**Proceedings of the**
**International Conference on Mechanical Engineering and Renewable Energy 2015**
**(ICMERE2015) 26 – 29 November, 2015, Chittagong, Bangladesh**

**ICMERE2015-PI-214**

# COMMERCIAL-SCALE COAL-TO-SNG PLANT: MODELING, SIMULATION AND PREFERENCE EVALUATION USING ILLINOIS #6 COAL AND IBC LOW RANK COAL BY ASPEN PLUS

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***Abstract***- *In this study, the entire process of Coal-to-SNG plant had been modeled and simulated by five sections utilizing Illinois #6 coal and IBC low rank coal as feed stocks. Shell's coal gasification process (SCGP) and Haldor Topsøe's recycle energy-efficient methanation process (TREMP$^{TM}$), in particular, were adopted in modeling of the gasification and methanation processes. Two drying methods were utilized for drying the IBC coal because of its higher moisture content. When only changing the feedstock from Illinois #6 coal to IBC coal in a Coal-to-SNG plant, the $CH_4$ purity and yield were 83.5 mol% and 0.264 kg/kg-coal (db); however, the $CH_4$ purity and yield could reach 94.4 mol% and 0.306 kg/kg-coal (db) when using IBC-CASE 2 drying concept in a Low Rank Coal-to-SNG plant, showing a higher $CH_4$ purity and an approximately equal yield compared with simulation results for a Coal-to-SNG plant by using Illinois #6 coal as feedstock. The Low Rank Coal-to-SNG process with IBC-CASE 2 drying concept becomes more feasible and attractive.*

**Keywords:** Synthetic natural gas, Coal-to-SNG, Drying concept, Low rank coal, Aspen Plus

## 1. INTRODUCTION

In the current state of energy production, natural gas is among the most clean, flexible and versatile fuels. While it is often used for producing heat and power, it can also be applied as a fuel in the transportation sector. It is well known that the reserves of oil and natural gas are limited to about 55 years, however, the reserve of coal is limited to 109 years [1][2]. Synthetic natural gas (SNG) production from coal is considered again due to rising prices for natural gas, the wish for less dependency from natural gas imports and the opportunity of reducing greenhouse gases by $CO_2$ capture and sequestration (CCS) [2][3]. Thus, for both energy security and $CO_2$ emission reduction, SNG production from coal is an important path to implement clean coal technologies. What's more, the Coal-to-SNG technology is proven, and with modern technology coupled with lessons learned from the gasification industry, it can be a reliable source of natural gas [2]. The Coal-to-SNG process utilizing low rank coal (LRC) as feedstock is referred to as the LRCoal-to-SNG process. It is generally expected that LRC will play a significant role as the major energy source, mainly because it is the most abundant and cheapest fossil fuel available, and LRC can be upgraded into SNG which can be transported and further used in high efficient power systems coupled with $CO_2$ sequestration technologies. Therefore, given the potential applications of Coal-to-SNG technologies, it is necessary to develop accurate methods of process modeling and performance evaluation on LRCoal-to-SNG plants.

## 2. PROCESS MODELING WITH ASPEN PLUS

### 2.1. The basic analyses of feed stocks

Two different ranks of coal were adopted in this research, one was Illinois #6 coal and another one was Indonesia LRC, which was named as IBC coal. The proximate and ultimate analyses and the higher heating values of these two feed stocks are shown in

Table 1.

### 2.2. Process modeling with Aspen Plus

The simulated Coal-to-SNG plant in this study will be developed based on SCGP and TREMP$^{TM}$. The whole plant process, presented in

Fig. 1, includes five sections: 1-coal preparation process, 2-gasification process, 3-gas cleaning process, 4-WGS process and 5-methanation process. Process Modeling software programs, such as Aspen Plus, are widely used in the simulation of carbonaceous fuel conversion processes [4][5][6][7].

2.2.1. Illinois # 6 feedstock preparation process modeling

Based on characteristics of Shell's coal gasification process (SCGP) technology utilized in gasification process [8], it is essential for dry-coal feed entrained-flow gasifier, thus the feedstock should be dried and pulverized in feedstock preparation process. Feedstock preparation process consisted of coal pulverizing, drying and transporting system.

2.2.2. Gasification, Gas cleaning, WGS, and methanation process modeling

The four sections that constitute the Shell gasifier [8][9][9] were simulated using Aspen Plus: thermal decomposition, fine & slag generation, coal gasification, raw syngas generation. In addition, gasifier input conditions of Illinois #6 coal are listed and showed in Table 2 according to the Shell gasifer conditions in the commercial case [11]. The gas cleaning section composed of ash removal (AR) and acid gas removal (AGR) processes. The water-gas shift reaction is a classic reaction for shifting $H_2$/CO ratio of the syngas, which is shown in Eq. (1) [12][13][14][15]. Methanathion process has been investigated with lots of researches [3], and the principle of catalytic synthetic production of methane from carbon monoxide and hydrogen was discovered in 1902 by Sabatier and Senderens [16], which can be described by Eqs. (2) and (3). Each process modeling simulation on coal preparation process, gasification process, gas cleaning process, WGS process, and methanation process had been modeled and shown in

Fig. 1.

$$\mathrm{CO} + \mathrm{H_2O} \rightarrow \mathrm{CO_2} + \mathrm{H_2}\ \Delta\mathrm{H} = -41.21\,\mathrm{kJ/mol} \quad (1)$$

$$\mathrm{CO} + 3\mathrm{H_2} \rightarrow \mathrm{CH_4} + \mathrm{H_2O} \quad \Delta\mathrm{H} = -206\ \mathrm{kJ/mol}$$

$$\mathrm{CO_2} + 4\mathrm{H_2} \rightarrow \mathrm{CH_4} + 2\mathrm{H_2O} \quad \Delta\mathrm{H} = -165\ \mathrm{kJ/mol} \quad (3)$$

Table 1: Proximate and ultimate analyses and HHV of Illinois #6 and IBC coal

| Sample | | Illinois #6 (wt%, arb*) | IBC (wt%, arb*) |
|---|---|---|---|
| Proximate analysis | Moisture | 11.12 | 34.05 |
| | Ash | 9.70 | 1.50 |
| | F.C. | 44.19 | 30.03 |
| | V.M. | 34.99 | 34.42 |
| Ultimate analysis | Ash | 9.70 | 1.50 |
| | C | 63.75 | 48.22 |
| | H | 4.50 | 2.61 |
| | O | 7.17 | 12.91 |
| | N | 1.25 | 0.67 |
| | S | 2.51 | 0.04 |
| HHV (Btu/lb) | | 6416.00 | 4102.00 |

arb*: as received basis.

2.2.3. Methods of data processing

In this study, CC and CGE were calculated using Eqs. (4) and (5): $CC$ (%) =

$$\frac{(mol_{CO} + mol_{CO_2} + mol_{CH_4})\ of\ syngas\ [kmol/h]}{mol_C\ of\ input\ fuel\ [kmol/h]}\ 100 \quad (4)$$

$$CGE\ (\%) = \frac{(mol_{CO} * HHV_{CO} + mol_{H_2} * HHV_{H_2} + mol_{CH_4} * HHV_{CH_4})\ of\ syngas\ [k}{HHV\ of\ input\ fuel\ [kcal/h]} * 100 \quad (5)$$

where $mol_{CO}$, $mol_{CH4}$, $mol_{CO2}$, and $mol_{H2}$ represent moles of CO, $CH_4$, $CO_2$, and $H_2$, respectively, and $HHV_{CO}$, $HHV_{CH4}$ and $HHV_{H2}$ represent the higher heating value of CO, $CH_4$, and $H_2$, respectively.

# 3. RESULTS AND DISCUSSION

## 3.1. Simulation results on entire Coal-to-SNG plant with Illinois #6 coal as feedstock

The gasification process modeling was verified from two aspects: comparisons with the reference data from Shell IGCC report and the sensitivity analyses. It can be concluded from Table 2 that the simulated results were consistent with the reference data received from Shell gasifier IGCC report [11].

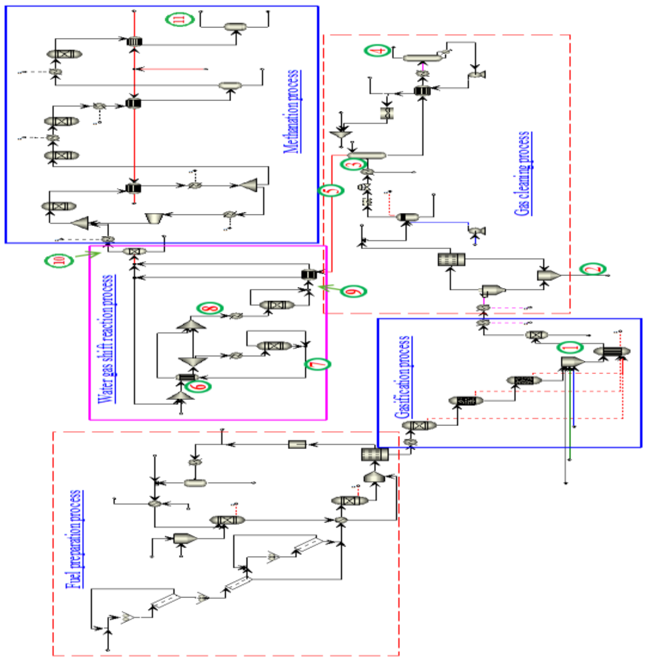


Fig. 1: The entire process modeling of Coal-to-SNG plant with Illinois #6 coal as feedstock by Aspen Plus

The results of the simulation experiment that modeled the WGS process are summarized in

Table 4. By comparing the gas flow rate before and after the reactors, the mole ratio of H2/CO had been adjusted to 3.07 from 0.378 in order to meeting the requirement of stoichiometric ratio in Eq. (1), it can be concluded that this WGS process modeling could provide an appropriate proportion of feed gases into methanation process.

The results of the simulation experiment that modeled the methanation process, using the gas feed composition adopted from **Module 3.0** of the Topsøe Company report, are shown in Table 7. It can be seen that the CH4 purity could reach 97.4 mol% after passing through these four adiabatic reactors.

Each process modeling simulation on coal preparation process, gasification process, gas cleaning process, WGS process, and methanation process had been simulated and shown well-matched with relative reference/report, thus the entire Coal-to-SNG process modeling (

Fig. 1) had also been run. The CH4 purity and yield were calculated and can reach 85.2 mol%, 0.324 kg/kg-coal (db), respectively. The reason why CH4 purity was much lower than 97.4 mol% of **Module 3.0** was that there was no extra N2 removal process in the entire Coal-to-SNG plant. Based on the simulation results of the entire Coal-to-SNG plant, the CC and CGE can reach 99.4 %, 80 %, respectively, while the CH4 purity and yield can reach 85.2 mol%, 0.324 kg/kg-coal (db), therefore, it can be concluded that the entire process modeling of Coal-to-SNG plant is feasible to be commercialized, even though without extra N2 removal process modeling.

Table 3 shows the results of the modelled gas cleaning process simulation. It can be clearly seen from Table 5 that changes of the flow rate before and after the gas cleaning process. Mole flow rate of $H_2S$, $NH_3$ and COS were lowered to trace amounts and mole flow rate of $CO_2$ was reduced into 6.7 from 130.6 kmol/h.

Table 2: The gas comparisons of reference and simulation data on Illinois #6 and IBC coals after gasification process

| Syngas composition (mol%) | Reference* | Simulation | |
|---|---|---|---|
| | Illinois #6 | Illinois #6 | IBC-CASE 1 |
| CO | 0.627 | 0.6312 | 0.654 |
| $CO_2$ | 0.0206 | 0.0172 | 0.077 |
| $H_2$ | 0.297 | 0.2982 | 0.213 |
| $CH_4$ | 0.0004 | 0.0004 | 35PPM |
| $N_2$ | 0.0432 | 0.0416 | 0.045 |
| AR | 0.0092 | 0.0097 | 0.011 |
| $H_2S$ | 430PPB | 440PPB | 3PPB |
| COS | 120PPB | 32PPB | TRACE |
| $NH_3$ | 0 | 4PPB | 383PPB |
| $H_2O$ | 0.003 | 0.0018 | 0.0002 |

*reference data is from the Shell gasifier IGCC report PED-IGCC-98-002.

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Table 3: The stream parameters at different positions in gas cleaning process modeling

| Stream | | ①* | ③* | ④* | ⑤* |
|---|---|---|---|---|---|
| Total gas flow (kmol/h) | | 7337.2 | 6591.7 | 2972.1 | 5525.8 |
| Mole flow for gas compositions (kmol/h) | $N_2$ | 303.9 | 303.9 | 39.3 | 264.7 |
| | AR | 73.5 | 73.5 | 19.9 | 53.6 |
| | $H_2O$ | 745.4 | 1.4 | 1772.0 | 7.6 |
| | $CO_2$ | 512.9 | 512.8 | 512.4 | 0.5 |
| | CO | 4275.8 | 4275.8 | 500.6 | 3775.2 |
| | $H_2$ | 1424.2 | 1424.2 | 0.0 | 1424.2 |
| | $CH_4$ | 0.009 | 0.009 | 0.007 | 0.001 |
| | $H_2S$ | 19.5ppm | 19.4ppm | 19.4ppm | Trace |
| | $NH_3$ | 0.003 | 0.002 | 0.002 | Trace |
| | COS | 2.16ppm | 2.16ppm | 2.16ppm | Trace |
| | SULFUR | 1.44 | 0.06 | Trace | 0 |
| Mass flow (kg/h) | ASH | 96.5 | - | - | - |
| | FINE | 107.3 | - | - | - |

*①, ③, ④ and ⑤ were marked in Fig. 1.

Table 4: The gas compositions at the different positions in WGS process modeling

| Gas composition | ⑤* | ⑥* | ⑦* | ⑧* | ⑨* |
|---|---|---|---|---|---|

| (mol%) | | | | | |
|---|---|---|---|---|---|
| CO | 0.683 | 0.315 | 0.049 | 0.004 | 0.233 |
| $H_2$ | 0.258 | 0.119 | 0.385 | 0.43 | 0.716 |
| $CO_2$ | 85ppm | 39ppm | 0.266 | 0.311 | 0.005 |
| $H_2O$ | 0.001 | 0.54 | 0.274 | 0.228 | 0 |
| $CH_4$ | 215ppb | 99ppb | 99ppb | 99ppb | 217ppb |
| $N_2$+Ar | 0.058 | 0.026 | 0.026 | 0.026 | 0.047 |

*⑤, ⑥, ⑦, ⑧ and ⑨ were marked in Fig. 1.

**3.2. Simulation results on entire Low Rank Coal-to-SNG plant with IBC coal as feedstock**

Following the entire Coal-to-SNG process modeling, the feedstock was changed to IBC coal from Illinois #6 coal so that the LRC-to-SNG plant model was built. How to dry or upgrade the IBC coal is becoming a more and more important issue, two different drying concepts of IBC coal was investigated here: IBC-CASE 1 and IBC-CASE 2, in order to improve the utilization efficiency of IBC coal: 1) IBC-CASE 1: Generally, the most commonly used coal drying process is referred as the conventional drying process in the IGCC plant, which was also utilized for drying the Illinois #6 coal; 2) IBC-CASE 2: If taking the $CH_4$ purity factor into consideration, the use of $N_2$ as the carrier gas should be controlled or switched to another carrier gas ($CO_2$).

Table 5: Mole fractions of syngas compositions and total flow rates in the different positions by using IBC-CASE 1 drying concept

| Syngas Compositions (mol%) | ①* | ③* | ⑤* | ⑩* | ⑪* |
|---|---|---|---|---|---|
| CO | 0.607 | 0.654 | 0.69 | 0.233 | 1ppm |
| $CO_2$ | 0.072 | 0.077 | 200ppm | 0.005 | 831ppm |
| $H_2$ | 0.197 | 0.213 | 0.252 | 0.717 | 0.003 |
| $CH_4$ | 35ppm | 38ppm | 8ppm | 8ppm | 0.835 |
| $N_2$ | 0.041 | 0.045 | 0.046 | 0.037 | 0.132 |
| AR | 0.01 | 0.011 | 0.01 | 0.008 | 0.028 |
| $H_2O$ | 0.073 | 205ppm | 0.001 | 0 | 0.001 |
| $H_2S$ | 3ppb | 3ppb | Trace | 0 | 0 |
| COS | Trace | Trace | Trace | 0 | 0 |
| $NH_3$ | 455ppb | 383ppb | Trace | 0 | 0 |
| Flow rate (kmol/h) | 7453.80 | 6911.40 | 5823.90 | 5775.90 | 1641.20 |

*①, ③, ⑤, ⑩ and ⑪ were marked in Fig. 1.

3.2.1. The entire LRCoal-to-SNG plant with IBC-CASE 1 as drying concept

All the data were entered in the LRCoal-to-SNG plant simulation and the process ran well. Several results are summarized in Tables 2 and 5. Table 2 shows that the mole fraction of syngas (CO + $H_2$) was about 87% after IBC coal gasification process, which is 6% lower than that after Illinois #6 coal gasification process. Table 5 shows that the $CH_4$ purity could reach 83.5 mol% after passed the methanation process. For the entire of the LRCoal-to-SNG process utilizing IBC coal as the feedstock, the CC and CGE, the $CH_4$ purity and yield were selected as performance evaluation parameters. Based on Eqs. (1) and (2), the CC and CGE can reach 99.8 %, 78.6 %, respectively. It can be seen from Table 5 that $CH_4$ purity was 83.5 mol% of the end-product and $CH_4$ yield was 0.264 kg/kg-coal (db).

3.2.2. The entire LRCoal-to-SNG plant with IBC-CASE 2 as drying concept

Table 6: Mole fractions of syngas compositions and total flow rates in the different positions by using IBC-CASE 2 drying concept

| **Syngas composition** (mol%) | ①* | ③* | ⑤* | ⑩* | ⑪* |
|---|---|---|---|---|---|
| CO | 0.646 | 0.681 | 0.702 | 0.24 | 2ppm |
| $CO_2$ | 0.05 | 0.052 | 417ppm | 0.005 | 0.001 |
| $H_2$ | 0.233 | 0.245 | 0.278 | 0.74 | 0.004 |
| $CH_4$ | 119ppm | 125ppm | 29ppm | 28ppm | 0.944 |
| $N_2$ | 0.01 | 0.01 | 0.011 | 0.008 | 0.031 |
| AR | 0.009 | 0.009 | 0.008 | 0.006 | 0.024 |
| $H_2O$ | 0.053 | 0.002 | 0.001 | 0 | 0.001 |
| $H_2S$ | 186ppb | 195ppb | Trace | 0 | 0 |
| COS | 17ppm | 18ppm | Trace | 0 | 0 |
| $NH_3$ | 10ppb | 7ppb | Trace | 0 | 0 |
| Flow rate (kmol/h) | 7331.4 | 6956.7 | 6145.5 | 6354.9 | 1659.4 |

*①, ③, ⑤, ⑩ and ⑪ were marked in Fig. 2.

IBC-CASE 2 drying concept was that the carrier gas of the LRCoal-to-SNG simulation plant was changed to $CO_2$. Thus, the IBC-CASE 2 drying concept was used in the whole LRCoal-to-SNG plant (Fig. 2).

After the data were entered in the upgraded simulation process and the simulation was run, the results from the five parts of the process are summarized in Table 6. When making the comparison clear with the simulation results utilizing $N_2$ as the carrier gas (Table 5), it can be founded in Table 6 that the $CH_4$ purity increased to 94.4 mol%, from 83.5 mol%, in the end-product stream.

3.2.3. Comparisons on $CH_4$ purity and yield by utilizing Illinois #6 and IBC coals as feedstock

Gasification performances were calculated based on Eqs. (1) and (2) and the simulation results obtained from the LRCoal-to-SNG plant (Fig. 3). It can be obtained from Fig. 3 that when changing the drying concept of IBC coal, all of the CCs can reach 99.8 % after gasification process. In addition, the CC and CGE of the LRCoal-to-SNG with the IBC-CASE 2 drying concept also showed a higher CC and equivalent CGE when compared with the CC and CGE of Illinois #6 Coal-to-SNG process. Methanation performances were also conducted and are also shown in Fig. 3. When using IBC coal as feedstock in LRCoal-to-SNG process, the IBC-CASE 2 showed the highest $CH_4$ purity of 94.4 mol% and yield of 0.306 kg/kg-coal (db), mainly caused by using $CO_2$ as carrier gas, and among these two drying concepts, production capability of $CH_4$ can be summarized as: IBC-CASE 1 < IBC-CASE 2. Therefore, it can be concluded that LRC had a very good gasification performance when utilized in the LRCoal-to-SNG with IBC-CASE 2 drying concept.

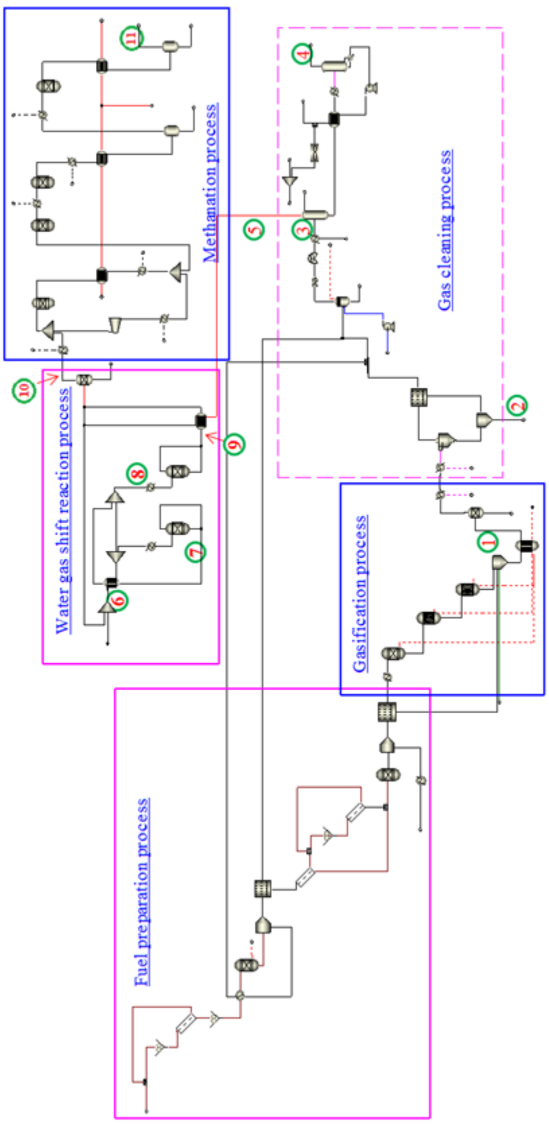


Fig. 2: The entire process modeling of LRCoal-to-SNG plant with IBC-CASE 2 drying concept by Aspen Plus

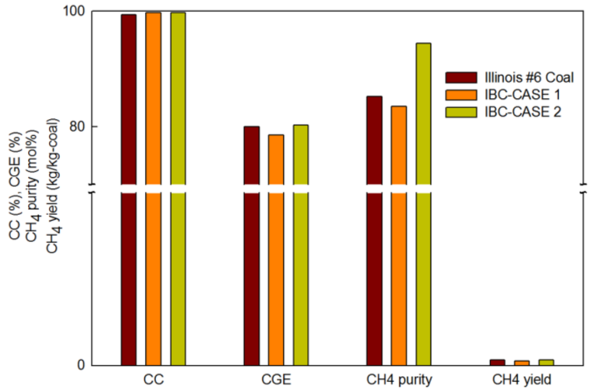


Fig. 3: The CC, CGE, $CH_4$ purity and yield changes utilizing different feedstocks in a Coal-to-SNG plant (Illinois #6 Coal: reaction conditions from reference report, IBC-CASE 1: the same reaction conditions (input and output temperature and heat loss) as Illinois #6 and also the same moisture content (5.33 wt%), and IBC-CASE 2: the same reaction conditions (input and output temperature and heat loss) as Illinois #6, but the upgraded drying concept was used and the moisture content was set at 7 wt%)

## 4. CONSLUSIONS

(l) After ran the entire Coal-to-SNG plant utilizing Illinois #6 coal as feedstock, the $CH_4$ purity and yield could reach 85.2 mol%, 0.324 kg/kg-coal (db), and was 12.2 % lower than that by using Module 3.0 because there was no extra $N_2$ removal process.

(2) When only changing the feedstock to IBC coal from Illinois #6 coal in the Coal-to-SNG plant, the $CH_4$ purity and yield were 83.5 mol% and 0.264 kg/kg-coal (db); however, the $CH_4$ purity and yield could reach 94.4 mol% and 0.306 kg/kg-coal (db) when applying the IBC-CASE 2 drying concept in LRCoal-to-SNG plant.

(3) When changing drying concepts of IBC coal, all of the CCs can reach 99.8 % after gasification process and shown a little higher than CC of Coal-to-SNG utilizing Illinois #6 coal as feedstock. Moreover, there is no apparent difference in CGE.

In conclusion, the LRCoal-to-SNG process with IBC-CASE 2 drying concept becomes more feasible and attractive.


## 5. ACKOWLEDGEMENT

This research was sponsored by the New & Renewable Energy of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant founded by the Korea Government Ministry of Trade, Industry & Energy (20113020050010).


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