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Çan Kömürü Gazlaştırılmasının Sürüklemeli Akış Gazlaştırıcıda Aspen PLUS® Kullanılarak İncelenmesi

Investigation of Çan Coal Gasification in Entrained Flow Gasifier by using Aspen PLUS®

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Abstract

Excessive consumption of fossil fuels due to energy demand leads to an increase in the amount of CO_2 emitted to the environment. Gasification technology enables clean and efficient use of fossil fuels such as coal, which cause CO_2 emissions predominantly. Gasification can be utilized under several atmospheres such as air, steam, O_2/CO_2 mixture, etc. The reduction of inert gases (N_2) and the increase of CO concentration at high temperatures in syngas provides high-quality gas. Among the commercial gasifiers, entrained flow gasifiers have many advantages such as obtaining tar-free synthesis gas, high carbon conversion efficiency, and production in high capacities. In addition, there is no limitation to the type of coal to be used. The performance of the entrained flow gasifiers can be examined by simulation programs and design optimization can be performed at a low cost. This study aims to develop a new entrained flow gasifier model for Turkish Lignite (Çan coal) using the Aspen Plus® thermodynamic simulation program and the effects of various parameters on the synthesis gas were investigated by sensitivity analysis.
Keywords: *Gasification, Çan Coal, Entrained Flow Gasifier, Aspen Plus*

Öz

Enerji talebi nedeniyle aşırı fosil yakıt tüketimi, çevreye yayılan CO_2 miktarında artışa neden olmaktadır. Gazlaştırma teknolojisi, CO_2 emisyonuna neden olan kömür gibi fosil yakıtların temiz ve verimli kullanılmasını sağlar. Hava, buhar ve O_2/CO_2 karışımı gazlaştırma atmosferi olarak kullanılabilir. İnert gazların azaltılması (N_2) ve sentez gazında yüksek sıcaklıklarda CO konsantrasyonunun artması yüksek kaliteli gaz elde edilmesine olanak tanır. Ticari gazlaştırıcılar arasında, sürüklemeli gazlaştırıcılarının katransız sentez gazı elde etme, yüksek karbon dönüşüm verimliliği ve yüksek kapasitelerde üretim gibi birçok avantajı bulunmaktadır. Ayrıca, sürüklemeli gazlaştırıcılarda kullanılacak kömür çeşidine bağlı olarak herhangi bir sınırlama yoktur. Sürüklemeli gazlaştırıcılarının performansı genellikle simülasyon programları ile incelenirken, düşük maliyetlerle tasarım ve optimizasyon yapılabilmektedir. Bu çalışmanın amacı Aspen Plus termodinamik simülasyon programını kullanarak Türk Linyitleri (Çan

kömürü) için yeni bir sürüklemeli akış gazlaştırıcı modeli geliştirmektir ve gazlaştırıcıya ait çalışma parametrelerinin sentez gazı üzerindeki etkilerini parametrik çalışma yaparak incelemektir.

Anahtar Kelimeler: *Gazlaştırma, Sürüklemeli Akış Yataklı Gazlaştırıcı, Aspen Plus*

1. Introduction

Energy is essential for maintaining human life. Fossil fuels such as oil, gas, and coal provide about 80 % of the energy demand in our society [1, 17, 29]. Coal is the primary source of energy for developing countries, especially in Turkey. However, the required energy provided by coal causes excessive CO_2 release [18, 41].

Coal gasification is an effective method to reduce environmental and health problems caused by CO_2 emissions [9, 24, 37]. Coal gasification is the process of converting coal into synthesis gas (H_2, CO, CO_2, CH_4, and N_2) with gasification atmosphere such as air, steam, oxygen, carbon dioxide, hydrogen or mixture of agents under high temperature and pressure [4, 30, 39].

Although there is a tendency to classify gasification processes according to the calorific value of the gas produced, it is also possible and more likely to classify according to the reactor type used in the gasification process. Gasification is mainly carried out in three types of reactors: fixed bed gasifiers, fluidized bed gasifiers, and entrained flow bed gasifiers [26, 40].

It is a convenient option to use an entrained flow gasifier to obtain tar-free synthesis gas and to achieve high carbon conversion efficiency with high production capacities [10, 22]. The entrained flow gasifier is the leader in the gasifier market worldwide due to the ease of handling feedstock. Furthermore, since there is no limitation on the type of coal used in entrained flow gasifiers, it is suitable for gasification of cheap and abundant low-rank coals such as lignite and brown coal [15, 16, 45].

Coal can be fed to the gasifier as dry or as slurry [36]. In the entrained flow gasifier, the dense solid or liquid phase particles are dispersed into a moving gaseous medium, whereby the particles are entrained along the bed. This provides a large solid-gas reactive surface area and reduces the diffusion resistance of the gas phase. Thus, chemical reactions between phases can occur rapidly [25]. Small particle size is preferred in entrained flow gasifiers to achieve a high conversion efficiency [19, 38, 44].

Mathematical models and simulations are necessary to understand the behavior of a process and to predict the effect of operating conditions on process performance. They are also cost-efficient and allowing easy analysis of different time-consuming scenarios by using sensitivity analysis [6, 7, 14].

There are many gasification simulators used in chemical engineering processes. One of the most widely used is the Aspen Plus® simulator [35].

Aspen Plus® is an equation-oriented and sequential modular simulation program used to simulate various processes [42] including gasification of coal and biomass-based on mass and energy balance relationships [5, 11, 23].

The aim of this study is to develop a new entrained flow gasifier model for Turkish Lignite (Çan coal) using Aspen Plus®. The effect of operating conditions on the synthesis gas composition such as gasifier pressure and temperature, equivalence ratio, and steam/fuel ratio was investigated by using sensitivity analysis.

2. Material and Method

2.1. Sample

Çan coal used in this study was provided by the Turkish Coal Enterprises Institution. Coal samples were pulverized to the desired particle size of < 250 μm using mortar grinder Retsch RM 200.

Proximate analysis of Çan coal was determined according to ASTM Standard D 5142-04 (Netzsch 409 PC). The ultimate analysis was performed with the test method of ASTM Standard D5373 standards in Advanced Technologies Application and Research Center, Hacettepe University by using LECO brand

Truspec elemental analyzer. Proximate and ultimate characteristics of Çan coal are presented in Table 1.

Table 1. Proximate and ultimate analysis results of Çan coal

Proximate analysis (wt%)	
Ash	41.83
Fixed carbon	26.30
Moisture	3.04
Volatile matter	28.83
Ultimate analysis (wt%)	
Carbon	30.15
Oxygen	60.25
Hydrogen	2.85
Nitrogen	0.69
Sulfur	6.06

2.2. Entrained Bed Gasifier Model

Due to the complex reaction pathways in the entrained flow bed gasifier, some assumptions were made and the main parts of the gasification of coal were taken into consideration.

When the particles of coal take part in an entrained flow bed gasifier, drying, decomposition of volatiles, char and volatile combustion & gasification reactions occur consequentially. The accepted assumptions in the developed entrained flow bed gasifier model are listed below:

- The gasification process is isothermal and steady-state.
- Volatile products of Çan coal after the decomposition zone majorly include H_2, CH_4, H_2O, CO_2, and CO [3, 21, 33, 34].
- Whole reactions reach the chemical equilibrium in the gasification process.
- Char includes only ash and carbon.
- Ash is regarded as inert and does not affect the reactions.

2.2.1. Aspen Plus® Model

The development of the entrained bed gasifier model was performed in Aspen Plus® V11 software. DCOALIGT was used for coal density calculations and HCOALGEN was used for enthalpy calculations. For accurate thermodynamic calculations in the gasification process, RK-SOAVE was determined as the thermodynamic method and STEAM-TA was preferred as the free-water method. The main flowsheet of the entrained bed gasifier model is given in Figure 1.

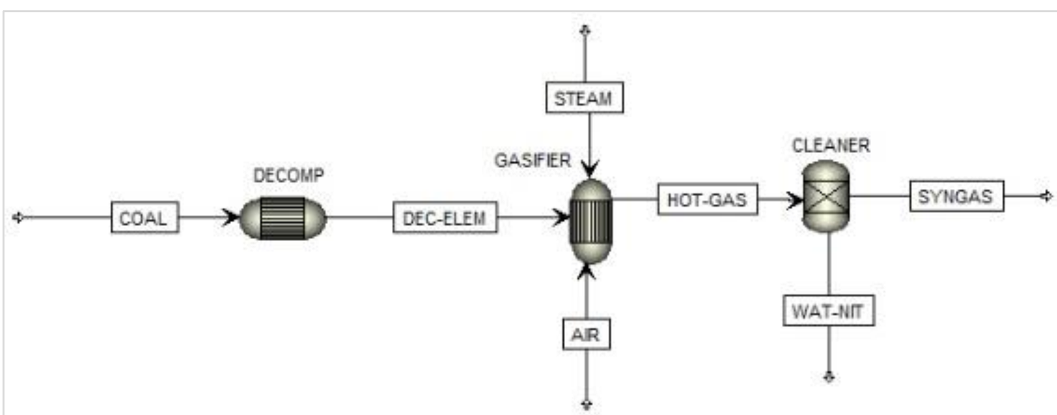

Figure 1. Aspen Plus® flowsheet of the entrained bed gasifier model.

During the development process of the entrained bed gasifier model, one yield reactor (DECOMP), one Gibbs reactor (GASIFIER), and one separator were used. The yield reactor called “DECOMP” decomposes the coal into its subcomponents. Since coal is a "non-conventional" solid structure, it must be converted to a "conventional" structure in order to simulate reactions and execute other thermodynamic calculations. The decomposition of coal into the chemicals in the "DECOMP" reactor is calculated using proximate and ultimate analysis results of Çan coal, which are defined as input variables to the "COAL" stream. Afterward, the coal feed flows into the "GASIFIER" reactor, where gasification reactions take place. "GASIFIER" is a Gibbs reactor, reacts components under defined temperature and pressure and produces possible chemical components by minimizing Gibbs free energy. In addition to coal, air and steam are also supplied to the "GASIFIER" reactor and are named "AIR" and "STEAM", respectively. "HOT-GAS" produced as a result of gasification and flows into the separator named "CLEANER". In this separator, undesired components such as water and nitrogen in the "HOT-GAS" are separated and adjusted to ensure that the "SYNGAS" flow is on the desired basis in this study. Table 2. represents a brief explanation of the blocks used in the model.

Table 2. Description of blocks in the gasification model.

Block Name Aspen ID	**Description**
DECOMP RYIELD	Decomposes coal (non-conventional solid) into conventional components using calculator block
GASIFIER RGIBBS	Minimizes the Gibbs free energy and simulates whole gasification reactions
CLEANER SEP	Separator of the H_2O and N_2

3. Results

3.1. Model Validation

To validate the newly developed entrained bed gasifier model developed in Aspen Plus®, the published experimental data from literature [27, 43] including feedstock characteristics, operating conditions and syngas compositions were used. Experimental parameters from the literature can be seen in Table 3.

Table 3. Operating Conditions of the gasifier taken from the literature

Reference [27]	**Literature**	**Model**
Temperature	1300 °C	1300 °C
Gasifier Pressure	2 MPa	2 MPa
Coal Feed Rate	1503 kg/h	1503 kg/h
Oxygen Feed Rate	753 N m^3/h	753 N m^3/h
Steam Feed Rate	233 kg/h	233 kg/h
Reference [43]	**Literature**	**Model**
Temperature	1217 °C	1217 °C
Gasifier Pressure	1 bar	1 bar
Coal Feed Rate	478 kg/h	478 kg/h
Equivalence Ratio	0.5	0.5

As shown in Figure 2 and Figure 3, the results of the newly developed entrained flow bed (EFB) gasifier model successfully shows similarity with experimental studies when they are run under the same operating conditions and with the same input variables. The Gibbs reactor used in the simulation program assumes that reactions occur rapidly and reach chemical equilibrium which makes it easier to simulate EFB gasifiers.

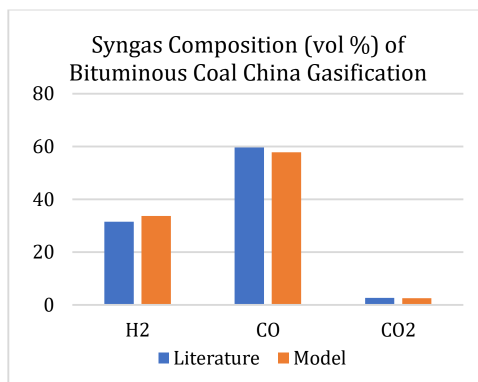

Figure 2. Comparison of syngas composition between literature and model

The reason that EFBs operate at high temperatures and reactions occur very quickly, they produce similar results to those produced by the Gibbs reactor in the model.

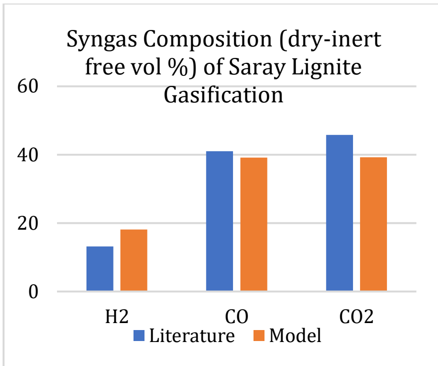

Figure 3. Comparison of syngas composition between literature and model

A low fraction of heavy hydrocarbons and tar produced in EFBs are present in trace amounts in the syngas as in the Gibbs reactor. In addition, the design parameters of the reactor vary depending on the type of coal to be used, but the new model can be used for different types of coal; these results in the model achieving different acceptable results during the gasification of different coals.

3.2. Effect of Gasifier Temperature

The temperature has a considerable effect on the equilibrium state of reactions that affects the syngas composition. The gasification temperature in the Aspen Plus® model was changed between 1000 °C and 1600 °C and the change in syngas composition was given in Figure 4. The steam/coal ratio and equivalence ratio were kept constant at 1.0 – 2.0 and 0.2 – 0.3, respectively.

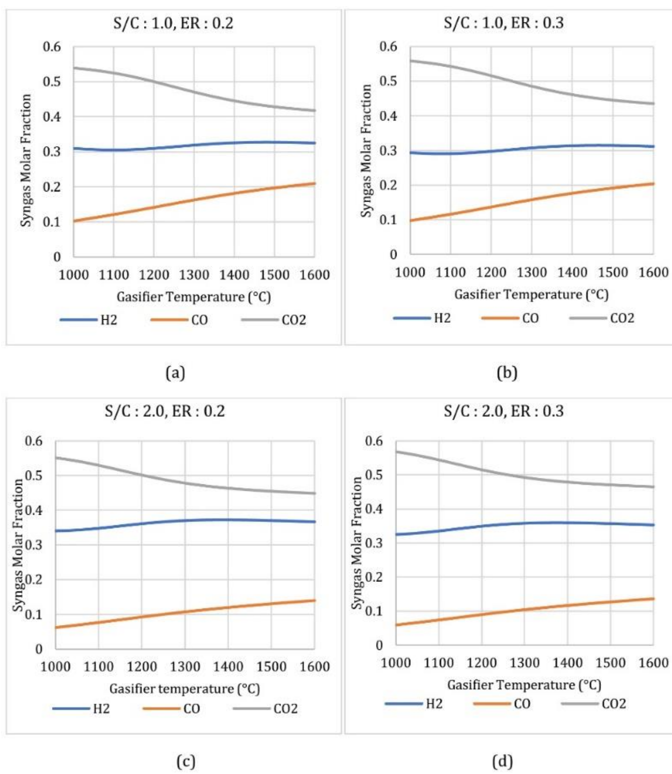

Figure 4. Effect of gasifier temperature on syngas composition (a) Steam/Coal : 1.0, ER : 0.2; (b) Steam/Coal : 1.0, ER : 0.3; (c) Steam/Coal : 2.0, ER : 0.2; (d) Steam/Coal : 2.0, ER : 0.3

One of the behaviors can be clearly seen in Figure 4 is that as the gasifier temperature increases, the CO concentration increases as well, but the CO_2 concentration decreases. This can be explained by the driving forward of the Boudouard reaction. Hydrogen fraction increases until a certain temperature and then it starts to decrease. As mentioned above, the concentration of favorable chemicals increases at high temperatures. Furthermore, as the ER increased, CO_2 fraction was reaching higher values and CO fraction was lowering oppositely. This can be explained by the formation of oxidized products due to the increased amount of oxidant in the reactor. In addition, when a higher steam/coal ratio exists in the gasifier, a higher fraction of H_2 and a lower fraction of CO was observed. The increasing amount of H_2O drives the water-gas shift reaction forward and increases steam gasification reactions.

3.3. Effect of Gasifier Pressure

The gasifier pressure significantly affects the dynamic equilibrium states of the gasification reactions. The gasification pressure was changed between 1 bar and 20 bar and the syngas composition was examined that is given in Figure 5. As seen in Figure 5, the steam/coal ratio and equivalence ratio were kept constant at 1.0 – 2.0 and 0.2 – 0.3, respectively.

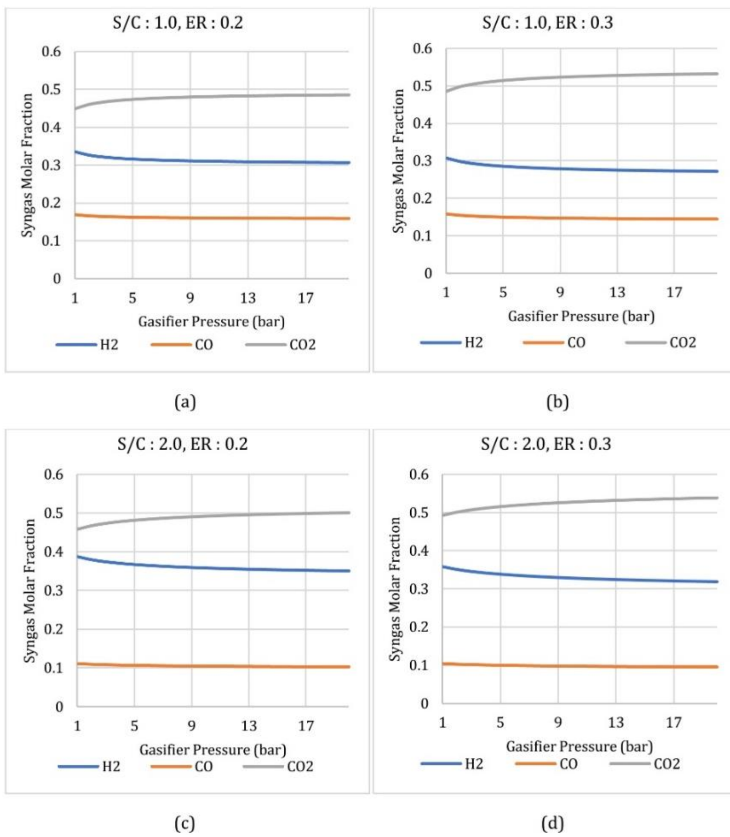

Figure 5. Effect of gasifier pressure on syngas composition. (a) Steam/Coal : 1.0, ER : 0.2; (b) Steam/Coal : 1.0, ER : 0.3; (c) Steam/Coal : 2.0, ER : 0.2; (d) Steam/Coal : 2.0, ER : 0.3

According to the Le Chatelier Principle, when a dynamic equilibrium is changed by a disturbing factor, the system moves in a direction to minimize this effect. Since the gasification reactions are also equilibrium reactions, the gasifier pressure changes the direction of the reactions and the composition of synthesis gas. As the gasifier pressure increases, the concentrations of H_2 and CO gases decrease, and the evolution of CO_2 gas increases. The decrease in CO gas formation and an increase in CO_2 gas concentration can be explained by the Boudouard reaction. The increase of ER boosts the complete combustion reactions which can be seen as an increase in the amount of CO_2 in the syngas. Moreover, the higher steam/coal ratio appears to be a high fraction of H_2 gas in the syngas.

3.4. Effect of Equivalence Ratio

The equivalence ratio (ER) is defined as the ratio of actual air-fuel ratio to the stoichiometric air-fuel ratio; thus, the ER has an important effect on the syngas composition. In this study, the equivalence ratio was ranged from 0.1 to 0.5, and the gasifier temperature was constant at 1300 °C. The effect of ER on syngas composition is given in Figure 6.

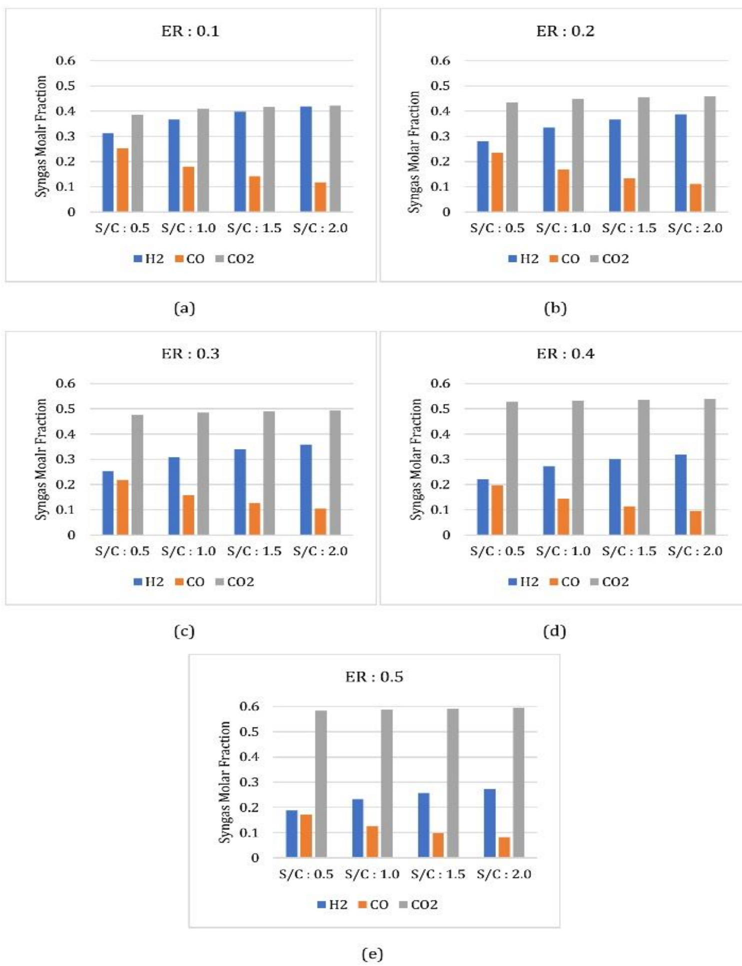

Figure 6. Effect of equivalence ratio on syngas composition (a) ER : 0.1; (b) ER : 0.2; (c) ER : 0.3; (d) ER : 0.4; (e) ER : 0.5

As the equivalence ratio increases in the system, the H_2 and CO concentrations decrease, but the CO_2 concentration increases. An increase in ER leads complete combustion reaction which reduces favorable chemicals in the syngas. Therefore, a rapid increase in CO_2 concentration is observed. Similar behaviors were observed by other researchers [12, 28].

3.5. Effect of Steam/Coal Ratio

The increase in S/C ratio promotes the evolved H_2 gas in the syngas because of the heterogeneous char steam gasification reactions [8, 20, 31]. Figure 7 demonstrates the syngas composition while the S/C ratio varies between 0.25 – 1.50. The gasifier temperature was kept constant at 1300 °C and the ER ranged from 0.1 to 0.5.

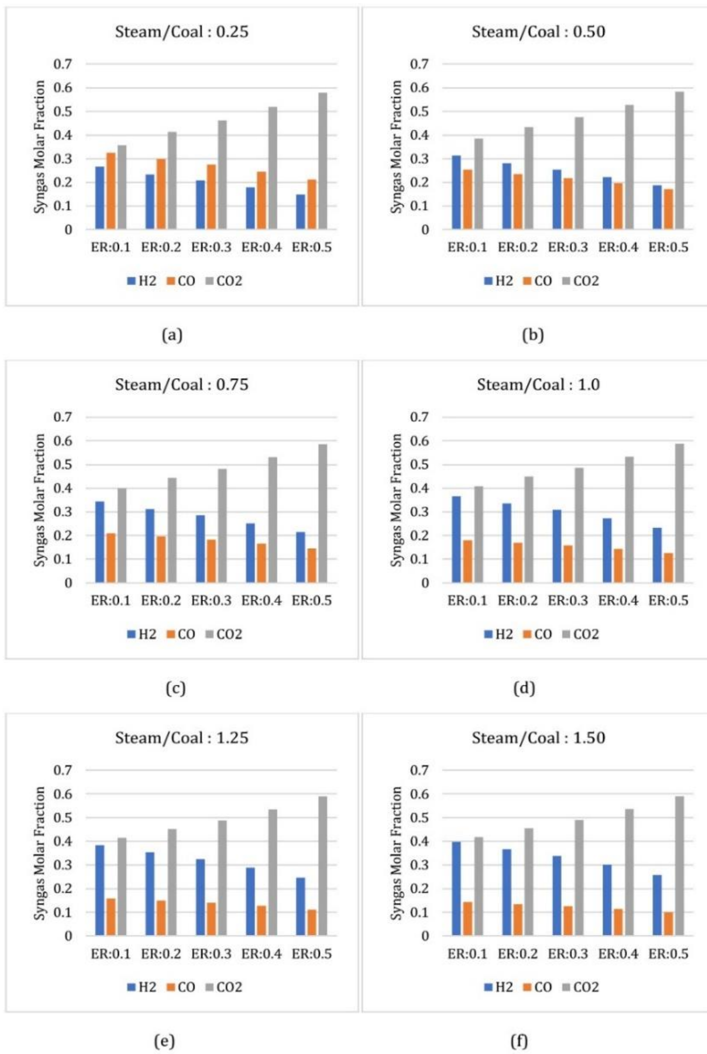

Figure 7. Effect of S/C ratio on syngas composition (a) Steam/Coal : 0.25; (b) Steam/Coal : 0.50; (c) Steam/Coal : 0.75; (d) Steam/Coal : 1.0; (e) Steam/Coal : 1.25; (f) Steam/Coal : 1.50

As can be seen in Figure 7, the increasing attitude of H_2O drives the water-gas shift reaction to the products side which provides a higher fraction of H_2 and CO_2. The reducing attitude of CO fraction can also be explained by the water-gas shift reaction. These behaviors were observed by other authors [2, 13, 32].

4. Discussion and Conclusion

In this study, an entrained bed gasifier model was developed in Aspen Plus® software by using a thermodynamic equilibrium model. Before examining the gasification performances of Turkish coal which is Çan Lignite, the model was validated by using the operating conditions and syngas compositions of the coals gasified experimentally in the entrained bed reactor from the literature. Tiny particle size and high-temperature requirement during the gasification process in entrained bed gasifiers make the reactions rapid thus, gasification reactions reach chemical equilibrium mostly. Likewise, the Gibbs reactor used in the model performs reactions assuming that the components have reached chemical equilibrium. The results show that the syngas compositions in the literature and the syngas compositions produced by the model are similar to an acceptable margin of error. Sensitivity analysis can be performed on the model to determine the appropriate operating conditions. As a result of this study, it has been seen that the entrained bed gasifier can be an options for the gasification of Turkish Lignites.

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