evaluation of performance of the process. The effects of steam rate of water gas shift reactor, bypass ratio and coal composition on synthesis gas produced were analyzed. Moreover, integration of the gasifier with water-gas shift reactor was also investigated to obtain the desired H_2/CO ratio using different coals. The model developed in this work can be used for choosing the proper set of operating parameters to produce the synthesis gas with the desired composition suitable for the purpose of its end use.

Keywords: *Coal gasification, synthesis gas, sensitivity analysis*

1. Introduction

The gasifier converts coal into a synthesis gas. The synthesis gas produced is predominately composed of carbon monoxide (CO) and hydrogen (H_2) and has a much lower heating value than natural gas[1]. Heat evolved from the exothermic reaction of oxygen with the fuel serves to maintain the gasifier at the operating temperature and drives certain endothermic reactions taking place inside it.

Gasification of coal offers certain important advantages over direct combustion. The most important advantage is related to equipment size. Equipment size is much smaller as compared to that of combustion system due to the reduction in volume of synthesis gas from gasification. Drop in size of equipment reduces overall costs and thus, gasification provides an attractive option for remote small capacity power units.

The combination of a gasifier and a combined cycle is called the integrated gasification combined cycle (IGCC). Such a system results in a greater reduction in emissions from coal-based energy systems compared to that with direct combustion of the coal for power generation. An IGCC system offers a generating efficiency (40%), higher than that for a conventional direct combustion pulverized coal fired plant (34%) [2].

Rising natural gas prices and a desire for fuel diversification represent some of the reasons why power developers are reexamining their power generation portfolios. As a result, more inquiry recently has gone to clean-coal technologies to alleviate these concerns. A particular clean-coal technology, integrated gasification combined cycle or IGCC, has been moved to the forefront of coalbased technology choices. IGCC, in its simplest form, is a technology that converts coal to synthesis gas or syngas for combustion in a gas turbine. IGCC's benefits lie in its resemblance to natural gas combined cycle (NGCC) in that it has very low emissions and uses mature combined cycle technology. IGCC has an advantage over NGCC in its much lower operating costs, similar to pulverized coal (PC) [3].

As we enter into the 21st century, there is an increasing need for energy due to global economic growth. Fossil fuels will continue to dominate the world energy supplies into the 21st century and coal as a fuel must play an increasing role [4]. However, there has also been increasing environmental concern directed towards utilising coal, for example, CO_2 emissions, pollutant emissions and particulate disposal. Therefore, there is a need for clean coal burning technologies. Clean coal technologies are now becoming popular because of their high efficiencies and minimal environmental impacts [5]. Several technologies, such as integrated gasification combined cycle (IGCC), pressurised fluidised bed combustor (PFBC) and pulverised coal injection (PCI), have been identified as the most viable alternatives for the clean utilisations of coal due to the use of combined cycles [5–8]. These advanced clean coal technologies have gained increased technological and scientific interest over the last few decades [5]. Higher operating pressures have been applied to these technologies, for instance, 10–15 atm for PFBC, 15–25 atm for IGCC and less than 5 atm for PCI. Higher pressure operations will inherently result in an increase in coal throughput, a reduction in pollutant emissions and an enhancement in the intensity of reaction [7].

There are so many contemporary studies in production of synthesis gas for power generation. Some of them can be found in the study of Casleton et al. [9]; a review of the basic technology of coal gasification, with particular application to the production of synthesis gas for power generation.

In this study, aim is oriented on the effect of operational parameters on the composition of produced synthesis gas to be able to use it in power production. Furthermore, by using a couple of water gas shift (WGS) reactors, a refinement process is developed. In combining the gasifier with WGS reactors, a bypass line is constructed connecting the gas at the exit of gasifier with the gas at the exit of WGS reactors to be able to control the properties of the synthesis gas produced more effectively.

2. Description of the problem

In this study, a gasification process is modeled to produce synthesis gas for power production and a two-stage WGS reactor is used to refine the synthesis gas from the gasifier and a bypass line to control the composition of synthesis gas at the exit of cascade reactor as shown in Fig. 1. Synthesis gas from the gasifier is fed into the refinement system and mixed with steam at the WGS Reactor I. Some portion of the Synthesis gas from the gasifier is mixed with the exiting stream via bypass line connecting inlet and exit streams. Synthesis gas at the exit of WGS Reactor-I is mixed with a second stream of steam. Synthesis gas at the exit of WGS reactor II is mixed with a bypass stream to produce resulting composition.

Gasification model is constructed using the following nine simultaneous reactions under equilibrium condition;

$$C + 1/2\,O_2 \rightarrow CO \tag{1}$$

$$C + O_2 \rightarrow CO_2 \tag{2}$$

$$CO + 1/2\,O_2 \rightarrow CO_2 \tag{3}$$

$$H_2 + 1/2\,O_2 \rightarrow H_2O \tag{4}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{5}$$

$$C + H_2O \rightarrow CO + H_2 \tag{6}$$

$$C + CO_2 \rightarrow 2CO \tag{7}$$

$$C + 2H_2 \rightarrow CH_4 \tag{8}$$

$$CH_4 + H_2O \rightarrow CO + 3H_2 \tag{9}$$

The first four reactions are combustion reactions, and reactions numbered between 5 and 8 are gasification reactions; 5th reaction is the WGS reaction, 6th reaction is water gas reaction, 7th reaction is Boduard equilibrium reaction, 8th reaction is hydrogenating gasification (methanation) reaction, and 9th reaction is methane decomposition reaction.

The equilibrium constants of gasification reactions [1]; water-gas-shift (WGS), Eq. (5), heterogeneous WGS, Eq. (6), Boduard, Eq. (7), and hydrogenating gasification reactions, Eq. (8) are given in Table 1 in the temperature range of 400 and 1500 K.

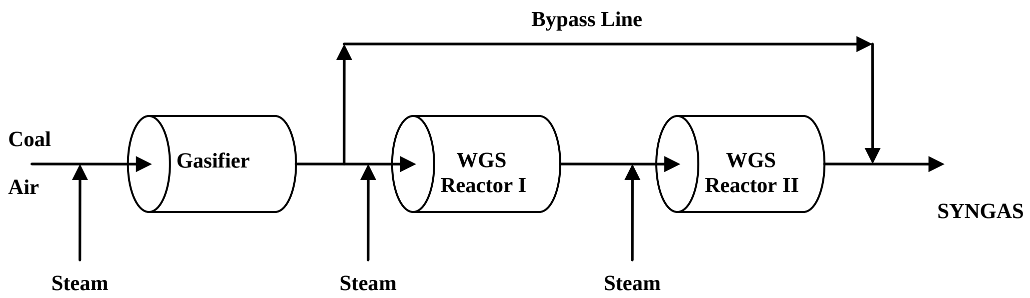

Figure 1. Schematic view of the gasifier

Table 1. Equilibrium constants of gasification reactions [1]

Temperature (K)	$K_{p,s}$ Eq. (5)	$K_{p,w}$ Eq. (6)	$K_{p,b}$ Eq. (7)	$K_{p,m}$ Eq. (8)
400	4.05×10^{3}	7.7×10^{-11}	5.2×10^{-14}	2.99×10^{5}
600	2.70×10^{1}	5.1×10^{-5}	1.9×10^{-6}	9.24×10^{1}
800	4.04×10^{0}	4.4×10^{-2}	1.1×10^{-2}	1.34×10^{0}
1000	1.38×10^{0}	2.62×10^{0}	1.90×10^{0}	9.6×10^{-2}
1500	3.7×10^{-1}	6.08×10^{2}	1.62×10^{3}	2.5×10^{-3}

The effect of coal types on the production of synthesis gas is examined under the conditions mentioned earlier. Coals are taken from different districts in Turkey and analyzed in the laboratories of Turkish Coal Enterprises. Results of analyses are presented in Table 2 for four different coal types. Ilgın-1 and Ilgın-2 named coals are taken from Çavuşçu Göl district, Yatağan coal from Yatağan and Tunçbilek from Tunçbilek Tavşanlı district. Ilgın-2 lignite has the highest ash content as shown in Table 2.

Table 2. Properties of coals from four different districts in Turkey

Constituents	**ILGIN-1**	**ILGIN-2**	**YATAGAN**	**TUNCBILEK**
C (%)	27.14	24.82	32.48	56.89
H (%)	2.05	2.82	2.79	4.28
O (%)	10.16	4.17	12.91	7.97
N (%)	0.61	0.62	0.66	2.16
S (%)	1.36	5.35	0.88	1.47
Ash (%)	5.42	16.58	6.44	13.72
Moisture (%)	53.26	45.64	43.84	13.51
LHV (Kcal/kg)	2056	2284	2694	5424
HHV (Kcal/kg)	2475	2698	3096	5728

3. Solution methodology

Two different types of software are developed for the solution of gasification equations: FORTRAN and MATLAB. In FORTRAN software, the model equations are solved using Gauss–Seidel iteration; successful relaxation method and combined relaxation Newton–Raphson methods. In MATLAB software, constrained optimization - sequential quadratic programming (SQP) based on least squares error minimization- method is used. Flowchart of the computational steps is shown in Figure 2 for the gasification model. A new calculation scheme is implemented into the code for the refinement process as shown in Figure 3.

There are many parameters affecting the composition of synthesis gas both in gasification and refinement processes. The amount of coal, coal properties, gasification temperature and pressure, air/fuel ratio, and steam/fuel ratio are gasification parameters. Simulation model calculates synthesis gas composition for aimed H_2/CO ratio at the gasifier exit for given gasifier operating conditions. The synthesis gas refinement process can be controlled by adjusting the synthesis gas, bypass ratio, bp, temperature of WGS reactors, T_1 and T_2, and the steam to synthesis gas ratios, SR_1 and SR_2. Therefore, simulation model also calculates optimum values of bypass ratio, temperature of WGS reactors, steam to synthesis gas ratio of WGS reactors for aimed H_2/CO ratio.

During synthesis gas refinement process, the model requires SYNGAS composition to be known at the beginning of calculation and after entering the operation parameters such as the steam ratios, SR_1 and SR_2, reactor temperatures, T_1 and T_2, and the H_2/CO ratio expected, the model performs calculations for SR_1 and SR_2. If the calculations converged to a solution, the program saves the results to a file and stops. Otherwise perform the following operations; updating the values of SR_1 and SR_2 and giving an initial value to the bypass ratio, the WGS reaction is solved to get a SYNGAS composition. As a final step, the desired H_2/CO ratio is checked. If this ratio satisfies the criteria, the program computes the HHV of the resulting SYNGAS composition, hot and cold gas efficiencies of the system.

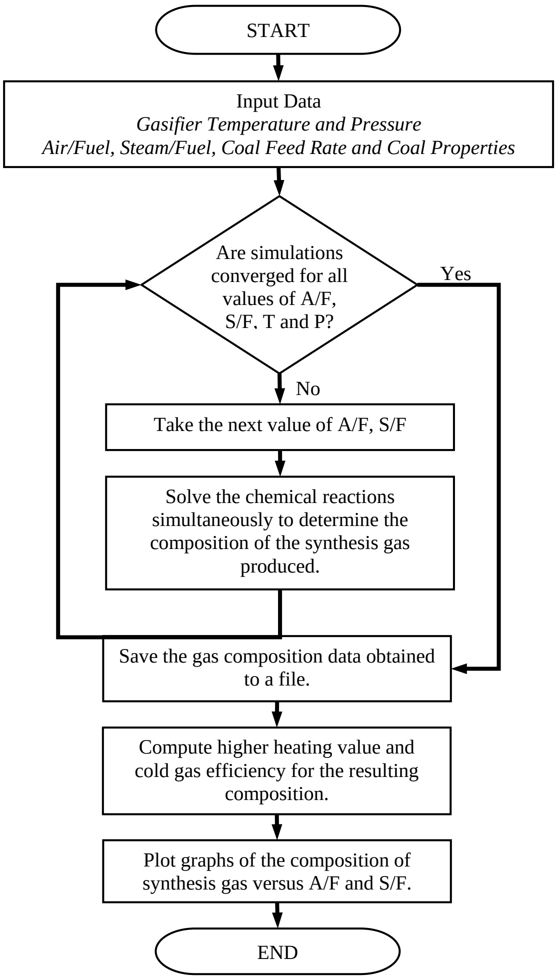

Figure 2. Flowchart of the gasification model

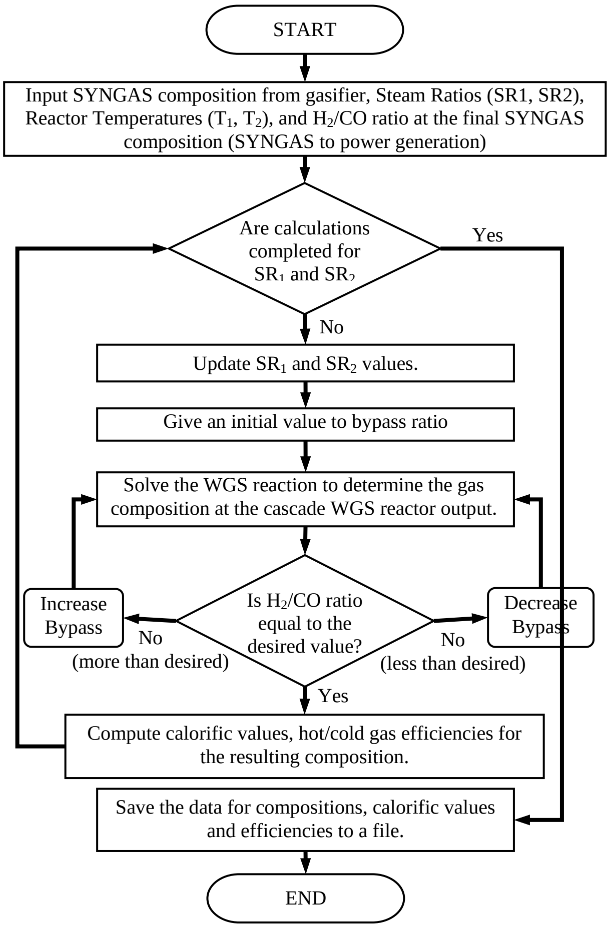

Figure 3. Flowchart of the cascade WGS reactor model

4. Results and discussion

There are many parameters effecting the composition of synthesis gas which makes the problem more complex. In this study, the most appropriate operational parameters in the gasification process which are obtained from earlier studies [10-12] are used in the calculations of the refinement process. The gasification pressure and temperature [10] are selected as 1 atm. and 1400 K, air to fuel ratio and steam to fuel ratio [11] in the gasifier on mass basis as 1.2 and 0.4, and the temperature of WGS-1 and WGS-2 reactors [12] as 350 K and 200K, respectively. We have learnt from the earlier study [12] that one can obtain the most appropriate result at all operating conditions balancing the amount of one of the steam rates and bypass ratio, therefore all the computations are done by adjusting the steam rate at WGS-1 reactor and eliminating the steam rate at WGS-2 reactor. The detailed information on the selection of these gasification parameters can be found in the relevant studies [10-12]. In this study, the results are obtained under these conditions for 1 kg of coal and four different Turkish coals, i.e. Ilgın-1, Ilgın-2, Yatağan and Tunçbilek.

In Figure 4, the variation of H_2/CO ratio with steam ratio for four types of Turkish coals are presented changing bypass ratio from 0 to 1 by step of 0.2. In Figure 4(a), the variation of H_2/CO ratio with steam ratio for four types of Turkish coals is presented at bypass ratio of 0.0. There is a linear increase in H_2/CO ratio with steam ratio for all type of coals having different slopes. Therefore, there is no optimum value for steam ratio of WGS reactor giving highest H_2/CO ratio. In this respect, looking at Figure 4 between (b) and (e), one can observe an optimum value for steam ratio of WGS reactor at each graph. These optimums are independent from the coal types. In Figure 4(b), the variation of H_2/CO ratio with steam ratio is presented for four types of Turkish coals at bypass ratio of 0.2. The optimum value for steam ratio of WGS reactor occurs at the value of 1. In Figure 4(c), the variation of H_2/CO ratio with steam ratio is presented for four types of Turkish coals at bypass ratio of 0.4. The optimum value for steam ratio of WGS reactor occurs at the value of 0.9. In Figure 4(d), the variation of H_2/CO ratio with steam ratio is presented for four types of Turkish coals at bypass ratio of 0.6. The optimum value for steam ratio of WGS reactor occurs at the value of 0.8. In Figure 4(e), the variation of H_2/CO ratio with steam ratio is presented for four types of Turkish coals at bypass ratio of 0.8. The optimum value for steam ratio of WGS reactor occurs again at the value of 0.8. Examining figures between 5 and 8, one can see that this optimum shifts left hand side by increasing bypass ratio from 0.2 to 0.6. In Figure 4(f), the variation of H_2/CO ratio with steam ratio is presented for four types of Turkish coals at bypass ratio of 1.0. There is no change in H_2/CO ratio with steam ratio as seen from Figure 4(f). Therefore, there is no optimum value for steam ratio of WGS reactor giving highest H_2/CO ratio independent from the coal type. From these figures, one can observe that Ilgın-2 has produced the highest H_2/CO ratio at WGS output and sorting from the highest to the lowest, Ilgın-1, Yatağan, and Tunçbilek come after Ilgın-2, respectively.

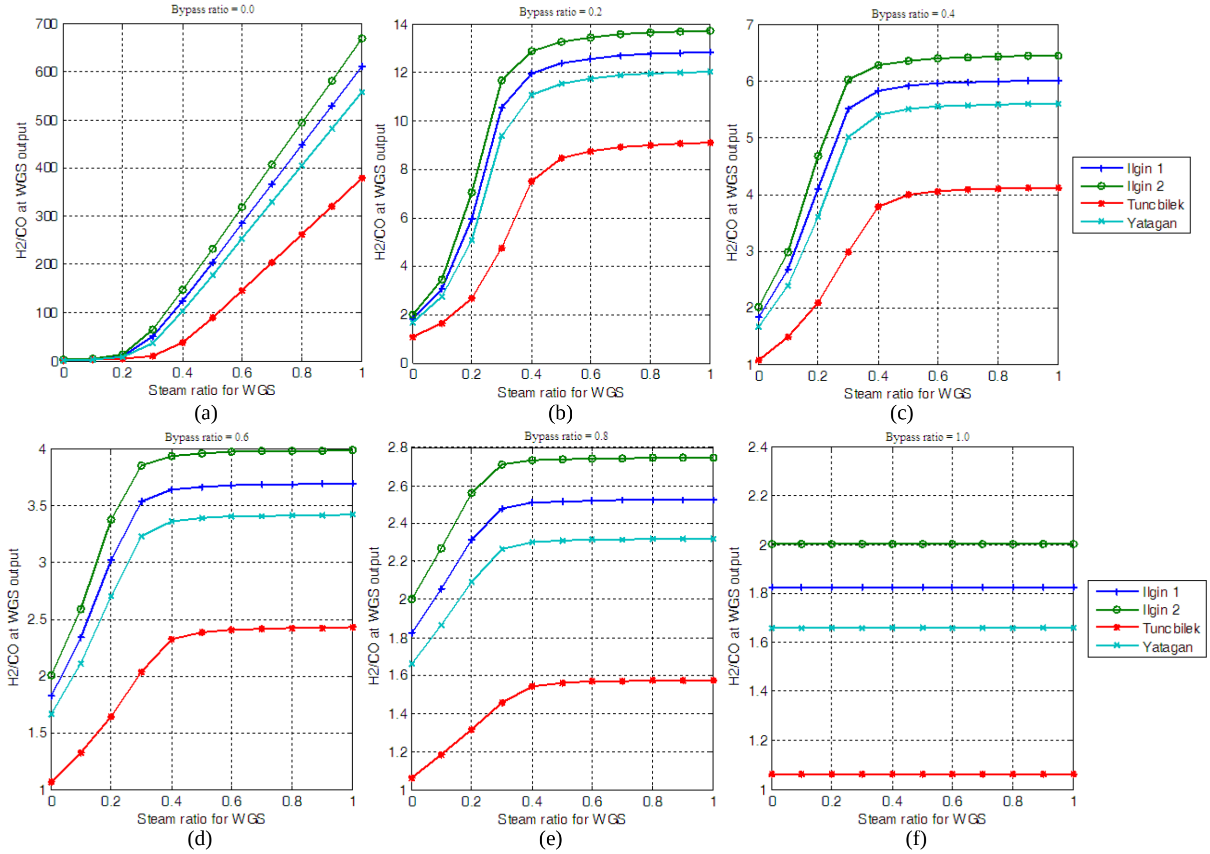

Figure 4. The variation of H_2/CO ratio with steam ratio and bypass ratio for four types of Turkish coals

Although the optimum value for steam ratio of WGS reactor shifts to the left hand side of the graph by increasing bypass ratio, one can fix the optimum value in the view of economic reasons. In each graph between Figures 4(b) and 4(e), there are two regions having steepest slope and smaller slope. The transition point between regions occurs at steam ratio of 0.3 for Ilgın-1, Ilgın-2 and Yatağan coals and 0.4 for Tunçbilek lignite regardless of bypass ratio. Following the steepest slope region, smaller slope region becomes and the optimum may be shifted in the lower slope region at a reasonable range. Let's put forth a criterion lowering the optimum value to a reasonable level from economic point of view. Criterion is that the optimum is the point where the change in H_2/CO ratio less than 2% is observed at first between successive points in the smaller slope region. Under this definition, the optimum value for steam ratio of WGS reactor may be taken as 0.4 independent from the bypass ratio.

Ilgın-1, Ilgın-2 and Yatağan coals present similar results with respect to the production of H_2/CO ratio except Tunçbilek lignite. The distinction is clearly shown on the Figures between 4(a) and 4(f). In Figure 4(b), the maximum value of H_2/CO ratio reaches about 14 for Ilgın-2, 13 for Ilgın-1 and 12 for Yatağan. Examining Figures between 4(b) and 4(f), one can see this maximum decreases while increasing bypass ratio. The maximum value of H_2/CO ratio for Ilgın-2 reaches about the value of 14 for bypass ratio of 0.2, 6.5 for bypass ratio of 0.4, 4 for bypass ratio of 0.6, 2.75 for bypass ratio of 0.8 and finally 2 for bypass ratio of 1.0. The maximum value of H_2/CO ratio for Ilgın-1 reaches about the value of 13 for bypass ratio of 0.2, 6 for bypass ratio of 0.4, 3.7 for bypass ratio of 0.6, 2.5 for bypass ratio of 0.8 and finally 1.8 for bypass ratio of 1.0. The maximum value of H_2/CO ratio for

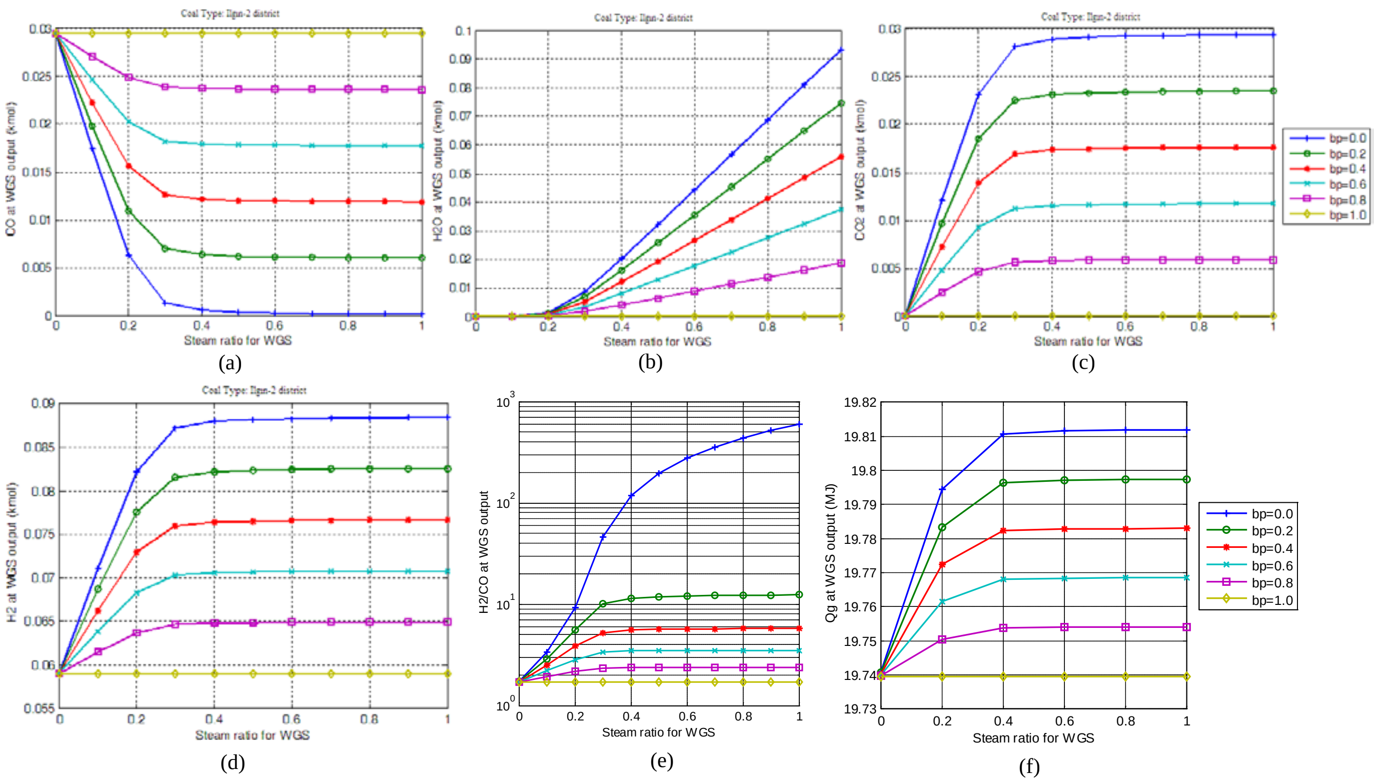

Figure 5. The variation of CO, H_2O, CO_2, H_2, H_2/ CO and HHV of SYNGAS with steam ratio and bypass ratio at the exit of WGS reactors

Yatağan reaches about the value of 12 for bypass ratio of 0.2, 5.5 for bypass ratio of 0.4, 3.4 for bypass ratio of 0.6, 2.3 for bypass ratio of 0.8 and finally 1.65 for bypass ratio of 1.0. The maximum value of H_2/CO ratio for Tunçbilek reaches about the value of 9 for bypass ratio of 0.2, 4 for bypass ratio of 0.4, 2.5 for bypass ratio of 0.6, 1.6 for bypass ratio of 0.8 and finally 1.1 for bypass ratio of 1.0.

The maximum value of H_2/CO ratio is reduced by 7% for bypass ratio of 0.2 changing the optimum for steam ratio from 1 to 0.4 regardless of coal type. The maximum value of H_2/CO ratio is reduced by 3% for bypass ratio of 0.4 changing the optimum for steam ratio from 0.9 to 0.4 regardless of coal type. The maximum value of H_2/CO ratio is reduced by 2.5% for bypass ratio of 0.6 changing the optimum for steam ratio from 0.8 to 0.4 regardless of coal type. The maximum value of H_2/CO ratio is reduced by 0.4% for bypass ratio of 0.8 changing the optimum for steam ratio from 0.8 to 0.4 regardless of coal type. As a result of changing optimum for steam ratio to 0.4 for all bypass ratios, the loss in the production of H_2/CO ratio is in allowable limits. Therefore, the optimum value of steam ratio of WGS reactor should be taken as 0.4 regardless of bypass ratio and coal type. It seems the most preferable coal type is Ilgın-2 between four types of coals for the production of H_2/CO ratio.

In Figure 5, the variation of CO, H_2O, CO_2, H_2, Cold gas efficiency and HHV of SYNGAS with steam ratio is shown for bypass ratio at the exit of WGS reactors. The results are obtained for 1000 kg Ilgın-2 lignite. In Figure 5(a), the variation of carbon-monoxide with steam ratio is shown at different bypass ratio for Ilgın-2. At steam ratio of 0.4, carbon-monoxide level reaches approximately zero without using bypass fluid. In Figure 5(d), the variation of hydrogen with steam ratio is shown at different bypass ratio for Ilgın-2. At steam ratio of 0.4, hydrogen amount reaches its maximum level and is about 0.087 kmol per 1 kg of coal feed. In Figure 5(b), the variation of water with steam ratio is shown at different bypass ratio for Ilgın-2. At steam ratio of 0.4, water level reaches 0.02 kmol per 1 kg of coal feed. In Figure 5(c), the variation of carbon-dioxide with steam ratio is shown at different bypass ratio for Ilgın-2. At steam ratio of 0.4, carbon dioxide level reaches its maximum for bypass ratio of zero and is about 0.029 kmol per 1 kg of coal feed. In Figure 5(e), the variation of H_2/CO with steam ratio is shown at different bypass ratio for Ilgın-2. At steam ratio of 0.4, H_2/CO value reaches a hundred levels for bypass ratio of zero. In Figure 5(f), the variation of HHV of synthesis gas with steam ratio is shown at different bypass ratio for Ilgın-2 at the exit of WGS reactor. At steam ratio of 0.4, the HHV of synthesis gas reaches its maximum level for bypass ratio of zero and is about 19.81 MJ per 1 kg of coal (4739 kcal/kg).

Conclusion

In this study, the most appropriate operating conditions for the production of synthesis gas which will be used in power production are determined. There are nine operating parameters in the gasification and refinement process which are the gasification pressure and temperature, air to fuel ratio and steam to fuel ratio in the gasifier, the temperatures of WGS-1 and WGS-2 reactors, steam rate at WGS-1 reactor, bypass factor in the refinement system, and coal type. The optimum value of steam ratio of WGS reactor can be taken as 0.4 regardless of bypass ratio and coal type. It seems the most preferable coal type is Ilgın-2 between four types of coals for the production of power. HHV of synthesis gas for bypass value of zero is always higher than that of bypass value of higher than zero. As a result of this fact, one can conclude that if primary aim is to generate electricity using the synthesis gas, we should not employ any bypass, i.e. bypass ratio should be zero. However, if the final use of synthesis gas is to produce different chemicals, then H_2/CO ratio can be pre estimated depending on the chemical and the bypass ratio can be adjusted accordingly.

References

[1] Basu P., Combustion and Gasification in Fluidized Beds, Taylor and Francis, CRC Press 2006.
[2]Schimmoller, B. K., Coal gasification: striking while the iron is hot, Power Eng., 30–40, March, 2005.
[3] R. Aiken, K.H. Ditzel, F. Morra and D.S. Wilson , “Coal-Based Integrated Gasification Combined Cycle: Market Penetration Strategies and Recommendations,” Final Report, Department of Energy (DOE), National Energy Technology Laboratory (NETL), Gasification Technologies Council (GTC), DE-AM26-99FT40575, September 3, 2004.
[4] L.D. Smoot, “International research centers' activities in coal combustion,” Progress in Energy and Combustion Science, Volume 24, Issue 5, 1998, Pages 409-501.
[5] Takematsu T, Maude C. Coal gasification for IGCC power generation. Gemini House, London: IEA Coal Research; 1991.
[6] Smoot LD, Smith PJ. Coal gasification and combustion. New York: Plenum Press; 1985.
[7] Harris DJ, Patterson JH. Aust Inst Energy J 1995;13:22.
[8] Kristiansen A. Understanding of coal gasification. Gemini House, London: IEA Coal Research; 1996.
[9] Casleton, K.H., Breault, R. W., Richards, G.A. “System Issues and Tradeoffs Associated with Syngas Production and Combustion”, *Combust. Sci. and Tech,* 180, 1013-1052, (2008).
[10] A. Bıyıkoğlu, C. Kasnakoğlu, M.Özbayoğlu, A. Güngör, D. Ö. Özgür, B.Z. Uysal, “Determination of coal gasification parameters for the production of synthesis gas,” 9th National Chemical Engineering Congress (UKMK-9) June 22-25, 2010, Gazi University, Ankara, Turkey.
[11] A. Güngör , M. Özbayoğlu, C. Kasnakoğlu , A. Bıyıkoğlu, B. Z. Uysal, “Determination Of Air/Fuel And Steam/Fuel Ratio For Coal Gasification Process To Produce Synthesis Gas,” The Second International Conference on Nuclear and Renewable Energy Resources, July 5th-7th, 2010, Golbasi Convention Center, Ankara, Turkiye.
[12] A.M.Özbayoğlu, C. Kasnakoğlu, A. Güngör, A. Bıyıkoğlu, B.Z. Uysal, “An Analysis of Water Gas-Shift Reactor Battery System For Synthesis Gas Refinement”, 11th International Combustion Symposium, June 24th - 27th 2010, SARAJEVO