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Energy



Energy Procedia 63 (2014) 421 - 430

GHGT-12

Equation-Oriented Optimization of Cryogenic Systems for Coal Oxycombustion Power Generation

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Abstract

Efficient separation systems are essential to the development of economical CO_2 capture system for fossil flue power plants. Air Separation Units (ASU) and CO_2 Processing Units (CPU) are considering the best commercially available technologies for the O_2/N_2 and CO_2/N_2 , O_2 , Ar separations in coal oxycombustion processes. Both of these systems operate at cryogenic temperatures and include self-integrated refrigeration cycles, making their design challenging. Several researchers have applied sensitivity tools available in the commercial flow sheet simulators to study and improve ASU and CPU systems for oxy-fired coal power plants. These studies are limited, however, as they neglect important interactions between design variables.

In this paper, we apply an advanced equation-based flowsheet optimization framework to design these cryogenic separations systems. The key advantage of this approach is the ability to use state-of-the-art nonlinear optimization solvers that are capable of considering 100,000+ variables and constraints. This allows for multi-variable optimization of these cryogenic separations systems and their accompanying multi-stream heat exchangers. The effectiveness of this approach is demonstrated in two case studies. The optimized ASU designs requires 0.196 kWh/kg of O₂, which are similar to a "low energy" design from American Air Liquide and outperforms other academic studies. Similarly, the optimized CPU requires 18% less specific separation energy than an academic reference case. Pareto (sensitivity) curves for the ASU and CPU systems are also presented. Finally, plans to apply the framework to simultaneously optimize an entire oxycombustion process are discussed.

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Keywords: air seperation unit; CO2 processing unit; coal oxycombustion; optimization; carbon capture

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1. Introduction

Coal oxycombustion is a promising technology for efficient and economical electricity generation with carbon capture. In this type of power plant, pulverized coal is combusted in a N₂ lean environment, resulting in flue gas primarily composed of CO₂ and H₂O, along with small amounts of N₂, O₂, pollutants (*e.g.* particulate matter, SO_x, *etc*) and inert gasses (*e.g.* Ar). After processing to remove pollutants and optionally H₂O, some of the flue gas recycled to regulate the boiler temperature (CO₂ acts as a dilutent). The remaining flue gas is processed to remove H₂O, N₂, O₂ and Ar, leaving a purified CO₂ stream which is compressed for utilization and/or sequestration in geological formulations. Thus, the major separation process in an oxy-fuel process (N₂/O₂ separation) is performed before combustion, opposed to after combustion (N₂/CO₂ separation) with other technologies such as amine-based flue gas scrubbing. See Scheffknecht et al [1] for a review of state-of-the-art oxycombustion technology.

Numerous research projects have focused on the development of oxycombustion technologies in the past decade, with an emphasis on numeric process simulation, thermodynamic assessment, economic analysis and redesign/retrofit of boilers for a different combustion atmosphere. Fu & Gundersen used pinch and exergy analysis to identify a 10 percentage point efficiency penalty associated with the cryogenic systems in the power plant [2]. Follow-up work investigated the best strategies for using heat integration to increase the efficiency of the oxycombustion plant [3]. For example, they considered the impact of using waste heat generated during compression for boiler feed water preheating, determining isothermal compression is more efficient than adiabatic compression with heat integration [4,5]. Several other researched utilized process simulation tools to investigate trade-offs in oxy-combustion power plants. Xiong et al [6] confirmed the efficiency penalty of the air separation unit and carbon dioxide processing equipment is approximately 10 percentage points using Aspen Plus. They also investigated the sensitivity of the oxycombustion process to several variables, including the flue gas recycle ratio, air ingress assumptions and O₂ purity produced by the ASU. Similarly, Besong et al [7] used Aspen HYSYS to compare and calculate power consumption benchmarks for two CO2 processing unit design from patents (single and triple flash vessel systems). In another study, Li et [8] al discuss the trade-offs between the air separation unit and carbon dioxide processing unit. They demonstrate it is beneficial from an energy perspective to relax the O_2 purity requires for the ASU away from the standard 95 mol% and increase the size of the CPU. This type of trade-off analysis in critical to reducing the separation systems' energy demands and ensuing oxycombustion is a cost effective means of carbon capture.

Unfortunately most systems analysis studies are flawed in two ways. First, they do not utilize advanced optimization methods that are becoming popular in academia and industry for improve process designs, control, operations and enterprise-wide decision making. Instead these studies rely on sensitivity analysis by individually perturbing key design parameters. Zebian et al [9,10] demonstrated the importance of simultaneously optimizing several variables, highlighting efficiency improvements missed in sensitivity analysis studies due to the interaction of decision variables. They only considered 17 design variables, however, using the Sequential Quadratic Programming (SQP) optimization methodology available in Aspen Plus, a technology which is 25+ years old and known to have several shortcomings. In contrast, state-of-the-art optimization algorithms are capable of handling 100,000+ variables and constraints, by exploring sparsity and exact derivatives.

The second major shortcoming of these process simulator based studies is the reliance of built-in reactor models (such as *Gibbs reactor block* in Aspen Plus). In a coal boiler over 90% of the heat transfer is radiative. Due to the difference in the radiative heat transfer properties of CO_2 and N_2 , oxycombustion boilers are expected to behave significantly different than their equivalent (same geometry, etc) air-fired counterparts. Thus it is essential to consider a detailed boiler model when studying the performance of the overall oxycombustion system. Recognizing this, Edge et al [11,12] have developed a method for incorporating data generated from computational fluid dynamic (CFD) simulations into flowsheeting tools. There work is restricted to only simulation, not numerical optimization.

In this paper and its companion [13], we present a methodology for optimization of an entire oxycombustion power plant with advanced boiler models (*e.g.* CFD simulations) using advanced optimization methods. We

ultimately seek to consider several trade-offs in the separation systems, boiler, compression trains and steam cycle simultaneously. This paper focuses on the application the equation-based flowsheet optimization framework to design cryogenic separation systems for coal oxycombustion, and is organized as follows: in Section 2, the modeling and optimization methodology is summarized. In Sections 3 and 4, optimized results for the ASU and CPU, respectively, are presented and compared with literature. Finally in Section 5, ongoing work to link this framework with a CFD boiler model is discussed. Details regarding boiler and steam cycle optimization are covered in [13].

2. A Framework for Advanced Flowsheet Optimization

The essential ingredient to modern, efficient large-scale nonlinear programming (optimization) algorithms is the availability of exact, sparse first and second derivative information for the objective function (overall goal) and constraints (inequality and equality). This information is not utilized in flowsheet simulation tools, such as Aspen Plus (sequential modular mode) and instead approximate derivatives are used (from perturbations or matrix updates). Using approximate derivatives deteriorates the performance of these optimization algorithms, resulting in slow convergence and limiting the problem size. In contrast, modern nonlinear programming algorithms such as IPOPT [14] and CONOPT [15] are capable of efficiently solving problems with 100,000+ variables and constraints (equality or inequality). Exact first and second derivatives are automatically calculated in optimization modeling environments, such as GAMS [16]. Thus to leverage these tools, we created a framework for flowsheet optimization in GAMS (*i.e.* independent of a commercial flowsheet simulator). The development effort is justified, as the new framework is capable of investigating trade-offs through optimization that are too challenging for commercial process optimization tools.

Below three important aspects of the framework are summarized. For additional details, see [17].

2.1. Embedded Thermodynamic Models and Flash Calculations

Thermodynamic models, including flash calculations, are written as constraints in the framework, making derivatives available via automatic/symbolic differentiation in GAMS. The outlet streams of a flash calculation are determined by solving (1), where y_i and x_i are the liquid and vapor compositions, respectively; *T* and *P* are the outlet temperature and pressure; K_i is an equilibrium coefficient for component *i*; *L*, V and F are the liquid outlet, vapor outlet and feed flowrates, respectively; z_i is the feed composition; and, H_L , H_V and H_F are enthalpies.

$$F = L + V \tag{1a}$$

$$Fz_i = Lx_i + Vy_i, \quad \forall i \in \{Components\}$$
(1b)

$$y_i = K_i(T, P, x_i, y_i) x_i, \ \forall i \in \{Components\}$$
(1c)

$$FH_F(T_{in}, P_{in}, \vec{z}) + Q = LH_V(T, P, \vec{x}) + VH_V(T, P, \vec{y})$$
(1d)

(1c) must be relaxed if a phase disappears due to changes in the flash operating conditions (such as T, P or Q). This is modeled in the framework using a combination of slack variables (s^L and s^V) and complementarity constraints, as shown in (2). " \perp " is the complementarity operator, which ensures that at least one of the complementing variables is zero. Thus in the phase disappearance example, either V = 0 (no vapor phase) or $s^V = 0$. See [18] for a derivation of this approach based on minimizing Gibbs free energy in a flash calculation.

$$y_i = \beta K_i(T, P, x_i, y_i) \ x_i, \ \forall i \in \{Components\}$$
(2a)

$$s^{L} \le \beta - 1 \tag{2b}$$

$$\beta - 1 \le s^{\vee} \tag{2c}$$

$$0 \le L \perp s^{L} \ge 0 \tag{2d}$$

 $0 \le V \perp s^V \ge 0 \tag{2d}$

Determining the phase of a stream typically involves heuristic, non-differentiable routines in flowsheet simulators (especially sequential modular codes). This is problematic for an equation-based optimization

framework, as exact derivatives are essential for efficient optimization algorithm performance. With this motivation, Kamath et al [19] proposed algebraic rules for selecting the liquid and vapor roots in a cubic equation of state (e.g. Peng Robinson), which are shown below for liquid (3) and vapor (4) streams,

$$f(Z_l) = a_0 + a_1 Z_l + a_2 Z_l^2 + Z_l^3$$
(3a)

$$f'(Z_l) \ge 0 \tag{3b}$$

$$f''(Z_l) \le Ms^2 \tag{3c}$$

$$f(Z_{\nu}) = a_0 + a_1 Z_{\nu} + a_2 Z_{\nu}^2 + Z_{\nu}^3$$
(4a)

$$f'(Z_v) \ge 0 \tag{4b}$$

$$f''(Z_l) \ge -Ms^V \tag{4c}$$

$$T(Z_l) \ge -Ms^{\nu} \tag{4c}$$

where f(Z) = 0 is the cubic equation of state in dimensionless form, Z is the compressibility factor and f'(Z) & f''(Z) are the first and second of derivatives f(Z) with respect to Z. The first derivative constraint ensure the spurious middle root is not selected, whereas the second derivative constraint distinguishes between the vapor and liquid roots. The later constraint is also relaxed with s^L and s^V to accommodate phase disappearance. This formulation, (1) - (4), allows for cubic equations of state thermodynamics to be directly embedded in optimization framework without calls to third party packages (that typically do not provide 1st and 2nd derivative information).

2.2. Simultaneous Process Optimization and Heat Integration

In mathematical programming (optimization) based heat integration literature, the following problem is typically considered: given fixed stream data (flowrates and temperatures), automatically synthesize the "best" heat exchanger network, measured by a combination of capital and operating costs [20]. This approach is inadequate for cryogenic system design, as adjusting stream data (flowrates, pressures, temperatures, etc.) impacts the operation of multistream heat exchangers. Thus this work features an extension of the Duran and Grossmann [21] pinch-location heat integration model, which allows for simultaneous heat integration (by calculating minimum utility demands) and process optimization (adjustment of stream data). This approach essentially embeds the famous pinch heat integration method (see [22]) into an optimization problem. For brevity, the model is not repeated here. See [21] for the original model, [17] for a small extension to improve numerical performance and [20,23] for an overview of optimization based integration methods. As discussed in [17,24] the model is very effective for primarily design multistream heat exchangers.

2.3. Distillation Column Optimization without Integer Variables

Distillation column design using mathematical programming (optimization) has been well studied for the past three decades [23]. Many models have been proposed to optimize both distillation column sequences and individual columns, and more recently include advance technologies such as heat integrated distillation sequences, reactive distillation columns and hybrid systems (distillation coupled with other separation technologies). Design of cryogenic systems for advance energy processing, such as the ASU and CPU, can benefit from these optimization technologies. However, the traditional models for single column optimization, which address important aspects of column sizing such as optimizing the number of trays and feed tray location(s), require the use of integer variables [25-27]. Reliably solving mixed integer nonlinear programs (MINLPs), especially with embedded non-convex thermodynamic models, remains an open challenge. Instead this framework includes a new, alternate model for distillation column optimization. Integer variables are avoided by using bypass streams around each possible equilibrium tray. This allows for the number of trays, number of feed streams and location of feed(s) to be optimized in a distillation column while considering equilibrium-based models for each theoretical tray (comparable to the RADFRAC model in Aspen Plus). For brevity, the detailed model is not included in this paper. See [17,28] for additional details.

2.4. Multistart Initialization

A variation of the multistart algorithm described in [17] is used for both case studies. Due to the non-convex equations (such as thermodynamic departure functions), deterministic global optimization algorithms (such as BARON [29]) are unable to prove global optimality with these models. Multistart initialization combine with deterministic local optimization solvers provides a practical alternative to global optimization for these systems.

3. Air Separation Units for Oxycombustion

Cryogenic distillation of air is consider the most viable, commercially available separation technology to produce large quantities of purified O_2 for coal oxycombustion power plants. Air Separation Unit (ASU) designs include three components: (1) two (or three) distillation columns, (2) a compression train and throttle valves, and (3) multistream heat exchanger(s). Air enters the process and is compressed to high pressures (up to 40 bar), cooled using heat exchangers and throttle to column operating pressures (slightly above ambient to 8 bar). The decrease in pressure causes a drop in temperature and/or (partial) condensation due to the Joule-Thomson effect. A majority of the air feed enters the high pressure column, which produces O_2 and N_2 rich intermediate streams that are sent to the low pressure column (in addition the remainder of the feed air). The pressure difference between the columns allows the high pressure column's condenser and low pressure column's reboiler to be heat integrated. In some popular ASU configurations, the N_2 rich stream from the high pressure column acts as reflux for the low pressure column, eliminating the need for a second condenser. In the multistream heat exchanger(s), the products are used to cool the feed air, reducing the compression energy required to drive the self-refrigeration cycle. Designing, simulating and optimizing ASUs is particularly difficult because of this tight heat integration (with approach temperatures below 2 °C in many systems).



Figure 1. ASU superstructure (left) and the configuration selected by the optimizer (right).

The optimization framework (see Section 2) is applied to the design of ASUs for oxycombustion, which is formulated as the following problem:

Minimize	Shaft Work/O ₂ Recovery + Complementarity Penalties			
s.t.	Flowsheet Connectivity	(see Fig. 1)		
	Peng-Robinson Thermodynamics	(3) & (4)		
	Distillation Models			
	Heat Integration Models			
	Ideal Gas Compression Model			
	Other Unit Operation Models			
	O_2 Purity > 95 mole %			

A superstructure, shown in Figure 1, is used to accommodate several popular ASU configurations. The optimizer selects the best reflux/recycle strategy. The energy optimized ASU requires 0.16 to 0.26 kWh/(kg O_2) of compression energy, depending on approach temperature. See [17] for a Pareto curve showing the minimum ASU separation energy depending on assumed minimum approach temperature (used for heat integration). The optimization problem above was resolved at various O_2 purities, resulting in another Pareto curve (see Figure 2). The results are consistent with low energy designs from American Air Liquide/NETL [30]. Interestingly, the results from other academic studies [6,31] require similar specific energy as the low capital case from American Air Liquide/NETL [30].



Figure 2: Pareto optimal front for O2 purity with a linear regression fit and comparison to literature.

4. CO₂ Processing Units and Compression Trains for Oxycombustion

In the oxycombustion flowsheet, treated flue gas is sent to the CO₂ Processing Unit (CPU) for further purification and compression to 150 bar for utilization and/or sequestration. Due to the large differences in boiling points, a sequence of flash vessels is typically used to separate O₂, N₂ and Ar from CO₂. Similar to the ASU, compression and expansion are used to drive the self-contained cryogenic refrigeration cycle. The flowsheet topology, adapted from [32], is shown in Figure 3. It includes two heat integration zones. The first is serviced by cooling water and the second represents a multi-stream heat exchanger (and is self-heat integrated). See [17,33] for detailed equipment equations. A special mathematical models using complementarity constraints is used to toggle on and off zone 1 heat exchangers, as they cannot cool below the cooling water utility temperature. See [33] for details. The following optimization problem is solved to design the CPU:



Figure 3. Flowsheet topology for the two flash vessel CPU, based on [32]. F603 acts as a mixer and does not contribute to the seperation.

Minimize	Shaft Work/O ₂ Recovery + 0.01 Cooling Water Demand + Complementarity Penalties		
	s.t.	Flowsheet Connectivity	(see Fig. 3)
		Flash Equipment Models	(1) & (2)
		Peng-Robinson Thermodynamics	(3) & (4)
		Heat Integration Models	
		Complementarity Equation for Heat Exchangers	
		Compressor Models	
		Other Unit Operation Models	
		2% Pressure Drops in Heat Exchangers	
		CO_2 Purity \geq 94.6 mole %	
		CO2 Recovery \geq 96.3 mole %	

4.1. Case Study: Comparison with Literature

The CO₂ purity and recovery specifications shown above correspond with the work by Fu & Gundersen [32]. Neglecting the small pressure drop in heat exchangers (approx. 2%), the above system was optimized and the optimized solution had a shaft work requirement which was 18% less compared to the requirement calculated by Fu & Gundersen [32] (0.093 vs 0.114 kW/kg of purified CO₂). The cooling water duty for the optimized system is 0.155 kW/kg of CO₂. See [33] for additional details.

4.2. Sensitivity Analysis: Pareto Curves

Similar to the ASU, the CO_2 outlet purity and recovery requirements will be adjusted in context of the entire oxycombustion flowsheet. Thus the CPU optimization problem, shown above, was re-optimized at a variety of conditions to create two Pareto curves, shown in Figure 4. These results assume an inlet stream composition of 83.5 mole % CO_2 , 3% O_2 , 10% N_2 and the remainder Ar and include 2% pressure drops in each heat exchanger. (Water is assumed to be removed beforehand by condensation, a packed bed, glycol scrubber or another technology.). As future work, the sensitivity of the CPU model at changes in the inlet stream composition will also be quantified.



Figure 4. Pareto curves for weighted specific energy (1 kW shaft work = 100 kW cooling water = 100 kW steam) vs CO₂ outlet purity and CO₂ recovery.

5. Conclusions and Future Work

In this paper, we present the application of an equation-oriented flowsheet optimization framework to design cryogenic systems for coal oxycombustion. By using equation-based models and exact derivatives, efficient advanced optimization algorithms are used to design these system with 10,000+ equations and constraints (ASU). By incorporating pinch-based heat integrations into the optimization problem, multistream heat exchangers are designed in tandem to the separation systems.

As future work, these models will be coupled with the remainder of the oxycombustion flowsheet. This will allow for several trade-offs between systems to be balances. Also, the companion paper in these proceedings describes integrated boiler and steam cycle optimization strategies [13]. Regarding these separation systems, two particular questions will be evaluated:

- 1. What is the optimal O_2 product purity from the ASU? This requires balancing the separation work in the ASU and CPU, while taking into account the boiler and steam cycle.
- 2. What are the advantages of heat integrating the ASU and CPU together? Is it possible to use cold products from the ASU to liquefy CO₂ and drastically reduce pressurization costs in the CPU? How does this strategy compare with heat integrating the compression trains in the ASU and CPU with the steam cycle?

Using an optimization framework allows these questions to be answered systematically and rigorously.

Acknowledgements

This work is supported as part of the Carbon Capture Simulation Initiative, a joint project between several universities and five US National Laboratories, sponsored by the US Department of Energy. The aim of CCSI is to develop computational tools to advance and support the development, scale-up and adoption of carbon capture

technologies (see www.acceleratecarboncapture.org for additional information). We would like to thank David Miller at the National Energy Technology Laboratory for the opportunity to work on this exciting project.

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