



## PREDICTION OF UNDERGROUND COAL GASIFICATION PERFORMANCE OF TURKISH LIGNITE RESERVES USING STOICHIOMETRIC EQUILIBRIUM MODEL

Engin Deniz CANBAZ\* and Mesut GÜR\*\*

\*Istanbul Technical University, Department of Mechanical Engineering  
34437 Beyoğlu, İstanbul, canbaze@itu.edu.tr, ORCID: 0000-0002-6287-8770

\*\*Istanbul Technical University, Department of Mechanical Engineering  
34437 Beyoğlu, İstanbul, mesutgur@itu.edu.tr, ORCID: 0000-0002-0407-0298

(Geliş Tarihi: 20.06.2019, Kabul Tarihi: 13.04.2020)

**Abstract:** Underground coal gasification (UCG) is a coal conversion process that enables the utilization of coal reserves in-situ, and it is an alternative technique to conventional mining methods. Previous experimental studies showed that UCG is a suitable method for the usage of low-rank coal or lignite reserves, which have the major part in the Turkish coal reserves. In this study, a thermochemical equilibrium model of UCG process is developed to predict syngas composition and to compare UCG-performance of the selected lignite reserves in Turkey. The lignite sites are chosen according to the described UCG site selection criteria. The equilibrium model consists of gasification reactions and water-gas shift reaction and it considers the effect of the drying process. The model is validated using the results of the lab-scale experimental UCG study. The predictions are made for both oxygen and steam-gasification processes. Results show that the lignite reserves which have high moisture content but low carbon content are suitable for hydrogen-rich syngas production and hydrogen production capabilities of all reserves can be enhanced significantly by the additional steam supply as the gasification agent.

**Keywords:** Underground Coal Gasification, Equilibrium Model, Lignite

## TÜRK LİNYİTLERİNİN YERALTINDA KÖMÜR GAZLAŞTIRMA PERFORMANSLARININ STOKİOMETRİK DENGE MODELİ İLE BELİRLENMESİ

**Özet:** Yeraltında kömür gazlaştırma (YKG) işlemi, kömürlerin yeraltındayken işlenmesine olanak sağlayan ve bu yönüyle, geleneksel madencilik yöntemlerine alternatif oluşturan bir kömür işleme prosesidir. Son deneysel çalışmalar ile YKG işleminin, ülkemizde de yüksek miktarda bulunan, düşük kaliteli kömürlere uygulanması durumunda da etkili olduğu ortaya konmuştur. Bu çalışma kapsamında ise, YKG işlemi sonucu üretilen sentez gazın içeriğini tahmin edebilecek bir termodinamik denge modeli oluşturulmuş ve oluşturulan model düşük kalitedeki kömür rezervlerinden üretebilecek sentez gazının özelliklerinin tahmini için kullanılmıştır. Denge modeli, gazlaştırma reaksiyonlarının ve su-gazı dönüşümü reaksiyonunun etkisini dikkate almakta ve kömür kuruması sonucu ortaya çıkan su buharının yapay gaz üzerindeki etkisini belirleyebilmektedir. Oluşturulan denge modeli, literatürde yer alan laboratuvar ölçekli deneysel YKG çalışmasının sonuçları ile doğrulanmıştır. Daha sonrasında ülkemizdeki linyit rezervlerinden YKG işlemi için uygun olduğu belirlenen rezervler, modelde girdi olarak kullanılmış ve rezervler için elde edilen YKG performans çıktıları birbirleriyle karşılaştırılmıştır. Performans analizi için her rezervin oksijen ve buhar ile gazlaştırma çıktıları incelenmiştir. Değerlendirme sonucu yüksek nem ve düşük karbon içeriğine sahip linyitlerin yüksek hidrojen yüzdeli sentez gaz üretimine elverişli olduğu, gazlaştırma ajanı olarak buhar beslemesi yapılması halinde ise tüm rezervlerin hidrojen üretim kapasitelerinin artırılabilceği belirlenmiştir.

**Anahtar Kelimeler:** Yeraltında Kömür Gazlaştırma, Denge Modeli, Linyit

### NOMENCLATURE

$C_{coal}$	Mole fraction of carbon in coal [-]	$n_{agent}$	Amount of gasification agent supplied to the system [mol]
$C_{agent}$	Mole fraction of carbon in gasification agent supplied [-]	$n_{coal}$	Amount of coal consumed by the system [mol]
$H_{coal}$	Mole fraction of hydrogen in coal [-]	$n_i$	Amount of each species in syngas [mol]
$H_{agent}$	Mole fraction of hydrogen in gasification agent supplied [-]	$n_{total}$	Total amount of the produced syngas [mol]
$K$	Equilibrium constant	$O_{coal}$	Mole fraction of oxygen in coal [-]
$N_{coal}$	Mole fraction of nitrogen in coal [-]	$O_{agent}$	Mole fraction of oxygen in gasification agent supplied [-]
$N_{agent}$	Mole fraction of nitrogen in gasification agent supplied [-]	$p_i$	Partial pressure of each compound in syngas [atm]
		$p_{total}$	Total pressure of the produced syngas [atm]
		$R_a$	Coal to agent (consumed) ratio [mol/mol]

$R_c$	Moisture to carbon ratio [kg/kg]
$T$	Equilibrium temperature [K]
$y$	Amount of change of species due to drying [mol]

## INTRODUCTION

The last estimations state that Turkey has 17.480 billion tons of lignite reserves, which is the largest share amongst the domestic fossil fuel sources (MTA, 2020). Unfortunately, approximately 21% of the lignite reserves have calorific value above 10.5 MJ/kg. This situation makes them unfeasible to utilize in energy production compared to imported energy sources. The percentage of domestic coal in total energy consumption proves this point. In 2013, domestic coal production covered only 12.8% of the total energy consumption, while the imported sources covered 73.4% of the total energy consumption (TKİ, 2014). Moreover, the decrease in the number of coal reserves that are available for feasible open-pit operations and concerns about the negative effects of coal on the environment hinders the competitiveness of domestic lignite reserves. However, recent developments in clean coal technologies and, also, growing energy-security problem in the world draw attention on the domestic coal reserves and possible alternative exploitation methods.

Underground coal gasification is one of the alternative coal technologies that can be an option to utilize the lignite reserves. Many experimental studies have shown the efficiency of the UCG process when it is applied to low-quality coals (Daggupati et al., 2010, Gür et al., 2017, Kapusta and Wiatowski, 2016, Stańczyk et al., 2011, Stańczyk et al., 2010). In the UCG process, the first phase is drilling injection and production wells into the coal seam that supply gasification agents and collect the syngas, respectively. Then, a connection needs to be established between those two wells to allow gas flow inside the seam. This connection is named as gasification channel, and that is the place where the chemical reactions and gas flow occur. In the UCG process, coal is converted into syngas in-situ via exothermic combustion and endothermic gasification reactions (Reactions 1-8). Reaction 4 is the water-gas shift reaction, and it is an essential reaction that balances  $H_2/CO$  ratio in syngas as the temperature and pressure changes during the process. Therefore, it is vital to have when modeling the gasification process. The produced syngas consists of  $CO$ ,  $H_2$ ,  $CO_2$ ,  $CH_4$  and other components and it can be utilized in electricity generation, liquid fuel production via Fischer-Tropsch synthesis, hydrogen production for fuel cells and in other chemical processes (Pei et al., 2016, Shafirovich & Varma, 2009, Shoko et al., 2006).

Syngas composition depends on many conditions such as gasification agent choice, coal properties, seam properties, gasifier design, etc. (Perkins, 2018a). For example, agent selection directly affects the process and syngas production properties. Air usage as the gasification agent decreases the calorific value of the produced syngas and temperature levels inside the combustion zone, but it

significantly lowers the operational costs compared to pure oxygen feed (Perkins et al., 2016, Swanson et al., 2010).

*Homogeneous reactions:*

*Oxidation reactions:*



*Water-gas shift reaction:*



*Heterogeneous reactions:*

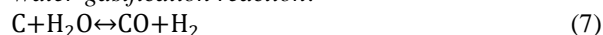
*Oxidation reaction:*



*Boudouard reaction:*



*Water-gasification reaction:*



*Methanation reaction:*



Coal properties also affect the syngas composition. In order to specify syngas production capabilities of specific coal depending on its properties, experimental and theoretical studies can be conducted. In lab-scale studies, ex-situ UCG reactors, where coal block sample and surrounding strata are placed, are used to simulate underground conditions and to test different gasification agent schemes that optimum process outputs can be achieved with (Fallahi et al., 2019, Gür et al., 2017). Additionally, highly valuable temperature measurements inside the reactor can be obtained during the ex-situ studies, which is not an easy process during an in-situ operation (Stańczyk et al., 2010).

Theoretical studies of UCG consist of mathematical models that include specific equations and relations representing the process. They can be divided into two groups: kinetic models and equilibrium models (Żogała, 2014a). The kinetic models use the kinetic reaction models, such as Arrhenius type equations, to predict mass conversion rates. The kinetic models of UCG are generally time-dependent and they are able to determine the gas properties in each phase of the process (Jowkar et al., 2018, Samdani et al., 2016, Żogała, 2014b). Integration of kinetic models with momentum, heat, and mass transport equations creates computational fluid dynamic (CFD) models which can calculate the spatial and temporal distribution of each component and the coal conversion at the same time (Perkins and Sahajwalla, 2007, Perkins and Sahajwalla, 2008, Sarraf Shirazi et al., 2013, Żogała and Janoszek, 2015).

Equilibrium models, on the other hand, relies on the thermochemical equilibrium principle. This type of mathematical model determines the equilibrium chemical composition of a specific amount of coal and gasification agent, which are considered as contained in an arbitrary control volume at the predetermined temperature and pressure. There are two different approaches to determine

the equilibrium point. The first one is the non-stoichiometric model that calculates the gas composition in the equilibrium state by minimizing the Gibbs free energy of the mixture (Altafini et al., 2003, Jarungthammachote and Dutta, 2008, Li et al., 2001). The second one is the stoichiometric model that uses equilibrium constants of the related chemical reactions to determine the composition while satisfying the mass conservation (Watkinson et al., 1991).

In this study, a two-stage stoichiometric equilibrium model, which contains gasification reactions (Reactions 6, 7, and 8) and water-gas shift reaction (Reaction 4), is used to evaluate the possible syngas composition of the chosen lignite sites in case of UCG application. The input parameters for the model are the elemental composition and moisture content of the selected lignite samples, the gasification agent composition, and the reaction equilibrium constants at the specific operation temperature. The selection of lignite sites has been made according to the selection criteria that are based on the suggestions made in the previous studies (Klimenko, 2009, Pana, 2009, Perkins, 2018a, 2018b, Shafirovich and Varma, 2009, Tunç, 2015). Eventually, nine different lignite sites have been chosen for the study. Pure oxygen, steam, and steam-oxygen mixture are supplied as the gasification agents. Results show that the moisture content of the coal directly increases the hydrogen content in the syngas when oxygen is supplied as the gasification agent. However, it does not affect the hydrogen content of the product gas when steam is supplied. Results also show that Edirköy lignite site has the greatest hydrogen production potential which is relevant to its higher moisture content and lower carbon content. Also, comparison of predicted consumption rate of coal and gasification agent indicates that UCG process can be conducted more efficiently in Edirköy and Eskihisar reserves.

## THE EQUILIBRIUM MODEL

The developed equilibrium model consists of two stages as shown in Figure 1, and it is based on mass conservation and equilibrium constants of the reactions as mentioned earlier. Conservation of carbon (C), hydrogen (H), oxygen (O), nitrogen (N) elements are taken into account for mass conservation. The model assumes that all those elements contained in coal and in gasification agents must be in the product gas after conversion in the form of carbon dioxide (CO<sub>2</sub>), carbon monoxide (CO), water (H<sub>2</sub>O), methane (CH<sub>4</sub>), hydrogen (H<sub>2</sub>), and nitrogen (N<sub>2</sub>) to satisfy the mass continuity. While satisfying the continuity, reaction equilibrium constants determine the composition of the product gas (syngas). Then, the equilibrium of water-gas

shift reaction, which directly affects the carbon monoxide and hydrogen ratio in the syngas as the temperature changes, determines the final composition with H<sub>2</sub>O addition that comes from coal drying.

As explained in Figure 1, in the first stage, it is assumed that coal is stationed in an arbitrary control volume. Then, gasification agents are added to the volume. At the end of the process, it is assumed that all gasification agents and coal contents are converted into 1 mole of syngas. In other words, neither coal nor gasification agents remain in the control volume. Therefore, the total number of moles,  $n_{total}$ , is equal to 1. This assumption results in two new unknowns ( $n_{agent}$ ,  $n_{coal}$ ) besides the molar fractions of syngas components. The amount of the consumed coal ( $n_{coal}$ ) and supplied gasification agent ( $n_{agent}$ ) need to be known to construct the mass balance and to specify the syngas composition. With the help of the mass conservation equations and equilibrium relations of Reaction 6, 7, and 8, the syngas composition and the amount of consumed gasification agent and coal are calculated.

It is assumed that gasification occurs at the atmospheric pressure ( $p_{total} = 1$  atm), and the end product is an ideal-gas mixture. Therefore, the molar fractions of the components in syngas can be expressed as the partial pressure values of each component. By applying a mass conservation law for the first gasification stage, it yields 8 equations (Equations 9-16) and 8 unknowns ( $p_{CO_2}$ ,  $p_{CO}$ ,  $p_{CH_4}$ ,  $p_{H_2O}$ ,  $p_{H_2}$ ,  $p_{N_2}$ ,  $n_{agent}$ ,  $n_{coal}$ ). The equilibrium constants of the gasification reactions are calculated using the temperature-dependent relations given below (Cempa-Balewicz et al., 2013) (Equation 17, 18, and 19).

$$(n_{agent}C_{agent} + n_{coal}C_{coal})/n_{total} = (p_{CO_2} + p_{CO} + p_{CH_4})/p_{total} \quad (9)$$

$$(n_{agent}H_{agent} + n_{coal}H_{coal})/n_{total} = (2p_{H_2O} + 2p_{H_2} + 4p_{CH_4})/p_{total} \quad (10)$$

$$(n_{agent}O_{agent} + n_{coal}O_{coal})/n_{total} = (2p_{CO_2} + p_{CO} + p_{H_2O})/p_{total} \quad (11)$$

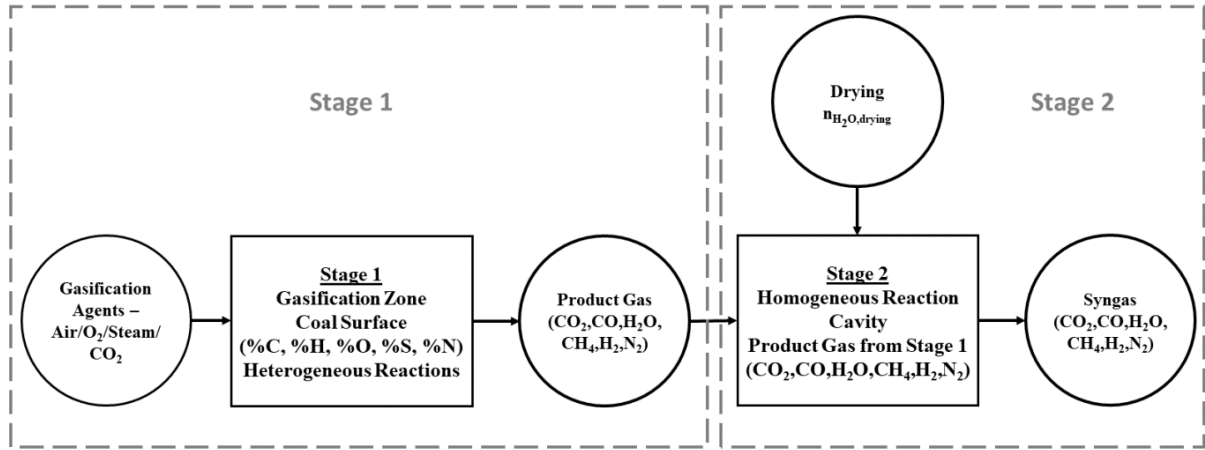
$$(n_{agent}N_{agent} + n_{coal}N_{coal})/n_{total} = 2p_{N_2}/p_{total} \quad (12)$$

$$K_{r6} = \frac{p_{CO}^2}{p_{CO_2}} \quad (13)$$

$$K_{r7} = \frac{p_{CO}p_{H_2}}{p_{H_2O}} \quad (14)$$

$$K_{r8} = \frac{p_{CH_4}}{p_{H_2}^2} \quad (15)$$

$$p_{CO_2} + p_{CO} + p_{H_2O} + p_{CH_4} + p_{H_2} + p_{N_2} = 1 \quad (16)$$



**Figure 1.** Flow scheme of the two-stage UCG equilibrium model.

$$\log K_{r6} = 3.2673 - 8820.7T^{-1} - 1.2087 \times 10^{-3}T + 0.1537 \times 10^{-6}T^2 + 2.2954 \log T \quad (17)$$

$$\log K_{r7} = 0.8255 \times 10^{-6}T^2 + 14.5158 \log T - 4825.986T^{-1} - 5.6711 \times 10^{-3}T - 33.4578 \quad (18)$$

$$\log K_{r8} = 4662.8T^{-1} - 2.0959 \times 10^{-3}T + 0.3863 \times 10^{-6}T^2 + 3.0343 \log T - 13.0636 \quad (19)$$

In the second gasification stage of the equilibrium model, the effect of the additional moisture content on the syngas composition is calculated using the equilibrium relation of the water-gas shift reaction. This stage intends to determine the change of syngas composition as the product gas advances in the gasification channel and interacts with the unaltered coal, which has higher moisture content.

$$n = n_{CO_2} + n_{CO} + n_{CH_4} + n_{H_2} + n_{H_2O} + n_{H_2O,drying} + n_{N_2} \quad (20)$$

$$K_{r4} = \frac{(n_{CO_2} + \gamma)(n_{H_2} + \gamma)}{(n_{CO} - \gamma)(n_{H_2O} + n_{H_2O,drying} - \gamma)} \quad (21)$$

$$\log K_{r4} = 3994.7T^{-1} - 4.4624 \times 10^{-3}T + 0.6718 \times 10^{-6}T^2 + 12.2203 \log T - 36.7251 \quad (22)$$

Equation 20 calculates the total number of moles of change after water vapor addition that comes from drying of the unaltered coal. At the end of the first stage, there was 1 mole of product gas, as previously mentioned. Additional water vapor changes the total number of moles in the product and shifts the equilibrium. The final composition is determined by Equation 21, which specifies the equilibrium point for water-gas shift reaction at 1 atm. The equilibrium constant is calculated from Equation 22 (Cempa-Balewicz et al., 2013). Other details about the model and calculation procedure are given here (Cempa-Balewicz et al., 2013; Gür et al., 2018).

## VALIDATION STUDY

For the validation study, the results of experimental UCG study conducted with Malkara/Pirinççeşme lignite are used. That experiment was conducted in an ex-situ UCG experimental setup built in Mechanical Engineering Faculty of Istanbul Technical University. Details about

the experiment and the setup were given in here (Gür et al., 2017).

Before the experiment, coal blocks, that were extracted from the mining site in Pirinççeşme, stayed in the UCG laboratory in open to atmospheric conditions. This situation led to loss of humidity and partially drying of the samples. Therefore, dry in air analysis results of Pirinççeşme is used as the inputs in the equilibrium model. Proximate and ultimate analysis results of Pirinççeşme lignite are listed in Table 1.

**Table 1.** Analysis results of Pirinççeşme lignite sample.

	Tekirdağ/Malkara Pirinççeşme	Dry in Air (wt. %)
Proximate Analysis	Moisture	15.27
	Ash	20.33
	Volatiles	32.55
	Fixed Carbon	31.86
Ultimate Analysis	C	48.32
	H	3.38
	O	6.91
	N	1.22
	S	4.58

For the comparison, the syngas composition results from the oxygen-gasification experiment are averaged. Then, syngas composition obtained from the equilibrium model is compared, and similar results are observed at 600 °C. That temperature level seems to be attainable since the temperature measurements from the reference study shows the highest temperature of 1000 °C during the process, which can be considered as the temperature level inside the combustion zone. The gasification zone follows the combustion zone, and temperature level drops toward the unreacted parts of the coal. The results are given in Table 2. CO<sub>2</sub>, CO, and H<sub>2</sub> percentage predictions are in good agreement with the experimental data but the model poorly estimates CH<sub>4</sub> percentage. But this situation is ignored because of the low percentage of methane in the product gas.

**Table 2.** Comparison of experimental and theoretical results that validates the equilibrium model.

Gasification Agent Equilibrium Temperature Results	Oxygen	
	600 °C	
	Experimental (Gür et al., 2017)	Equilibrium Model
CO%	21.0	21.4
H <sub>2</sub> %	23.9	26.5
CH <sub>4</sub> %	5.8	1.2
CO <sub>2</sub> %	49.1	50.7

## THE SELECTION CRITERIA

Underground coal gasification is a transient thermo-chemical process. It depends on many parameters such as coal properties, depth of the coal to be gasified, geological properties and presence of aquifers around the coal seam, supply rate of gasification agents, dimensions of the gasification channel, etc. Early UCG trials have shown the need to choose the correct UCG site for efficient operation, as well as the selection of the appropriate coal for the process (Sarhosis et al., 2017).

The specific conditions of the coal and its reservoir condition must be considered to choose an appropriate UCG site. First of all, the rank of coal is an important aspect. High-rank coals are not suitable for the UCG process due to low reactivity and sudden termination of

the process because of agglomeration that occurs at high temperatures. Coals with high volatile matter tend to have higher reactivity. Moisture content is also essential to have a high hydrogen production rate. Another important aspect is the thickness of the coal seam. The thickness of the coal seam should be in between 2 m and 15 m (Shafirovich and Varma, 2009). The permeability of the coal is the key factor when establishing the connection between injection and the production wells. High-permeability makes the connection between the wells easier. On the other hand, high-permeability leads to gas losses and contaminant leakage from the reactor to the surrounding strata and the surface. Coals surrounded by water-saturated rocks that have low-permeability should be chosen to avoid losses (Sarhosis et al., 2017).

In case of transportation, the UCG site needs to be accessible for the equipment transfer and the installations. Usually, the produced gas is utilized near the production site to decrease the costs. Therefore, surface conditions must be appropriate to build the syngas utilization facilities.

In light of the factors mentioned above, nine lignite reserves were selected in Turkey. Their proximate and ultimate analysis results are given in Table 3. The other details on the selection of the reserves are explained here (Tunç, 2015).

**Table 3.** Proximate and ultimate analysis results of the selected lignite sites.

Ref.	Location	Proximate Analysis (wt. %)				Ultimate Analysis (wt. %)				
		Moisture	Ash	Volatiles	Fixed Carbon	C	H	O	N	S
Gür et al., 2016	Pirinççeşme-Malkara Tekirdağ	25.17	17.95	28.47	28.14	42.66	2.99	6.10	1.08	4.05
	Çobanköy-Seyitömer Kütahya	40.81	8.77	25.48	24.94	34.05	2.49	10.33	1.21	2.34
	Ömerler-Tunçbilek Kütahya	14.96	26.92	26.58	31.54	41.21	2.82	10.17	1.42	2.50
Tuncalı et al., 2002	Eskihisar-Yatağan Muğla	39.04	14.21	27.32	19.43	30.55	2.42	11.57	1.16	1.05
	Himmetoğlu-Göynük Bolu	30.86	11.72	28.45	28.97	34.24	3.15	18.47	0.96	0.60
	Harmanalan-Keles Bursa	37.94	19.84	22.92	19.30	28.61	2.35	9.67	0.32	1.27
	Edirköy-Saray Tekirdağ	43.59	13.91	23.11	19.39	26.45	2.34	9.01	0.42	4.28
	Eynez-Soma Manisa	13.56	13.43	32.86	40.15	51.60	3.89	15.51	1.48	0.53
	Işıklar-Soma Manisa	11.17	24.32	33.06	31.45	44.03	3.53	16.16	0.47	0.32

## RESULTS & DISCUSSION

Using the developed stoichiometric equilibrium model, the pure oxygen supply for the reserves is discussed as the first case. Figure 2 presents the syngas compositions calculated for each reserve by the model. These results were obtained at 600 °C, which was the validation temperature of the model, as explained earlier in the validation study section. Edirköy stands out as it had the highest hydrogen content with a value of 49.18%. High moisture content (Table 3) of Edirköy reserve led to relatively high hydrogen production. High hydrogen percentage in syngas was also seen in the results of Eskihişar and Harmanalan reserves. The hydrogen percentages of the Eskihişar and Harmanalan lignites were calculated as 45.43% and 44.73%, respectively. It was an expected result as they also have relatively high moisture content. Although Çobanköy lignite reserve has a high moisture content, its higher carbon content than the reserves mentioned above makes the hydrogen percentage in the produced syngas lower and carbon dioxide percentage higher.

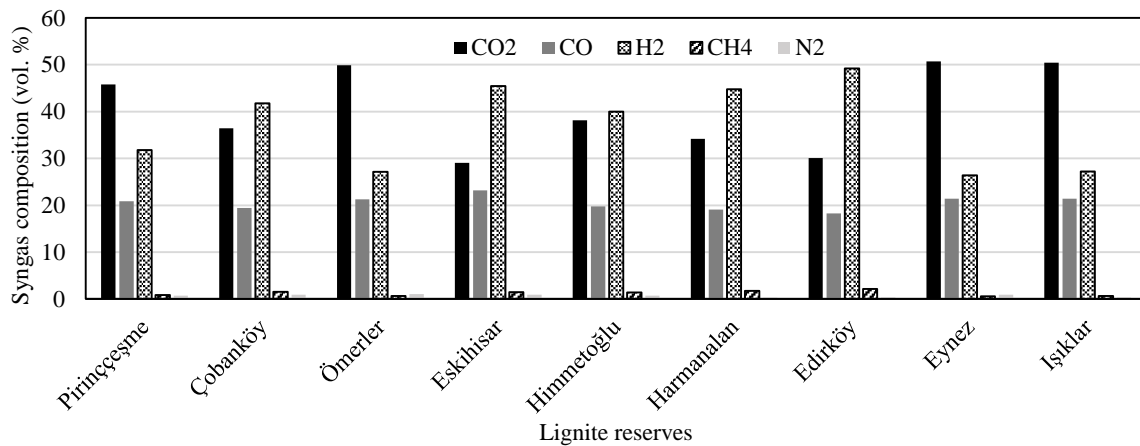


Figure 2. Resulted syngas compositions from the selected lignite reserves in case of oxygen supply.

Even though the higher moisture ratio led to an increase in the hydrogen production in the simulation, it is hard to expect hydrogen-rich syngas production from these reserves in reality. High moisture ratio decreases the reactivity of coal, and it delays the ignition of coal and the process development by weakening the heat accumulation and forming a film on the coal surface that inhibits O<sub>2</sub> transfer and reactions (Xuyao et al., 2011).

The predicted CO ratio in syngas was almost the same for all reserves, around 20%, but Eskihişar lignite reserve had the highest percentage with 23.17%. In case of CO<sub>2</sub> production, the reserves with higher carbon content, such as Ömerler, Eynez, and Işıklar, resulted in carbon dioxide of 50%.

For the oxygen supply case, a new variable,  $R_a$ , was defined to show how efficient the supplied gasification agent was used.  $R_a$  is the ratio of consumed coal to consumed gasification agents which were determined by the equilibrium model. Since the consumed amount of

coal is hard to determine in the UCG process, defining a ratio that can give a prediction about the coal consumption based on the supplied amount of gasification agent is highly valuable. The relation for the new variable is given below.

$$R_a = n_{coal}/n_{agent} \quad (23)$$

Here,  $n_{coal}$  is the amount of coal consumed in the process to produce 1 mole of syngas, and it is an unknown which was calculated by the equilibrium model.  $n_{agent}$  is the amount of gasification agent consumed in the process and it is another unknown that was calculated by the model. The ratio of these two variables gives valuable information about the effective use of the gasification agent. With the help of the ratio,  $R_a$ , coal consumption rate can be estimated based on the gasification agent supply rate.

In Figure 3, the resulted  $R_a$  values are given for all lignite reserves. Edirköy reserve is showing apparent difference indicating much more coal can be converted into syngas by the same amount of oxygen supply.

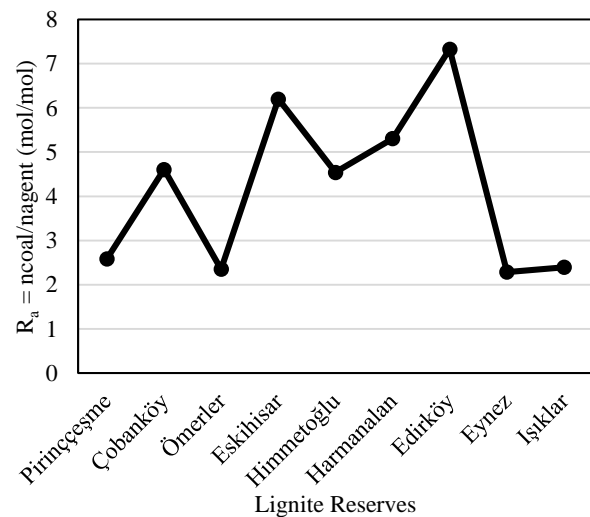
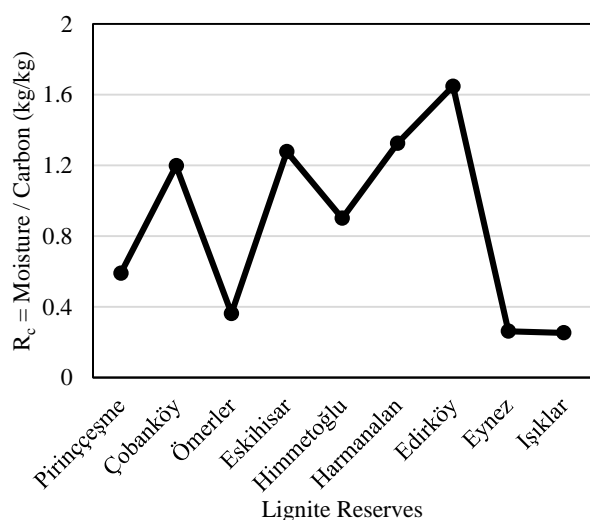


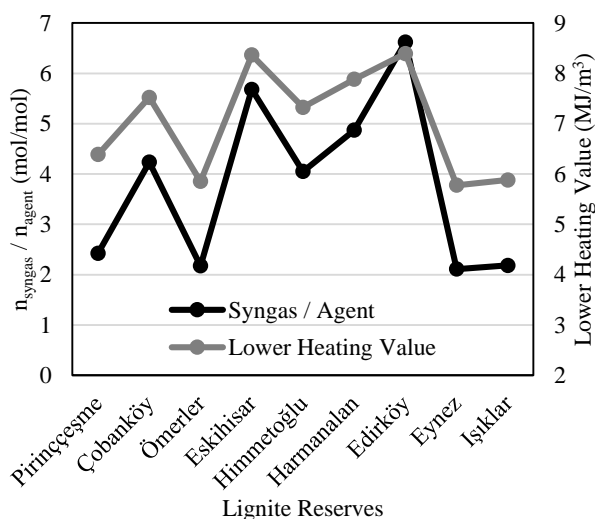
Figure 3.  $R_a$  ratios of all reserves in case of oxygen supply showing the effectiveness of the oxygen supply.

In Figure 4, moisture content of reserves, as stated in proximate analysis results in Table 3, were divided by carbon content, which was given in the ultimate analysis results, to get a better explanation of the effects of moisture and carbon content on hydrogen production. This new ratio was named as  $R_c$ , and its trend of change over the reserves, which is given in Figure 4, resembles the trend of the consumed coal to agent ratio,  $R_a$ . This resemblance indicates that higher moisture and lower carbon content resulted in higher hydrogen yield.



**Figure 4.** Moisture to carbon ratio of the reserves.

Also, the produced syngas to the consumed gasification agent ratio was higher for Edirköy and Eskihisar reserves, meaning much more syngas can be produced per consumed gasification agent. In Figure 5, the syngas to gasification agent ratio and syngas calorific value in case of oxygen supply is presented for all reserves.



**Figure 5.** Produced syngas amount with respect to consumed gasification agent and lower heating value of syngas in case of oxygen supply.

Results show that 6.6 mol of syngas with a heating value of 8.4 MJ/m<sup>3</sup> can be produced per 1 mol of gasification agent used in Edirköy reserve. High H<sub>2</sub> yield capability of Edirköy and Eskihisar reserves was presented in Figure 2. In addition to that, syngas production with a greater rate and less coal consumption means a more efficient UCG process for those reserves.

In case of pure steam supply, results in Figure 6 show that coal content is not crucial for the syngas composition. Hydrogen content for all reserves was around 50% for all reserves, and other contents in syngas didn't show any significant difference from each other. Steam supply is an effective technique to produce hydrogen from coal, but it is not a thermally sustainable process due to the endothermic nature of the gasification reactions. However, results obtained from the equilibrium model showed that, with the steam supply, syngas with high hydrogen content could be produced from the reserves. Equilibrium temperature was again 600 °C for the steam supply case. Several studies show that this temperature level is achievable if oxygen (or air) is supplied prior to the steam supply (Gür and Canbaz, 2020, Hongtao et al., 2011, Stańczyk et al., 2010). Oxygen supply before the steam supply creates the thermal energy needed for the gasification reactions with the help of combustion reactions, and that energy allows high hydrogen production from the water-gasification reaction.

Figure 7 shows the resulted syngas content when the steam-oxygen mixture was supplied as the gasification agent. Here, the properties of both pure-oxygen supply and pure-steam supply are observable. Edirköy reserve still had the highest hydrogen content, but all other reserves had the hydrogen content around 50%. However, carbon monoxide percentages were lower compared to the oxygen supply case. Steam-oxygen mixture ratio was 2.5:1 in this case. The supply of steam-oxygen mixture is a promising technique to produce hydrogen-rich syngas. Still, continuation of the process can be a problem when this technique is applied in-situ. Oxygen content should be enough for the continuation of the UCG process. Yang et al. showed that the continuation of the UCG process during the steam-oxygen supply is possible with a certain ratio (Yang et al., 2009). Yet, the continuation of the process is dependent on the coal properties and each lignite reserve would respond differently to a specific steam-oxygen ratio. Starting with the oxygen supply then switching to steam-oxygen mixture can be a reliable procedure for a long-term process without interruptions.

In Figure 8, lower heating values for calculated syngas compositions of each reserve are presented. Lower heating value changed according to the supply scheme for each reserve. Edirköy's results almost didn't vary as the gasification agent changes. However, lower heating values of the reserves with higher carbon content increased with the presence of steam in the gasification agent.

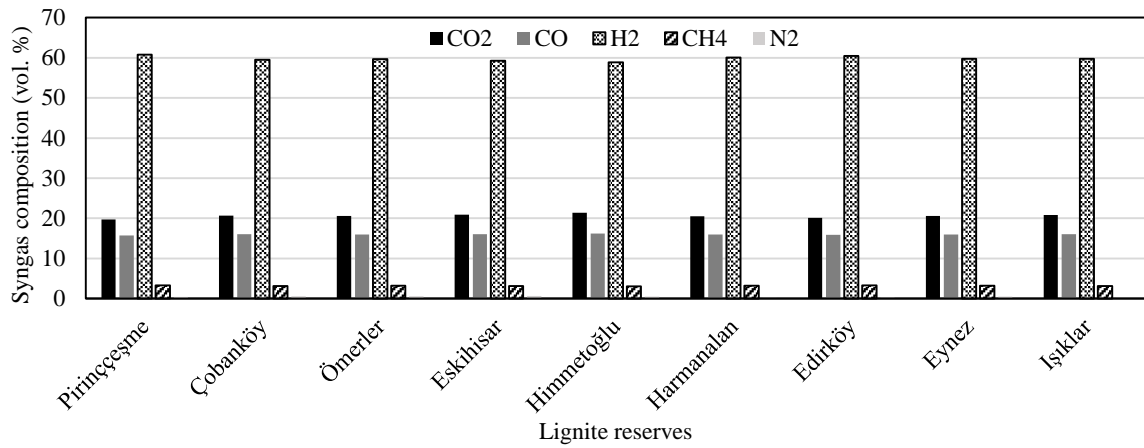


Figure 6. Resulted syngas compositions from the selected lignite reserves in case of steam supply.

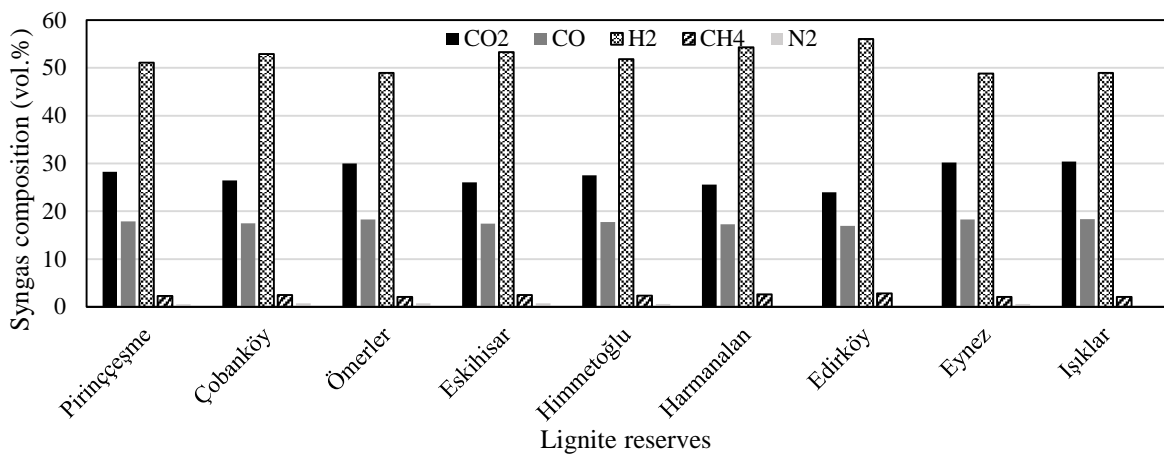


Figure 7. Resulted syngas compositions from the selected lignite reserves in case of steam-oxygen mixture supply.

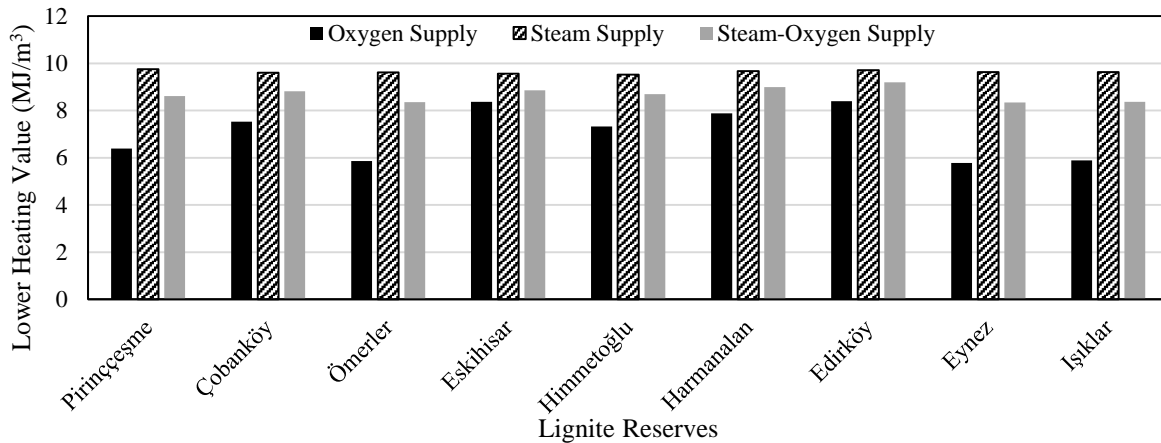


Figure 8. Calculated lower heating values for calculated syngas compositions.

## CONCLUSION

The UCG equilibrium model was used to predict the produced syngas compositions from the Turkish lignite reserves that were selected for a possible UCG application. Oxygen, steam, and steam-oxygen mixture were considered as the supplied gasification agents and used as input in the model. Results showed that:

- In case of oxygen supply, moisture content of the coal became crucial to produce hydrogen-rich syngas.

- Edirköy lignite reserve showed the greatest hydrogen production capability for oxygen-gasification.
- Edirköy had also the highest coal to agent ratio ( $R_a$ ) indicating much more coal can be converted with the same amount of oxygen.
- Change of  $R_a$  value was directly related to the moisture to carbon ratio of the coal sample.
- In case of oxygen supply, carbon dioxide percentage changed according to carbon content of the lignite reserves, but carbon monoxide percentage didn't vary and stayed on the same level for all reserves.



- When steam was supplied as the gasification agent, results showed that the coal content didn't affect the syngas composition.
- Steam-gasification is not a thermodynamically favorable process due to the endothermic nature of the water-gasification reaction. Therefore, the steam-oxygen mixture supply can be considered as the oxygen presence can make the continuation of gasification process possible.
- Results of steam-oxygen mixture supply showed that improvement in carbon monoxide and hydrogen content in syngas could be achieved for all reserves with the steam addition into the gasification agent. Enhancement in lower heating values, especially for the reserves with higher carbon content, also showed the positive effect of the steam addition.
- The equilibrium model explained here provides valuable primary estimations for the syngas production properties of Turkish lignites.

As the future study, by implementing the first law analysis of thermodynamics into the model, questions related to thermal stability and sustainability of the gasification process and effects of the moisture content on the UCG process can be answered.

## REFERENCES

- Altafini, C. R., Wander, P. R., and Barreto, R. M., 2003, Prediction of the working parameters of a wood waste gasifier through an equilibrium model. *Energy Conversion and Management*, 44(17), 2763–2777
- Cempa-Balewicz, M., Jacek Łączny, M., Smoliński, A., and Iwaszenko, S., 2013, Equilibrium Model of Steam Gasification of Coal. *Journal of Sustainable Mining*, 12(2), 21–28
- Daggupati, S., Mandapati, R. N., Mahajani, S. M., Ganesh, A., Mathur, D. K., Sharma, R. K., and Aghalayam, P., 2010, Laboratory studies on combustion cavity growth in lignite coal blocks in the context of underground coal gasification, *Energy*, 35(6), 2374–2386
- Fallahi, Y., Aydın, A. A., Gür, M., and Okutan, H., 2019, Investigation of the pollution risk of residues from a laboratory-scale underground coal gasification of Malkara (Turkey) lignite, *International Journal of Environmental Science and Technology*, 16(2), 1093–1102
- Gür, M., Eskin, N., Okutan, H., Arısoy, A., Böke, E., Altıntaş, Ü., ... Yıldırım, O., 2016, *Experimental and computational studies on underground gasification of Turkish lignite*, In 33rd Annual International Pittsburgh Coal Conference: Coal - Energy, Environment and Sustainable Development, PCC 2016 (Vol. 2016-August).
- Gür, M., Eskin, N., Okutan, H., Arısoy, A., Böke, E., Altıntaş, Ü., ... Yıldırım, O., 2017, Experimental results of underground coal gasification of Turkish lignite in an ex-situ reactor, *Fuel*, 203, 997–1006
- Gür, Mesut, and Canbaz, E. D., 2020, Analysis of syngas production and reaction zones in hydrogen oriented underground coal gasification, *Fuel*, 269, 117331
- Gür, Mesut, Eskin, N., Büyüksirin, O., and Canbaz, E. D., 2018, Kimyasal Denge Modeliyle Yeraltında Kömür Gazlaştırılmasının İncelenmesi, *IV. Uluslararası Katılımlı Anadolu Enerji Sempozyumu*, Edirne
- Hongtao, L., Feng, C., Xia, P., Kai, Y., and Shuqin, L., 2011, Method of oxygen-enriched two-stage underground coal gasification, *Mining Science and Technology (China)*, 21(2), 191–196
- Jarungthammachote, S., and Dutta, A., 2008, Equilibrium modeling of gasification: Gibbs free energy minimization approach and its application to spouted bed and spout-fluid bed gasifiers. *Energy Conversion and Management*, 49(6), 1345–1356
- Jowkar, A., Sereshki, F., and Najafi, M., 2018, A new model for evaluation of cavity shape and volume during Underground Coal Gasification process, *Energy*, 148, 756–765
- Kapusta, K., Wiatowski, M., and Stańczyk, K., 2016, An experimental ex-situ study of the suitability of a high moisture ortho-lignite for underground coal gasification (UCG) process, *Fuel*, 179, 150–155
- Klimenko, A., and Y., A., 2009, Early Ideas in Underground Coal Gasification and Their Evolution. *Energies*, 2(2), 456–476
- Li, X., Grace, J. R., Watkinson, A. P., Lim, C. J., and Ergüdenler, A., 2001, Equilibrium modeling of gasification: A free energy minimization approach and its application to a circulating fluidized bed coal gasifier. *Fuel*, 80(2), 195–207
- Pana, C., 2009, *Review of Underground Coal Gasification with Reference to Alberta's Potential. ERCB/AGS Open File Report 2009-10*, Energy Resources Conservation Board Alberta Geological Survey, Canada
- Pei, P., Korom, S. F., Ling, K., and Nasah, J., 2016, Cost comparison of syngas production from natural gas conversion and underground coal gasification, *Mitigation and Adaptation Strategies for Global Change*, 21(4), 629–643
- Perkins, G., and Sahajwalla, V., 2007, Modelling of Heat and Mass Transport Phenomena and Chemical Reaction in Underground Coal Gasification, *Chemical Engineering Research and Design*, 85(3), 329–343

- Perkins, G., and Sahajwalla, V., 2008, Steady-State Model for Estimating Gas Production from Underground Coal Gasification. *Energy & Fuels*, 22(6), 3902–3914
- Perkins, G., 2018a, Underground coal gasification – Part I: Field demonstrations and process performance, *Progress in Energy and Combustion Science*, Elsevier Ltd
- Perkins, Greg., 2018b, Underground coal gasification – Part II: Fundamental phenomena and modeling, *Progress in Energy and Combustion Science*, 67, 234–274
- Perkins, G., du Toit, E., Cochrane, G., and Bollaert, G., 2016, Overview of underground coal gasification operations at Chinchilla, Australia. *Energy Sources, Part A: Recovery, Utilization and Environmental Effects*, 38(24), 3639–3646
- Samdani, G., Aghalayam, P., Ganesh, A., Sapru, R. K., Lohar, B. L., and Mahajani, S., 2016, A process model for underground coal gasification - Part-I: Cavity growth, *Fuel*, 181, 690–703
- Sarhosis, V., Lavis, S., Mostade, M., and Thomas, H. R., 2017, Towards commercialising underground coal gasification in the EU, *Environmental Geotechnics*, 4(2), 113–122
- Sarraf Shirazi, A., Karimipour, S., and Gupta, R., 2013, Numerical simulation and evaluation of cavity growth in situ coal gasification, *Industrial and Engineering Chemistry Research*, 52(33), 11712–11722
- Shafirovich, E., and Varma, A., 2009, Underground coal gasification: A brief review of current status, *Industrial and Engineering Chemistry Research*, 48(17), 7865–7875
- Shoko, E., McLellan, B., Dicks, A. L., and da Costa, J. C. D., 2006, Hydrogen from coal: Production and utilisation technologies, *International Journal of Coal Geology*, 65(3–4), 213–222
- Stańczyk, K., Howaniec, N., Smoliński, A., Świdrowski, J., Kapusta, K., Wiatowski, M., ... Rogut, J., 2011, Gasification of lignite and hard coal with air and oxygen enriched air in a pilot scale ex situ reactor for underground gasification, *Fuel*, 90(5), 1953–1962
- Stańczyk, Krzysztof, Smoliński, A., Kapusta, K., Wiatowski, M., Świdrowski, J., Kotyrba, A., and Rogut, J., 2010, Dynamic experimental simulation of hydrogen oriented underground gasification of lignite, *Fuel*, 89(11), 3307–3314
- Swanson, R. M., Platon, A., Satrio, J. A., and Brown, R. C., 2010, Techno-economic analysis of biomass-to-liquids production based on gasification. *Fuel*, 89(1), 11–19
- Tuncalı, E., Çiftçi, B., Yavuz, N., Toprak, S., Köker, A., Gencer, Z., ... Şahin, N., 2002, *Türkiye Tersiyer Kömürlerinin Kimyasal ve Teknolojik Özellikleri*, Maden Tetkik ve Arama Genel Müdürlüğü (MTA), Ankara, Turkey
- Tunç, İ., 2015, *Yarı Pilot Ölçek Yer Altı Kömür Gazlaştırma Deney Düzeneginde Malkara Pirinççeşme Kömür Sahasına Ait Blok Kömür Örneklerinin Gazlaştırılması*, M.Sc. Thesis, Istanbul Technical University, Istanbul, Turkey
- Turkish Coal Enterprises (TKİ), 2014. *2015-2019 Stratejik Plan*, Ankara.
- Watkinson, A. P., Lucas, J. P., and Lim, C. J., 1991, A prediction of performance of commercial coal gasifiers. *Fuel*, 70(4), 519–527
- Xuyao, Q., Wang, D., Milke, J. A., and Zhong, X., 2011, Crossing point temperature of coal, *Mining Science and Technology*, 21(2), 255–260
- Yang, L. H., Zhang, X., and Liu, S., 2009, Underground coal gasification using oxygen and steam, *Energy Sources, Part A: Recovery, Utilization and Environmental Effects*, 31(20), 1883–1892
- Żogała, A., 2014a, Critical Analysis of Underground Coal Gasification Models. Part I: Equilibrium Models – Literary Studies. *Journal of Sustainable Mining*, 13(1), 22–28
- Żogała, A., 2014b, Critical Analysis of Underground Coal Gasification Models. Part II: Kinetic and Computational Fluid Dynamics Models, *Journal of Sustainable Mining*, 13(1), 29–37.
- Żogała, A., and Janoszek, T., 2015, CFD simulations of influence of steam in gasification agent on parameters of UCG process. *Journal of Sustainable Mining*, 14(1), 2–11
- Internet, 2020, General Directorate of Mineral Research and Exploration (MTA), *Kömür Arama Araştırmaları*, <http://www.mta.gov.tr/v3.0/arastirmalar/komur-arama-arastirmalari>



**Prof. Dr. Mesut GÜR** is currently a Professor of Mechanical Engineering at the Istanbul Technical University (ITU), which he joined in 2011. He received his first B.E. in Mechanical Engineering in 1977 from SDMMA (Sakarya University, Turkey) and his second B.E. in Process Engineering from the Hamburg Technical University. He graduated from the Hamburg-Harburg Technical University (Germany) Process Engineering program with a M.Sc. in 1986 and received his Ph.D. degree in 1992 in Mechanical Engineering from Clausthal Technical University (Germany). After working several years in the industry and simultaneously teaching at the Istanbul University, he joined the Sakarya University Mechanical Engineering Department as an Associate Professor. He became a full professor in the same department in 1999 and was appointed as the vice president of the Sakarya University in the same year. During his sabbatical leave (2004-2005) he worked as a visiting faculty/researcher in the Department of Mechanical Engineering and Material Science at the University of Pittsburgh (USA), focusing on super conducting materials. Prof. Mesut Gür's current research areas are coal and biomass gasification and combustion. He is specialized in the field of high temperature ventilators, pumps, cyclone heat exchangers, flow and heat transfer in microchannels, drying and combustion in fluidized bed applications. He has worked as the project manager and researcher in numerous international projects in Germany and USA. He has over 120 publications, including SCI indexed journal papers, conference proceedings, books and book chapters.



**Engin Deniz CANBAZ, M. Sc.**, received his B.Sc. and M.Sc. degree in mechanical engineering from Istanbul Technical University in 2016 and 2018, respectively. In his master's thesis, he studied mathematical modeling of underground coal gasification. Currently, he is a Ph.D. student at Istanbul Technical University and continuing his study on underground coal gasification.