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Study on co-feed and co-production system based on coal and natural gas for producing DME and electricity

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Abstract

China, an oil and NG scarcity country, is coal dependent, and this situation will remain for a long time. DME, as an ideal replacer of liquid fuel, is considered to develop. The efficient way of producing DME from coal is under research. Considering the components of coal and natural gas (NG), we choose co-feed (coal and NG) and co-production (electricity and DME) system (Co–Co system) to be studied on. Three systems which are the standalone system, co-generation system and Co–Co system are simulated by Aspen-Plus. The simulation results concerning material flows, exergy flows, CO_2 emission and the evaluation indexes are obtained. It is found that Co–Co system has higher exergy efficiency, higher economic benefit, and it is environmental friendly because of releasing the least CO_2.The analysis illustrates that Co–Co system has obviously advantage over the other two kinds of systems.

Keywords: Coal; Natural gas; DME; Co-feed and co-production; Simulation

1. Introduction

China has imported 136 million ton oil in 2005, and now it is the world's second-largest importer. However, China imports only 12% of the energy it consumes. But 12% has been too high for China [1]. Energy structure of China is characterized as "full of coal while lack of oil and natural gas". With the fast development, much more energy will be needed in the future. Although proportion of oil, natural gas and other clean energy sources in consumption is increasing year after year, coal still remains the most essential component of the energy mix. Coal, with important meaning, is the most important energy resource in China. It should be recognized that China is a coal dependent country and will remain for a long time. In coal utilization, the principal conflicts are overall enormous amount against low efficiency and demand of sustainable development against serious pollution. All of these can cause serious problems in both social and economic aspects.

How to utilize coal and to resolve oil scarcity has become a hot topic in both industrial and scientific research area. In oil consumption, automobile fuel takes the most part. Accordingly, resolving oil scarcity means in fact how to resolve fuel scarcity. Some reports [2,3] have proposed that DME (dimethyl ether, CH_3OCH_3) produced from coal can be taken as the replacer of liquid petroleum gas (LPG) and diesel. It is predicted that it is the one and the only carbon-based energy carrier in the long term next to electricity and hydrogen. DME is widely used for chemical product and clean fuel. Its cetane number (55–60) is even higher than diesel oil, having excellent compressibility; it goes with relatively low engine noise; it needs less oxygen intake during combustion; it has about the same mileage as diesel. It is the most superior candidate fuel for diesel motor. The liquid fuel market in China is growing very quickly compared to the rate of increase in liquid fuel production capacity. If DME price is reasonable and could replace LPG, about 19.2 million ton DME will be needed for China in 2010 [4]. Consequently, DME as a kind of clean diesel motor fuel is called an idea substitude for liquid fuel in 21st century.

How to produce DME from coal is being considered. Some people have suggested that integrated polygeneration system is an efficient way using limited resources to produce DME in energy conversion and end-use system. This integrated system is large and encompasses a number of options in the industry and energy sectors. These systems are flexible, amenable to the input of different raw materials and have the ability of cascading and recycling outputs in order to minimize environmental impacts.

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Nomenclature

ASU	air separation units
CC	co-production and co-feed system
DME	dimethyl ether, CH_3OCH_3
IGCC	integrated gasification combined cycle
MeOH	methanol, CH_3OH
NG	natural gas
OT	co-generation system
ST	the standalone system
UBC	unburned carbon

It has been proved that such polygeneration system producing DME, electricity and steam can realize more benefits in energy, economy and environment [5].

However, because coal is a kind of carbon rich material, C/H ratio of syngas from coal is much higher than that needed for producing DME. There are increasing concerns over the CO_2 emission effects of fossil fuel use in general, and coal in particular. In response to these problems, we suggest adding natural gas as hydrogen rich material to complement the use of coal as a feedstock. This means, C/H ratio can be adjusted by the ratio of coal and natural gas prior to synthesis according to the need of DME composing. Coal feedstock produces high carbon content syngas, while natural gas produces high hydrogen content syngas. It is a multi-feed and multi-product system, and is more efficient and incorporate. We name it co-feed and co-production system (Co–Co for short) based on syngas, using coal and natural gas as feedstock and co-producing electricity, heat and DME.

Based on such idea, a Co–Co system is built and simulated by Aspen-Plus. The potential energy, economic and CO_2 reduction advantages that can be realized through the development of the integrated, multiplex system are discussed. The simulation results indicate how such system is organized pursuing maximum benefit, and how it behaves in 3-E analysis including energy, economic and environmental aspects.

The remainder of this article is organized as follows. Section 2 illustrates the concept and technology of Co–Co system. Section 3 explains how to set up modular flowsheet and simulate the whole system by Aspen-Plus to get the simulation results for the following analysis. For comparing, another two systems, which are the standalone system and co-generation system, are simulated as well. Section 4 examines the systems from three aspects: energy, economy, and environment separately and furthermore from comprehensive analysis. Through such analysis, evaluation and some relative conclusions can be drawn out at last.

2. Concept and technology of Co–Co system

2.1. Conception

In co-feed and co-production system [6], natural gas is used to supplement the use of coal as one feedstock. The system gasifies coal and natural gas into syngas (mainly consisting CO and H_2) by gasification, and produces various productions based on syngas. Main products include: liquid fuel (DME, F-T fuel, methanol, etc.), electricity, heat, town gas and chemical products. Other more, H_2, a future fuel, and CO_2 can be produced through a gas shifting process and gas separation.

Few of high concentrated CO_2 (as high as 99%) can be used for carbon fertilization or other industrial utilization which means CO_2 could contribute to keeping captured CO_2 out of the atmosphere by storing in anthropogenic carbon products. Most of CO_2 can be sequestrated referring to the provision of a long-term storage of carbon. There are mainly three categories [7]. First is called underground geological sequestration like enhance coal-bed methane (ECBM), enhance oil recovery (EOR), enhance gas recovery (EGR), storage in abandoned oil and gas fields, and saline aquifer storage. The second is ocean storage, which means captured CO_2 could be deliberately injected into the ocean at great depth, where most of it would remain isolated from the atmosphere for centuries. And the other is mineral carbonation which means captured CO_2 is reacted with metal-oxide bearing materials, forming the corresponding carbonates and a solid byproduct, silica for example.

The configuration of Co–Co system is shown schematically in Fig. 1. Coal and natural gas, with water and pure oxygen, are converted into clean syngas by two steps as gasification and carbon and sulfur removal, and then made into different kinds of products.

Although Co–Co system may have many different patterns, all of them have a common character, taking gasification as the key technology. Sulfur, nitrogen, metal element, and particulate matter are all removed during gasification, in order to realize nearly "zero emission". Additionally, variety products are in series or parallel made from syngas. It is anticipated that such integrated system cannot only reduce investment, but can also use energy effectively and logically. It can gain benefits in energy, economy and environment, realizing concordant development of the 3-E aspects.

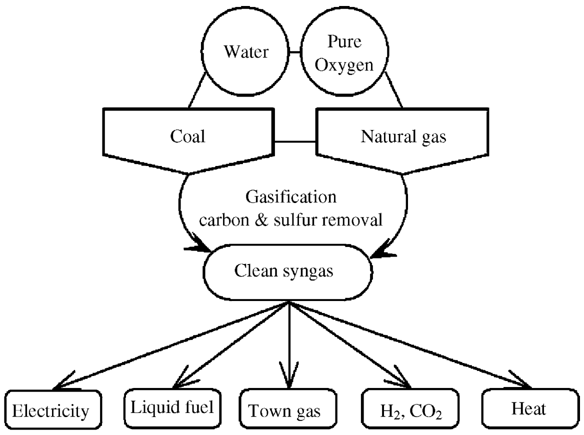

Fig. 1. Configuration of Co–Co system.

2.2. Gasification

Syngas can be produced from two kinds of feedstock by coal gasification and natural gas reforming. The gasification process is a well-established technology that converts feedstock to synthetic gas using steam and oxidant. Although there are many kinds of patterns or assembled modes, gasification, as the key technology, is necessary for any Co–Co system. And energy efficiency as well as investment of gasification plays an important role in evaluating polygeneration system's rationality and feasibility.

There are mainly three kinds of coal gasification technology [8,9]: spouted bed (Shell and Texaco), steam fluidized bed (KRW and U-gas) and fixed bed (BGL). In all of these technologies, spouted bed, developed by Shell and Texaco, is the best choice for Co–Co system for three reasons [10]. First, throughput of unit cubage is higher. Second, there are no tar and phenolic matter, with simple post treatment. And the last reason is inert slag is discharged with lower carbon content less than 1%.

Natural gas reforming technology [10], converting natural gas into syngas, is an important technology as well to utilize conventional resource. There are mainly four kinds of it: steam reforming, catalytic partial oxidation, partial oxidation and autothermal reforming. Through comparing among these technologies, autothermal reforming behaves the best and is applicable for Co–Co system. Its simple configuration achieves lower investment, and ratio of hydrogen/carbon can be adjusted in a wide range with favorable flexibility.

So in this article, spouted bed coal gasification and natural gas autothermal reforming are chosen to simulated and discussed in Section 3.

2.3. DME

DME is called clean diesel motor fuel in 21st century. Many research institutes, such as American Air Production & Chemical [11], Japanese NKK [12], and China Tsinghua University [13] dedicate in developing or improving DME production technology in industrialization in large-scale process. At present, DME production technology is mainly two-step process. It is limited by low conservation of CO because of thermodynamic equilibrium. A new one-step DME process has been developed by Tsinghua University and small-scale industrialization has been implemented [13]. Its primary character is combining both composing methanol by syngas and hydrolyzing methanol reactions, realizing one-step composing DME in slurry bed reactor. It is more convenient and efficient. So in this article, we will choose one-step DME synthesis technology in our proposed Co–Co system.

2.4. IGCC

Integrated gasification combined cycleI (GCC) produces power with theoretical highest efficiency through gas turbine and steam turbine by syngas from coal [14]. Its main process is "coal → gasification → syngas purification → gas turbine → steam turbine". The advantages of IGCC include [6]: considerable flexibility in fuel selection; advanced emissions control; improved thermal efficiency; better prospects for waste minimization. Many aspects of IGCC technology make plant sitting appreciably more flexible than that of conventional fire power plants.

However, only for generating electricity, the implementation of IGCC has met some barriers because of its higher investment and cost compared with traditional plants. Thus, its adoption and implementation has been limited in the near future, and its developing speed is lower than expected. IGCC should combine with other production systems to reduce its high investment and cost. In Co–Co system, IGCC is proposed to share infrastructures like gasification and raw gas purification, cutting the investment and cost. Only combined cycle section (gas turbine and steam turbine) are added in to use exhausted gas and residual heat, and this power generation section is simply simulated with the corresponding conversion and efficiency. Co–Co system with IGCC section is under detailed studied to see whether IGCC's advantages can be well represented.

3. Modular flowsheet and simulation

In this article, Aspen-Plus is used to simulate the whole systems. In order to explain how the Co–Co system behaves, we choose another two systems to be simulated: the standalone system (ST) which only produces DME and co-generation system (OT) which produces DME, electricity only based on coal. The consideration in this article is based on China's situation. Consequently, we do not choose the co-generation system (OT), which produces DME, electricity only based on NG, because energy structure of China is characterized as "full of coal while lack of oil and natural gas" as described before. But in the future, it is hoped that coal-bed gas can be utilized and replace NG, as technology developing. After feedstock is given, detailed data of each stream including components, temperature, pressure and enthalpy can be obtained for the following analysis.

3.1. Flowsheet simulation

Three kinds of systems including co-production and co-feed system (CC), the standalone system (ST) and co-generation system (OT) are simulated in our study. All the systems are divided into several parts called subsystem, as gasification, water gas shift, carbon and sulfur removal, synthesis and separation. Gasification model is classified into coal gasification and natural gas reforming. Fig. 2 presents the Co–Co system in which the whole system and subsystem modules are represented. All the models of each part are built in semi-mechanism model.

3.1.1. Coal gasification

The process of spouted bed coal gasification has been simulated with the method reported [15]. In our work, input data is based on Texaco and Shell technologies. First, coal is divided into three kinds of nonconventional matter as coal, ash and unburned carbon (UBC). Then nonconventional matter coal is decomposed in RYIELD model by element analysis and carbon conservation. After this, decomposed composition, decompos-

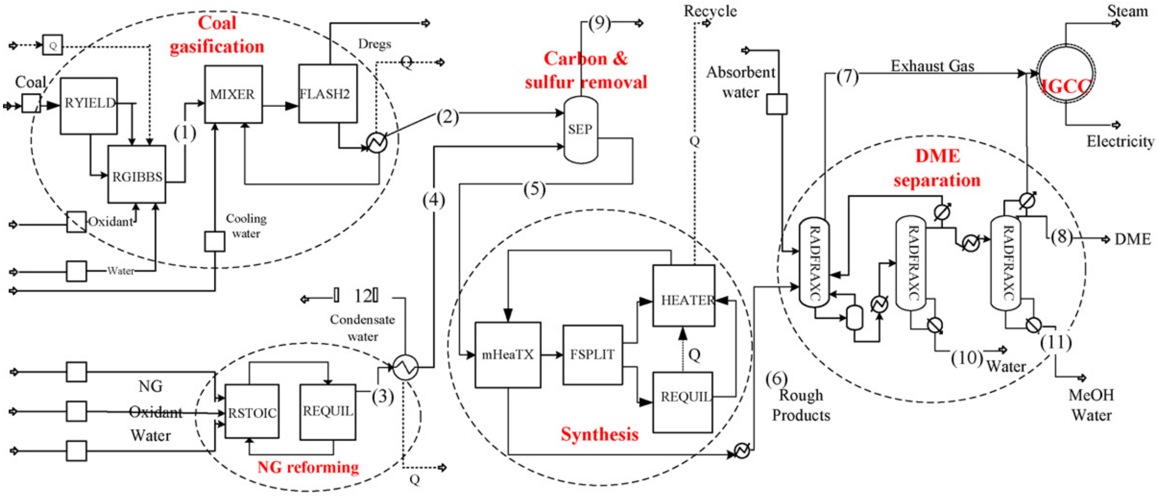

Fig. 2. Flowsheet for the simulation of DME·CC system.

ing heat, O_2, water, etc. are all fed into RGIBBS model. This model calculates chemical equilibrium by Gibbs energy minimization with certain thermal loss (Q-loss) for a given atomic population. At last, MIXER and FLASH2 models can separate raw syngas and dregs into two outlet streams using rigorous vapor liquid equilibrium calculation.

3.1.2. Natural gas reforming

Natural gas autothermal reforming can be simulated by RSTOIC and REQUIIL model [16]. In RSTOIC model which is used as the burning room, sub-stoichiometric burning reaction is realized using Eq. (1) [17] and it simulates stoichiometric reactor with specified reaction conversion. In model REQUIL, two parts can realize reforming reactions, as strong endothermic steam reforming Eq. (2) and weak exothermic water gas shift reaction Eq. (3).

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O \tag{1}$$

$$CH_4 + H_2O \rightarrow CO + 3H_2 \tag{2}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{3}$$

This REQUIL model performs chemical and phase equilibrium by stoichiometric calculation. It represents excessive methane and outputs are mixed together achieving autothermal reforming in catalyze bed.

3.1.3. DME synthesis

DME synthesis process can be described by three reactions as Eqs. (4)–(5).

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{4}$$

$$CO + H_2 \rightarrow CH_3OH \tag{5}$$

$$2CH_3OH \rightarrow CH_3OCH_3 + H_2O \tag{6}$$

DME synthesis is simulated by mHeaTX, FSPILT, REQUIL and HEATER model, according to reaction conversion and DME characters [18,19]. Inputs with defined H_2/CO ratio of 1 should pass through preheater (mHeaTX) exchanging heat first, and then enter reaction processes (FSPILT, REQUIL and HEATER). It is supposed that the synthesize reaction is under constant temperature and reactive heat is recycled by residual heat process. FSPLIT model divides feed steam based on splits specified for outlet steams, REQUIL simulates chemical and phase equilibrium by stoichiometric calculation and HEATER determines thermal and phase conditions of outlet steams.

3.1.4. DME separation

Raw output of DME is consisted by CO, H_2, CO_2 and DME, with little H_2O and MeOH. DME can dissolve in water or methanol easily. So complex DME separation can consist of three columns [20–22]. In Aspen-Plus, three RADFRAC models can express three column equipments. This model performs rigorous rating and designs calculation for single column. Water is chosen as absorbent to absorb DME in the first RADFRAC model. DME can be physical separated from water by rectification in the second RADFRAC model, and can be separated from MeOH in the third RADFRAC model. In this way, not only high-pure DME can be produced, but removed water can also be circularly used, avoiding wastewater pollution and reducing charge of public projects.

3.2. Feedstock

In the simulation, detailed components of coal and natural gas are necessary. Luzhou city, in south west of China, is rich in coal and NG. It is suitable for developing Co–Co system [23]. Hence, we take representative components of coal and NG in Luzhou as an example (Table 1). And all kinds of feedstock for Co–Co system are shown in Table 2.

3.3. Simulation results of DME·CC system

Through simulation and calculation by Aspen-Plus, data of each stream can be gain for the following analysis, as compo-

Table 1
Components of coal and NG in Luzhou [23]

Coal	Ash	C	H	N	S	O
Mass fraction (%)	22	64	4.3	1.1	3.6	5

NG	CH_4	CO_2	N_2	H_2S
Mass fraction (%)	98	0.6	1	0.4

Table 2
Feedstock for the DME·CC system

	Temperature (°C)	Pressure (bar)	Mass flow (kg/s)
Coal	30	68	1
$Oxidant_{coal}$ (94.3% mol O_2)	100	68	0.79
$Water_{coal}$	30	68	0.35
Cooling $water_{coal}$	20	68	1
Absorbent (water)	20	15	3.427
NG	300	25	0.160
$Oxidant_{NG}$ (94.3% mol O_2)	300	25	0.201
$Water_{NG}$	300	25	0.246

nents, temperature, pressure, enthalpy and so on. Table 3 lists the detailed simulation results of DME·CC system.

4. Analysis and evaluation

4.1. Energy analysis

When natural resource becomes economically scary, resource efficiency becomes a competitive advantage. Since there are two products (DME and electricity) with different exergy values, a second law (exergy) analysis could be used to compare among different systems. Exergy efficiency is identified as Eqs. (7) and (8).

$$\text{Exergy efficiency} = \frac{\text{output chemical exergy values} + \text{output electricity exergy values}}{\text{input exergy values}} \times 100\% \tag{7}$$

$$\begin{aligned}\text{Input exergy values} &= \text{input coal exergy value} + \text{input NG exergy value} \\ &\quad + \text{input water exergy value} + \text{input oxygen exergy value} \\ &\quad + \text{input electricity exergy value}\end{aligned} \tag{8}$$

Coal exergy value can be calculated by Eq. (9) [24].

$$\begin{aligned}\mathrm{Ex}_{\mathrm{Coal}}\,(\mathrm{CNHSO}) &= 34215.87\mathrm{C} + 21.97\mathrm{N} + 116702.76\mathrm{H} + 18260.36\mathrm{S} \\ &\quad - 13278.59\mathrm{O} - 298.15 \times 0.71768\mathrm{M} \\ &\quad + 0.6276\mathrm{O}\{32792.8\mathrm{C} + 141791.11\mathrm{H} \\ &\quad - 17723.84\mathrm{O} + 16019.49\mathrm{S}\}\ \mathrm{kJ/kg}\end{aligned} \tag{9}$$

Ex represents exergy value, and C, H, O, S, N, ash represent mass fraction of each element separately. Then we get the exergy value of raw coal as 27703.303 kJ/kg.

NG can be considered as gas fuel, and reaction exergy of fuel takes up a large proportion of chemical exergy. Then the exergy value of NG can be approximate calculated by caloric value as Eq. (10) [24].

$$\mathrm{Ex}_{\mathrm{G}} = 0.95 \times \mathrm{HHV} \tag{10}$$

HHV can be calculated by caloric value of combustible components multiply corresponding volume percentage. Using Eq. (10), exergy value of NG is 51742.396 kJ/kg.

Table 3
Calculation results of the DME·CC system

Mole fraction	1	2	3	4	5	6	7	8	9	10	11	12
CO	0.420	0.500	0.149	0.217	0.478	0.372	0.416	0.004	0.000	0.000	0.000	0.000
H_2	0.284	0.338	0.449	0.652	0.478	0.368	0.412	0.000	0.000	0.000	0.000	0.000
CO_2	0.102	0.120	0.071	0.103	0.013	0.116	0.122	0.061	0.906	0.000	0.000	0.000
H_2O	0.160	0.001	0.312	0.001	0.002	0.002	0.002	0.000	0.000	1.000	0.866	1.000
N_2	0.007	0.008	0.004	0.006	0.009	0.012	0.013	0.000	0.000	0.000	0.000	0.000
AR	0.012	0.014	0.007	0.010	0.015	0.020	0.023	0.000	0.000	0.000	0.000	0.000
CH_4	0.003	0.003	0.007	0.011	0.006	0.008	0.009	0.000	0.000	0.000	0.000	0.000
H_2S	0.012	0.013	0.001	0.001	0.000	0.000	0.000	0.000	0.089	0.000	0.000	0.000
COS	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.006	0.000	0.000	0.000
CH_4O	0.000	0.000	0.000	0.000	0.000	0.003	0.000	0.000	0.000	0.000	0.133	0.000
C_2H_6O	0.000	0.000	0.000	0.000	0.000	0.098	0.003	0.935	0.000	0.000	0.001	0.000
Mole flow (mol/s)	93.13	78.16	42.32	29.17	95.00	68.01	60.81	6.92	12.33	188.9	1.57	13.15
Mass flow (kg/s)	1.945	1.672	0.607	0.370	1.509	1.509	1.184	0.318	0.533	3.404	0.031	0.237
Temperature (°C)	1160	40	951	40	40	46	22	11	40	171	142	40
Pressure (bar)	68	68	25	68	68	57	6	6	68	8	6	68
Caloric value (MW)	18.28	18.25	6.66	6.66	24.31	22.59	13.90	8.55	0.60	0.00	0.14	0.00
Reaction exergy (kJ)	18,179	18,020	6659	6546	23,695	23,053	13,722	9178	870.7	1629	164.1	113.3
Diffusion exergy (kJ)	−325	−225	−136	−71.2	−213	−239	−181	−4.5	−10.2	0.0	−1.6	0.0
Temperature exergy (kJ)	2203	0.9	746.7	0.3	1.0	1.3	0.0	0.0	0.2	174.7	0.8	0.2
Pressure exergy (kJ)	971.1	815.0	336.3	304.2	990.6	679.4	268.1	30.5	128.5	967.7	6.9	137.1

Table 4
The values of Ex_0 and S_0 used for calculating water exergy

Temperature t (°C)	Pressure (bar)	Ex_0 (kJ/kg)	S_0 (kJ/kg/K)	Ex (kJ/kg)
20	68	13.18	0.4344	2.3
30	68	9.69	0.2949	2.3
300	25	1194.7	6.647	1028.5
20	15	4.42	0.296	−3.0
510	60	1557.6	6.9119	1384.8
200	5	926.8	7.0592	750.3

Table 5
Reference station of oxygen exergy value

Component	H_2	CO	CO_2	H_2O	N_2	H_2S	Ar	O_2
Fraction	0	0	0.0003	0.0312	0.756	0	0.0091	0.2034

Table 6
The exergy values of two kinds of oxygen

Component	O	N	Ar	Exergy value (kJ/mol)
1	0.943	0.012	0.045	3.6406
2	0.995	0.001	0.004	3.8910

Water exergy value can be calculated by Eq. (11) [25].

$$\mathrm{Ex} = \mathrm{Ex}_0 - 25 \times S_0 \tag{11}$$

Ex (kJ/kg) represents exergy value at some temperature and pressure; Ex (kJ/kg) and S_0 (kJ/kg/K) represent standard exergy value and standard entropy at some temperature and pressure, and their data can be searched and obtained as offered in Table 4 [25].

The exergy value of oxygen used for gasification actually is pressure exergy. When the system pressure is different from reference pressure, its exergy can be calculated by Eq. (12)

$$\mathrm{Ex}_\mathrm{p} = RT_0 \ln \frac{P}{P_0} \tag{12}$$

The reference station of oxygen is given in Table 5. Then we can get exergy values of two kinds of oxygen used as shown in Table 6.

Chemical exergy values can be obtained directly from Aspen-Plus simulation results. And electricity exergy value is actually equal to its electric quantity. Electricity consumption in the whole system can be divided into four parts, as ASU (air separation units), synthesis, recycle and others. And these four parts can be calculated by the following equations [26].

$$\begin{array}{lll} \text{ASU} & 94.5\%\ O_2 & \text{electricity consumption (MW)} = 1.35 \times O_2 \text{ mass flow (kg/s)} \\ [26] & 99.5\%\ O_2 & \text{electricity consumption (MW)} = 1.5 \times O_2 \text{ mass flow (kg/s)} \\ \text{Synthesis} & & \text{electricity consumption (MW)} = 0.002 \times \text{DME caloric value (MW)} \\ \text{Recycle} & & \text{work of cycle machine calculated by Aspen} \\ \text{Others} & & \text{electricity consumption (MW)} = 0.01 \times \text{material caloric value (MW)} \end{array} \tag{13}$$

Table 7
Exergy efficiency for DME synthesis systems based on 1 kg/s coal feed

System	CC	OT	ST	IGCC
Input				
Coal (kJ)	27703.303	27703.303	27703.303	27703.303
NG (kJ)	7832.356	0	0	0
H_2O (kJ)	245.440	−4.477	−22.229	2.320
O_2 (kJ)	684.863	544.068	521.362	544.068
Electricity (kJ)	1663.778	1311.626	1876.529	1000.000
Total (MJ)	38.130	29.555	30.079	29.250
Net output (MJ)				
Chemicals	9.204	6.603	14.953	0
Electricity	8.690	6.090	0.664	10.220
Total	17.894	12.693	15.617	10.220
Efficiency (%)	46.93	42.95	51.92	34.94

Table 8
Exergy efficiencies for DME synthesis systems based on same products

System	CC	OT (+IGCC[a])	ST + IGCC
Net output (MJ)			
Chemicals	9.204	9.204	9.204
Electricity	8.690	8.690	8.690
Total input (MJ)	38.130	41.773	42.215
Total efficiency (%)	46.93	42.84	42.39

[a] When the same chemical product is produced, OT produces less electricity than CC, as shown in front of parenthesis. So IGCC is added into calculation, and the result is shown in parentheses.

As IGCC system is complex, we did some simplified calculation. Referring typical IGCC systems made by Siemens, ABB and GE [27], efficiencies of gas turbine and steam turbine can be obtained. Comparing these data, efficiency of gas turbine is always between 0.3 and 0.35, while that of steam turbine is always between 0.25 and 0.3. Thus 0.33 for gas turbine and 0.285 for steam turbine are chosen to calculate electricity generation. And during the whole IGCC calculation, its process is “coal → gasification → syngas purification → gas turbine → steam turbine”.

By simulation and calculation, input and output exergy values, electricity consumption, and electricity generation are obtained. Then exergy efficiencies for different systems, based on same amount of coal feed, can be obtained and compared in Table 7. OT, ST and IGCC are all based on 1kg/s coal, while CC is based on 1 kg/s coal plus matching NG.

From Table 7, ST reveals the highest exergy efficiency. However, considering the exergy efficiency differences between electricity and chemicals, it is more practical to compare based on same outputs. Consequently, when producing the same amount of chemical and electricity, exergy efficiencies are calculated in Table 8. Conveniently, for comparing, OT and ST are assumed to add whole IGCC for producing the same electricity

Table 9
Data for equipment investments [31]

Equipment	Benchmark	Scale	Unit	Investment Benchmark (M$)	Size factor
Coal cleaning	Raw coal	27.4	kg/s	29.10	0.67
Coal gasification	Material caloric value	716	MW	61.90	0.67
NG reforming	Material caloric value	716	MW	61.90	0.67
Air separation unit	Pure O_2	21.3	kg/s	45.70	0.50
WGS	Material caloric value	1450	MW	39.30	0.67
H_2S removal	Element S	29.3	mol/s	44.44	0.67
COS removal	CO_2 absorption	2064.4	mol/s	32.80	0.67
S recycling	Element S	29.3	mol/s	22.90	0.67
Residual heat system and steam turbine	Outlet electricity	200	MW	94.70	0.67
Gas turbine	Outlet electricity	30.6	MW	58.83	0.67
DME·OT synthesize and separation	Feed gas	2910	Mol/s	36.79	0.65
DME·ST synthesize and separation	Feed gas	8680	mol/s	87.37	0.65

as CC. From Table 8, it can be clearly seen that CC system has the highest exergy efficiency, about 5% higher than ST + IGCC. And OT and ST + IGCC are near to each other.

4.2. Economic analysis

Whether Co–Co system can be received and applied in chemical industry in the future mostly lies on whether the system can bring economic benefit. Accordingly, it is necessary to make economic evaluation. In our study, investment and cost are analyzed.

4.2.1. Static system investment

Investment budgetary is estimated by plant cost index [28] and exponential coefficient method as Eq. (14).

$$\text{Equipment investment} = \text{domestic made factor} \times \text{investment} \times \left(\frac{\text{equipment capacity}}{\text{basic equipment capacity}}\right)^{n} \qquad (14)$$

Exponent n is related with kinds of equipment. When large sale is realized by parallel small scales, the exponent is usually set to be 0.85–0.90. Static system investment is calculated by adding up all the separate equipments. Table 9 offers the data for equipment investments. In our work, domestic-made factor is set to be 0.65 [29,30]. Besides fixed investment [31], all the other unexpected investment is set together as 20% of total investment. In order to compare the investment of CC, OT and ST systems when the same DME and electricity are produced, whole IGCC is added into ST as "ST + IGCC", and so is OT system. Then we get the following Fig. 3 to compare the investment at different DME outputs of 5, 25, 50 and 100 × 10^4 t/year separately.

From Fig. 3, it is clear to find that the investment will increase as the output increases. Although the investment of ST is much lower than that of the other systems, the point is, when the same amount of chemical and electricity is produced, OT and CC are lower than ST plus IGCC. In other words, OT and CC are better than ST plus IGCC. In order to explain why investment of ST + IGCC is much higher, Fig. 4 summarizing subsystems investment of each system is given. Gasification is consisted of coal pretreatment, coal gasification and natural gas reforming; synthesis is consisted of water gas shift, carbon and sulfur removal, product synthesis and separation. It can be found the reason why ST + IGCC spends more investment is because of its investment of gasification equipment, while CC spends much lower investment without water shift equipment.

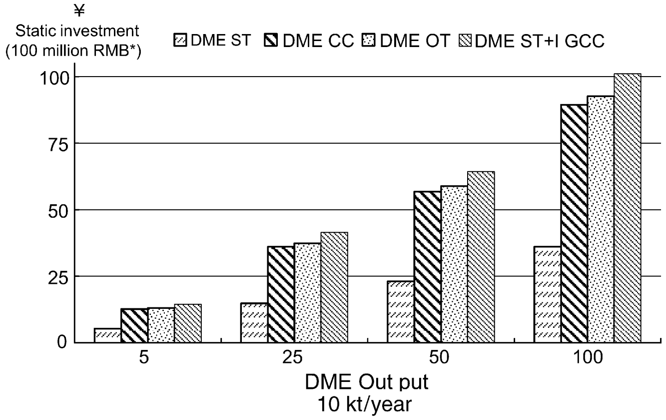

Fig. 3. Different DME system investments. RMB*: The exchange rate of RMB against the US dollar ranged from 8.0608 to 7.8087, and against the euro ranged from 9.8447 to 10.2665 in 2006.

4.2.2. Cost of DME

Besides investment, the cost of product is similarly an important index to evaluate a process or system in practical project. In

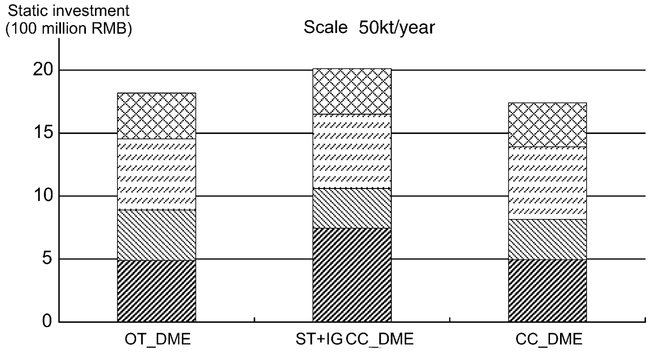

Fig. 4. DME subsystem investments analysis (50 kt/year) (▨, gasification; ▧, composing; ▤, electricity; ☒, others).

Table 10
Material cost

	Coal	NG	Water	Electricity
Unit	RMB/t	RMB/N m^3	RMB/t	RMB/kWh
Price	200	0.6	2	0.30

this article, cost is calculated by Eqs. (15) and (16).

DME product cost

$$= \frac{\text{annual investment} + \text{material charge} \\ + \text{maintenanc charge} - \text{electricity income}}{\text{DME product output}} \quad (15)$$

Annual investment

$$= \text{investment} \times \text{capital recovery factor (CRF)},$$

$$\text{CRF} = \frac{i}{1-(1+i)^{-n}} \quad (16)$$

n means useful life, and is set to be 25, while i means discount rate, and is set to be 0.1 in our calculation. Material cost is offered in Table 10, and maintenance expense is 4% of the total investment. When material cost is the same, costs of chemical product and IGCC electricity generation with reasonable limits in the small size field are calculated under different electricity capacities (see Fig. 5). Fig. 5 compares different chemical output scales of DME at 5, 25, 50 and 100 × 10^4 t/year separately. From this figure, we can see as the scale is bigger, the cost decreases sharply for each system. It is clear that ST is better than OT and CC when the scale is not big enough.

"coal → gasification → syngas purification → gas turbine → steam turbine" is the process of whole IGCC considered. We can calculate static system investment using Eq. (14), and the cost of electricity from IGCC similarly to DME, considering electricity as the only product. Fig. 6 shows the cost of the electricity from IGCC. As illustrated in Fig. 6, it can be found that when the capacity of IGCC electricity generation is bigger, the cost of electricity from IGCC decreases obviously. Thereupon, when the DME scale is big enough, as big as over 25 × 10^4 t/year, the DME cost of OT and CC can be lower, and will reveal advantage gradually.

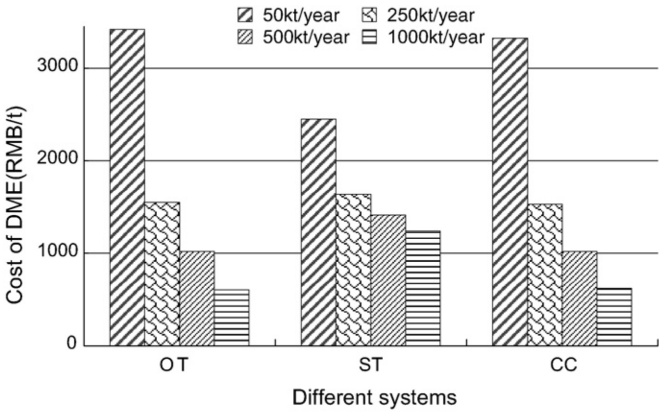

Fig. 5. DME cost of different systems.

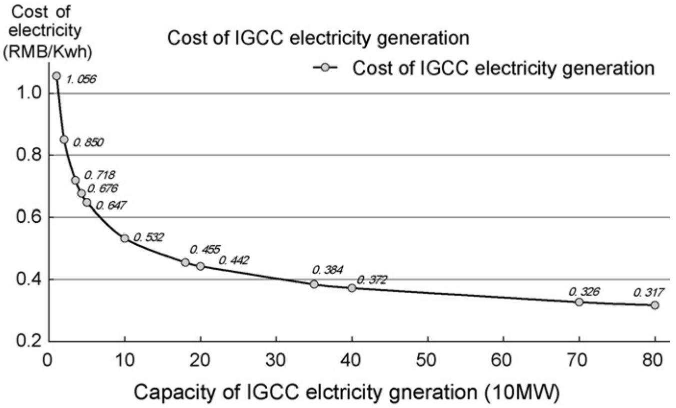

Fig. 6. Cost of the electricity from IGCC.

Thus, only considering economic factors upwards, CC system should be the best choice.

4.3. Environmental analysis

Much use of fossil energy causes great environmental pollution, especially great greenhouse gas emissions like CO_2. Therefore, study on the amount of CO_2 emission has great meaning in environmental analysis. In our study, it is supposed that CO_2 removed is not utilized, and emission ratio of CO_2 is identified as Eqs. (17) and (18).

Emission ratio of CO_2

$$= \frac{\text{carbon element amount in emission } CO_2}{\text{carbon element amount in feedstock}} \times 100\% \quad (17)$$

$$\text{Emission } CO_2 = CO_2 \text{ removed} + CO_2 \text{ in tail gas} \quad (18)$$

In order to predict the CO_2 emission amount in ST + IGCC system, CO_2 emission factor of IGCC is set to be 0.9159 kg CO_2/kWh, and coal consumption of IGCC is set to be 0.3903 kg coal/kWh.

Under the same scale of 5 × 10^4 t/year, Fig. 7 gives comparison of CO_2 emission among three systems. Although IGCC system cannot use CO_2 effectively, OT and CC can absorb CO_2 during synthesis inherently after DME water shift process. From Fig. 7, it is obviously that comparing with other two systems; CC system releases the least amount of CO_2, being the most

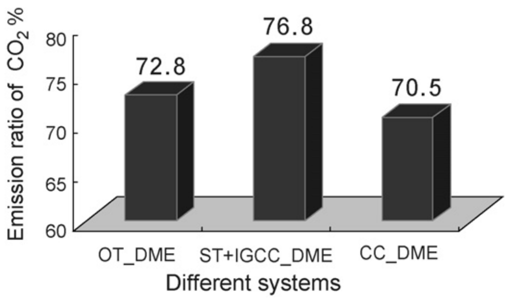

Fig. 7. CO_2 emission ratio of three systems.

Table 11
Normalization indexes of evaluation among different DME systems

Item		Energy index (1/3)	Economic index (1/3)			Environmental index (1/3)	Comprehensive evaluation
System	Scale (10^4 t/year)	Thermal efficiency	Investment (0.5)	Cost (0.5)	Total index	Emission ratio of CO_2	
CC	5	1	1	0.1	0.55	1	0.85
	25	1	1	1	1	1	1.00
	50	1	1	1	1	1	1.00
	100	1	1	0.98	0.99	1	1.00
OT	5	0.123	1	0	0.5	0.63	0.42
	25	0.123	0.8	0.81	0.805	0.63	0.52
	50	0.123	0.71	1	0.855	0.63	0.54
	100	0.123	0.67	1	0.835	0.63	0.53
ST + IGCC	5	0	0	1	0.5	0	0.17
	25	0	0	0	0	0	0
	50	0	0	0	0	0	0
	100	0	0	0	0	0	0

environmental friendly. With no environmental policy considered, effective CO_2 emission reducing can be realized directly and effectively.

4.4. Comprehensive analysis

Different single indexes illustrate different aspects. However, single index cannot delegate the whole situation. To quantify the overall advantages of CC system, it is necessary to compare it by a comprehensive index. We have analysis the CC system from three different aspects, including energy, economy, and environment, comparing with the other two systems. Then we try to choose a normalization index combining them.

For those indexes that are as bigger as better, we use Eq. (19). And for those indexes that are as lower as better, we use Eq. (20).

$$I' = 1 - \frac{\max(\mathbf{I}) - I}{\max(\mathbf{I}) - \min(\mathbf{I})} = \frac{I - \min(\mathbf{I})}{\max(\mathbf{I}) - \min(\mathbf{I})} \qquad (19)$$

$$I' = \frac{\max(\mathbf{I}) - I}{\max(\mathbf{I}) - \min(\mathbf{I})} \qquad (20)$$

If considering the scale is an important aspect in economic analysis, there are total 12 kinds of choices, which are under different scales of different systems for evaluating. However, when the scale increases, the investment will increase and the cost will decrease naturally. So in this article, such normalization is considered among different systems under the same scale. Table 11 lists the results of the comprehensive index as the integration of weighted 3-E indexes. The weights of investment and cost are both set to be 0.5, and energy, economy and environment is considered equally.

Then we get Fig. 8, comparing the comprehensive evaluation indexes intuitively. From this figure, results presents that comprehensive evaluation index of CC under the same scale is always higher than that of OT and ST + IGCC obviously. Further, OT system is always the second one. Although CC production cost is nearly the most expensive one when the scale is 5×10^4 t/year, its total economic index is still the best one under this scale. Additionally, as the scale is bigger (over 25×10^4 t/year), CC system behaves better. A conclusion can be drawn that CC system has more advantage when exergy efficiency, investment, cost and emission ratio of CO_2 are considered simultaneously, comparing with OT and ST + IGCC.

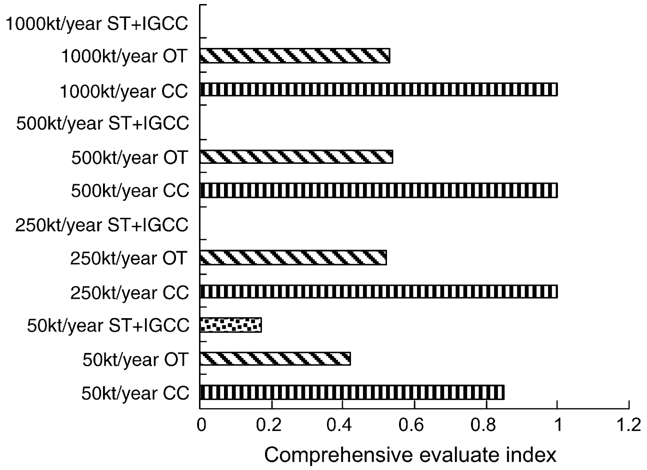

Fig. 8. Comprehensive evaluation indexes of each DME system.

5. Conclusions

The concept of Co–Co system is proposed and evaluated in this article. Coal, carbon rich material, is combined with natural gas, a hydrogen rich material as feedstock. Then standalone system for DME, co-generation system for DME and electricity, and the co-feed (from coal and NG) and co-production system for DME and electricity are simulated and discussed. All concerning systems are divided into subsystems. And different advanced technologies are discussed and chosen including one-step DME synthesis and IGCC.

All the system consisting of several unit processes have been built with the software Aspen-Plus on the basis of analyzing key technologies. And simulation results concerning material flows and exergy flows of the systems are obtained. Those data are in fact necessary and the base for the subsequent analysis.

Whether a system is practical and whether it is promising should be proved by actual data and analysis. 3-E analysis is considered in this work, including energy, economy and environment. Through analysis and comparison, we can get four conclusions on this. First, Co–Co system has higher exergy efficiency when producing the same electricity and chemical product. Second, it has higher economic benefit, and such advantage is clearer when the scale is as big as over 25×10^4 t/year. Third, Co–Co system is environmental friendly releasing the least CO_2 when CO_2 removed and CO_2 in tail gas are all considered. Besides, OT and CC can absorb CO_2 during synthesis process. Then comprehensive evaluation index is calculated at last. Co–Co systems under different scales all reveal the best benefit in overall.

From all the analysis results, it illustrates that Co–Co system has obviously advantages over the other two systems, standalone system for DME + IGCC (ST + IGCC) and co-production system for DME and electricity (OT). Such as described, it has high resource utilization efficiency, and is much more environmental friendly. Further, Co–Co system can be used to produce DME as fuel to mitigate the energy source problem in China in the future. With the fast development of China and much more requirement for energy, it can be expected that such Co–Co polygeneration system can lead to new opportunities for the commercialization of advanced coal utilization generation, and will play an important role in research area and practical industry in the near future.

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