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Design concept for coal-based polygeneration processes of chemicals and power with the lowest energy consumption for CO_2 capture

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ABSTRACT

Single coal based chemicals production processes emit large amount of CO_2 during conversion of the syngas to the high H_2/CO ratio feed gas for chemicals synthesis. However, the feed gas is with a low CO_2 molar fraction, leading to high energy cost for CO_2 capture. In this work, we try to reduce energy consumption for CO_2 capture by improving its molar fraction. A new methanol and power polygeneration process is designed and analysed based on process modeling and simulation. The hierarchical conceptual design methodology is introduced to design the polygeneration more reasonably. In this process, the shifted syngas exiting from the water gas shift unit first goes into the CO_2 capture unit to remove CO_2. Then, the purified H_2-rich syngas is mixed with the unshifted syngas and fed into the methanol synthesis to produce methanol. Then, unreacted syngas out from the methanol synthesis unit is moderately recycled to use, while the rest is used to generate power. Energy consumption for CO_2 capture of the polygeneration process is 0.7 GJ/t-CO_2, which is a 40.6% reduction compared to that of the single coal-to-methanol process and a 22.2% reduction to that of coal-to-hydrogen for power generation process. Techno-economic analysis shows that energy saving ratio and primary cost saving ratio are 16.5% and 13.2%, respectively.

1. Introduction

Coal is the dominant resource for chemicals production or power generation in China. This is as known due to lack of natural gas and oil. This energy structure brings severe green house gas (GHG) emissions since the production processes transfer carbon rich resource to hydrogen rich product or to power [1,2]. According to reports, CO_2 emission of a coal-to-methanol (CTM) process is about 3.85–4.3 t CO_2/t-methanol and that of an IGCC process is 0.68–0.85 t/MW h [3,4]. Carbon capture and storage (CCS) technology is broadly accepted as a feasible approach to reduce CO_2 emission [5]. However, a CCS process adds large amount of energy consumption and increases operational cost much. In the CCS process, energy for CO_2 capture takes the largest proportion, accounting for 70–80% of the total. For example, the energy efficiency of an IGCC plant with CO_2 capture is 10 percentage points lower than that of the original IGCC [4].

Increasing CO_2 molar fraction can effectively reduce energy for CO_2 separation. Zhang et al. [6] studied energy consumption for CO_2 capture using membrane separation process. Results showed that the energy for CO_2 capture was reduced from about 1.8 GJ/t to 0.1 GJ/t CO_2 as the molar fraction increases from 0.025 to 0.5, as shown in Fig. 1.

Some research attempts to increase the CO_2 molar fraction in coal based chemical process, Li et al. [7] proposed a coal based natural gas (SNG) and power polygeneration process. Coal based syngas is sent directly to the methanation reactor to produce SNG without H_2/CO ratio adjustment. The active gas is reacted and the molar fraction of CO_2 is increased after the reaction. The unreacted gas is separated and the corresponding energy for the CO_2 separation is reduced. This theoretical process seems reasonable to reduce the energy for CO_2 capture. However, the syngas with an insufficient H_2/CO ratio is not suitable for SNG synthesis, leading to catalyst deactivation and a low reaction rate. In this case, the loss in product yield outweights the energy saving from CO_2 capture.

As to a coal based chemicals synthesis process, the original H_2/CO ratio is only about 0.7. The H_2/CO molar ratio is increased by the water gas shift (WGS) reaction and prepare for chemical synthesis. For methanol synthesis, the ratio has to be increased up to 2.0–2.1, while to 3.1–3.3 for SNG synthesis [8,9]. In the WGS unit, part of CO is converted to CO_2 and the same amount of H_2 is produced. After the adjustment, the ratio is sufficient for chemical synthesis. CO_2 in the syngas is then separated. However, the CO_2 molar fraction is as low as 31%. The energy for CO_2 capture is high 1.07 GJ/t-CO_2 [10]. As for coal based hydrogen power generation process, all CO in the syngas is converted to CO_2. The CO_2 molar fraction is higher than that in other

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Nomenclature

Notations in formulation

C	production cost
C_F	cost of fuel
E_F	apparent activation energy (kJ/kmol)
F_{cap}	flowrate of the syngas (kmol/h)
G	Gibbs free energy (kJ)
I	total capital cost
k	kinetic factor (kmol/(s m^3 Pa^2))
K_{eq}	equilibrium constant
P	pressure (Pa)
Q	production scale
r	rate of reaction (kmol/(s m^3))
T	temperature (°C)

Abbreviations

ASU	air separation unit
CCS	carbon capture and storage
CRF	capital recovery factor
CTM	coal-to-methanol process
CTME	coal to methanol and power polygeneration process
ESR	energy saving ratio
GHG	green house gas
HRSG	heat recovery steam generator
IGCC	integrated gasification combined cycle
MIXCINC	conventional and nonconventional solids
O&M	operating and maintenance coefficient
PCS	primary cost saving ratio
RGibbs	Gibbs reactor
RPlug	plug flow reactor
SR	split ratio
WGS	water gas shift
WHB	waste heat boiler

Subscripts

ci	construction interest
oc	overnight capital
PG	polygeneration process
SG	single-product process

Superscripts

sf	scale factor

Greek letters

α	interest rate in the constructing period
η	energy efficiency

chemical synthesis pathway. Thus, the energy for CO_2 capture is low.

Inspired by the above idea, we introduce a polygeneration process design concept for chemicals and power production with the lowest CO_2 capture energy consumption. It follows the principles of efficient resource utilization and energy cascade utilization and integration.

Till now, a number of design concepts for chemical processes are reported. In general, design concept follows the procedure of choosing batch or continuous processes, designing vapor and liquid recovery systems, determining separation system and sequence, and evaluating benefit of heat integration [11]. Douglas et al. [12] proposed a systematic procedure for conceptual design of vapor-liquid-solid processes. It follows the steps of selecting process unit, identifying equipment configuration, and determining the important design variables and the associated economic trade-offs. The physical and chemical properties of the involved chemical system play an important role. A thermodynamic hybrid method to select the separation process was proposed by Jaksland et al. [13]. Smith [14] proposed a hierarchical conceptual design method named "onion" model. In this model, a chemical process is decomposed into four layers, starting from reaction, followed by separation process, heat exchanger network and utility system, as shown in Fig. 2.

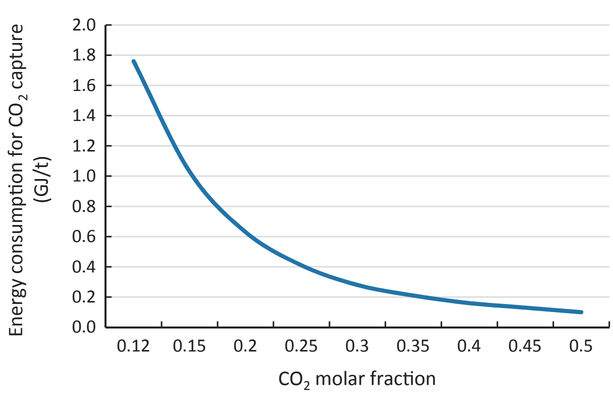

Fig. 1. Energy for CO_2 capture using membrane separation.

2. Design concept for coal based chemicals and power polygeneration process

2.1. Process design concept

Different from design concept for chemical processes, there is few design concept for polygeneration processes. Based on the above concept, this paper proposes a design concept for polygeneration processes of chemical and power. It can pursue energy cascade utilization and resource efficient utilization. For chemicals production processes, focus is paid on resource transformation from feedstock to products, while for power generation, focus is on energy conversion from chemical energy to physical energy. In addition, degree of resource transformation is increased by recycling part of unreacted gas [15].

To convert fuel into power, fuel is usually burned to release chemical energy, power is then generated by Brayton cycle and/or Rankine cycle [16]. Previous studies showed that fuel combustion leads to large exergy destruction, accounting for more than 30% of fuel energy [17]. Recycling of unreacted gas can increase the resource transformation. This recycle brings additional energy consumption and this increase is

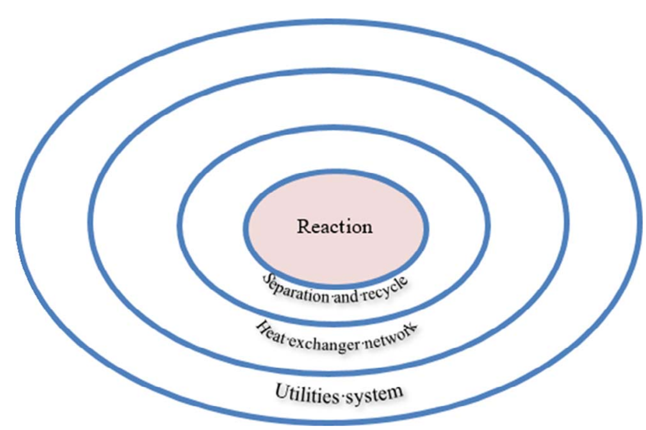

Fig. 2. Onion diagram for process design.