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Optimal operation of cryogenic air separation systems with demand uncertainty and contractual obligations

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ABSTRACT

Cryogenic air separation is an efficient technology for supplying large quantities of nitrogen, argon, and oxygen to chemical, petroleum and manufacturing customers. However, numerous uncertainties make effective operation of these complex processes difficult. This work addresses the problem of determining an optimal operating strategy to maximize the total profit of a cryogenic air separation process while considering demand uncertainty and contractual obligations. A rigorous process model is included as constraints in a nonlinear programming formulation. Uncertain demands are assumed to be normally distributed with known mean and standard deviation, and expected profit in the objective function is evaluated using the standard loss function. A probabilistic fill-rate expression, also based on the loss function, is used to model the contractual obligations by providing a lower bound on the expected product sales. In the single period case with one customer satisfaction constraint, the nonlinear programming formulation can be solved efficiently using the general purpose nonlinear optimization package, IPOPT. This formulation is then extended to include multiple time periods, the potential for product storage, and customer satisfaction constraints on multiple products. To solve the large-scale nonlinear programming formulation that considers a seven-day operating horizon, a tailored parallel nonlinear programming algorithm is used. This approach makes use of a Schur complement decomposition strategy to exploit the block structure of the problem and allow efficient solution in parallel. Using these tools, we solve for a set of optimal operating strategies over the complete space of different fill rates. This produces planning figures that identify key trade-offs between profitability and contractual obligations.

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1. Introduction

Cryogenic air separation is the dominant process for supplying significant quantities of high-purity industrial gas, such as nitrogen, argon and oxygen, to steel, chemical, petroleum, semiconductor, and aeronautical industries. The major operating cost of a cryogenic air separation process is electricity, and high energy costs drive increased mass and energy integration in these processes. Given uncertainty in product demands and changing electrical prices, maintaining contractual obligations while improving profitability may require frequent load changes and switches in the operating conditions. However, highly integrated flowsheets make the process more complex and challenging to operate, especially given the coupled interactions between multiple products. Therefore, it is important to use rigorous model-based tools to determine an operating strategy that maximizes profitability while considering demand uncertainty and contractual obligations to customers.

Previous research on optimization of cryogenic air separation systems focuses on detailed process optimization and control, as well as high level planning and scheduling. Dynamic optimization strategies, linear model predictive control, and nonlinear model predictive control techniques have all been applied to cryogenic air separation systems (Bian et al. 2005a,b; Huang et al., 2009; Roffel et al., 2000; White et al., 1996; Zhu et al., 2001; Zhu and Laird, 2008). These studies have focused primarily on the use of rigorous models for improving controller performance, and on determining optimal operating profiles targeting specific load changes. However, formulations like these, with detailed process models, typically do not consider high level operating concerns like uncertainty in product demands. On the other hand, planning and scheduling studies (Daryanian et al., 1989; Ierapetritou et al., 2002; Sirdeshpande and Ierapetritou, 2005; Karwan and Keblis, 2007; Miller et al., 2008) do consider market uncertainty and product inventory when planning operating strategies. To enable efficient solution of these challenging problems, simplified or linearized models are often used, which may ignore the integrated nature of the system and the nonlinear interactions between multiple products.

Several of these formulations directly address uncertainty in product demand. Multi-scenario approaches are often adopted in stochastic programming to deal with problems that contain

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uncertainties in the objective function or constraints (Pistikopoulos, 1995; Rooney and Biegler, 2003). While previous research using this approach has been successful for optimal planning and operation of air separation systems (Ierapetritou et al., 2002; Sirdeshpande and Ierapetritou, 2005), adopting a purely multi-scenario approach that requires the satisfaction of customer demands over all the scenarios can lead to solutions that are too conservative (Li et al., 2004; Nahmias, 2005; Li et al., 2008). To relax the constraints, the feasible region can be expanded and the objective function can be modified to penalize failure to satisfy all scenarios. However, the exact formulation and penalty parameter values may be difficult to determine or tune. As an alternative, probabilistic approaches (Wendt et al., 2002; Li et al., 2008) have been used. Coupled with known probability density distributions, probabilistic constraints can be reformulated as equivalent deterministic forms. Since the original constraints are only required to be satisfied with a given probability, solutions using these approaches can be significantly less conservative (Li et al., 2008).

This paper addresses the problem of determining optimal operating strategies to maximize the total profit of a cryogenic air separation system while considering rigorous nonlinear process models, uncertain product demands, and contractual obligations in the form of probabilistic fill-rate constraints. A first principles model of an air separation system is developed for three coupled columns to capture the nonlinear interactions in this highly integrated flowsheet. This model includes the necessary mass and energy balances as well as rigorous phase equilibrium and physical property expressions. In this paper, we adopt the probabilistic loss function developed in Li et al. (2004) and Nahmias (2005) to address the uncertainty associated with product demands. Uncertain demands are assumed to be normally distributed with known mean and variance, and the loss function is used to evaluate the expected revenue in the objective function.

To include contractual obligations, two types of service levels are typically considered (Li et al., 2004; Nahmias, 2005). The Type 1 service level only focuses on the number of scenarios that fail to satisfy demands. It does not consider the magnitude of the demand deficit in stock-out scenarios. In contrast, the Type 2 service level explicitly considers the amount of the demand that is not satisfied by plant. The *fill rate*, or customer satisfaction level, provides a lower bound on the ratio of the expected product sales to the expected product demand. The Type 2 service level is used in this work to capture contractual obligations since it is typically more consistent with actual contracts (Nahmias, 2005).

The complete nonlinear programming formulation can be used to identify optimal operating strategies for a particular facility with given contractual obligations in the form of fill-rate constraints. As well, solving the optimization problem repeatedly over the complete space of fill-rate values for different products provides valuable planning information. In particular, three regions can be identified. In the first region, the *profit defined region* (PDR), all the fill-rate constraints are inactive and the operating conditions are determined by profit considerations alone. As the required fill rates are increased, at least one of these constraints becomes active. Profits begin to deteriorate since the operating strategies are now constrained by contractual obligations. This region is called the *fill-rate constrained region* (FCR). The third region, the *infeasible region* (IR), identifies the space of fill rates that cannot be met by the plant without the use of inventory. These figures can be generated for a particular facility and used to assist management in analyzing the trade-offs between contractual obligations and expected profit.

The paper is organized as follows. Section 2 describes the cryogenic air separation and the rigorous nonlinear model of the process under study. Section 3 introduces the complete nonlinear programming formulation. This formulation includes the use of the loss function to evaluate the expected profit in the objective function. The loss function is also used in probabilistic fill-rate constraints to address contractual obligations. The formulation is presented for the multiperiod case with and without the potential for inventory. Single period formulations are solved using the interior-point nonlinear programming solver Ipopt (Wächter and Biegler, 2006), and the algorithm is briefly described. For multiperiod case studies, the problem is significantly larger, and a parallel approach is used based on the Schur-complement decomposition of the Newton step. Section 4 presents a case study that determines the optimal operating conditions for a single time period with a fill-rate constraint on a single product only. This study includes optimal results with and without available inventory. In Section 5, product interactions are considered with fill-rate constraints on multiple products. In Section 6, the case study is extended to include multiple time periods, the possibility of product inventory, and fill-rate constraints on all three products. Section 7 presents a summary and conclusions.

2. Cryogenic air separation process model

A typical cryogenic air separation system includes a double-effect heat-integrated distillation column with a side column of crude argon. The double distillation column is the common part of all cryogenic air separation systems, while a crude argon column (CAC) is adopted in some systems for co-production of argon. Addition of the argon column increases the complexity of the system significantly through additional coupling and recycling, and makes operation more difficult than the system with a double-effect distillation column alone. Fig. 1 shows the process flowsheet for the system studied in this paper. The crude air feed stream is compressed and primary impurities such as water and carbon dioxide are removed. After cooling, a portion of the air feed stream is expanded and introduced into the low-pressure distillation column (LPC) containing 70 theoretical stages. The remaining feed air stream enters the bottom of the high-pressure distillation column (HPC) with 36 theoretical stages. In the combined condenser/reboiler, the partially liquefied stream in the bottom of the LPC is vaporized, while the nitrogen vapor stream in the top of the HPC is condensed. A liquid nitrogen stream from the top of the HPC is introduced into the top of the LPC as the reflux stream. A portion of the oxygen-rich liquid from the bottom of the HPC is introduced into the 17th tray of the LPC in order to produce oxygen product with high purity. The remainder of the oxygen-rich liquid is used by the condenser at the top of the CAC to condense the argon-rich stream and produce the reflux for the CAC. A side vapor stream primarily composed of oxygen and argon is withdrawn at the 28th tray of the LPC and separated in the CAC. Liquid oxygen product is directly taken from combined condenser/reboiler and gas oxygen product is taken from the bottom of the LPC. Liquid nitrogen product is taken from the top of the HPC while gas nitrogen product is from the top of LPC. Nominal operating conditions for the air separation process under study are listed in Table 1.

The detailed air separation model is derived using the following four assumptions: (1) complete mixing on each tray and 100% tray efficiency; (2) negligible heat losses in the tray; (3) constant pressure drop on each tray; (4) uniform pressure and temperature on each tray.

The model includes mathematical expressions for the three distillation columns, two main heat exchangers, two integrated exchangers (one between the HPC and the LPC, another between the CAC and the HPC), and several throttle valves. The model contains mass and energy balances for all the exchangers and throttle valves. We assume that there is no energy loss in the exchangers, and that the pressure drops are constant across these units. The three distillation columns are all modeled using the following tray-by-tray equations, physical property expressions, and phase equilibrium.

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