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Optimal design of cryogenic air separation columns under uncertainty

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ABSTRACT

Cryogenic air separation, while widely used in industry, is an energy intensive process. Effective design can improve efficiency and reduce energy consumption, however, uncertainties can make determination of the optimal design difficult. This paper addresses the conceptual design of cryogenic air separation process under uncertainty. A rigorous, highly nonlinear model of three integrated columns is developed to capture the coupled nature of the process. The multi-scenario approach is used to incorporate the uncertainty, giving rise to a nonlinear programming problem with over half a million variables. Nevertheless, this problem is solved efficiently using Ipopt, demonstrating the effectiveness of interior-point methods on complex, large-scale nonlinear programming problems. The optimal design from the multi-scenario approach is compared against the optimal design using nominal parameter values. As expected, the results using the multi-scenario approach are more conservative than the nominal case; however, they may be less conservative than traditional overdesign factors.

1. Introduction

Large quantities of high-purity air products are used in several industries, including the steel, chemical, semiconductor, aeronautical, refining, food processing, and medical industries. Methods of air separation include cryogenic and non-cryogenic approaches (Castle, 2002). Although non-cryogenic processes such as pressure swing adsorption and membrane separation have become more competitive, cryogenic distillation technology is still the dominant choice for producing large quantities of very high-purity and liquefied air products (Baukal, 1998). Cryogenic air separation is an energy intensive process that consumes a tremendous amount of electrical energy. The U.S. industrial gas industry consumed approximately 31,460 million kilowatt hours in the USA in 1998, which accounts for 3.5% of the total electricity purchased by the manufacturing industry (Karwan & Keblis, 2007).

Optimal operation and control of cryogenic air separation processes has received significant attention, with the primary goal of reducing energy consumption and improving economic performance during operation. Load switching in air separation columns are analyzed by White, Perkins, and Espie (1996), and multivariable control schemes for cryogenic air separation are developed in Zhu, Henson, and Megan (2001) and Roffle, Betlem, and Ruijter (2000). Trierweiler and Engell (2000) investigated the selection of an appropriate control structure based on dynamic behavior analysis. Seliger, Hanke, Hannemann, and Sundmacher (2006) integrated an air separation process model with an IGCC power plant and analyzed the combined process dynamics. Control strategies such as nonlinear model predictive control (NMPC) are difficult to implement for these systems because of the high computational cost associated with optimization of a large, complex dynamic model. Approaches have been developed that promote efficient NMPC for these systems by reducing the size and complexity of the model. Bian, Henson, Belanger, and Megan (2005) developed a strategy for nonlinear model predictive control by adopting a dynamic wave model for the single nitrogen column. The advanced step NMPC controller (Zavala & Biegler, 2009), an alternative approach based on NLP sensitivity, has also been used in Huang, Zavala, and Biegler (2009) to perform efficient nonlinear model predictive control of a cryogenic air separation column as a part of an IGCC. Considering offline dynamic optimization, Zhu and Laird (2008) proposed an effective parallel nonlinear solution to deal with optimal control and operation under uncertainty for two highly coupled cryogenic air separation columns.

In addition to process control, previous research has also focused on planning and scheduling for air separation columns. Karwan and Keblis (2007) use a mixed integer programming formulation to optimize operating decisions under real time pricing. Miller, Luyben, and Blouin (2008) use thermodynamic ideal work to predict the energy requirements when production rates of cryogenic air separation columns change under varying electrical prices. Ierapetritou, Wu, Vin, Sweeney, and Chigirinskiy (2002) use an ARIMA model to predict future power prices and minimize operating cost using a two stage stochastic programming formulation.

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Nomenclature

F	feed flow rate (mol/s)
K	ideal vapor–liquid equilibrium constant
V	vapor flow rate (mol/s)
L	liquid flow rate (mol/s)
S	side flow rate (mol/s)
H	vapor or liquid enthalpies
T	tray temperature
P	tray pressure
Q	transferred heat
UA	heat transfer rate (W/K)
x	liquid flow composition
y	vapor flow composition
z	feed flow composition
U_1	air feed flow rate in HPC (mol/s)
U_2	expand air flow (mol/s)
U_3	nitrogen reflux from HPC to LPC (mol/s)
U_4	waste nitrogen (mol/s)
U_5	feed flow rate of crude argon column (mol/s)
D	diameter of distillation columns (m)
k	adiabatic index number in compressor

Greek letters

γ	activity coefficient
η	compression efficiency

Abbreviation

HPC	high-pressure distillation column
LPC	low-pressure distillation column
CAC	crude argon column
TAC	total annual cost
EC	electricity cost
BHP	brake horsepower of the compressor
CPC	capital cost of main compressor
HEC	capital cost of heat exchanger
CSC	capital cost of column shells
CTC	capital cost of column trays

Because of the complexity associated with handling uncertainty, much of the existing research regarding design and operation under uncertainty of air separation systems makes use of simplified or linear process models. However, when considering the entire coupled system and the potential for varying operating conditions, air separation plants can exhibit highly nonlinear behavior. There is a need for strategies that can consider uncertainties and provide rigorous optimization of these complex nonlinear models.

Optimizing the design of the cryogenic air separation system has the potential to significantly affect not only the capital investment, but also the future economic performance. In practice, most current design schemes focus on specialized column structures and opportunities for energy and mass integration. Agrawal and coworkers simulate and analyze various thermal coupling methods (Agrawal & Yee, 1994), structured packing on packed columns for argon production (Agrawal, Woodward, Ludwig, & Bennett, 1993), and multiple component distillation sequences (Agrawal, 1995, 1996) in order to improve energy efficiency and separation performance. Egoshi, Kawakami, and Asano (2002) address the problem of predicting practical separation performance and obtaining the optimal design of cryogenic air separation plants using a rigorous transport model for structured packing. Regardless of the design strategy used, in order to retain future process flexibility it is important to consider potential uncertainties during the design phase. These include uncertainty in process performance, uncertainty in product demands and pricing, and uncertainty in availability and pricing of process inputs.

One example of uncertainty in the model arises in the selection of thermodynamic methods and parameters. The primary components are separated under extremely low temperatures, and standard packages may not adequately describe the behavior of the system under these conditions. Indeed, many companies specializing in air separation have spent significant resources developing specialized thermodynamic methods for their systems.

A second form of uncertainty relates to unknown demands on the process. Air separation systems can produce three component products of various grades in both vapor and liquid phases. Different customers have different product and purity demands, and these demands can change with seasons and other external factors. It is important to consider this product demand uncertainty during the design phase and develop a process that is flexible enough to meet future product demands.

A third form of uncertainty comes from unknown or varying availability of process inputs and pricing. The dominant operating expense in cryogenic air separation systems is the electricity required by the process. Peak versus off-peak costs and real-time pricing changes, can significantly affect the economic performance of the process. This uncertainty is well studied in a number of articles (Ierapetritou et al., 2002; Karwan and Keblis, 2007; Miller et al., 2008).

To handle potential uncertainties in the design phase, the traditional approach is to design the process according to nominal values of the uncertain parameters and then overdesign based on empirical factors. However, this approach may result in infeasible or conservative design decisions. The development of systematic design methods that explicitly consider process uncertainty has been an important research topic for many years (Grossmann & Sargent, 1978; Halemane & Grossmann, 1983). The two dominant approaches for rigorous consideration of uncertainty in optimization are the stochastic programming approach and the chance-constrained approach. Grossmann and Guillén-Gosálbez (2009) recently discussed the opportunities for the use of these approaches in the synthesis and planning of sustainable processes.

In the stochastic programming approach, individual scenarios are included in the optimization formulation for each discrete realization of the uncertain parameters. Continuous uncertainty spaces are usually approximated by appropriate sampling. The problem can be formulated using multiple stages with potential for decisions (or recourse) at each stage. Several good textbooks describe this approach in detail (e.g. Birge & Louveaux, 2000).

In chance-constrained programming, constraints need not be satisfied over the entire uncertainty space, but instead they are required to be satisfied with a given probability. While this explicit description is often desirable, these formulations can be very difficult to solve in the general case.

Multi-scenario optimization is a popular approach for design of chemical processes under uncertainty. Several researchers have investigated effective formulation and solution strategies for this class of problems (Paules & Floudas, 1992; Pistikopoulos & Grossmann, 1988a, 1988b; Pistikopoulos & Ierapetritou, 1995; Raspanti, Bandoni, & Bielger, 2000; Rooney & Biegler, 1999, 2001, 2003; Varvarezos, Biegler, & Grossmann, 1994), and several well known reviews are available (Biegler, Grossmann, & Westerberg, 1997; Pistikopoulos, 1995; Sahinidis, 2004). Two stages are typically considered in these formulations: the design stage and the operation stage. Values for the design variables must be determined, whereas values of the control variables can be determined during the operational stage when some uncertainties may have been resolved.