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Integrated Simulation and Optimization for Carbon Capture and Storage System

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Abstract**—**CO_2 capture and storage/sequestration (CCS) is a key technology for addressing the global warming issue. This paper proposes an integrated model for the whole chain of CCS, from a power plant to a reservoir. The integrated model is further utilized to determine optimal operating conditions and study responses to various changes in input variables.

Keywords**—**CCS, Caron Dioxide, Carbon Capture and Storage, Simulation, Optimization.

I. Introduction

CARBON capture and storage/sequestration (CCS) have emerged as a key issue since CO_2 was identified as a major source of global warming problem. Generally CCS technology consists of three main activities: capture, transmission, and storage/sequestration. Most research has focused on a certain part of the whole chain only. However, an integrated view of the whole chain is essential for its practical implementation. This is because the whole chain is interconnected with significant interactions among different stages. In addition, an optimal condition obtained without considering the interactions may not be the true optimum for the entire chain. For example, the amount and composition of flue gas emitted from power plant depend on the power generation, which is determined according to the power demand.

This study proposes an integrated model of the whole CCS chain, from a power plant to a reservoir. Power plant, capture, compression, liquefaction, transmission and storage models are constructed using a commercial process simulator, Pro/II. With this integrated model, sensitivity analysis is conducted to evaluate the effect of changes in input variables and determine control variables and proper control schemes for dynamic simulation. The ultimate goal of this study is to construct an optimal configuration, which is automatically changed according to a variety of options of scenarios.

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II. Design Basis

Pro/II with the Soave-Redlich-Kwong (SRK) equation of state was employed except for CO_2 and H_2O of capture process, for which amine package and NRTL equation were employed, respectively. The SRK equation predicts the behavior of CO_2 mixture with good precision at high pressure [1].

Since power plants using natural gases have gas turbine and usually are constructed as integrated gasification combined cycle (IGCC), only conventional coal power plant was simulated. Coal was simulated as a solid material and assumed to be Illinois No.6bituminous coal. The capacity of power plant was set to be 550MW.

In capture process, only wet capture process was considered due to the high complexity of dry process as well as its difficulty in commercialization. 30wt% MEA was selected for capturing CO_2 with 90% the capture ratio.

Compression and liquefaction process was designed to achieve the following product condition: 7 bar and 198K. During the CO_2 liquefaction, the water content was restricted below 50 vppm, which was much lower than 500 vppm reported by Aspelund and Jordal [2].

Only transmission using pipeline was simulated and the condition for transmission was obtained from [1]. The location of reservoir was assumed to be at 2000m below sea level.

III. Process Design

A. Power Plant Model

Conventional coal power plant was designed with 550 MW power capacity. Illinois No.6 coal was simulated as a solid material and it was mixed with process water. The coal composition is shown in Table I. Boiler, steam turbine chain, feed water heater, and condenser were included. Basic input variables for power plant were obtained from [3].

TABLE I
COAL COMPOSITION FOR POWER PLANT MODEL

Parameter	Value	Units
	Coal Composition	
C	71.73	wt%
H	5.06	wt%
N	1.41	wt%
S	2.82	wt%
Cl	0.33	wt%
Ash	10.91	wt%
O	7.74	wt%

B. Capture Model

CO_2 in the flue gas was captured by using 30 wt% MEA. The pressure of absorption column and regeneration column were1 bar and 1.5 bar respectively. With the amine package, the specification for CO_2capture performance was 90%.Energy for regenerating MEA was calculated as 3.9 GJ/tonCO_2 shown in Table II.

TABLE II
FLUE GAS COMPOSITION AND OUTPUT DATA FOR CAPTURING MODEL

Parameter	Value	Units
	Flue Gas Composition	
Ar	0.0083	mol%
CO_2	0.1354	mol%
H_2O	0.1508	mol%
N2	0.6815	mol%
O2	0.0240	mol%
	Process Output Data	
CW Temperature	308.15	K
CO_2 Concentration	94	mol%
Regeneration Energy	3.9	GJ/tonCO2
CO_2 Lean Loading	0.257	-

C. Compression and Liquefaction Model

Multistage compression was designed with 4 compressors. For water removal, triethylene glycol (TEG) was employed to control the water concentration below 50 vppm for preventing hydrate formation [4]. The pressure and temperature condition of product from liquefaction process were7 bar and198K respectively. Table III shows the input and output data for the compression and liquefaction model.

TABLE III
INPUT AND OUTPUT DATA FOR COMPRESSION AND LIQUEFACTION MODEL

Parameter	Value	Units
	Feed Gas Composition	
CO2	0.94	mol%
H_2O	0.05	mol%
H2	Trace	mol%
O2	Trace	mol%
	Process Output Data	
Temperature	198	K
Pressure	7	Bar
Energy	105	kWh/ton CO_2
H_2O Concentration	50	vppm

D. Transmission and Storage Model

After the liquefaction process, CO_2 rich gas was compressed to 180bar for pipeline transmission. It was assumed that CO_2 reservoir was located at 2000m below sea level. The output data for transmission and storage model is shown in Table IV.

IV. RESULT AND DISCUSSION

This section presents the optimization results of power generation, regeneration energy, liquefaction energy with the sensitivity analysis with the integrated model. Process flow diagram (PFD) for the integrated model is shown in Fig. 2.

TABLE IV
OUTPUT DATA FOR TRANSMISSION AND STORAGE MODEL

Parameter	Value	Units
	Process Output Data	
Temperature	209.15	K
Pressure	379	bar
CO_2 Concentration	99.93	mol%
H_2O Concentration	50	Vppm

A. Power Generation

Since regeneration energy for MEA is high, it has been suggested that using part of the steam from power plant to supply energy to the reboiler of regeneration column. However, optimal point of capturing steam varied case by case. We compared the following two cases: capturing steam between intermediate pressure (IP) and low pressure (LP) turbine and after the 1st LP turbine.

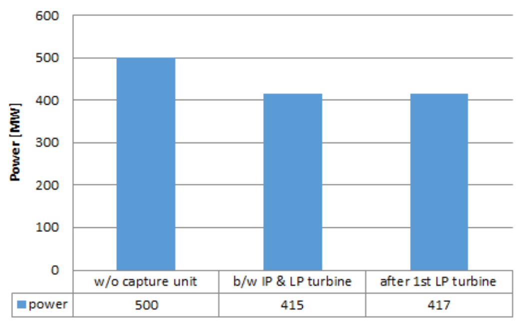


Fig. 1 Power generation comparison

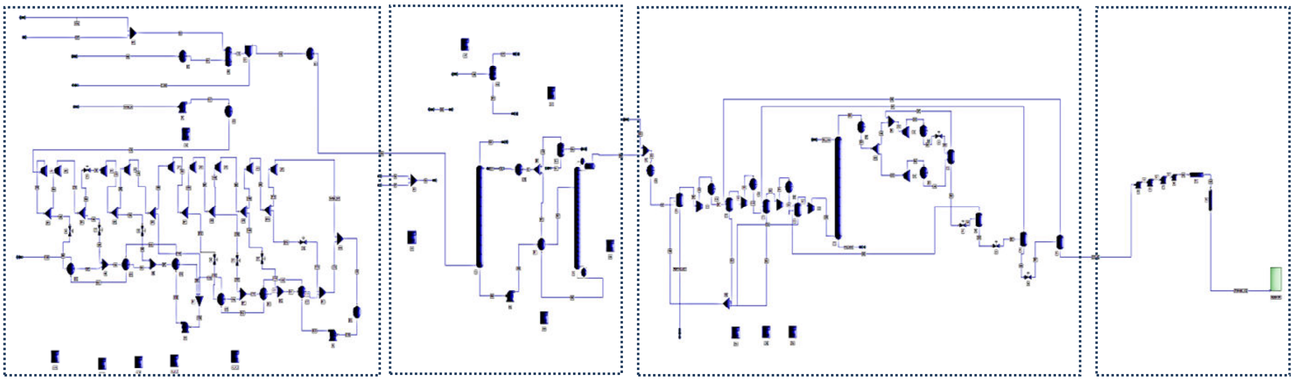
It was found that capturing steam after the 1st LP steam turbine was more effective than capturing between IP and LP turbine. Net efficiency in terms of higher heating value (HHV) was reduced from 45% to 28% due to the addition of capturing process.

B. Regeneration Energy

Regeneration energy varied from column pressure, liquid/gas (L/G) ratio and CO_2lean loading value. For prevention of MEA impairment, temperature of the bottom of regeneration column should be maintained below 400.15 K. As the column pressure increased from 1 bar to 2 bar, required energy for MEA regeneration decreased from 5.2 GJ/tonCO_2 to 2.7 GJ/tonCO_2.

Column pressure was set to be 1.3 bar considering both heat exchanger MTA (minimum temperature approach)of 5 K from heuristic method and bottom temperature. Regeneration energy change in according to column pressure is shown in Fig. 3.

Fig. 4 showed that optimal L/G ratio was around 3.0. However, it varied case by case due to its sensitivity to input change.



Power plant Capture Compression and liquefaction Transmission and storage

Fig. 2 Process flow diagram of integrated carbon capture and storage system

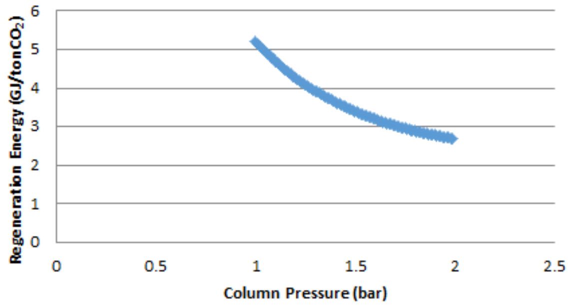


Fig. 3 Regeneration energy as a function of column pressure

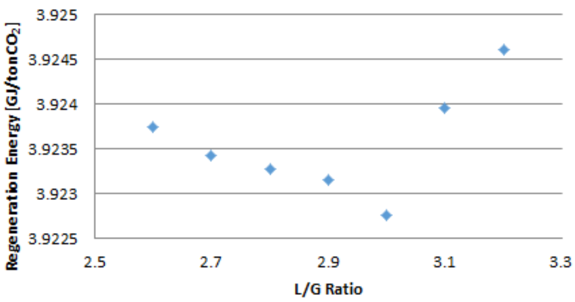


Fig. 4 Regeneration energy as a function of L/G ratio

Optimal CO_2 Lean Loading value was obtained as 2.57 from sensitivity analysis shown in Fig. 5.

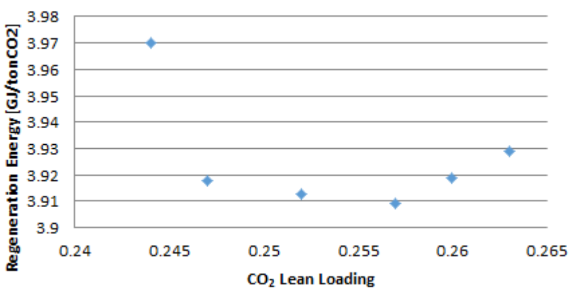


Fig. 5 Regeneration energy as a function of L/G ratio

C. Liquefaction Energy

Liquefaction energy was reduced from 119.3 kWh/tonCO_2 to 105.0 kWh/tonCO_2 by using optimizer solver from Aspen HYSYS and 105.03 kWh/tonCO_2 was obtained via Pro/II and it was corresponding with the result from [5]. The initial value and optimal value is shown in Table V.

TABLE V
INITIAL VALUE AND OPTIMAL VALUE FOR LIQUEFACTION ENERGY

Parameter	Initial value	Optimal value	Unit
	Compression Ratio		
C1	3.5	3.94	-
C2	3.5	3.85	-
C3	3.5	2.84	-
C4	3.5	1.77	-
	Liquefaction Energy		
Total Energy	119.31	105.03	kWh/tonCO_2

D. Sensitivity Analysis

In real situation, power generation changes according to the power demand. Assuming this scenario, the amount of coal in power plant was varied by 5%. The resulting regeneration energy, CO_2 emission, compression energy and capture ratio are presented in Fig. 6.

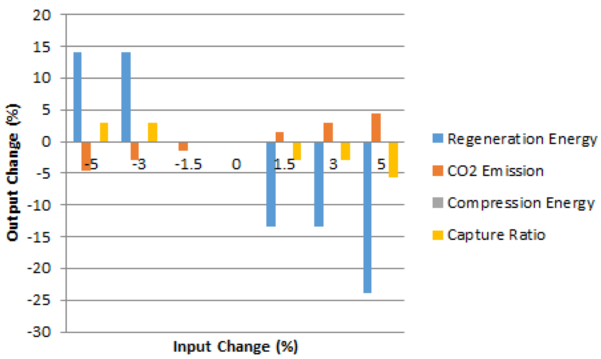


Fig. 6 Sensitivity analysis

Depending on the value of input, regeneration energy showed the most significant changes followed by CO_2 emission, capture ratio and compression energy. This means that a controller may be required to maintain the feed flow rate to the regeneration column and prevent energy loss in reboiler. Sudden reduction of feed gas could lead to higher regeneration energy. Meanwhile, the changes of compression energy and capture ratio were not significantly affected by the feed change. Based on these results, the most sensitive part of the process was concluded to be the capture process.

V. Conclusion

In this paper, the integrated simulation model for whole CCS chain was suggested and used for optimization and sensitivity studies. In this model, each process was optimized to reduce required energy as well as an integrated process: power plant and capture unit. Sensitivity analysis shows that the most sensitive part in the whole CCS chain was the capture process with the change in regeneration energy over 200% to input change.

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