Separation and Purification Technology 67 (2009) 262–270

Contents lists available at ScienceDirect

Separation and Purification Technology

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

Simulation and optimization of cryogenic air separation units using a homotopy-based backtracking method

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ARTICLE INFO

Article history:
Received 28 November 2008
Received in revised form 10 February 2009
Accepted 11 March 2009

Keywords:
Cryogenic air separation
Homotopy method
Backtracking
Automatic load change

ABSTRACT

In response to frequently changing demands on gaseous products of cryogenic air separation units, an automatic load change (ALC) system is desired to optimally change the products and recycle rates under widely variable load conditions. However, due to the complex heat integration in the process, simulation and optimization of cryogenic air separation units (ASUs) often fails to converge with traditional Newton-based algorithms. A homotopy-based backtracking method (HBM) is presented and applied to the process operation of a cryogenic ASU under wide changes in load conditions. Different from traditional process simulation, a load vector is introduced to denote the variation of the operation point due to the load change. The HBM solves the process in a way that heads toward the target and backtracks at failure. The results show that a large number of operating points that failed to converge with traditional algorithms can be successfully optimized with the proposed method.

1. Introduction

A cryogenic air separation unit (ASU) produces large volumes of oxygen, nitrogen, and argon at high purity. It is always connected to a manufacturing process such as production of primary metals or chemicals, or gasification. If the ASU is supplying gaseous products to a batch process like a steel furnace, it must automatically and rapidly respond to changing demands from the terminal user. Accurate predictions of the steady states at various operating points during load changes are essential for process operation. This requires a simulation and optimization technique that can always converge quickly and successfully.

A number of research reports on the process simulation and control of cryogenic air separation units have been published. Vinson [1] discussed air separation control technologies and considered the installation of model predictive control (MPC) as the best industry practice. Zhu et al. [2] developed a reduced order model for nitrogen purification using nonlinear wave theory. As an extension of this study, Bian et al. [3] established a dynamic simulation of the column and the integrated condenser/reboiler using Aspen Dynamics® and applied it to study the dynamic characteristics of the nitrogen plant. Bian et al. [4] also proposed compartmental modeling of high purity air separation columns by simplifying the stage-by-stage balance equations to compartment-by-compartment balance equations. These studies normally focused on columns. However, the separation of air into its components is energy-intensive and most units used in this process are highly thermally coupled. Therefore, the whole plant needs to be considered to reveal its true characteristics. Sirdeshpande et al. [5] described the mass and energy balances of the air separation cycle with a simplified algebraic model. However, the rigorous equilibrium-based method for a multi-components distillation column is much more effective for providing basic data to design and optimize this application. The traditional sequential modular (SM) method with iterating and tearing techniques often fails to converge quickly for this complex process with sensitive heat-coupling flowsheeting features under such widely varied operating conditions. The equation-oriented (EO) method based on Newton's algorithm, on the other hand, typically converges quickly. However, the EO method requires a good initial guess close to the solution, especially for complex process simulations. Therefore, Newton's method has difficulties in cases with wide and frequent load change requirements.

Homotopy methods [6] are a class of robust and globally convergent algorithms. The idea of these algorithms is to continuously deform a simple (easy) problem into the given (hard) problem with a homotopy index changing from zero to one. If the family of deformed problems converges easily, the method is particularly suitable for highly nonlinear problem for which good initial solution estimates are difficult to obtain. This kind of method has been successfully applied to chemical engineering process simulations [7–15]. Unlike the traditional homotopy methods for static process simulations, we propose in this paper a homotopy-based backtracking method (HBM) for real time optimization of a cryogenic ASU under widely varying load conditions. This method uses the opera-

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doi:10.1016/j.seppur.2009.03.032

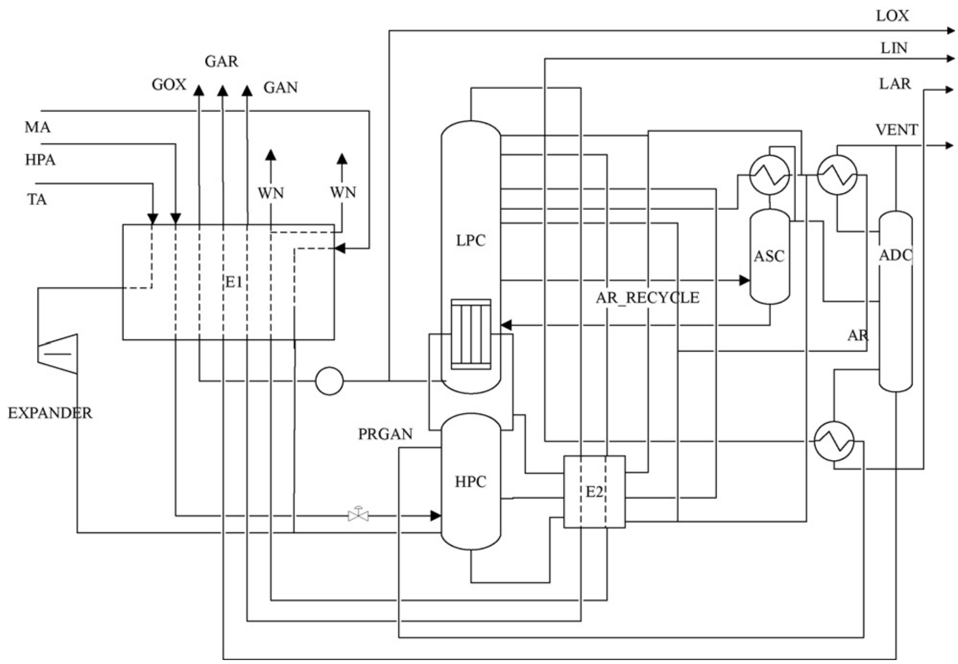

Fig. 1. Flow diagram of an internally compressed cryogenic air separation unit.

tional difference between the base and target points during a load change to define the homotopy parameter. Moreover, a backtracking technique is applied during the transition from the base point to the target point to improve efficiency.

2. Problem description

In this project, the flowsheeting study focuses on an internally compressed cryogenic air separation plant with a nominal capacity of 20,000 Nm^3/h gaseous oxygen. As illustrated in Fig. 1, the flowsheet consists of cooling and separating sections in a cold box. The air compression and CO_2 removal sections are not under discussion in this project.

In the plant, the compressed and cooled air streams are distilled in an integrated four-column distillation system, which consists of a high-pressure column (HPC), a low-pressure column (LPC), an argon sidearm column (ASC), and an argon distillation column (ADC). The cleaned air is split into three fractions: high-pressure air (HPA), main air (MA), and turbine air (TA). All the feeds are sent to a multi-stream heat exchanger, E1, to exchange heat with exit products and the waste nitrogen. HPA is mostly liquefied through a throttle valve and sent to an intermediate location of the HPC. MA and TA are directly fed into the bottom of HPC as saturated vapors. In HPC, the air is separated into high purity liquid nitrogen, nitrogen-rich liquid, and oxygen-rich liquid streams. LPC produces high purity gaseous nitrogen (GAN) at the top and liquid oxygen (LOX) at the bottom. After part of the LPC bottom stream is withdrawn as the liquid oxygen product, the remaining portion is pumped with an elevated pressure and vaporized in E1 to produce gaseous oxygen (GOX). Waste nitrogen (WN) is a side product of LPC drawn below the first section of the packing. A sub-cooler, E2, is designed to cool the HPC product streams against WN and GAN. The crude argon (AR) in this flowsheet is produced at the top of the ASC. High purity gaseous argon (GAR) and liquid argon (LAR) products are distilled in the ADC equipment. The process is a highly energy-integrated system. All columns and heat exchangers are thermally coupled without any utility inputs. HPC and LPC are designed to share a common condenser/reboiler. The overhead of the ASC is condensed by the oxygen-rich liquid air. ADC is reboiled by nitrogen vapor, called the pressure nitrogen (PRGAN) and condensed by liquid nitrogen. Gaseous products are evaporated and warmed by recycles and feeds in the heat exchangers E2 and E1.

The ASU is expected to optimally change its operating point in response to demand changes with an advanced control system. To maximize profit, a process simulation and optimization system is developed in this project for setting variables during load changes. In this system, the liquefied nitrogen and both the gaseous and liquefied argon products are set to constant flow rates. The product mix, therefore, is determined by three other variables, $\{F_{GOX}, F_{LOX}, F_{GAN}\}$, which represent the flow rates of gaseous oxygen, liquefied oxygen and gaseous nitrogen, respectively. Each product mix represents the online gas and liquid demand of a customer. Besides the demands of the product mix, the economic objective of minimizing the compression cost on feeds is also desirable for the process operation. With a steady state process model (f) described by the balance equations of the material, equilibrium, summation, and enthalpy (MESH) for all units and an additional work equation for the expander, the following process optimization problem can be built to locate the optimal operating point at various loads.

$$\begin{aligned}&\min_{X_{opt}} k_1 F_{HPA} + k_2 F_{MA} + k_3 F_{TA}\\ &s.t.: f(X_{prd}, X_{opt}, X_{fix}, X_{\exp}, X_{cal}) = 0\\ &X_{prd} = \{F_{GOX}, F_{LOX}, F_{GAN}\}\\ &X_{cal}^L \le X_{cal} \le X_{cal}^U\\ &X_{opt}^L \le X_{opt} \le X_{opt}^U\end{aligned} \qquad (1)$$

where k_1, k_2, and k_3 are cost coefficients of compressing HPA, MA and TA, respectively; X_{prd} is the desired product mix at a changing load; X_{opt} represents the optimized variables; X_{fix} represents the fixed parameters; X_{exp} represents the empirical variables; X_{cal} represents the calculated variables; X_{cal}^L and X_{cal}^U are the bounds on the calculated variables, such as the product purity specifications, operating pressure and temperature limits, etc.; and X_{opt}^L and X_{opt}^U are the bounds on the optimized variables.

The mathematical model of the process is built in Aspen Plus by a set of nonlinear algebraic equations with a total of 7447 variables. Among these variables, the fixed parameters include equipment structure parameters and hypothetically constant variables such