VERSITA

Chemical Papers 66 (7) 677–683 (2012)
DOI: 10.2478/s11696-012-0164-0

ORIGINAL PAPER

A parametric study on coal gasification for the production of syngas

[a]Afsin Gungor*, [b]Murat Ozbayoglu, [c]Cosku Kasnakoglu, [d]Atilla Biyikoglu, [e]Bekir Zuhtu Uysal

[a]*Department of Mechanical Engineering, Faculty of Engineering, Akdeniz University, Dumlupınar Bulvarı, Kampus, 07058 Antalya, Turkey*

[b]*Department of Electrical Engineering,* [c]*Department of Computer Engineering, TOBB University of Economics and Technology, Sogutozu Caddesi, 43 Sogutozu, 06560 Ankara, Turkey*

[d]*Department of Mechanical Engineering,* [e]*Department of Chemical Engineering, Engineering Faculty, Gazi University, Eti Mh, Yukselis Sk, 5 Maltepe, 06500 Ankara, Turkey*

Received 25 August 2011; Revised 10 February 2012; Accepted 17 February 2012

In this parametric study, the effects of coal and oxidiser type, air-to-fuel ratio, steam-to-fuel ratio, reactor temperature, and pressure on H_2 and CO amounts at the gasifier output, H_2/CO, and higher heating value of the syngas produced have been calculated using a coal gasification model. Model simulations have been performed to identify the optimum values which are assumed to be 100 % for both cold gas efficiency and carbon conversion efficiency in the gasification process. From this study, it may be observed that the moisture content of the coal type is of crucial importance for the air gasification process; the O_2 content of similar coals (taking into consideration the moisture and H_2 content) is of significant importance for the air gasification process. When compared with air gasification, air-steam gasification becomes a more effective coal gasification method. The optimum working condition for air-steam gasification is to carry out the process at one atmosphere. High gasifier temperatures are not needed for the air-steam gasification of coal.

Keywords: coal gasification, syngas production, gasification simulation, chemical process optimization

Introduction

There are numerous current studies devoted to syngas production for power generation in the literature (Li et al., 2001; Lin et al., 2002; Huang et al., 2003; Shi et al., 2006). In the study of Casleton et al. (2008), the basic technology of coal gasification is reviewed, giving a detailed account of the production of syngas in power generation. The numerical simulation of coal gasifiers is an important tool in the prediction of its gasification behaviour. The modelling of coal gasifiers aims at creating a system which maximises gasification efficiency and thus minimises investment, operational costs, and emissions of pollutants.

From this perspective, reactor temperature and pressure, steam-to-fuel ratio, air-to-fuel ratio, and the effects of coal and oxidiser type are investigated using the coal gasification model developed. Steam and air are used as the coal gasification agent (oxidiser). Model simulations were carried out with the optimum values which are assumed to be 100 % both for cold gas efficiency and carbon conversion efficiency in the gasification process. The novelty of this study is that it gives consideration to four different types of Turkish coal and investigates the effect of coal grade on the gasification process. Coal used in this study is provided by Turkish Coal Enterprise (TKI) from different locations of Turkey.

*Corresponding author, e-mail: afsingungor@hotmail.com

Theoretical

Achieving the best synthesis gas (syngas) composition for power generation and the production of coal chemicals represents a challenge. An accurate understanding of the gasification phenomena is needed for a reliable prediction of performance by way of modelling. From this perspective, the present study seeks to develop a model for the coal gasification process. The most significant reactions used in the model are as follows:

$$C + 1/2O_2 \leftrightarrow CO \quad (1)$$

$$C + O_2 \leftrightarrow CO_2 \quad (2)$$

$$CO + 1/2O_2 \leftrightarrow CO_2 \quad (3)$$

$$H_2 + 1/2O_2 \leftrightarrow H_2O \quad (4)$$

$$C + H_2O \leftrightarrow CO + H_2 \quad (5)$$

$$C + CO_2 \leftrightarrow 2CO \quad (6)$$

$$C + 2H_2 \leftrightarrow CH_4 \quad (7)$$

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \quad (8)$$

where Eq. (5) represents heterogeneous water-gas-shift (WGS) reaction, Eq. (6) Boudouard equilibrium, Eq. (7) hydrogenating gasification, and Eq. (8) methane decomposition.

The model is based on the assumption that the gasifier is operated isothermally, and chemical equilibrium is achieved. The equilibrium constants of Boudouard, heterogeneous WGS, and hydrogenating gasification reactions are given in Table 1 (Tsui et al., 2002).

The higher heating value of the synthesis gas is computed from the sum of the heating values of the individual combustible constituents, being H_2, CO, 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 (Kaushal et al., 2007). In this case, the amounts of H_2S and CH_4 are negligible, hence they are not included in the calculations of heating value.

In the model, a combined relaxation Newton–Raphson method is used, with Fortran as the computer code. The following equation is used in the solution of matrix with three bands:

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

where X and F represent the variable and function vectors, respectively, and B is iteration number. The elements of the matrix with three bands are calculated using the Jacobian term, $\partial F/\partial X$. The flow-chart of the computations in the model is presented in Fig. 1.

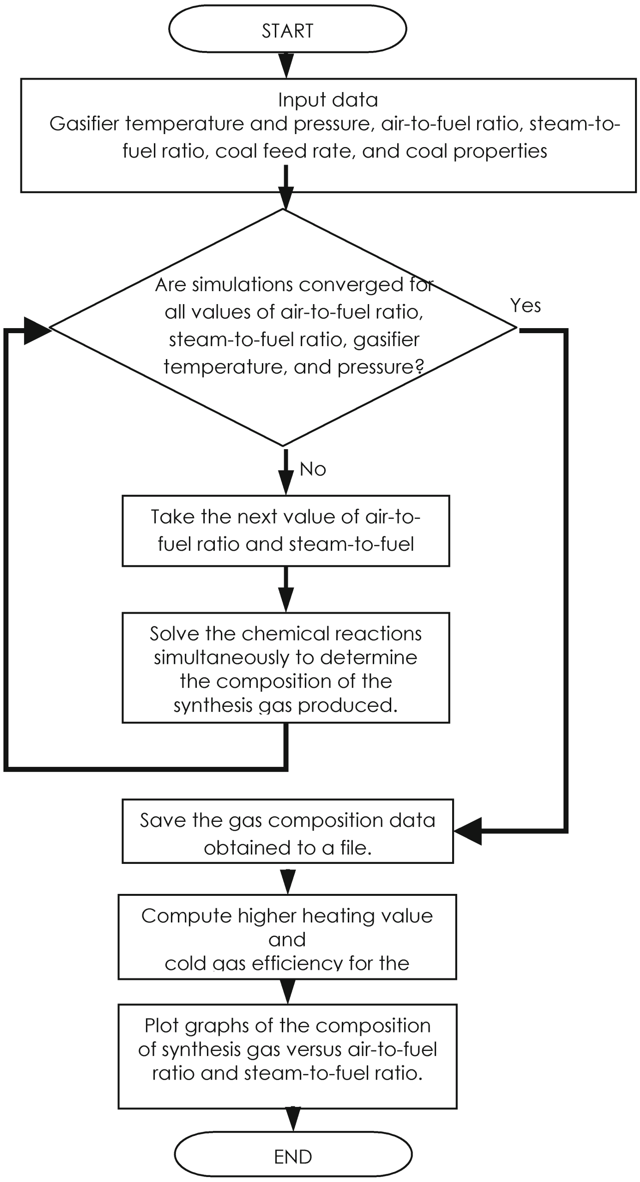

Fig. 1. Flow-chart of gasification model.

Table 1. Equilibrium constants

Temperature	$K_{p,w}$	$K_{p,b}$	$K_{p,m}$
K	Eq. (5)	Eq. (6)	Eq. (7)
400	7.70×10^{-11}	5.20×10^{-14}	2.99×10^{5}
600	5.10×10^{-5}	1.90×10^{-6}	9.24×10^{1}
800	4.40×10^{-2}	1.10×10^{-2}	1.34×10^{0}
1000	2.62×10^{0}	1.90×10^{0}	9.60×10^{-2}
1500	6.08×10^{2}	1.62×10^{3}	2.50×10^{-3}

$K_{p,w}$, $K_{p,b}$, and $K_{p,m}$ represent the equilibrium constants for water-gas-shift, Boudouard, and methane formation reactions, respectively.

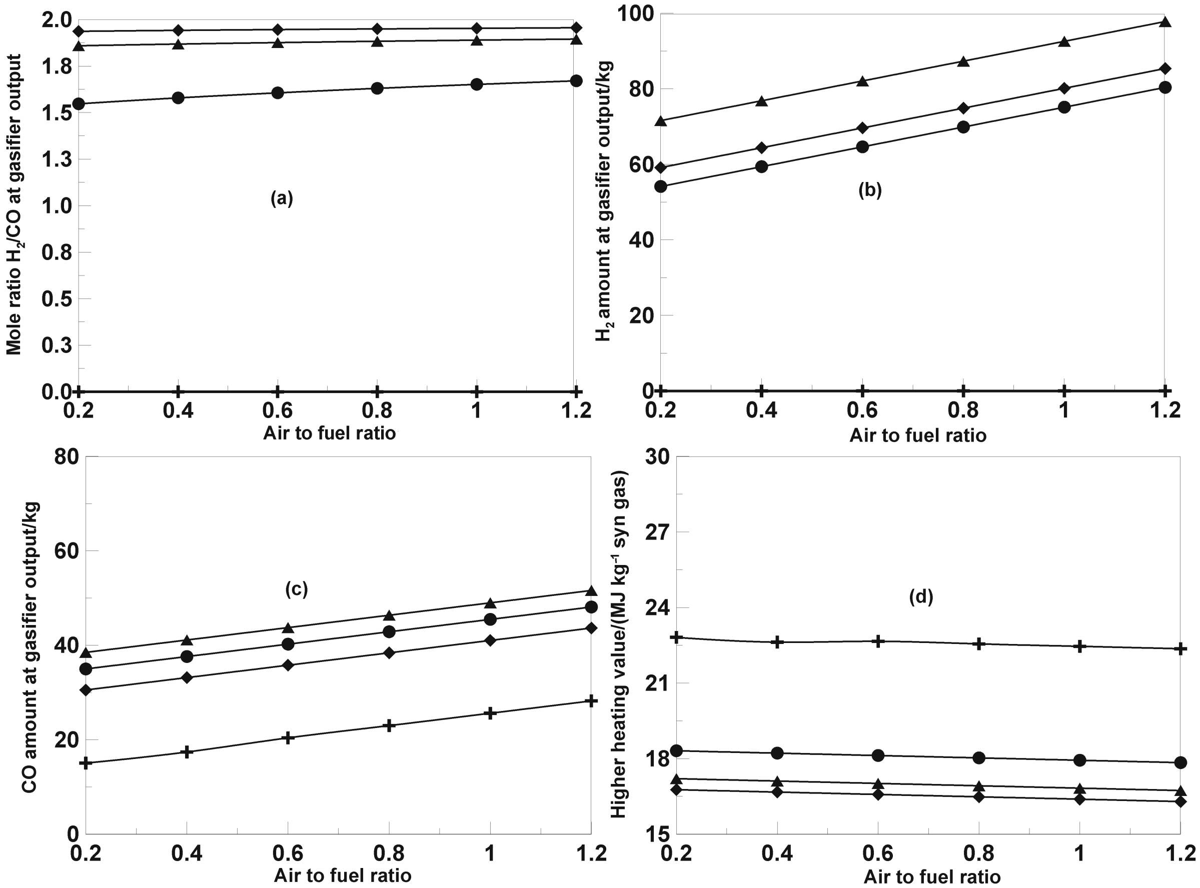

Fig. 2. Effect of air-to-fuel mass ratio on H_2/CO at gasifier output (a), H_2 (b) and CO (c) amounts at gasifier output, and higher heating value of syngas (d) for four different kinds of Turkish coal; ▲ – ILGIN-1, ♦ – ILGIN-2, ● – YATAGAN , + – TUNCBILEK.

Table 2. Coal properties

Property	ILGIN-2	ILGIN-1	YATAGAN	TUNCBILEK
C (mass %)	24.82	27.14	32.48	56.89
H (mass %)	2.82	2.05	2.79	4.28
O (mass %)	4.17	10.16	12.91	7.97
N (mass %)	0.62	0.61	0.66	2.16
S (mass %)	5.35	1.36	0.88	1.47
Ash (mass %)	16.58	5.42	6.44	13.72
Moisture (mass %)	45.64	53.26	43.84	13.51
LHV (MJ kg^{-1})	9.5	8.6	11.2	22.7
HHV (MJ kg^{-1})	11.2	10.3	12.9	23.9

LHV – Lower heating value, HHV – higher heating value.

The input parameters for the model are coal-feed rate, coal properties, gasification temperature and pressure, air-to-fuel ratio, and steam-to-fuel ratio. The simulation model calculates the synthesis gas composition, H_2/CO and higher heating value for the air-to-fuel ratio and steam-to-fuel ratio under the given operating conditions.

Results and discussion

There are many parameters affecting the composition of synthesis gas which render the problem more complex. In this study, the reactor temperature and pressure, steam-to-fuel ratio, air-to-fuel ratio, and the effects of coal and oxidiser type are investigated using the coal gasification model developed. Steam and air are used as the coal gasification agent (oxidiser). All model simulations were carried out for the optimum

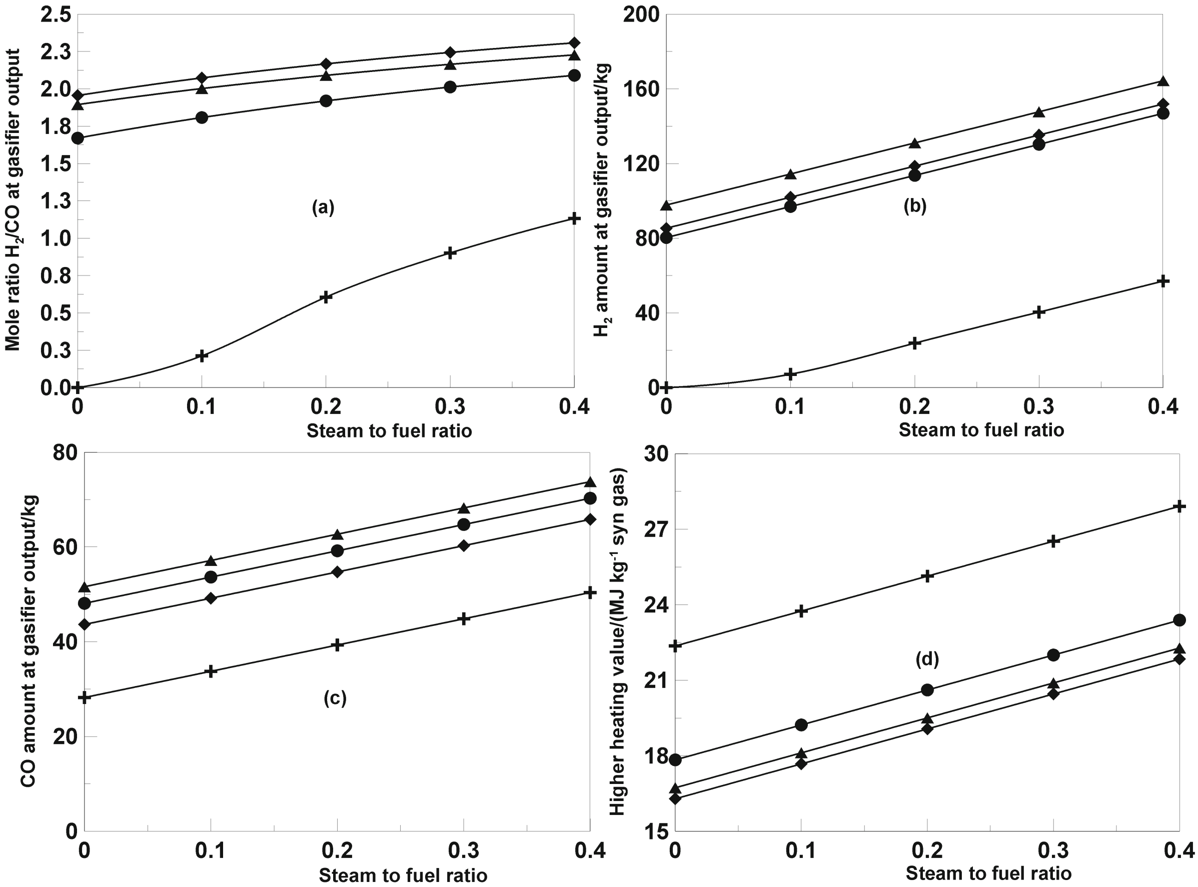

Fig. 3. Effect of steam-to-fuel mass ratio on H_2/CO at gasifier output (a), H_2 (b) and CO (c) amounts at gasifier output, and higher heating value of syngas (d) for four different kinds of Turkish coal; ▲ – ILGIN-1, ♦ – ILGIN-2, ● – YATAGAN , + – TUNCBILEK.

values, which are assumed to be 100 % both for carbon conversion efficiency and cold gas efficiency of the gasification process. The coal properties used in the model are given in Table 2. It should be noted that hydrogen and oxygen are assumed to be present as H_2 and O_2.

Fig. 2 shows the effect of the air-to-fuel ratio on the H_2/CO at the gasifier output, on H_2 and CO amounts at the gasifier output, and the higher heating value of syngas for four different kinds of Turkish coal. Fig. 2 plots the predicted modelling results for six air-to-fuel mass ratios (0.2, 0.4, 0.6, 0.8, 1.0, and 1.2). Under this assumption, the steam-to-fuel mass ratio is 0 kg steam per kg of fuel, gasifier temperature is 1400 K, gasifier pressure is 101.325 kPa, and coal feed is 1000 kg. Therefore, air is used as the coal gasification agent. As can be seen in Fig. 2, the increase in H_2 and CO amounts at the gasifier output is caused by the increase in the air-to-fuel ratio. Increasing the air-to-fuel ratio has a negative effect on the syngas higher heating value. When the air-to-fuel ratio is increased, a decrease in the higher heating value of syngas is observed, mainly due to a decrease in methane content and concentrations of other light hydrocarbons with high heating values. At higher equivalence ratios, the higher concentration of nitrogen causes low gas higher heating values. Nitrogen dilutes the product gas and reduces its energy content. On the other hand, the air-to-fuel ratio does not substantially influence the H_2/CO at the gasifier output.

ILGIN-1 has the highest moisture content of all the coal types, resulting in the higher H_2 and CO amounts seen in Fig. 2b. This phenomenon shows that the moisture content of the coal type is of crucial importance for the air gasification process. When we consider the coal types with similar C content, it is observed that the gasifier output CO amount is higher in coal which is richer in O_2 content under the same air-to-fuel ratio. This proves that the O_2 content of similar coals is of significant importance for the air gasification process. When we consider coal with a high C content, it is observed that the coal with high moisture and volatile matter also has higher H_2 and CO amounts at the gasifier output, given the same air-to-fuel ratio. However, when the higher heating value is taken into consideration, it is observed that coals that are higher in C concentration have the highest higher heating value, which is also observed in Fig. 2d. This is a major indicator that the coal grade exerts a great effect on gasification behaviour.

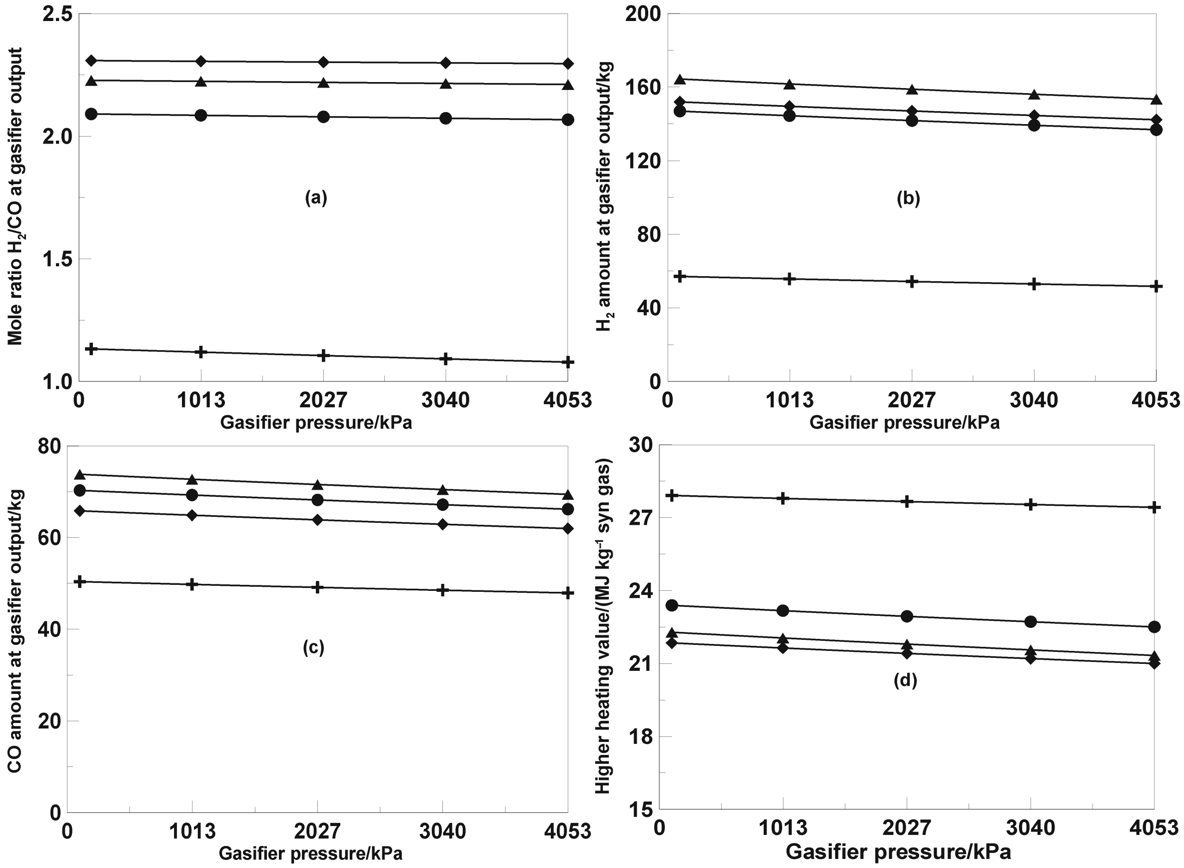

Fig. 4. Effect of gasifier pressure on H_2/CO at gasifier output (a), H_2 (b) and CO (c) amounts at gasifier output, and higher heating value of syngas (d) for four different kinds of Turkish coal; ▲ – ILGIN-1, ♦ – ILGIN-2, ● – YATAGAN , + – TUNCBILEK.

Fig. 3 shows the effect of the steam-to-fuel ratio on the H_2/CO at the gasifier output, on H_2 and CO amounts at the gasifier output and the higher heating value of syngas for four different kinds of Turkish coal. Fig. 3 plots the predicted model results for five steam-to-fuel mass ratios (0, 0.1, 0.2, 0.3, and 0.4). Under this assumption, the air-to-fuel ratio is 1.2 kg air per kg of fuel, gasifier temperature is 1400 K, gasifier pressure is 101.325 kPa, and coal feed is 1000 kg.

Steam gasification has become a favoured method as it maximises the product with high heating rates. Moreover, it has good residence time characteristics and effective tar-char reduction resulting from steam-reforming. As the steam is introduced to steam gasification, the gas quality is improved. This study also proves that air-steam gasification is a more effective coal gasification method than air gasification, as can be clearly observed in Fig. 3. Increasing the steam-to-fuel ratio has a considerably positive effect on H_2 and CO compositions, H_2/CO at the gasifier output and higher heating value of the syngas.

Fig. 4 shows the effect of gasifier pressure on H_2/CO at the gasifier output, on H_2 and CO amounts at the gasifier output, and the higher heating value of syngas for four different kinds of Turkish coal. Fig. 4 shows the predicted results for 5 gasifier pressure values (101 kPa, 1013 kPa, 2027 kPa, 3040 kPa, and 4053 kPa). Under this assumption, the air-to-fuel ratio is 1.2 kg air per kg of fuel, the steam-to-fuel ratio is 0.4 kg steam per kg of fuel, the gasifier temperature is 1400 K, and the coal feed is 1000 kg. The gasification pressure influences the reaction kinetics and equilibrium; as the pressure increases, the equilibrium of H_2 and CO production decreases. In this study, it is observed that high pressure reduces the H_2 yield and low pressure does not substantially improve the H_2 yield. The highest H_2 yield occurred at atmospheric pressure. Therefore, it may be concluded that the optimum working condition for air-steam gasification is to carry out the process at one atmosphere.

Fig. 5 shows the effect of gasifier temperature on the H_2/CO at the gasifier output, on H_2 and CO amounts at the gasifier output, and the higher heating value of syngas for four different kinds of Turkish coal. Fig. 5 plots the predicted modelling results for five gasifier temperature values (1100 K, 1200 K, 1300 K, 1400 K, and 1500 K). Under this assumption, the air-to-fuel mole ratio is 1.2 kg air per kg of fuel, the steam-to-fuel ratio is 0.4 kg steam per kg of fuel, the gasifier pressure is 101 kPa, and

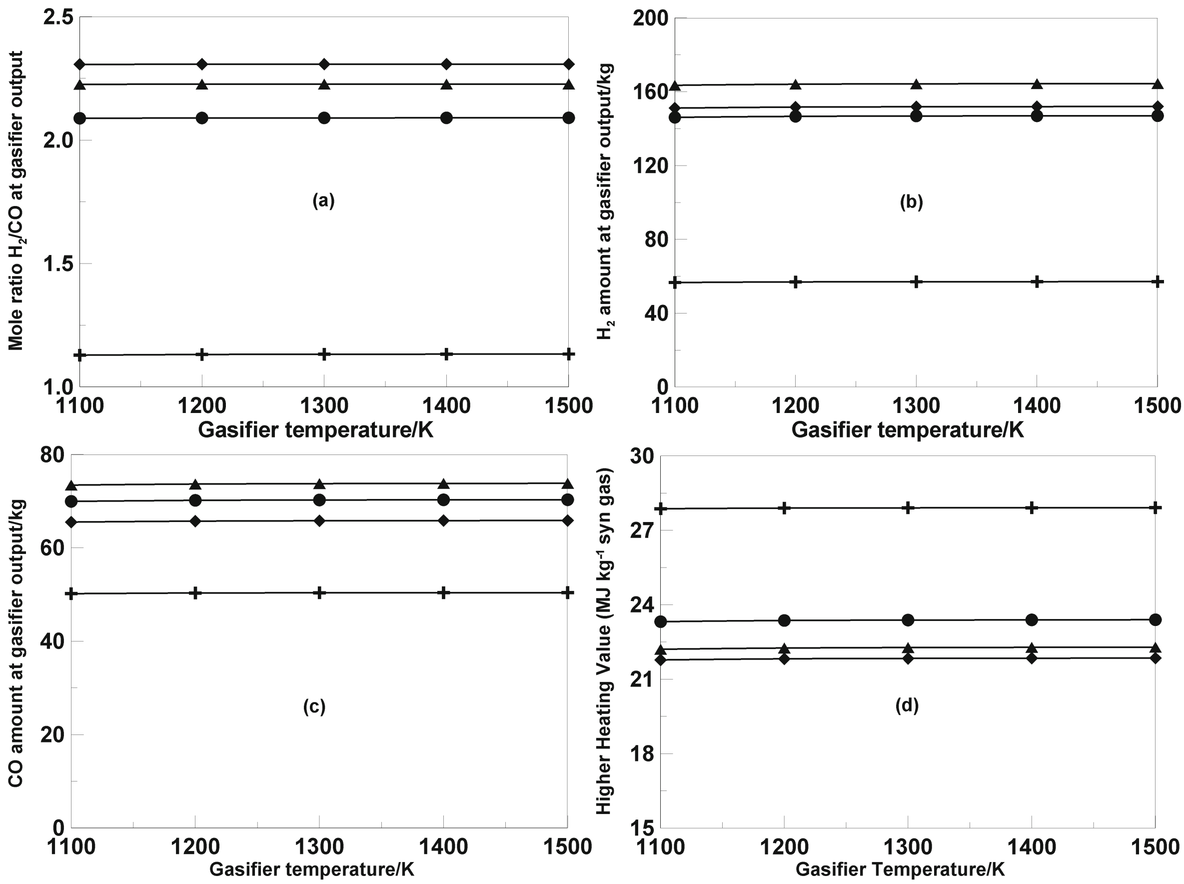

Fig. 5. Effect of gasifier temperature on H_2/CO at gasifier output (a), H_2 (b) and CO (c) amounts at gasifier output, and higher heating value of syngas (d) for four different kinds of Turkish coal; ▲ – ILGIN-1, ♦ – ILGIN-2, ● – YATAGAN , + – TUNCBILEK.

the coal feed is 1000 kg. Fig. 5 shows that the gasifier temperature does not have a significant effect on the air-steam gasification process. It may be assumed that higher gasifier temperatures are not needed for the air-steam gasification of coal. Therefore, a temperature of 1100 K may be considered as the optimum working condition for air-steam gasification.

Conclusions

In this parametric study, the effects of coal and oxidiser type, air-to-fuel ratio, steam-to-fuel ratio, reactor temperature, and pressure on H_2 and CO amounts at the gasifier output, H_2/CO, and higher heating value of the syngas have been estimated using the coal gasification model developed. Model simulations were performed for the optimum values, which are assumed to be 100 % both for cold gas efficiency and carbon conversion efficiency in the gasification process. The results observed in this study are as follows: (i) the moisture content of the coal type is of crucial importance for the air gasification process, (ii) the O_2 content of similar coals (considering moisture and H_2 content) is of significant importance for the air gasification process, (iii) high pressure reduces the H_2 yield and low pressure does not provide any substantial improvement in the H_2 yield; it may therefore be concluded that the optimum working condition for air-steam gasification is for the process to be conducted at one atmosphere, (iv) higher gasifier temperatures are not necessary for the air-steam gasification of coal.

Acknowledgements. Financial support from the Turkish Coal Enterprise (TKI) is gratefully acknowledged. The authors also express their thanks to Canan Gungor for her contribution to this work.

References

Casleton, K. H., Breault, R. W., & Richards, G. A. (2008). System issues and tradeoffs associated with syngas production and combustion. *Combustion Science and Technology*, *180*, 1013–1052. DOI: 10.1080/00102200801962872.

Huang, J., Fang, Y., Chen, H., & Wang, Y. (2003). Coal gasification characteristics in a PFB. *Energy Fuels*, *17*, 1474–1479. DOI: 10.1021/ef030052k.

Kaushal, P., Pröll, T., & Hofbauer, H. (2007). Model development and validation: co-combustion of residual char, gases and volatile fuels in the fast fluidized combustion chamber of a dual fluidized bed biomass gasifier. *Fuel*, *86*, 2687–2695. DOI: 10.1016/j.fuel.2007.03.032.

Li, X., Grace, J. R., Watkinson, A. P., Lim, C. J., & Ergüdenler,

A. (2001). Equilibrium modeling of gasification: a free energy minimization approach and its application to a circulating fluidized bed coal gasifier. *Fuel*, *80*, 195–207. DOI: 10.1016/s0016-2361(00)00074-0.

Lin, S. Y., Harada, M., Suzuki, Y., & Hatano, H. (2002). Hydrogen production from coal by separating carbon dioxide during gasification. *Fuel*, *81*, 2079–2085. DOI: 10.1016/s0016-2361(02)00187-4.

Shi, S. P., Zitney, S. E., Shahnam, M., Syamlal, M., & Rogers, W. A. (2006). Modeling coal gasification with CFD and discrete phase method. *Journal of the Energy Institute*, *79*, 217–221. DOI: 10.1179/174602206x148865.

Tsui, H., Yavuzkurt, S., & Scaroni, A. (2002). Thermodynamic analysis of the gasification of coal water slurry fuels for a circulating fluidized bed gasifier. *Journal of Power and Energy*, *216*, 343–353. DOI: 10.1243/095765002320877838.