Multi-energy Complementary System for Joint Production of Liquid Fuel and Power

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Abstract. By taking the energy complementation as an idea and the steam methane reforming as well as coal partial gasification and Fischer-Tropsch synthesis as the core technological means, this paper establishes a coal and methane to co-produce liquid fuels and power generation system using an ASPEN PLUS simulator, and realizes that the H₂/CO can be adjusted by directly changing the charging rate of raw materials with no need for additional equipment. At the same time, the coal char that has not yet been gasified is burned to provide the needed heat for the reaction of steam methane reforming, which can not only solve the demand of high heat of steam methane reforming, but also realize the gradient utilization of energy, thus reducing the loss in energy. In addition, some Fischer-Tropsch steam is used to generate power to further reduce the energy damage of the system. Two key parameters, namely coal input and Fischer-Tropsch recycle ratio, are discussed and their effects on system performances are analysed. At the optimum condition, the energy efficiency of this novel system reaches 52.5%, and the primary energy saving ratio reaches 30.4%.

1. Introduction
In the face of decreasing oil reserve and its rapid consumption, the research of synthetic oil technology will have great value and influence. At present, the indirect conversion method that is relatively mature and has the higher degree of industrialization, is a process of converting raw materials into synthesis gas and indirectly producing liquid fuel based on Fischer-Tropsch (F-T) synthesis technology. The technology of indirect conversion to synthetic oil is mainly composed of three units, including synthesis gas preparation, F-T synthesis and product purification. As the preparation unit before F-T synthesis, the synthesis gas preparation should try to meet the condition of F-T inlet amount of gas, that is, the H₂/CO ratio (H/C) should be 2, otherwise the output and yield of product oil will be seriously affected. According to different sources of synthesis gas feed, the routes of liquid fuel production have been mainly developed into two forms: natural gas to liquid fuel (GTL) and coal to liquid fuel (CTL) [1].

Steam methane reforming (SMR) is the most widely used process at present and obtains a synthesis gas having a H/C of syngas higher than 3[2]. In the process of CTL, the H/C of produced synthesis gas after coal gasification is low, which is not enough to meet the raw material requirements of F-T synthesis. It is required to improve H/C through removing CO from synthesis gas before carrying out F-T synthesis, thus obtaining high yield oil products [3]. It can be seen that both traditional GTL technology and CTL technology have the disadvantage of requiring to adjust the process of H/C. A reverse water-gas shift reaction (RWGS) is generally required for GTL process as well as a water gas shift reaction (WGS) for CTL [4, 5]. These two processes not only increase the technology difficulties,
but also enhance capital cost resulting from the further additionally supplemental CO₂ and steam source [6].

Multi-energy complementary system refers to the combination of different types of energy, and the advantages of each energy system are integrated into a new system. This paper uses ASPEN PLUS software to establish a coal and methane to co-produce liquid fuels and power generation system, which is efficient, practical and easy to control. The biggest feature of the system is that the low \( H/C \) of syngas from coal gasification and a high \( H/C \) of syngas from methane reforming are coupled for downstream F-T synthesis. In comparison with a traditional CTL or GTL process, the WGS or RWGS unit is correspondingly eliminated, and the acceptable syngas production becomes more stable. In addition, coal can be partially gasified by controlling gasification temperature, which provides probability on not only reducing excessive exergy destruction of gasification, but also offsetting the required heat of SMR by combusting the un-gasified coal char. Finally, through the evaluation methodology of thermodynamics, this paper analyses and discusses the influence of key parameters on the system performance.

2. Process description

A coal and methane to co-produce liquid fuels and power generation system is shown in figure 1. It mainly consists of three parts: Coal gasification & methane reforming unit, F-T synthesis & products distillation unit and heat recovery & power generation unit. By adjusting the charging rate of coal and methane, the coal gasification product with low \( H/C \) and the reforming product with high \( H/C \) are mixed, thus obtaining the synthesis gas that is suitable for F-T synthesis. In the meantime, by controlling the feed amounts of oxygen and steam that required for coal gasification to adjust the coal gasification temperature and conversion ratio, and un-gasified coal char is used for combustion to provide the heat required for methane reforming. After purification, the applicable syngas accesses F-T reactor for production, and the liquid fuels composed of various hydrocarbons from F-T reactor are sent to distillation tower to fractionate products. Some of the steam from F-T reactor is recycling back to F-T reactor, and the remained is used to turbine for generate power. The syngas with high temperature and flue gas from coal char combustor pass the waste heat boiler (WHB) to recover heat to generate high temperature and pressure steam, and the heat of F-T reaction can be recovered to generate low-pressure steam. The produced steam is used to meet system internal steam demand or generate power by means of steam turbine.

**Figure 1.** Schematic of a coal and methane to co-produce liquid fuels and power generation system process.
2.1. Coal gasification & methane reforming unit
The coal gasification and methane reforming process are used to produce synthesis gas. Raw coal material, pure oxygen and mid-pressure steam are fed into gasifier, and the gasification temperature and conversion rate of the coal are controlled by controlling the feed amount of the gasification agents (oxygen and steam). The pure oxygen needed for coal gasification is obtained by air separation unit (ASU) after the fresh air is compressed to 3 bar by C-Air, then the pure oxygen goes on further compression to 32 bar by multi-stage intercooling compressors and fed into gasifier to meet the operational pressure of 30 bar. In terms of SMR, the ratio of mid-pressure steam (30 bar) to methane input is fixed at 3, and methane is compressed to 32 bar by multi-stage intercooling compressors and fed into reformer operated at 30 bar. The un-gasified coal char goes through combustor to be burned to provide heat for methane reforming and enhance reformer temperature limited to 950 °C. The oxygen to carbon molar ratio is 0.2, and steam to carbon molar ratio is 0.1.

2.2. F-T synthesis & products distillation unit
The shifted syngas from upstream goes through F-T reactor after heat exchanging, condensation, acid gas removal and dehydration. The F-T reactor adopts RCSTR module to simulate the F-T slurry bed reaction with producing C1-C30 alkanes and C2-C20 olefins [7]. The liquid fuels from F-T steam three-phase flash together with F-T liquid fuels are directed to fractionating tower for three kinds of products: light (C1-C4), gasoline (C5-C11) and C11+ (C11-C30) product. Both the mass purities of gasoline and C11+ product is higher than 95%, and the mass purity of light product is kept around 60% correspondingly. The steam from flash is divided into two parts; one is recycled back to F-T reactor accounting for 90% of steam (molar fraction), and the rest is used to turbine for generating power.

2.3. Heat recovery & power generation unit
Taking the high temperature of syngas and flue gas into consideration, a heat exchanger network be used to recover heat. Heat exchanging medium is high-pressure water at 110 bar compressed by pump. High-temperature and pressurized steam produced declines to mid-pressure steam after high-pressure (HP) steam turbine, and some of the mid-pressure (MP) steam is reheated to meet the amount of steam required in the processes of coal gasification, methane reforming and distillation rectification stripping. The remaining is utilized for power generation by means of second stage (namely MP) steam turbine. The unreacted gas from F-T synthesis is utilized for power generation via gas turbine and downstream steam turbines. The excessive heat from F-T synthesis is also collected by low-pressure steam (5 bar), combining with the steam from the second-stage steam turbine and further introducing into condenser to enhance power generation.

3. Simulation
The whole co-production of liquid fuels and power, by using coal and methane process, is built and simulated by ASPEN PLUS software. The Peng-Robinson with Boston-Mathias function (PR-BM for short) is selected as property method, suitable for simulating coal gasification and methane reforming process [8]. In addition, PRMHV2 is selected for F-T and BK-10 for distillation as property method accordingly [7].

The step of coal gasification is composed of decomposition with Ryield and oxidation with RGibbs blocks in series. The products from Ryield bock are a variety of elements that make up coal (C, H, O, N, S and ash). Under the constraints of phase equilibrium, chemical equilibrium, and atomic balance, the conventional elements in coal can be converted to syngas based on the principle of Gibbs free energy minimization [9]. The reforming of methane adopts RGibbs as well.

F-T synthesis is simulated by RCSTR module (continuous stirring tank reactor) as slurry phase F-T reactor model based on linear kinetics. In the practical industry of F-T slurry phase reaction system, small particle catalysts (Co-based catalyst or Fe-based catalyst) is utilized for reaction [10]. Meanwhile the F-T reactor can remove heat operated at isothermal condition of 250 °C and 28.5 bar. Since F-T synthesis is not a highly selective process, a wide range of products from F-T synthesis reaches 100 species according to the Anderson-Schulz-Flory (ASF) products distribution [11]:
\[ \ln \left( \frac{W_n}{n} \right) = n \ln \alpha + \ln \left( \frac{1 - \alpha}{\alpha} \right) \]  

(1)

where \( W_n \) means weight fraction of molecules with \( n \)th carbons, \( n \) means carbon number of chain length and \( \alpha \) means chain growth probability.

Clearly, according to the ASF equation, the descent of \( \ln(W_n/n) \) is linear with increasing carbon number. Therefore, this process considers the generation of \( \text{C}_3-\text{C}_{30} \) alkanes and \( \text{C}_2-\text{C}_{20} \) olefins alone for the purpose of simulation simplification, and the generation of higher carbon chain, aromatics and oxygenates are ignored because of their trace content [12].

The distillation of F-T products adopts PetroFrac block with strict calculation on complex types of steam-liquid separation operation, and free water is detected and separated from fuels. WHB is simulated by MHeatX block with specifying multi-heat and cool streams heat exchanging for satisfying downstream units operating conditions and improving energy utilization. For all the power consumption devices, such as compressors and pumps, the power consumption is read from the simulation. As for the use of ASU and acid gas removal (AGR) blocks, the required energy consumption is obtained by calculating with values based on the practical separation processes.

4. Evaluation methods

Concerning on this process, the definition of energy efficiency (\( \eta_{en} \)) is the ratio of valuable outputs to system inputs. The valuable output include light, gasoline, \( \text{C}_{11+} \) products and net power, and the system inputs are associated with coal and methane, as shown in Equation (2).

\[ \eta_{en} = \frac{E_{\text{light}} + E_{\text{gasoline}} + E_{\text{C}_{11+}} + E_{\text{net}}}{E_{\text{coal}} + E_{\text{methane}}} \]  

(2)

where \( E \) means energy outputs (LHV), \( W \) means power output or input.

It is worth mentioning that all power consumption of devices that mentioned previously is not considered as input; as a result of the power consumption can be offset from system itself.

The net power output is calculated by Equation (3).

\[ W_{\text{net}} = W_{\text{GT}} + W_{\text{ST}} - W_{\text{compressors}} - W_{\text{pumps}} - W_{\text{ASU}} - W_{\text{AGR}} \]  

(3)

The exergy destruction (\( Ex_{\text{dest}} \)) of F-T unit is considered to assess the loss of the work potential of energy from a given thermodynamic state, which can be calculated by exergy balance as follows:

\[ Ex_{\text{dest}} = Ex_{\text{in}} - Ex_{\text{out}} \]  

(4)

Notably F-T heat can be utilized for raising steam and the exergy of heat (\( Ex_Q \)) is calculated by Equation (5).

\[ Ex_Q = Q \left( 1 - \frac{T_0}{T} \right) \]  

(5)

where \( T_0 \) means the reference temperature (298.15 K), \( T \) means reaction temperature, \( Q \) means the quantity of released heat.

In terms of this poly-generation system, primary energy saving ratio (\( PESR \)) is used to assess the primary energy saving potential of this system compared with the reference system by quantifying the same amount of outputs, which is shown in Equation (8). The reference systems considered in this study are a combination of a GTL system for liquid fuels production and a nature gas combined cycle (NGCC) system for power generation. The energy efficiencies of GTL system and NGCC system are 47% [13] and 55% [14], respectively.
where $PE_{\text{refer}}$ means the total consumption of primary energy of separation systems, $PE$ means the total consumption of primary energy of this novel system.

5. Results and Discussion

5.1. System performance

The thermodynamic performance of this process is shown in Table 1. At the designed conditions (coal input of 5 kg/s and methane input of 0.1 kmol/s), the output of liquid fuels (light, gasoline and $C_{11+}$ product) amount to 76.37 MW, accounting for 66.4% of all outputs. While the net power accounts for 33.6% as an additional product, the total energy efficiency of this process achieves 52.5%.

| Item                        | Unit | Value | Percentage |
|-----------------------------|------|-------|------------|
| Energy input                | MW   | 219.00| 100%       |
| Coal (LHV)                  | MW   | 139.00| 63.5%      |
| Methane (LHV)               | MW   | 80.00 | 36.5%      |
| Energy output               | MW   | 114.97| 1          |
| Light (LHV)                 | MW   | 22.47 | 19.5%      |
| Gasoline (LHV)              | MW   | 33.28 | 29.0%      |
| $C_{11+}$ (LHV)             | MW   | 20.62 | 17.9%      |
| Power                       | MW   | -38.60| 33.6%      |
| Energy efficiency           | %    | 52.50 | -          |
| Inherent work consumption   | MW   | 21.45 | 1          |
| ASU                         | MW   | 1.82  | 8.5%       |
| $O_2$ pre-compression       | MW   | 0.52  | 2.4%       |
| Methane compression         | MW   | 1.2   | 5.6%       |
| Acid gas removal            | MW   | 3.3   | 15.4%      |
| Recycle compression         | MW   | 0.61  | 2.8%       |
| Air 3 compression           | MW   | 13.75 | 64.1%      |
| Water 1 pumping             | MW   | 0.25  | 1.2%       |
| Water 2 pumping             | MW   | 0.002 | -          |

5.2. Effect of coal input

In this study, the methane input is fixed at 0.1 kmol/s, and steam needed for reforming is 0.3 kmol/s, with a favored steam to methane ratio of 3 for meeting economic-interest and avoiding coke formation for reforming. Therefore, for realizing material coupling and thermal coupling, the amount of coal input is the most essential parameters for meeting this goal. The appropriate amount of coal input can achieve the acceptable $H/C$ of syngas and provide proper heat for methane reforming simultaneously depending on the appropriate amount of coal input. When the amount of coal feed is insufficient, there exists an imbalance between the amounts of coal gasification for syngas production and un-gasified coal char to be combusted for methane reforming. The consequences of this problem are a high $H/C$ of syngas and a lack of heat required for methane reforming. Yet excessive coal inputs lead to an extremely low energy utilization of a waste of burning heat beyond the principle of heat and material coupling. The effect of coal input on $H/C$ of syngas is shown in figure 2, the effects of coal input on energy efficiency & $PESR$ and productions of liquid fuels & power are shown in figure 3 and figure 4, respectively.
Figure 2 clearly shows a decrease in H/C of syngas as the amount of coal feed increase, and it reflects the feasibility of coal input quantities for adjusting the H/C of syngas. When the coal input is chosen as 5 kg/s, the H/C of syngas required for F-T synthesis is obtained. Meanwhile, the heat required for methane reforming can be judged from methane reforming conversion and temperature (the methane reforming conversion and temperature are 92.7% and 950 °C, respectively). Accordingly, as shown in figure 3, the maximum value of system energy efficiency amounts to 52.5% based on coal input at 5 kg/s due to the energy of coal and methane are optimally utilized as well as PESR. In order to measure the effects of different amount of coal input on product outputs, i.e. liquid fuels and power, normalized ratio is proposed in this study to accurately measure the relationship between coal input and product outputs by means of quantifying the same amount of energy of fuels input based on LHV. As presented in figure 4, liquid fuels production peaks at 2.2×10^2 MW of energy input (i.e. the corresponding coal input is 5 kg/s), and it verifies that the optimal H/C of syngas for F-T is around 2 in this process, which conforms the practical industry operation [15]. For another, the valley value of power production appears at 5 kg/s of coal input as well as resulting from a decrease in GT power generation since a decrease in un-cycled F-T steam. Figure 5 shows the comparisons of PESR with separation systems (GTL and NGCC systems) at 5 kg/s of coal input, and this novel poly-generation system obtains a decrease of 30.4% comparing with total energy input of reference systems based on PESR.
5.3. Effect of F-T steam recycle ratio

F-T steam recycle ratio is defined as the molar quantity of steam in circulation to total molar quantity of steam from F-T synthesis. It is no doubt that unrestricted recycle increases the conversion ratio of F-T synthesis ceaselessly, however, increasing the recycle ratio results in an increase in exergy destruction of F-T synthesis and efficient utilization of system energy. As shown in figure 6, it is clearly that the exergy destruction trend increases sharply after the recycle ratio beyond 0.9, and the maximum energy efficiency appears at a recycle ratio of 0.9. Thus, the best value of recycle ratio for this process is set to be 0.9, and the remaining steam is used to generate power to achieve higher-energy efficiency.

![Figure 6. Effect of recycle ratio on system energy efficiency and F-T exergy destruction.](image)

6. Conclusion

In this work, a new system about co-production of liquid fuels and power by using coal and methane has been proposed by ASPEN PLUS software. The results show that the system model has outstanding advantages in work simplification, process regulation and energy utilization, and realizes the highly coordinated distribution and utilization of material, heat and electricity. At the same time, the target product can also meet the requirements of high quality. Several observations for the system model are summarized as follows:

(1) The energy efficiency of this coal and methane to co-produce liquid fuels and power generation system process achieves 52.5% based on designed conditions; this is a fact that the energy quality of coal has been improved greatly.

(2) The amount of coal input plays a decisive role in determining the material coupling and thermal coupling of the whole system. When the methane input is fixed at 0.1 kmol/s, the optimum system performance appears at 5 kg/s of coal input.

(3) Increasing F-T steam recycle ratio can enhance F-T conversion ratio, however, excessive recycle ratio results in huge exergy destruction in F-T synthesis process. Thus, a part of F-T steam is used to combust for power generation to improve energy utilization. And the recycle ratio is selected 0.9.

(4) Compared with separation systems of reference at the same product outputs, the energy efficiency of this novel system has been improved by 5.5% than that of conversional GTL process, and the PESR reaches to 30.4%.

7. References

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