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Simulation for Separation and Conversion Energy Consumption of Shale Gas

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Shale gas is an unconventional gas existing in organic-rich shale formations. The world is in a new energy revolution due to abundant shale gas reserve and thus its conversion and utilization has been a hot research topic in the field of chemical industry. Similar to natural gas, the primary component of shale gas is methane, with a little other alkane especially ethane, carbon dioxide and nitrogen. Through separation and conversion, the stream mainly contains methane can be the substitute of natural gas while that mainly contains ethane can be applied to produce ethylene by cracking reaction. So estimating the energy consumption for the aforementioned separation and conversion is of great significance to the application of shale gas. This paper carries on the research by establishing a shale gas separation and conversion process and performing a simulation by Aspen Plus and Aspen Hysys software. The total consumption is obtained by the simulation and heuristic energy integration is considered in this paper. The data indicates that this design is an energy saving process. The result of this paper can be a reference to practical shale gas separation and conversion energy consumption in chemical industries.

1. Introduction

With the relationship between natural gas supply and demand is becoming tenser, exploitation and utilization of unconventional gas has got intensively attention in recent years. Unconventional gas especially shale gas served as a new alternative energy is bringing convenience to energy requirement of the whole world. The primary differences between modern shale gas and conventional natural gas development are the extensive use of horizontal drilling and multi-stage hydraulic fracturing (Arthur, 2009). Besides, the success of the exploration technology has led to the rapid yield of commercial shale gas in many countries and increasing estimation of global natural gas reserves (Gregory et al., 2010). Shale gas mainly distributes over regions of North America, East Asia, North Africa and Australia (Xiao and Chen, 2015). North America is the only place that has realized large-scale shale gas commercialization, and shale gas rose from less than 1 % of domestic gas production in the United States in 2000 to over 20 % by 2010 (Stevens, 2012). According to Chen et al. (2011), there is abundant shale gas reserve in China. It is prospect to help China reduce natural gas import and CO_2 emission meanwhile (Chang et al., 2016). Though it is full of challenges for shale gas industry in China, the government still supports its development and offers subsidies (Hu and Xu, 2013). Thus, the great resource potentiality makes energy chemical industries full of expectations.

Usually, about 75 %-90 % component in shale gas is CH_4, and the remaining species vary from area to area and even well to well in the same area (He and You, 2015), but always are some or all of following constituents: natural gas liquids (namely NGLs that contains C_2H_6, C_3H_8, C_4H_{10},C_{5+}), acid gases (mainly CO_2 and H_2S), N_2, He and H_2O. In the U.S., it has been reported that most of the shale gas is rich in ethane and other NGL content whose market values are far higher than sales gas (mainly CH_4). Especially, due to economic and environmental advantage over naphtha, 99 % of the ethane from NGLs is used to produce ethylene (He and You, 2014). Thus, the process of shale gas separation and ethane cracking can take full advantage of shale gas and improve economic efficiency.

There is already research on developing novel shale gas processing to achieve the target of energy efficient and cost reduction. He and You (2014) designed a process integrating shale gas processing and bioethanol

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dehydration. Khojasteh et al. (2015) presented a process producing ethylene and electricity through methane oxidative coupling from shale gas. He and You (2015) developed such a process including three parts: shale gas sequential processing (SSP), ethane cracking gas recycling to NGLs recovery (CRN) and cracking gas recycling to dehydration (CRD). However, they did not focus on detailed energy conservation of the process.

This paper built components separation and ethane cracking processes for shale gas utilization and simulated them using Aspen Plus and Aspen Hysys. Meanwhile, heuristic heat integration is considered to conserve energy. The research is on shale gas integrated utilization and aims to conserve energy consumption of the process, so as to obtain a more effective process to utilize shale gas resource. This study can be primary insight to further research and future industrial application.

2. Process Simulation

2.1Simulation for separation process

This part of work aims to get the energy consumption of process separating ethane and propane from methane by simulation. Literature about separation process for shale gas is limited. Natural gas liquefaction process (Gu et al., 2003) and light hydrocarbon recovery process (Shang, 2006) that have been used practically can be the reference of this process simulation. The separation process method employed in this paper is cryogenic separation that is commonly applied in natural gas industry. The cryogenic separation process mainly contains three parts: heat transfer process, throttling expansion or adiabatic expansion process and cryogenic distillation process. A flow sheet of separation process for a specified material composition should be set up according to practical process and the whole process is shown in Figure1.

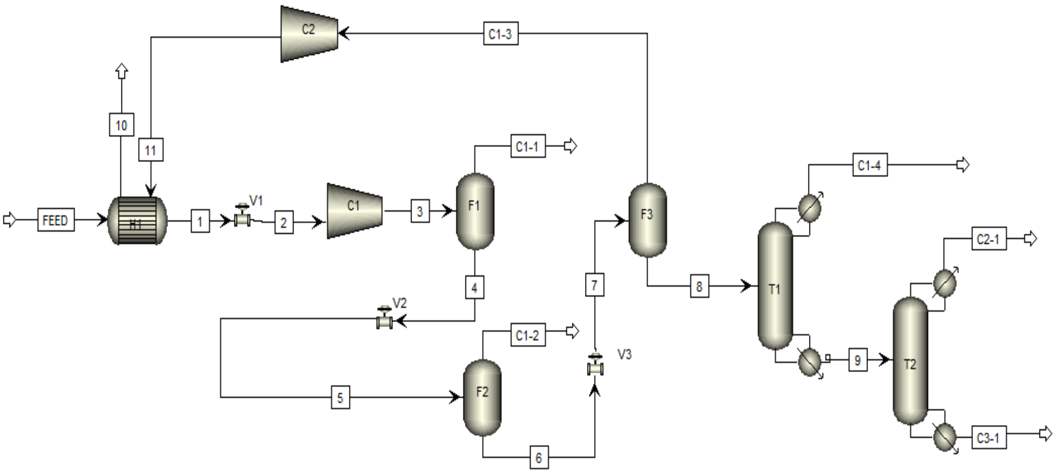

Figure 1: Process of shale gas cryogenic separation

Table 1 is the feed composition of shale gas (Xiao and Chen., 2015), feed pressure and temperature is 5 MPa and 40 ℃, the volume flow rate of the feed is 2,704 m^3/d. This process contains a heat exchanger (H1), two compressors (C1 and C2), three valves (V1, V2 and V3), three flashes (F1, F2 and F3) and two rectifying columns (T1 and T2). The feed is precooled by exchanger (heat transfer process). Then material flow 1 gets low temperature and low pressure by throttling of V1. After be compressed by C1, the material flow 3 is separated to two phases by flash vessel F1, the vapor phase C1-1 mainly contains methane while liquid phase is sent to next two throttling (V2 and V3) and phase separation units (F2 and F3) and get two other vapor phases C1-2 and C1-3 whose major component is methanol as well (throttling expansion process).The liquid phase (Material 8) is separated to C1-4, C2-1, C3-1 that mainly contains methane, ethane and propane respectively by rectifying column T1 and T2 (cryogenic distillation process). The process is simulated by Aspen Plus. Considering that the most part of energy consumption usually produced by compressors and rectifying columns, Table 2 provides the main parameters of these two kinds of equipment. Table 3 shows the separation results and the energy consumption data is shown in Table 4.

It can be seen that in such flow sheet, the three useful and key components methane, ethane and propane are separated individually with high recoveries.

Table 1: Feed composition

Components	Mole fraction(%)
CO_2	0.1
N_2	0.4
CH_4	79.4
C_2H_6	16.1
C_3H_8	4

Table 2: Main parameters of equipment

Parameters	Blocks		Parameters	Blocks	
	T1	T2		C1	C2
Number of stages	20	20	Discharge pressure(MPa)	4.5	0.5
Reflux ratio	2	2	Discharge Temperature (℃)	-69	-148
Distillate to feed ratio	0.30	0.79			

Table 3: Separation results

		Methane				Ethane	Propane
		C1-1	C1-2	C1-3	C1-4	C2-1	C3-1
	CO_2	0.036	0.018	0.002	0.029	0.584	0
Mole	N_2	0.812	0.622	0.185	0.009	0	0
Fraction	CH_4	93.956	97.055	99.437	99.051	0	0
(%)	C_2H_6	4.791	2.230	0.375	0.911	0	0
	C_3H_8	0.405	0.075	0. 001	0	0. 435	1
Temperature℃		-69	-94	-148	-144	-89	-41
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Liquid
Total flow m^3/h		11.970	40.602	575.732	221.127	577.431	0.00696

Table 4: Energy consumption results

Equipment	Blocks	Energy consumption(kW)	
Rectifying column		Condenser	Reboiler
	T1	183.65	289.89
	T2	306.34	459.39
Compressor	C1	432.31	
	C2	127.77	
Heat exchanger	H1	210.10	
Flash vessel	F1	0	
	F2	1.19	
	F3	1.84	

It can be concluded that the total energy consumption of this process is about 2,012.45 kW while in the process designed by He and You (2015) the shale gas process total consumption is about 11,665 kW using the same feed flow rate. Although the process in this paper is simpler, the important separation process takes up only 17 % of the mentioned literature. Though without systematic heat integration, this process can probably be expected better.

2.2 Simulation for ethane cracking process

Through previous separation the ethane product C2-1 got a high purity (up to about 0.99). However, economic value of ethane is much lower than ethylene. Using ethane to produce ethylene has the advantage of high productivity and less byproduct compared with other material. Thus, this paper uses the ethane product in shale gas separation process C2-1 to produce ethylene and get the high value byproduct H_2 in the meanwhile.

Ethane cracking process is so complicated that there is no literature can specify a practical condition that can achieve the highest conversion ratio of ethane or highest yield of ethylene. This paper will set up a kinetic model of ethane cracking reaction according to related literature and simulate the reaction process by Aspen Hysys.

According to Sundaram and Forment (1977), the reaction kinetics equations of this cracking reaction are listed below:

$$C_2H_6 \xrightleftharpoons{k_1} C_2H_4 + H_2 \tag{1}$$

$$2C_2H_6 \xrightarrow{k_2} C_3H_8 + CH_4 \tag{2}$$

$$C_3H_8 \xrightarrow{k_3} C_3H_6 + H_2 \tag{3}$$

$$C_3H_8 \xrightarrow{k_4} C_2H_4 + CH_4 \tag{4}$$

$$C_3H_6 \xrightleftharpoons{k_5} C_2H_2 + CH_4 \tag{5}$$

$$C_2H_2 + C_2H_4 \xrightarrow{k_6} C_4H_6 \tag{6}$$

$$2C_2H_6 \xrightarrow{k_7} C_2H_4 + 2CH_4 \tag{7}$$

$$C_2H_6 + C_2H_4 \xrightarrow{k_8} C_3H_6 + CH_4 \tag{8}$$

In the equations above, k is the reaction rate constant.

Due to the limit of kinetic model, it is impossible to know the product distribution of the ethane cracking reaction. But it can be predicted through choosing reaction models. Froment et al. (1976) predicted a product distribution by reaction models listed following:

$$C_2H_6 \xrightleftharpoons{k_1} C_2H_4 + H_2 \tag{1}$$

$$2C_2H_6 \xrightarrow{k_2} C_3H_8 + CH_4 \tag{2}$$

$$C_3H_6 \xrightleftharpoons{k_5} C_2H_2 + CH_4 \tag{5}$$

$$C_2H_2 + C_2H_4 \xrightarrow{k_6} C_4H_6 \tag{6}$$

$$C_2H_6 + C_2H_4 \xrightarrow{k_8} C_3H_6 + CH_4 \tag{8}$$

The data of activation energy E and frequency factor A in the models above are shown in Table 5 (Gujarathi et al., 2009).

Table 5: Data of activation energy E and frequency factor A

Reaction equations	A (sec-1)	E(kcal/kmol)
$C_2H_6 \xrightleftharpoons{k_1} C_2H_4 + H_2$	4.65×1013	65,210
$2C_2H_6 \xrightarrow{k_2} C_3H_8 + CH_4$	3.85×1011	65,250
$C_3H_6 \xrightleftharpoons{k_5} C_2H_2 + CH_4$	9.81×108	36,920
$C_2H_2 + C_2H_4 \xrightarrow{k_6} C_4H_6$	1.03×10^{12}	41260
$C_2H_6 + C_2H_4 \xrightarrow{k_8} C_3H_6 + CH_4$	7.08×1013	60,430

This paper chose tube furnace to simulate according the reactor model put forward by Froment et al. (1976). The process is shown in Figure 2.

The reactor inlet temperature and pressure are 680 ℃ and 303 kPa, dilution factor of the reactor is set as 0.4. Reactor model used in Hysys is three plug flow reactors. The flow rate and constitution of the feed refer to the data of material C2-1 shown in Table 1. In this process, the function of water is to inhibit coking. The constitution of product is related to many factors, and the reaction model is determined above with the product distribution and productivity conforming with that in the literature (Froment et al., 1976). This simulation studied the relationship between the ethylene yield and the length of each reactor (suppose that three reactors are in the same size) and got a fit curve shown in Figure 3.

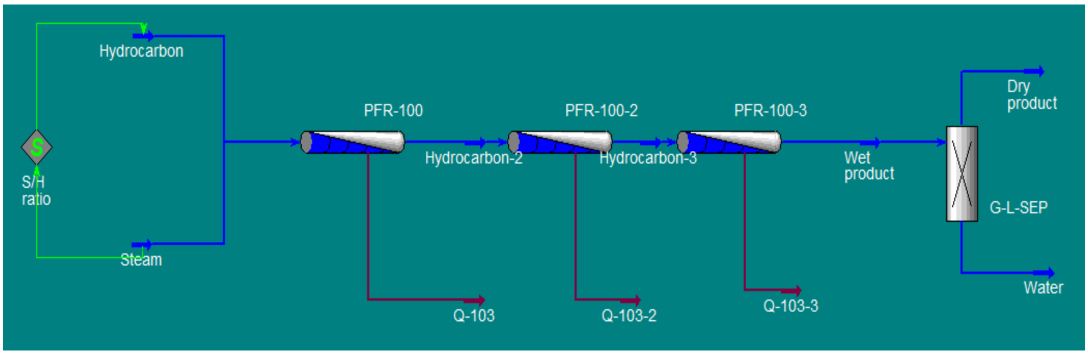

Figure 2: Ethane cracking process

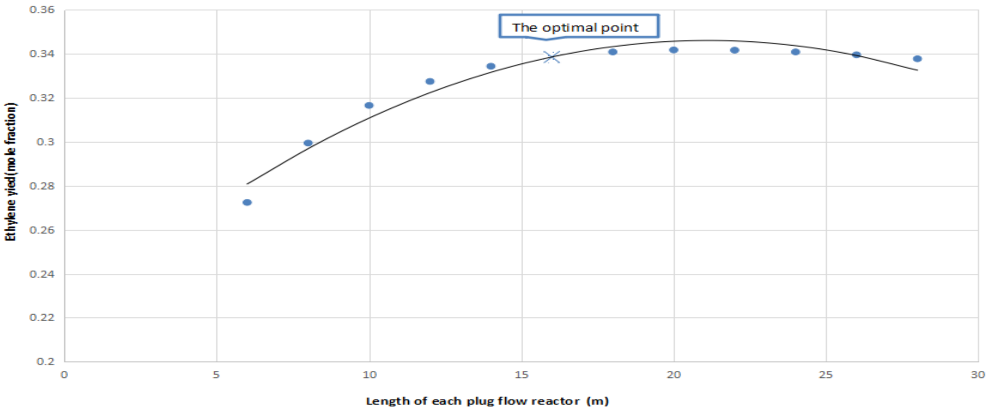

Figure 3: Relationship between ethane mole fraction and reactor length

It can be seen from the figure that when the length of reactor is less than 20 m, the ethylene yield increases with the increasing of length. However, when the length is larger than 20 m, the circumstances is just the opposite. Besides, it is obvious that when the length is between 16 - 20 m the growth of ethylene mole fraction is slow. Therefore, to ensure a reasonable ethylene productivity and decrease the investment, the simulation sets length of each plug flow reactor at 16 m (the overall length is 48 m), this setting is at the total flow of 34.928 kmol/h which conforms to the data got by Froment et al. (1976). (the overall length is 95 m while the total flow is 75.07 kmol/h), and the optimal point is highlighted in Figure 3. In this condition product distribution of the react is shown in Table 6 and the total energy consumption of this reacting process is 1,082.7 kW.

Table 6: Products distribution

Product	Mole fraction (%)	Product	Mole fraction (%)
Methane	4.76	Hydrogen	38.20
Ethylene	33.9	Propane	0.46
1,3-Butadiene	1.94	Ethane	20
Acetylene	0.26	Propene	0.18
CO_2	0.36		

2.3 Heuristic energy integration

Through simulation, this paper gives the energy consumption of shale gas separation process (2,012.45 kW) and ethane cracking process (1,082.7 kW). The result of total energy consumption is 3,095.15 kW.

To reduce the utilities and the investment cost, it is necessary to consider energy integration in this whole separation and reaction process. Since there are a few heat exchangers and columns, the energy conservation strategy involved in this paper is heuristic heat integration including three parts listed below:

(1) In the separation part, most precooling method previous works adopted are propane cycle refrigeration. Considering the low temperature of the product, this work uses one of the product C1-3 to precool the feed.

(2) For the condenser of rectifying column T2 is giving out heat in -89 ℃while flash vessel F2 is absorbing heat in -94 ℃, so the heat released by T2 can be used to afford to F2.
(3) In the reaction process, it is practicable to use the product except ethylene and hydrogen as the fuel to provide heat to reactor.

3. Conclusions

The shale gas separation and ethane cracking process were simulated by Aspen Plus and Aspen Hysys respectively in this paper to estimate overall energy consumption. Besides, possible heuristic energy integration is considered to conserve energy. Compared with existing process, this paper can save energy on the basis of the same throughput. The important point of this paper is the exploration of shale gas utilization which considers shale gas separation and ethane cracking process together, and the result can perform as reference to further practical industrial production.

Acknowledgments

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