MODELING AND OPTIMIZATION OF THE AIR- AND GAS-SUPPLYING NETWORK OF A CHEMICAL PLANT

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Abstract: This paper presents a novel optimization method for the air- and gas-supplying network comprised of several air compression systems and air and gas streams in an industrial chemical plant. The optimization is based on the hybrid model developed by Han and Han\textsuperscript{1} for predicting the power consumption of a compression system. A constrained optimization problem was formulated to minimize the total electric power consumption of all the compression systems in the air- and gas-supplying network under various operating constraints and was solved using a successive quadratic optimization algorithm. The optimization approach was applied to an industrial terephthalic acid manufacturing plant to achieve about 10% reduction in the total electric power consumption under varying ambient conditions.

Keywords: Hybrid Modeling, Optimization, Air Compression System, Utility Plant, Partial Least-Squares.

1. INTRODUCTION

Air is one of the essential utilities for operating chemical plants and is usually supplied by compressors of various types. Typically, the compressor is connected with a steam turbine, a gas expander, or an electric motor as drivers on a single rotor, thus constitutes a compression system together with auxiliary components such as bearings, coolers, and gears.\textsuperscript{2} For a large-scale chemical plant, the compression systems are interconnected to each other to form a complex air-and gas-supplying network. In some cases, such a network consumes a major portion of the electric power spent in the plants and is usually supplied by compressors of various types.\textsuperscript{3}

Many optimization studies have been carried out for the utility systems in chemical plants, but most of them have been focused on steam production networks rather than air- and gas-supplying systems.\textsuperscript{4-8} In industry, compressors and turbines are usually optimized on the basis of macroscopic mass and energy balances where the performances (efficiencies) of compressors and turbines are assumed to be constant or expressed as relatively simple correlations that fit the design diagrams.\textsuperscript{9, 10} These industrial practices may not lead to the true optimal conditions because the performances of industrial compression systems are affected by diverse operating conditions such as discharge flow rate, ambient temperature and humidity, pressure drop through an air filter, compressor blade fouling, gas composition, and so forth.\textsuperscript{4, 9}

This paper presents a novel optimization approach for the air- and gas-supplying network as well as its outcome when applied to the TPA manufacturing plant of Samsung Petrochemical Corporation in Ulsan, Korea. This work is based on and logically follows from the modeling study for the compression systems by Han and Han\textsuperscript{1}. First, we present brief descriptions of the supplying network and the modeling problem is formulated on the basis of the hybrid models and the mass balances on the network. Finally, the results of field application is presented and discussed.

2. DESCRIPTION OF THE AIR- AND GAS-SUPPLYING NETWORK

Figure 1 shows a schematic diagram of the air-compression system consisting of a multistage compressor, an electric motor, and a multistage expander in the air- and gas-supplying network of a chemical plant. The compressor consists of several compression stages in series with an intercooler installed between successive compression stages. Humid air enters the suction of the first compression stage and is pressurized up to a desired level through several stages.

| Table 2. Variables Used for the Hybrid Modeling of the Compression Systems |
|-----------------|-----------------|-----------------|-----------------|
| Compression System | (Manipulated Variables) | (Unknown Operating Variables) | (Ambient Conditions) |
| Comp 1 (k = 1) | | | |
| Comp 2 (k = 2) | | | |
| Comp 3 (k = 3) | | | |
| Comp 4 (k = 4) | | | |
| Comp 5 (k = 5) | | | |

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Figure 1. Schematic of the multistage air-compression system

Because an isothermal compression process requires the minimum power, the intercooler lowers the temperature of the air discharged from each stage. The expander is used as the primary driver of the compressor and is comprised of several expansion stages in series with a re-heater installed in-between to maximize the energy recovery. The electric motor makes up for the deficient portion of the total power requirement of the compression system which the expander cannot provide.

Figure 2 shows the air- and gas-supplying network comprised of five compression systems and the air and gas streams in the TPA manufacturing plant of Samsung Petrochemical Corporation in Ulsan, Korea. Table 1 lists the configuration of the compression systems in the network. The compressor of each compression system provides the compressed air to various users such as the p-Xylene oxidizers, the TPA crystallizers, and the instrumental air units. The oxidizers are the main users; oxidizers are the main users that take up about 90 percent of the total compressed air. The inert high-pressure nitrogen is recovered from the oxidizers along with some by-product gases. This off-gas is supplied for the pneumatic conveying of particles and the driving of the expanders through the interconnected gas-stream lines. The flow rates and pressures of the air and off-gas are kept regulated and balanced throughout the network by the control systems.

Figure 2. Air- and gas-supplying network of the TPA plant

3. MODELING OF THE COMPRESSION SYSTEMS

In this section we will only briefly outline the modeling approach for the compression systems in the network and refer the readers to the paper by Han and Han1 for the details. Figure 3 depicts the prediction procedure for the electric power consumption $W_c^{(k)}$ of the k-th compression system in the air- and gas-supplying network. $W_c^{(k)}$ is ultimately calculated using the thermodynamic equation

$$W_c^{(k)} = \frac{\sum_{i=1}^{n} P_i (\gamma - 1) M_v}{P}$$

where $W_c^{(k)}$ and $W_c^{(k)}$ are the minimum and maximum powers of all the compression stages and expansion stages, respectively, that can be theoretically obtained under adiabatic and reversible conditions by

$$W_c^{(k)} = \frac{\sum_{i=1}^{n} P_i (\gamma - 1) M_v}{P}$$

and $\eta_{C}^{(k)}$ is the overall efficiency that colligates the performances of all the components comprising the compression system and is to be predicted as a function of operating variables and ambient conditions. The variables affecting $\eta_{C}^{(k)}$ are classified into three categories: 1) the manipulated variables $x_{\text{in}}^{(k)}$ that can be set by the operator, 2) the unknown state variables $x_{\text{in}}^{(k)}$ that vary with other operating variables, and 3) the ambient conditions $x_{\text{in}}^{(k)}$. Table 2 lists the classified variables for each of the five compression systems in the network. The partial least squares (PLS) models are constructed for the prediction of the unknown variables and efficiency, respectively, on the basis of the operating data for the past nine months, and are combined with the thermodynamic equations (1)-(3) to form a hybrid model for predicting the actual power consumption. The typical performance of the hybrid model is demonstrated by Figure 4 that shows excellent agreement between the measured and predicted values of the electric power consumption for Comp 1 with 0.69% average prediction error. Similar performances were obtained for the other compression systems with the average errors ranging between 0.49% and 1.25%

Figure 3. Prediction procedure of the electric power consumption of the kth compression system
4. FORMULATION OF THE OPTIMIZATION PROBLEM

The objective of the optimization is to minimize the total electric power consumption of all the compression systems in the air- and gas-supplying network under various operating constraints. The objective is achieved by formally solving the following constrained optimization problem:

\[
\min J = \sum_{k} W_{k}^{(a)} = \sum_{k} \left[ W_{k}^{(a)} + W_{k}^{(g)} \right] / \eta_{k}^{(a)}
\]  

subject to

\[
A_{i} X_{i} = b
\]

\[
X_{i} \leq X \leq X_{i}
\]

\[
W_{k}^{(a)} \leq W_{k} \leq W_{k}^{(a)}
\]

\[
P_{k}^{(a)} = F_{k}^{(a)}(\alpha_{k}^{(a)} + B_{k}^{(a)}), \quad k = 1, 2, \ldots, N_{k}
\]

\[
P_{k}^{(g)} = F_{k}^{(g)}(\alpha_{k}^{(g)} + B_{k}^{(g)}), \quad k = 1, 2, \ldots, N_{k}
\]

\[
P_{k}^{(a)} = F_{k}^{(a)}(\alpha_{k}^{(a)} + B_{k}^{(a)}), \quad k = 1, 2, \ldots, N_{k}
\]

In the above, \( X_{i} \) denotes the vector of the optimization (decision) variables to be determined. It consists of most of the manipulated variables for all the compression systems (except the discharge pressures of the compressed air and the suction pressures of the off-gas which are predetermined by the operating conditions of the users) and the flow rates of the air and gas streams in the network. The equality constraint (5) represents the mass balances that allocate the air and gas streams to meet the demands of various users in the network. Equations (6) and (7) represent the lower and upper bounds on the optimization variables \( X_{i} \) and the other operating variables \( X_{i} \), which are imposed by hardware constraints, operating conditions, and safety considerations. Equation (8) confines the power loads of the electric motors between appropriate bounds. Equations (9) and (10) address the important safety limits in the operation of a compressor and prevent each compressor from being operated below a surge line and above a stonewall (or choke line), respectively. The parameters \( \alpha_{k}^{(a)} \), \( \alpha_{k}^{(g)} \), \( \beta_{k}^{(a)} \), and \( \beta_{k}^{(g)} \) in the equations can be obtained from the performance curves of compressors provided by vendors. Equations (11) and (12) address the similar safety considerations for the expanders. Tables 3 and 4 list the optimization variables and various bounds explained in the above.

![Comparison of the measured (dotted lines) and predicted (solid lines) values of the electric power consumption of Comp 1.](image)

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5. RESULTS AND DISCUSSION

The optimization problem defined in Equations (4) – (12) is a nonlinear programming (NLP) problem. In this study, a successive quadratic programming (SQP) algorithm was employed to solve this NLP problem. All the equations in the hybrid model are described in the objective function routine of the SQP algorithm.

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Table 3. Optimization (Decision) Variables and Their Operating Ranges

<table>
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<tr>
<th>Variable</th>
<th>Optimization Bound</th>
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<th>Upper</th>
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<td>Bound</td>
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<td>14</td>
<td>( \eta_{14}^{(a)} )</td>
<td>28.0</td>
<td>26.0</td>
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Table 4. Parameters of the Operating Bounds

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Comp 1</th>
<th>Comp 2</th>
<th>Comp 3</th>
</tr>
</thead>
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<tr>
<td>( W_{1}^{(a)} )</td>
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<td>10000</td>
<td>10000</td>
</tr>
<tr>
<td>( W_{2}^{(a)} )</td>
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<td>12000</td>
<td>12000</td>
</tr>
<tr>
<td>( \alpha_{1}^{(a)} )</td>
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<td>60.0</td>
<td>60.0</td>
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<tr>
<td>( \alpha_{2}^{(a)} )</td>
<td>60.0</td>
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<td>( \beta_{1}^{(a)} )</td>
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<td>( \eta_{4}^{(a)} )</td>
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<td>( \eta_{6}^{(a)} )</td>
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obtained within three seconds on a Pentium III-866 machine. Taking much time, the optimization results were typically function evaluation in the optimization algorithm does not.

Basic™ programming for field installation. Since the graphic user interface was constructed using Microsoft Visual 90 codes were prepared for the optimization engine and the optimization model is more reproducible and needs lower maintenance cost than closed-equation approaches. Fortran

the oxidizers, thus can be ignored in the optimization. On the other hand, since the ambient temperature and relative humidity change significantly between day and night as well as according to the seasonal and weather variations, they are regarded as the two major disturbance variables whose effects on the power consumption are to be examined in this study.

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Since the ambient conditions listed in Table 2 represent the systems, their effects on the optimization results were investigated. Among the ambient conditions, the off-gas composition varies little due to stable composition control in gas-supplying network, depicted in Figure 2, in the TPA plant of Samsung Petrochemical Corporation using the optimization engine and the optimization results were typically obtained within three seconds on a Pentium III-866 machine.

The optimization runs were carried out for the air- and gas-supplying network, depicted in Figure 2, in the TPA plant of Samsung Petrochemical Corporation using the optimization variables and their associated bounds listed in Tables 3 and 4. Since the ambient conditions listed in Table 2 represent the disturbance variables in the operation of the compression systems, their effects on the optimization results were investigated. Among the ambient conditions, the off-gas composition varies little due to stable composition control in the oxidizers, thus can be ignored in the optimization. On the other hand, since the ambient temperature and relative humidity change significantly between day and night as well as according to the seasonal and weather variations, they are regarded as the two major disturbance variables whose effects on the power consumption are to be examined in this study.

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Tables 5 and 6 compare the operating conditions and the electric power consumptions between before and after optimization. The optimizations were performed for two different sets of ambient conditions: the daytime operation ($T_a = 299.5 \, K$, $H_a = 59 \%$) and the nighttime operation ($T_a = 288.0 \, K$, $H_a = 71 \%$). Table 5 shows that the air and off-gas flow rates ($F_a$ and $F_e$) should be reallocated to the compression systems and the off-gas temperatures ($T_{eg}$) should be adjusted from the present operating conditions to reduce the total electric power usage at each operation mode. Table 6 demonstrates that such changes of operating conditions led to about 10% reduction in the total power consumption both for the day and night operations.

**NOMENCLATURE**

- $F_a$: flow rate of the air through a compression stage [kg/s]
- $F_e$: flow rate of the air through an interconnected line [kg/s]
- $\bar{F}_a$: average flow rate of the air through a multistage compressor [kg/s]
- $F_{gs}$: flow rate of the gas through an expansion stage [kg/s]
- $F_{gs}$: flow rate of the gas through an interconnected line [kg/s]
- $H_a$: relative humidity [%]
- $M_{ar}$: average molecular weight of ambient air [kg/kg-mole]
- $M_{gr}$: average molecular weight of the gas entering an expander [kg/kg-mole]
- $N_c$: total number of compression stages of a compression system
- $N_e$: total number of expansion stages of a compression system
- $N_k$: total number of compression systems installed in the air- and gas-supplying network
- $P_{ad}$: discharge pressure of the air from a compression stage [kPa]
- $P_a$: suction pressure of the air at to compression stage [kPa]
- $P_e$: atmospheric pressure [kPa]
- $P_{gs}$: discharge pressure of the gas from an expansion stage [kPa]
- $P_{gs}$: suction pressure of the gas to an expansion stage [kPa]
- $R$: universal gas constant [8.314 kJ/kg-mole-K]
- $S_k$: impeller rotating speed of a single expansion stage [RPM]
- $T_a$: ambient temperature of compression systems [K]
- $T_{ad}$: discharge temperature of the air from a compression stage [K]
- $T_{gs}$: suction temperature of the gas to an expansion stage [K]
- $W_{es}$: minimum power required for a multistage compressor under an adiabatic and reversible process [kW]
- $W_{es}$: maximum power generated by a multistage expander under an adiabatic and reversible process [kW]
- $W_{em}$: electric power delivered to an electric motor [kW]
- $X$: vector of optimization (manipulated) variables for the air- and gas-supplying network
- $x_{ki}$: vector of manipulated variables of a compression system
- $X_{ki}$: vector of unknown operating variables of a compression system
- $\alpha_c$: slope of the surge control line of a compressor [kPa-s/kg]
- $\alpha_e$: slope of the stonewall line of a compressor [kPa-s/kg]
- $\alpha_{es}$: slope of the lower operation line of an expander [kPa-s/kg]
- $\beta_c$: intercept of the surge control line of a compressor [kPa]
- $\beta_e$: intercept of the stonewall line of a compressor [kPa]
- $\beta_{es}$: intercept of the lower operation line of an expander [kPa]
- $\gamma_a$: average adiabatic exponent of the air through a multistage compressor
- $\gamma_e$: average adiabatic exponent of the gas through a multistage expander
- $\Delta P_e$: pressure drop through a compressor filter [kPa]
- $\eta$: overall efficiency of a compression system [0–1]
- $\lambda$: weight fraction of gas [0–1]
- $\phi_i$: position of the inlet guide vane of a compressor [degree]
- $\phi_i$: position of the inlet guide vane of an expander [degree]
- $\omega$: regression coefficient vector of the PLS model for the overall efficiency prediction
- $\omega$: regression coefficient vector of the PLS model for the unknown variable prediction

**Greek Letters**

- $\alpha$: air
- $C$: compressor or compression stage
- $CO$: carbon monoxide
- $CO_2$: carbon dioxide
- $E$: expander or expansion stage
- $e$: ambient condition
- $g$: gas
\( L = \text{lower} \)  
\( M = \text{electric motor} \)  
\( O_2 = \text{oxygen} \)  
\( U = \text{upper} \)  
\( W = \text{water} \)  
\( (i) = \text{compression or expansion stage } i \)  
\( (k) = \text{kth compression system in the air- and gas-supplying network} \)

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