Chapter 12

Robust Engineering Strategy for Solving Optimization Problems of Refinery Hydrogen System

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12.1 INTRODUCTION

In order to maintain business efficiency, refineries are increasingly concerned with improving the operational management of their complex process. In fact, there has been much effort that addresses problems in the management of production systems and steam power systems of refineries. Moro et al. (1998) developed a nonlinear planning model for refinery production, which is able to represent a general refinery topology and allowed the implementation of nonlinear process models as well as blending relations. This framework was later extended to support sequence decisions at the scheduling level by Pinto et al. (2000) and Joly et al. (2002). In the work of Neiro and Pinto (2005), uncertainties related to petroleum and product prices as well as demand are included in the model as a set of discrete probabilities. Based on a fast and robust online data reconciliation method, operational optimization of a utility system in a petrochemical plant was developed by Lee et al. (1998) and the fuel cost was reduced by 5.4%–9.2% compared with the former operation. In order to deal with the prediction errors of energy demands in multiperiod operational planning, Yi et al. (2003) proposed an integration methodology of periodic replanning and hierarchical repair. Micheletto et al. (2008) presented a conceptual modeling framework for operational optimization of utility systems. The MILP (mixed-integer linear programming) model was integrated with the refinery database for the planning of a refinery utility system and effectively optimized the financial performance of the thermoelectric plant without any capital investment.

In recent years, the management of refinery gas systems, such as fuel gas systems (Hasan et al., 2011; Iyer and Grossmann, 1997; Jagannath et al.,

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2012; Zhang and Rong, 2008; Zhang et al., 2010) and hydrogen networks (Ahmad et al., 2010; Alves and Towler, 2002; Elkamel et al., 2011; Hallale and Liu, 2001; Jiao et al., 2012; Liao et al., 2011; Liao et al., 2010; Liu and Zhang, 2004; Van den Heever and Grossmann, 2003; Xuan et al., 2010; Zhou et al., 2014; Zhou et al., 2012; Zhou et al., 2013), has drawn more and more attention. This is because they are the primary energy source in the refinery, while hydrogen is critical for improving product quality. However, relatively little research has focused on optimizing these systems, especially the hydrogen system. Hydrogen is continuously generated from the reformer and PSA units and is supplied to most of the hydrogen consumers around the refinery via compressors. Therefore, effective operational optimization of the hydrogen system can be very effective for energy cost reduction and emission reduction in the refining process. Liu and Zhang (2004) established simplified mathematical models for various purification devices and proposed a superstructure model of hydrogen network design with an integrated hydrogen purification scheme. In order to capture a richer network structure space, Liao et al. (2010) introduced a state space superstructure for integrating purifiers with compressors. Jiao et al. (2012) decomposed the optimization problem into two parts: hydrogen purification network and hydrogen supply network. They also linearized the original MINLP model into a MILP model.

The scheduling of hydrogen networks has also attracted wide attention. Van den Heever and Grossmann (2003) established two MINLP models to optimize the production planning and scheduling of the hydrogen systems. Xuan et al. (2010) and Ahmad et al. (2010) introduced a multiperiod hydrogen network optimization model based on their previous single period models. Elkamel et al. (2011) incorporated a hydrogen network with rigorous process models. Zhou et al. (2014) proposed detailed hydrogen pipeline models for the scheduling problem.

The rest of the paper is organized as follows: Section 12.2 describes the problem statement as well as the general features of the hydrogen system in a refinery. Section 12.3 presents the mathematical formulation of the operational optimization problem. Section 12.4 illustrates a systematic procedure to implement the method of Section 12.3 to a large-scale refinery. Conclusions of this work are given in Section 12.5.

12.2 PROBLEM STATEMENT AND DESCRIPTION OF THE HYDROGEN SYSTEM

Typical hydrogen-related streams in a refinery are shown in Fig. 12.1. The lines in red or blue in the figure represent the gas flow. For a hydrogen pipeline system, there are generally two categories: low-pressure hydrogen pipeline networks (LP network) and high-pressure hydrogen pipeline networks (HP network). The hydrogen inside an LP network can be compressed to the HP network, while the hydrogen from a HP network can be purged to the LP network

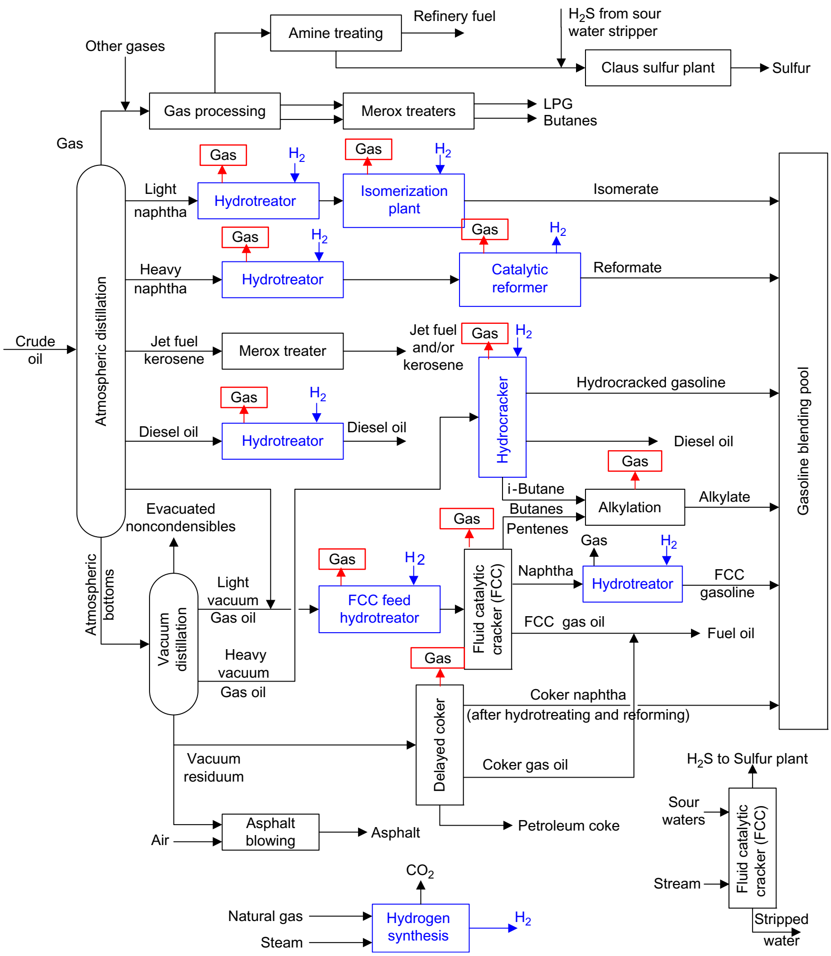

FIG. 12.1 Schematic representation of a refinery process.

via valves. Consequently, the LP network and HP network could be balanced by this two-way connection. Both an LP network and a HP network are critical to the hydrogen supply in a refinery. Therefore, the operational optimization of a hydrogen pipeline system should include both LP and HP networks. The optimization problem can be stated as follows: given a set of hydrogen generating/consuming processes and a network of interconnections among the processes, it is desired to determine a scheduling scheme so that the overall annualized cost is minimized while the processes receive adequate hydrogen resource.

Fig. 12.2 presents a simplified flowchart of an HP network system in which the pipeline network is represented by the red lines and each unit connected to the network is represented by a rounded rectangle that contains its identification.

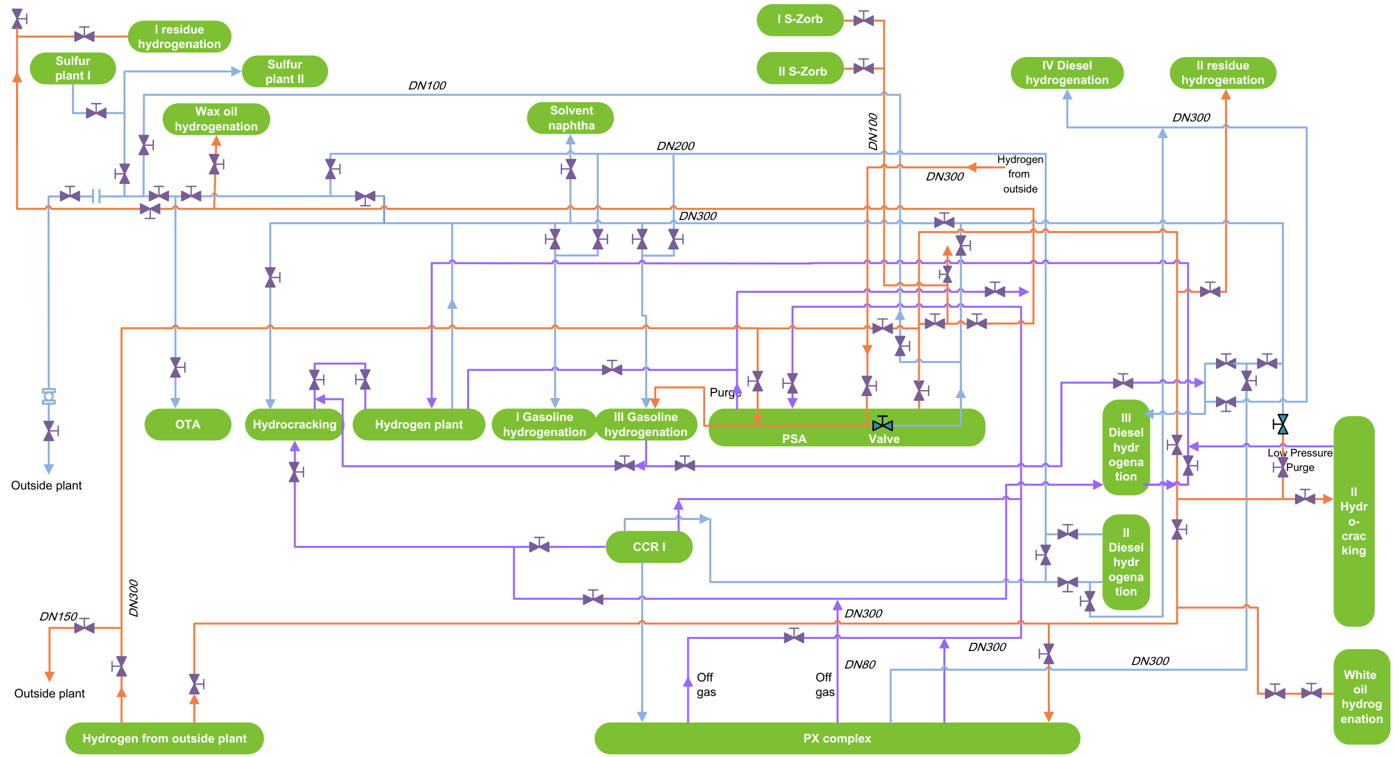

FIG. 12.2 Simplified flowchart of refinery's HP network system.

As illustrated in Fig. 12.2, the units in the HP network include a gasoline hydrotreating unit (GHU), diesel hydrotreating unit (DHU), hydrocracker (HC), s-zorb unit (SZU), wax oil hydrotreating (WHU), residue hydrotreating (RHU), and a hydrogen plant (HP). Despite the hydrogen plant, the units connected to the HP network only consume hydrogen, and they are called "hydrogen consuming units." The hydrogen consuming units are depicted in dark color, while the hydrogen producer—hydrogen plant is depicted in light color.

The units in the LP network include continuous reforming unit (CRU), pressure swing adsorption (PSA), hydrocracker (HC), diesel hydrotreating (DHU), and gasoline hydrotreating unit (GHU). The consumers of LP network are mainly supplied by hydrogen produced from CRU and PSA units. It should be noted that the HC, DHU, and GHU units can receive hydrogen from both the HP and LP network. Thus, we have a degree of freedom for practical hydrogen allocation and balance. The balancing tools are the compression of the surplus hydrogen of the LP network to the HP network and the relief of the surplus hydrogen of the HP network to the LP network. Because compressors consume a large amount of energy, they are the most important equipment for keeping the balance of the hydrogen pipeline network. If the above two tools cannot balance the hydrogen production and consumption instantly, an additional schedule to relieve hydrogen to the fuel gas system or to cut down the production rate of certain units will be employed. Of course, the additional schedules would cause economic loss, as they are not expected.

Hydrogen produced by the CRU cannot satisfy the demand of the whole refinery. The deficit of hydrogen demand is compensated by the hydrogen plant, which converts hydrocarbon resources, such as natural gas, liquefied petroleum gas (LPG), and refinery off gas, into hydrogen and carbon dioxide. As a result, it is desirable to minimize the hydrogen plant production for economic profit.

12.3 MATHEMATICAL MODEL AND SOLVING METHOD

In a previous work (Zhou et al., 2014), a hydrogen pipeline schedule model is proposed to optimize equipment operation. A modeling method called mathematical programming with equilibrium constraint (MPEC) is introduced to model the operation of compressors and the flow of a branching structure pipeline network, which replaces the MINLP formulation with a NLP problem and improves the solution efficiency.

The formulation of the operational optimization model of a hydrogen pipeline network in this research is based on the hydrogen pipeline network of Fig. 12.2, the scheduling model is formulated as follows.

12.3.1 Objective Function

The goal of the multiperiod scheduling model of hydrogen systems is to minimize the total cost. Because the hydrogen from the reforming unit is a byproduct, we only consider the hydrogen cost from the hydrogen plant. The objective function is as follows:

$$\text{Min} \quad obj = \sum_h \sum_t e_{h,t} F_{h,t} \tag{12.1}$$

where $F_{h,\,t}$ represents the production amount of the hydrogen plant in period t and e_{ht} stands for the production cost of the hydrogen plant. The efficiency and unit cost of the hydrogen plant depend on the production rate. In order to minimize the total cost and to keep the hydrogen plant running as smoothly and efficiently as possible, the operating schedule of the hydrogen plant should be optimized according to the efficiency curve. Let us introduce a penalty term, $e^{penalty}$, to the cases that are outside the optimal production range. The production cost of the hydrogen plant can be described by a segmentation function as follows:

$$e_{h,t} = \begin{cases} e + e^{penalty1} & \text{if} F_{h,t} < F_h{}^{Low} \\ e & \text{if} F_h{}^{Low} \le F_{h,t} \le F_h{}^{Up} \\ e + e^{penalty2} & \text{if} F_{h,t} > F_h{}^{Up} \end{cases} \tag{12.2}$$

12.3.2 Hydrogen Pipeline Model

A hydrogen pipeline network not only transfers hydrogen, but also stores hydrogen. Hydrogen transport in the pipeline should satisfy the following balance equations: mass balance equation, momentum balance equation, and energy balance equation. Because the hydrogen pipeline network is operated at room temperature, we assume the whole procedure is isothermal. Consequently, the energy balance of the pipeline can be ignored.

The mass balance equation reads:

$$\frac{MwA}{ZRT}\frac{\partial P}{\partial t} + \frac{\partial F}{\partial z} = 0$$

where Mw is the molecular weight of the gas flow inside the pipe, A is the cross-sectional area of the pipe, Z is the gas compression factor, R is a constant, T is the temperature inside the pipe, P is pressure, and F is the gas flowrate inside the pipeline. After manipulating the above formula, we obtain:

$$\frac{MwA_a\ell_a}{ZRT}\left(\overline{P}_{a,t+1} - \overline{P}_{a,t}\right) = \int_t^{t+1} \left(F_{a,in} - F_{a,out}\right)dt \quad \forall a \in A, t \in T$$

where ℓ is the length of the pipeline and $P_{a,t+1}$ is the average pressure of the pipeline in period t. In order to obtain a numerical mass balance equation, we integrate the above equation by the trapezoidal integral method. The result is as follows:

$$\frac{MwA_a\ell_a}{ZRT}\left(\overline{P}_{a,t+1}-\overline{P}_{a,t}\right)=\frac{1}{2}[(F_{a,in,t}-F_{a,out,t})+(F_{a,in,t+1}-F_{a,out,t+1})](t_{t+1}-t_t)$$
$$\forall a\in A,t\in T$$

Note that in the above equation, Mw does not vary with location a and period t. This equation is only suitable for gas transport systems with stable components. We have more than one hydrogen source in the hydrogen pipeline network and the flowrate and purity of the hydrogen injection varies with production period. Therefore, the Mw inside the hydrogen pipeline network is not constant. Accordingly, the above equation can be modified as follows:

$$\frac{A_a\ell_a}{RT}\left(\frac{Mw_{a,t+1}}{Z_{a,t+1}}\overline{P}_{a,t+1}-\frac{Mw_{a,t}}{Z_{a,t}}\overline{P}_{a,t}\right)$$
$$=\frac{1}{2}[(F_{a,in,t}-F_{a,out,t})+(F_{a,in,t+1}-F_{a,out,t+1})](t_{t+1}-t_t)\quad \forall a\in A,t\in T \tag{12.3}$$

where $Mw_{a,\,t}$ can be calculated by the composition of the source hydrogen streams:

$$Mw_{a,t}=\frac{1}{\sum_m {y_{a,m,t}}/{Mw_m}}\qquad \forall a\in A,t\in t \tag{12.4}$$

The compression factor of the mixed gas can be calculated by several methods. Because its hydrogen content is >80%, we calculate the compression factor based on the hydrogen content:

$$Z_{a,t}=\frac{\overline{P}_{a,t}Vm_{a,t}}{RT}\qquad a\in A,t\in T \tag{12.5}$$

where $Vm_{a,\,t}$ is the gas volume. The relationship between the average pressure and the gas volume is presented by the Peng-Robinson equation:

$$\overline{P}_{a,t}=\frac{RT}{Vm_{a,t}-b^{P-R}}-\frac{a^{P-R}\alpha^{P-R}}{Vm_{a,t}{}^2+2b^{P-R}Vm_{a,t}-\left(b^{P-R}\right)^2}\quad a\in A,t\in T \tag{12.6}$$

where a^{P-R} and b^{P-R} are coefficients.

$$a^{P-R}=0.45724\frac{R^2Tc^2}{Pc} \tag{12.7}$$

$$b^{P-R}=0.0778\frac{RTc}{Pc} \tag{12.8}$$

$$\alpha^{P-R}=\left(1+\left(1-\sqrt{T/Tc}\right)\left(0.37464+1.54226f^{Acentricity}-0.26992\left(f^{Acentricity}\right)^2\right)\right)^2 \tag{12.9}$$

The above simplification has been validated in our previous work.

12.3.3 Momentum Balance Equation

As the hydrogen pipe diameter is relatively large, the gas flow in the pipeline can be recognized as a one-dimensional flow, and the momentum conservation equation may be expressed as:

$$\frac{dP}{dz} = \frac{-fZRTF|F|}{2DA^2MwP}$$

If we only examine the pressure and flow changes at the inlet and outlet of the pipe section, then the above equation can be written as:

$$\left.\frac{dP}{dz}\right._{a,k,t} = \frac{-f_{a,k,t}Z_{a,t}RTF_{a,k,t}|F_{a,k,t}|}{2D_aA_a{}^2Mw_{a,t}P_{a,k,t}} \qquad \forall a \in A, t \in T, k \in K \tag{12.10}$$

where $K = \{\text{in, out}\}$ stands for the inlet and outlet of the pipeline section, respectively. Note that the absolute value is employed for reverse flow phenomena.

$$F_{a,in,t}F_{a,out,t} \geq 0 \qquad \forall a \in A, t \in T \tag{12.11}$$

The average pressure of the pipeline is calculated as:

$$\overline{P}_{a,t} = \frac{\int_0^{L_a} P(z')dz'}{\int_0^{L_a} dz} \qquad \forall a \in A, t \in T$$

We use the collocation method to solve this momentum balance equation:

$$P_{a,in,t} = h_{a,t}{}^1 \qquad \forall a \in A, t \in T \tag{12.12}$$

$$\left.\frac{dP}{dz}\right._{a,in,t} = h_{a,t}{}^2 \qquad \forall a \in A, t \in T \tag{12.13}$$

$$P_{a,out,t} = h_{a,t}{}^3 \qquad \forall a \in A, t \in T \tag{12.14}$$

$$\left.\frac{dP}{dz}\right._{a,out,t} = h_{a,t}{}^4 \qquad \forall a \in A, t \in T \tag{12.15}$$

$$h_{a,t}{}^3 = h_{a,t}{}^1 + \frac{L_a}{2}\left(h_{a,t}{}^2 + h_{a,t}{}^4\right) \qquad \forall a \in A, t \in T \tag{12.16}$$

where $h^1_{a,\,t}$, $h^2_{a,\,t}$, $h^3_{a,\,t}$ and $h^4_{a,\,t}$ are auxiliary variables. Now the average pressure calculation equation can be written as:

$$\overline{P}_{a,t} = \frac{\int_0^{L_a} P(z')dz'}{\int_0^{L_a} dz} = \frac{(1/2)h_{a,t}{}^1 + (1/12)h_{a,t}{}^2L_a + (1/2)h_{a,t}{}^3 - (1/12)h_{a,t}{}^4L_a}{L_a}$$

$$\forall a \in A, t \in T \tag{12.17}$$

So far, we have modeled the mass balance and momentum balance of the gas flow in the pipeline section. It should be pointed that the hydrogen streams inside the refinery are multicomponent streams. In addition, there is a composition distribution inside the pipeline network. Therefore, we need to calculate the composition of the hydrogen pipeline network in real time.

Assuming that the pipeline is filled with hydrogen at the beginning of the first period:

$$y_{a,m,0} = {y_{a,m,0}}^{in} \qquad \forall a \in A, m \in M \tag{12.18}$$

In actual production, the pipelines are connected by a flange, which forms physical nodes. For modeling convenience, we denote the flange by node $n \in N$, assuming that the pipelines and the hydrogen sources and demands are all connected by the nodes, as shown in Fig. 12.3. Because the flange (2-way or 3-way) is used only as a connection tool for the pipeline, no material accumulation occurs.

$$y_{i,m,t} = y_{n,m,t} \qquad \forall (i,n) \in Sup(I,N), m \in M, t \in T \tag{12.19}$$

$$y_{j,m,t} = y_{n,m,t} \qquad \forall (j,n) \in Dem(J,N), m \in M, t \in T \tag{12.20}$$

The concentration of the node is equal to the concentration of the stream that is flowing into the node.

$$y_{n,m,t} = \begin{cases} {y_{a,m,t}}^{in} & \text{if } F_{a,in,t} > 0 \quad \forall (a,n) \in A \text{ from } N(A,N), t \in T \\ {y_{a,m,t}}^{in} & \text{if } F_{a,out,t} < 0 \quad \forall (a,n) \in A \text{ to } N(A,N), t \in T \end{cases} \tag{12.21}$$

The mass balance equation at the node and the component mass balance equation are as follows:

$$\sum_{a:(a,n)\in AtoN(A,N)} F_{a,out,t} + \sum_{i:(i,n)\in Sup(I,N)} F_{i,t} = \sum_{a:(a,n)\in AfromN(A,N)} F_{a,in,t} + \sum_{j:(j,n)\in Dem(J,N)} F_{j,t} \quad \forall n \in N \tag{12.22}$$

$$\sum_{a:(a,n)\in AtoN(A,N)} F_{a,out,t} y_{a,m,t} + \sum_{i:(i,n)\in Sup(I,N)} F_{i,t} y_{i,m,t} = \sum_{a:(a,n)\in AfromN(A,N)} F_{a,in,t} y_{a,m,t} + \sum_{j:(j,n)\in Dem(J,N)} F_{j,t} y_{j,m,t} \quad \forall n \in N, m \in M \tag{12.23}$$

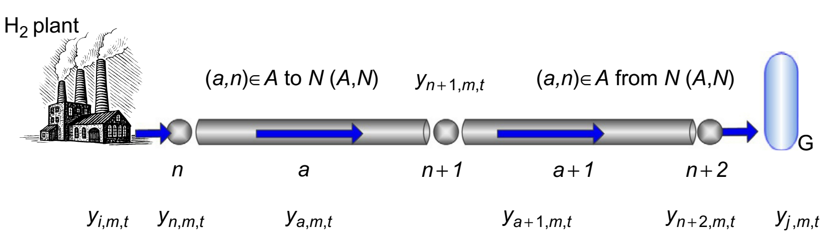

FIG. 12.3 Sketch map for the pipe segments, nodes, and the corresponding variables.

where $y_{a,m,t}$ denotes the concentration of component m at pipeline a in period t.

Once $t > 0$, there will be hydrogen streams with different compositions that flow into the pipeline, assuming that the pipeline hydrogen concentration is always uniform. As there may be reverse flow in the pipeline section, the pipeline composition calculation is divided into two cases:

(1) $F_{a,in,t+1} > 0$

$$y_{a,m,t+1}\left(F_{a,in,t+1}\Delta t + Inventory_{a,t}\right) = y_{a,m,t+1}{}^{in}F_{a,in,t+1}\Delta t + y_{a,m,t}Inventory_{a,t} \quad \forall a \in A, m \in M, t \in T \tag{12.24}$$

(2) $F_{a,out,t+1} < 0$,

$$y_{a,m,t+1}\left(|F_{a,out,t+1}|\Delta t + Inventory_{a,t}\right) = y_{a,m,t+1}{}^{in}|F_{a,out,t+1}|\Delta t + y_{a,m,t}Inventory_{a,t} \forall a \in A, m \in M, t \in T \tag{12.25}$$

Component concentration normalization equation:

$$\sum_m y_{a,m,t}{}^{in} = 1 \qquad \forall a \in A, t \in T \tag{12.26}$$

$$\sum_m y_{a,m,t} = 1 \qquad \forall a \in A, t \in T \tag{12.27}$$

$$\sum_m y_{n,m,t} = 1 \qquad \forall n \in N, t \in T \tag{12.28}$$

$$\sum_m y_{d,m,t} = 1 \qquad \forall d \in D, t \in T \tag{12.29}$$

where $Inventory_{a,t}$ indicates the amount of hydrogen stored in the pipeline section. The hydrogen pipe network has two major roles: (1) to move the hydrogen from the hydrogen source to the hydrogen trap transport; and (2) as the system of hydrogen buffer equipment. When the hydrogen production is greater than the consumption of a certain amount of hydrogen storage, the system hydrogen production is less than the consumption of hydrogen released. The initial hydrogen storage capacity in the pipe section is calculated according to the average pressure in the pipe section of the initial production cycle. After the start of the dispatching cycle, the hydrogen accumulation in the pipe section is the difference between the hydrogen injection and the consumption at the inlet and outlet.

$$Inventory_{a,0} = \frac{A_a \ell_a Mw_{a,0}\overline{P}_{a,0}}{RT} \qquad \forall a \in A$$

$$Inventory_{a,t+1} = \begin{cases} Inventory_{a,t} + (F_{a,in.t+1} - F_{a,out,t+1})\Delta t & \text{if } F_{a,in,t} > 0 \\ Inventory_{a,t} - (F_{a,in,t+1} - F_{a,out,t+1})\Delta t & \text{if } F_{a,in,t} < 0 \end{cases}$$
$$\forall a \in A, t \in T \tag{12.30}$$

The total hydrogen storage in the hydrogen pipeline network is:

$$Total\_inventory_t = \sum_{a \in A} Inventory_{a,t} \qquad \forall t \in T \tag{12.31}$$

In order to ensure the reliability of the scheduling results, to prevent the excessive storage of hydrogen stored in the pipeline, we specify that the ending hydrogen storage should be equal to or larger than the starting storage amount.

$$Total\_inventory_0 \le Total\_inventory_t \qquad \forall t = t^{End} \tag{12.32}$$

When the flowrate in the pipeline changes, the flow pattern may also change. The friction factor varies with flow pattern and the pressure drop varies either. Therefore, it is necessary to describe and calculate the flow pattern inside the pipe network system. The fluid flow pattern and its transformation can be judged by a dimensionless number—the Reynolds number.

$$\mathrm{Re}_{a,k,t} = \frac{|F_{a,k,t}| Dia_a}{\mu Area_a} \qquad \forall a \in A, k \in K, t \in T \tag{12.33}$$

When $Re_{a,k,t} < 2300$, the lamina friction factor should be calculated as:

$$f_{a,k,t}{}^{lam} = \frac{64}{\mathrm{Re}_{a,k,t}} \qquad \forall a \in A, k \in K, t \in T \tag{12.34}$$

When $Re_{a,k,t} > 2300$, the turbulent friction factor should be calculated by the Colebrook-White equation:

$$f_{i,k,t}{}^{turb} = 1.326 \left[\ln \left(\frac{1}{\varepsilon_a/(3.7Dia_a) + 2.51/\left(\mathrm{Re}_{i,k,t} \sqrt{f_{i,k,t}{}^{turb}} \right)} \right) \right]^{-2}$$
$$\forall a \in A, k \in K, t \in T \tag{12.35}$$

Similar to the concentration definition, the pressure of the pipeline network is defined as follows:

$$P_{a,out,t} = P_{n,t} \qquad \forall (a,n) \in A \text{ to } N(A,N), t \in T \tag{12.36}$$

$$P_{a,in,t} = P_{n,t} \qquad \forall (a,n) \in A \text{ from } N(A,N), t \in T \tag{12.37}$$

$$P_{i,t} = P_{n,t} \qquad \forall (i,n) \in Sup(I,N), t \in t \tag{12.38}$$

$$P_{j,t} = P_{n,t} \qquad \forall (j,n) \in Dem(J,N), t \in T \tag{12.39}$$

12.3.4 Constraints for Hydrogen Sources and Demands

The flowrate upper bounds for hydrogen plants and other hydrogen sources are:

$$F_{h,t} \le F_{h,t}{}^{Capacity} \qquad \forall h \in H, t \in T \tag{12.40}$$

$$F_{i,t} \leq F_{i,t}{}^{Max} \qquad \forall i \in I, t \in T \tag{12.41}$$

The flow rate, purity, and pressure constraints for the hydrogen consumption unit are:

$$F_{j,t} = F_{j,t}{}^{De} \qquad \forall j \in J, t \in T \tag{12.42}$$

$$y_{j,H_2,t} \geq y_{j,H_2}{}^{De} \qquad \forall j \in J, t \in T \tag{12.43}$$

$$P_{j,t} \geq P_j{}^{De} \qquad \forall j \in J, t \in T \tag{12.44}$$

12.3.5 The MPEC Method

The above mathematical model contains a large number of noncontinuous expressions, such as the sectional calculation of the hydrogen cost, the calculation of the friction factor, and the absolute value function. To solve this problem, the discontinuous variables in the complementary constrained model are introduced.

The MPEC method has been a research focus in recent years in the field of mathematical programming. Mathematical Programming with Equilibrium Constrained problems can be treated as two-level programming problems with variational inequalities or complementary constraints. The problems dealt with in this paper are complementary constraints.

The absolute functions have the following equality forms:

$$|F_{a,k,t}| = F_{a,k,t}{}^{positive} + F_{a,k,t}{}^{negative} \qquad \forall a \in A, k \in K, t \in T \tag{12.45a}$$

$$F_{a,k,t} = F_{a,k,t}{}^{positive} - F_{a,k,t}{}^{negative} \qquad \forall a \in A, k \in K, t \in T \tag{12.45b}$$

$$0 \leq F_{a,k,t}{}^{positive} \perp F_{a,k,t}{}^{negative} \geq 0 \qquad \forall a \in A, k \in K, t \in T \tag{12.CR-1}$$

where $F_{a,k,t}^{positive}$ and $F_{a,k,t}^{negative}$ are supplemental variables, Eq. (12.CR-1) denotes the relationship between $F_{a,k,t}^{positive}$ and $F_{a,k,t}^{negative}$. Namely, at least one of them should equal the boundary zero value.

The friction factor $f_{a,k,t}$ is calculated in two flow patterns: advection and turbulence.

$$f_{a,k,t} = {}^{a,k,ta,k,t} \begin{cases} f_{a,k,t}{}^{lam} & \text{Re} < 2300 \\ f_{a,k,t}{}^{turb} & \text{Re} > 2300 \end{cases} \qquad \forall a \in A, k \in K, t \in T$$

Converting the above equation to the complementary constraint form:

$$f_{a,k,t} = switch\_f_{a,k,t} f_{a,k,t}{}^{lam} + (1 - switch\_f_{a,k,t}) f_{a,k,t}{}^{turb} \qquad \forall a \in A, k \in K, t \in T \tag{12.46a}$$

$$(\text{Re}_{a,k,t} - 2300) - \lambda\_f1_{a,k,t} + \lambda\_f2_{a,k,t} = 0 \qquad \forall a \in A, k \in K, t \in T \tag{12.46b}$$

$$0 \le switch\_f_{a,k,t} \perp \lambda\_f1_{a,k,t} \ge 0 \quad \forall a \in A, k \in K, t \in T \tag{12.CR-2}$$

$$0 \le (1 - switch\_f_{a,k,t}) \perp \lambda\_f2_{a,k,t} \ge 0 \quad \forall a \in A, k \in K, t \in T \tag{12.CR-3}$$

where switch $-f_{a,k,t}$ is the shift variable, which is determined by the Reynolds number. When $Re < 2300$, it is laminar flow. If Eq. (12.46b) holds, the supplemental variable $\lambda\_f2_{a,k,t}$ should be positive. Therefore, we have $1 - \text{switch}\_f_{a,k,t} = 0$, switch$_f_{a,k,t} = 0$, $f_{a,k,t} = f^{lam}_{a,k,t}$. Similarly, when $Re > 2300$ we can obtain switch$_f_{a,k,t} = 0$ and $f_{a,k,t} = f^{turb}_{a,k,t}$.

The equivalent constraint form of the hydrogen cost calculation for the hydrogen plant is:

$$e_{H_2} = switch\_p1_{i,t}(e + e^{penalty1}) + switch\_p2_{i,t}e + switch\_p3_{i,t}(e + e^{penalty2}) \quad \forall i \in I, t \in T \tag{12.47a}$$

$$\left(F_{i,t} - F_i^{Low}\right) + \gamma\_p_{i,t} - \lambda\_p1_{i,t} = 0 \quad \forall i \in I, t \in t \tag{12.47b}$$

$$\left(F_{i,t} - F_i^{Low}\right)\left(F_{i,t} - F_i^{Up}\right) + \gamma\_p_{i,t} - \lambda\_p2_{i,t} = 0 \quad \forall i \in I, t \in T \tag{12.47c}$$

$$\left(F_i^{Up} - F_{i,t}\right) + \gamma\_p_{i,t} - \lambda\_p3_{i,t} = 0 \quad \forall i \in I, t \in T \tag{12.47d}$$

$$\gamma\_p_{i,t} \ge 0 \quad \forall i \in I, t \in T \tag{12.47e}$$

$$switch\_p1_{i,t} + switch\_p2_{i,t} + switch\_p3_{i,t} = 1 \quad \forall i \in I, t \in T \tag{12.47f}$$

$$0 \le switch\_p1_{i,t} \perp \lambda\_p1_{i,t} \ge 0 \quad \forall i \in I, t \in T \tag{12.CR-4}$$

$$0 \le switch\_p2_{i,t} \perp \lambda\_p2_{i,t} \ge 0 \quad \forall i \in I, t \in T \tag{12.CR-5}$$

$$0 \le switch\_p3_{i,t} \perp \lambda\_p3_{i,t} \ge 0 \quad \forall i \in I, t \in T \tag{12.CR-6}$$

12.4 ROBUST IMPLEMENTATION STRATEGY

The above modeling procedure is effective in small-scale refinery hydrogen systems, as illustrated in our previous work. However, applying it directly to large-scale refineries may cause instability problems. For instance, the solution procedure might have difficulty finding a feasible solution, and the obtained result may be far from optimal. The instability problems are induced by the parameter settings during the solution procedure. Therefore, in order to guarantee the performance of the proposed methods in large-scale refineries, we need a robust engineering strategy to make the solution procedure stable. In this paper, a systematic procedure is proposed to ensure the feasibility, necessity, and effectiveness of the implemented hydrogen system optimization. As shown in Fig. 12.4, the procedure involves a number of steps, which are informed by the real status and real decision parameters.

The first step is precision validation of the model in the proposed validation structure. It is the foundation of any industrial application of operational optimization. Reliability of the optimal decisions will be guaranteed only when the

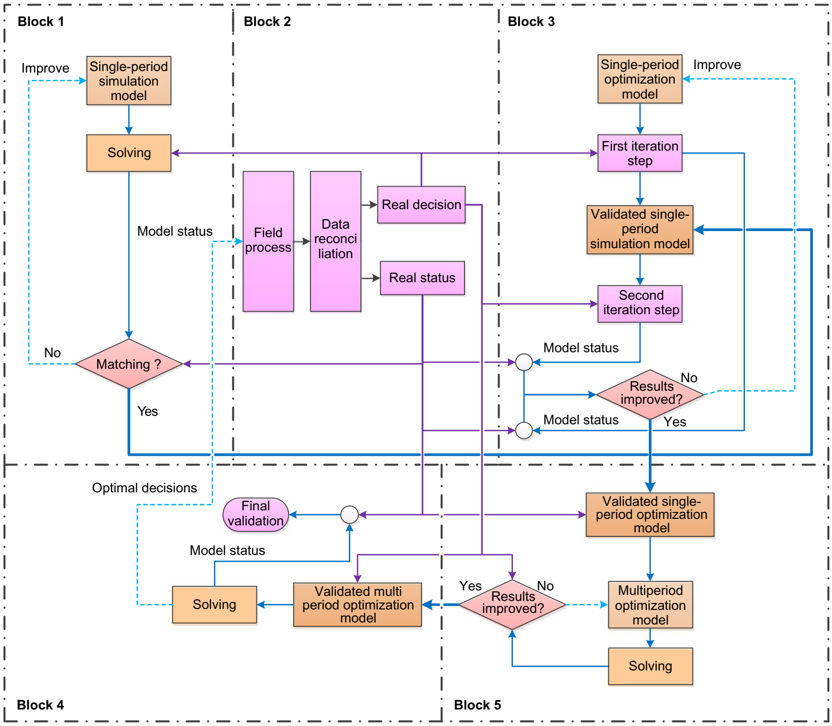

FIG. 12.4 Schematic representation of proposed implementation procedure.

precision of the model meets the requirement, and we need to check the precision of the collocation method. The second step is efficiency validation of the solution method. The proposed approach should be examined by real-time data in this section to explain its value for industrial application. The third step is effect validation of the operational optimization. It is used to indicate the potential economic benefit to refineries if operational optimization of the hydrogen system is executed. After the above three validation processes, the necessity of implementing operational optimization of the hydrogen system can be interpreted. However, these three validation processes are offline ones. In fact, online validation is needed to ensure its effect in industrial application. Based on offline validation, online validation called as "execution validation on field" is finally carried out to interpret the effectiveness of implementing operational optimization of the hydrogen system. The detailed procedures of these four steps are given in the following.

12.4.1 Precision Validation of the Model

The aim of precision validation of the model is to verify whether the optimization model can express the real hydrogen system. The procedure of the validation is illustrated in block 1 of Fig. 12.4. As shown in the figure, the precision validation involves four substeps.

1. Execute data reconciliation to eliminate measurement error in the initial data so that the processed data, which is called validation data, will satisfy mass and energy balances;
2. Input the validated real decisions into the single-period model;
3. Solve the model;
4. Compare the model status derived from step 1 with the validated real status. The precision of the model will be satisfied with the application requirement if and only if the error between these two statuses is small enough, and then this validation can be ended. If this is not the case, the model should be improved according to the comparison result, and then the validation procedure should be executed again.

12.4.2 Efficiency Validation of the Solution Method

Efficiency validation of the solution method is explained here to verify its value for industrial application by the real-time data. The procedure of the validation is illustrated in block 3 of Fig. 12.4 and is described in detail as follows.

1. Develop the multiperiod operational optimization model for the hydrogen system and extract the single-period optimization model from the multiperiod model;
2. Input the validated real decision data into the single-period optimization model and solve the problem.
3. Employ the result of the previous step as the initial value of the model to generate the new model parameters;
4. Refresh the new parameters in the optimization model and run the problem a second time;
5. Improve the single-period optimization model and repeat steps 2 to 4 until the average error tolerance $\overline{\varepsilon}_F$ and $\overline{\varepsilon}_H$ meet the requirements;
6. Examine the comparison results in each iteration step to verify the convergence of the solution method.

12.4.3 Effect Validation of the Operational Optimization

The destination of performing an operational optimization of the hydrogen system is to bring profit to the refinery by reducing its operating cost. The effects of the operational optimization are examined to illustrate whether the proposed optimal operation in the refinery can achieve this destination. The procedure of the validation is illustrated in block 5 of Fig. 12.4 and is described in detail as following.

7. Extend the validated single-period optimization model to the multiperiod model;

8. Input the real status, which consists of initial values of unit status, the production amount of hydrogen, and the energy demand of the units, to the multiperiod model of step 1;
9. Solve the validation model by NLP solvers to obtain the optimal decisions;
10. Compare the optimal decisions with the real decisions to investigate the variation of operating cost.

12.4.4 Execution Validation on Field

The above three offline validations verify the feasibility and necessity of the operational optimization of the hydrogen system in the refinery. However, online validation is required to guarantee its effect in industrial application. After these offline validations, execution validation on field is finally carried out to illustrate the effectiveness of implementing the operational optimization in the refinery. The procedure of the validation is illustrated in block 4 of Fig. 12.4, which involves the following 5 steps:

11. Install the operational optimization of the hydrogen system on field;
12. Obtain the hydrogen production flow rate and energy demand of each unit needed by the optimization model from the real-time data base.
13. Solve the problem by the proposed approach, and save the model status derived during the solution procedure;
14. Execute the optimal decisions on field;
15. Compare the model status derived from step 3 with the real status under the optimal decisions to investigate the effectiveness of implementing the operational optimization in the refinery.

12.4.5 Demonstration of the Execution Validation on Field

The above model and implementation strategy has been applied to a large-scale refinery case, as shown in Fig. 12.2. Due to the limited space, we briefly present the compressor scheduling result in Fig. 12.5. From the figure, we can see a more stable and relatively smaller load on the compressor. The compressor load is 7% smaller than the real-time case. The corresponding hydrogen production from the hydrogen plant is also reduced 5%.

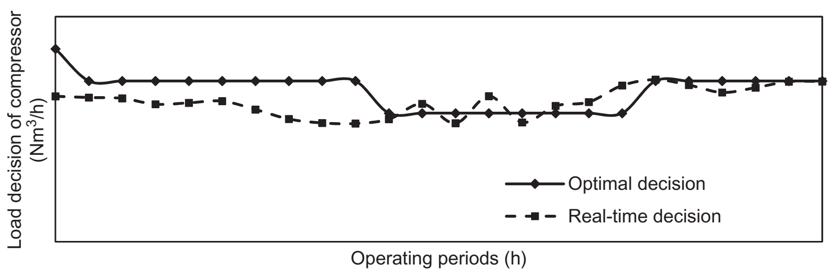

FIG. 12.5 Comparison of load decision of compressors.

12.5 CONCLUSION

This paper introduced a robust engineering strategy for implementing the previously developed optimization method to a hydrogen system in a refinery. Using four kinds of validation procedure, the feasibility, necessity, and effectiveness of implementing the operational optimization was presented. The proposed method has now been developed as a software system and integrated with the refinery database to effectively support the operational optimization of the hydrogen system of an oil refinery. A future effort will be to incorporate a more precise model of the compressor into the proposed formulation so that the work status of the hydrogen system can be expressed much more reasonably.

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