Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Design of carbon dioxide dehydration process using derivative-free superstructure optimization

Jinjoo An [a,1], *Jonggeol Na* [a,1], *Ung Lee* [b,*], *Chonghun Han* [a,*]

[a] *School of Chemical and Biological Engineering, Seoul National University, Gwanak-ro 1, Gwanak-gu, Seoul 08826, South Korea*

[b] *Clean Energy Research Center, Korea Institute of Science and Technology, 5, Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, South Korea*

ARTICLE INFO

Article history:
Received 13 August 2017
Received in revised form 12 November 2017
Accepted 18 November 2017

Keywords:
CO_2 dehydration
TEG absorption
Process design
Superstructure optimization
Genetic algorithm
Techno-economic optimization

ABSTRACT

A comprehensive optimal design for the CO_2 dehydration process created by decomposition-based superstructure optimization is proposed. To reach the most economical process configuration, the superstructure model has been developed including binary interaction parameter regression of the NRTL-RK thermodynamic model, unit operation modeling, and identification of the connectivity of each of the unit operations in the superstructure. The superstructure imbeds 30,720 possible process alternatives and unit operation options. To simplify the optimization problem, the process simulation was explicitly carried out in a sequential process simulator, and the constrained optimization problem was solved externally using a genetic algorithm and an Aspen Plus-MATLAB interface. The optimal process includes a five-stage contactor, a nine-stage still column (with the feed stream entering at the seventh stage), a lean/rich solvent heat exchanger, and a cold rich solvent split flow fed to the first stage of still column. The total annualized cost of the optimum process is 6.70 M\$/year, which corresponds to the specific annualized cost of 1.88 \$/t CO_2. As part of the process optimization, a Monte Carlo simulation was performed to analyze the sensitivity of utility cost volatility; the refrigerant and steam present the most influential utility costs.

1. Introduction

Carbon capture and storage (CCS) technologies have been extensively studied over the past few decades because they are considered a realistic option for mitigating climate change (IPCC, 2011, 2015). Research in this field often focuses on the CO_2 capture and liquefaction processes because of their high cost and energy consumption (Aspelund and Jordal, 2007; Figueroa et al., 2008; Lee et al., 2012; Lin and Chen, 2011; Padurean et al., 2011; Rubin et al., 2007; Scheffknecht et al., 2011; Versteeg and Rubin, 2011; Wall et al., 2011). The dehydration process, on the other hand, is approximated using simple models; consequently, it is often economically underestimated despite its importance in the CCS chain (Kemper et al., 2014). The dehydration of high-purity CO_2 streams is often necessary according to the quality of the captured CO_2 product. Excess water in CO_2-rich streams may cause operational problems like hydrate formation and corrosion in downstream transportation and injection systems. Low water content is, therefore, critical for the operation and safety of the process.

The dehydration process for lowering the water content of captured CO_2 includes several processes, including compressor interstage cooling, Joule–Thomson (J–T) cooling, refrigeration, supersonic separation, solid desiccant, and liquid desiccant (Kemper et al., 2014; Machado et al., 2012; Netusil and Ditl, 2011; Scholes et al., 2012). Some of these processes, such as compressor interstage cooling and J–T cooling, cannot achieve sufficiently low water content alone, necessitating additional dehydration to meet the specifications for CO_2 transportation. Triethylene glycol (TEG)-based absorption and molecular sieve adsorption are the best suited to meet the severe water content specifications for CCS purposes (Kemper et al., 2014). The glycol system is widely

---

* *Corresponding authors.*
E-mail addresses: ulee@kist.re.kr (U. Lee), chhan@snu.ac.kr (C. Han).

[1] These authors contributed equally to this work.

https://doi.org/10.1016/j.cherd.2017.11.028
0263-8762/

Nomenclature

AIC	Annualized capital investment cost
AOC	Annualized operation cost
C	Compressor
CCS	Carbon capture and storage
CSSF	Cold solvent slit flow
CW	Cooling water
E	Energy consumption
EIC	Equipment installation cost
EPC	Equipment purchase cost
GA	Genetic algorithm
HX	Heat exchanger, heater, or cooler
JT	Joule–Thompson valve
LB	Lower bound
L/R	Lean/rich
LVC	Lean vapor compression
MINLP	Mixed integer non-linear programming
MTA	Minimum temperature approach
NC	The number of components
NDG	The number of data group
NP	The number of points
NRTL	Non-random two-liquid
P	Pump
RK	Redlich–Kwong
RMSE	Residual root mean square error
TAC	Total annualized cost
TEG	Triethylene glycol
SG	Stripping gas
h	Equality constraints
H_s	Sensible heat requirement
H_R	Desorption heat
Q_{RB}	Reboiler heat requirement
Q_{Cond}	Condenser cooling requirement
r_i	Compression ratio at ith compression stage
T_{top}	Temperature at the top of the column
UB	Upper bound
x	Binary and integer variables
y	Continuous variables
γ	Penalty parameter
μ	Utility average cost
σ	Cost variance

and successfully used for natural gas dehydration due to its advantages such as simplicity in operation (GSAP, 2004). In particular, TEG has lower vapor pressure, evaporation loss, and thermal degradation than other glycol solvents.

The high energy requirement of the dehydration process has encouraged many researchers and companies to develop enhanced glycol processes for natural gas dehydration systems. Most of these processes regenerate the water-rich TEG to the water-lean TEG to minimize solvent usage and achieve low water concentrations. In addition, advanced lower-energy process configurations can achieve reasonably low water concentration. Among these, stripping gas injection is a common process alternative. A patented process, Drizo^{TM} by ProserNAT, is an alternative design to traditional stripping gas units which uses internally generated stripping gas. COLDFINGER$^{®}$ by Gas Conditioners International condenses and extracts water from the vapor phase using a cold coil or tube bundle (Netusil and Ditl, 2012). Alternatively, mixtures of TEG with lean oil (LO) and toluene or isooctane have been proposed by Rincón et al. (2016) and Paymooni et al. (2011). However, the transferability of these processes to CO_2 dehydration system has not yet been evaluated. Alternatives to absorption processes include column intercooling, interheating, split flow or staged feed, and vapor recompression (VRC). These lower the energy demands of solvent regeneration by reducing the latent or sensible heat requirement of the regeneration column reboiler. Implementation of column intercooling and feed gas split flow increases the solvent's absorption capacity and rich solvent loading by cooling the mid-bottom of the absorber (Biliyok et al., 2012; Chang and Shih, 2005; Jung et al., 2013; Le Moullec and Kanniche, 2011; Moser et al., 2011; NETL, 2011; Plaza et al., 2010). In addition, column interheating and a staged feed of cold rich solvent decrease the temperature of the inlet stream or top stage (Aroonwilas and Veawab, 2007; Karimi et al., 2012b; Soave and Feliu, 2002; Van Wagener and Rochelle, 2011). Lean, rich, and mechanical vapor recompressions (LVR, RVR, and MVR) decrease the temperature of the inlet stream by vaporizing the solvent under low pressure, recompressing it, and sending it to the column bottom (Fernandez et al., 2012; Jassim and Rochelle, 2006; Jeong et al., 2015; Jung et al., 2015; Karimi et al., 2011, 2012a; Le Moullec and Kanniche, 2011; Lee et al., 2016a). Some of these alternatives improve the energy efficiency of the system; however, they may also increase the overall cost by requiring capital investments in additional equipment or utilities.

Solid desiccants, including gels, alumina, and molecular sieves, are also candidates for dehydrating captured CO_2. Dehydration units using these desiccants can achieve very low dew point temperatures in the product or outlet streams. For example, molecular sieves can be used to achieve dew point temperatures of 172 K. However, they are generally more expensive than glycol units in terms of both operation and maintenance. Therefore, their use is recommended for applications where very low dew point temperature or water content is essential (GSAP, 2004; IEAGHG, 2014).

The design of the CO_2 dehydration process can be optimized using superstructure optimization. Since most process alternatives are included in a superstructure, this method enables the determination of the optimal process design through mathematical formulation and optimization. Recently, superstructure optimization using a rigorous process model has been applied to the optimization of a CO_2 capture and conditioning process design (Lee et al., 2016a,b) and a microchannel reactor (Na et al., 2017a). Trespalacios and Grossmann (2014) presented a comprehensive review of the superstructure optimization method of process design. To find the optimal process configuration in a given superstructure, mixed integer non-linear programming (MINLP) has been widely used (Grossmann, 1985; Grossmann, 1989; Grossmann, 1990).

In this study, a superstructure-based techno-economic evaluation of a CO_2 dehydration process with four-stage compression is performed. In Chapter 2, a detailed description of the results of thermodynamic modeling of the CO_2 dehydration process using TEG is given. The selected model with estimated parameters has been validated using an experimental data set. The superstructure design is described in Chapter 3, which gives detailed information on unit operations, including the rationale for considering each one. In the optimization-formulation section, Chapter 4, a derivative-free process simulator-based mixed integer nonlinear programming (MINLP) formulation is introduced. Finally, the resulting optimized CO_2 dehydration process is suggested, and the results of a sensitivity analysis and Monte Carlo simulation are presented with several suboptimal alternatives.

2. Modeling basis

2.1. *Design specifications*

Flue gas from power plants that combust hydrocarbon fuels contains impurities such as air components, SO_2, NO_2, CO, and H_2O. Many researchers have discussed the effect of these on CO_2 sequestration and the allowable concentrations in the stream (Skaugen et al., 2016; Wetenhall et al., 2014). Among these impurities, the presence of free water in gas and liquid CO_2 stream may cause problems in the operation and safety of the CO_2 sequestration, such as corrosion and hydrate formation. Without strict limitations on contaminants (e.g.