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A Multiperiod Optimization Model for Hydrogen System Scheduling in Refinery

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ABSTRACT: In a refinery, hydrogen, as a valuable resource, is also a byproduct and a significant raw material source of the petroleum refining and petrochemical hydrogenation process. To reduce costs and save energy for the petrochemical industry, the hydrogen system in a refinery should be operated under the optimal scheme to meet the varying hydrogen demands of hydrogen consumers. Optimal scheduling of the hydrogen system can help a refinery to achieve cost reduction and cleaner production. In this paper, a discrete-time mixed-integer nonlinear programming (MINLP) model that considers the penalties for abnormal situations in the hydrogen pipe network (HPN), compressors start−stop, and changes in hydrogen sources for hydrogen consumers is proposed for the optimal scheduling of the hydrogen system under multiperiod operation. The solution of the scheduling problem is obtained based on an iterative method between that of a mixed-integer linear programming (MILP) problem and that of a nonlinear programming (NLP) problem, avoiding the solution of the MINLP problem directly and the occurrence of composition discrepancy. A case study based on the data from a real refinery is presented to illustrate the effectiveness and feasibility of the proposed methodology.

1. INTRODUCTION

During the past decade, crude oil has become heavier and contains more sulfur and nitrogen, while the specifications of clean fuels have progressively tightened via the legislation for environmental protection. Hydrocracking and hydrotreating, which consume most of the hydrogen in a refinery, are used more and more widely to upgrade heavy oils, to obtain more-valuable products and remove sulfur and nitrogen compounds from the petroleum products, to satisfy the more-stringent quality requirements for fuel oil.[1,2] Hydrogen is now getting scarce and becoming a critical issue to the refiners worldwide. The cost of hydrogen has become the second-largest cost after the cost of crude oil in refineries.[3] To lighten the load of hydrogen production and save hydrogen cost, refiners must find effective hydrogen management techniques to satisfy the increasing hydrogen requirements.[4,5] Therefore, effective scheduling of the hydrogen system plays an important role in the reduction of hydrogen cost and a cleaner production process.

With the increasing demand for hydrogen, the hydrogen system in a refinery is now becoming larger and more and more complex. Consequently, effective scheduling in a big and complex hydrogen system is not easy. Schedulers must continuously watch both the pressure of the hydrogen pipe network (HPN) and the operational status of the hydrogen plant and match them to the fluctuating hydrogen demands. In most cases, under intense time pressure and low inventory flexibility, the schedulers rely highly on their experience, and select the first feasible solution for the scheduling problem, based on their experience. It is obvious that a scheduling approach based on experience cannot handle a complex hydrogen scheduling problem effectively. It is almost impossible for artificial scheduling to achieve the optimal scheduling for a hydrogen system. However, tremendous opportunities for economic and operability improvement exist in this process.

In some refineries, imbalance between the amount of the production and consumption of the hydrogen occurs frequently, because of the poor scheduling of the hydrogen system. This imbalance means an excess or shortage of hydrogen in the HPN, which will cause an increase in the operational cost and even a threat to the safe production. In fact, once the prediction of the hydrogen production is given, this abnormal situation can be avoided by appropriately adjusting the supply of hydrogen to the consumers.

Most research works have been focused on the design optimization of a hydrogen network in the refinery. Two main methods employed for the design optimization of hydrogen network are graphical and mathematical programming approaches. Towler et al.[1] first proposed a systematic approach to study the hydrogen network based on analyzing cost and value composite curves. Alves and Towler[2] proposed hydrogen pinch analysis for targeting the minimum amount of hydrogen consumption for the entire hydrogen system by using an analogy to pinch analysis for heat exchanger networks (HENs). Liao et al.[6,7] obtained the optimal conditions for pinch problems and proposed a rigorous targeting approach for

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hydrogen minimization, and this approach is more accurate and efficient than other published targeting methods in providing an overall optimal solution. Furthermore, mathematical programming methods were employed to solve these problems. Hallale and Liu[4] first developed a superstructure-based optimization method that accounts for the pressure constraints, as well as the existing equipment. Liu and Zhang[5] introduced a detailed model of purification units into the hydrogen network to evaluate possible purification scenarios. Khajehpour et al.[8] proposed a reduced superstructure based on experience and engineering judgment to retrofit the hydrogen network of an Iranian refinery and employed a genetic algorithm to address optimization problems, and a 22.6% reduction in hydrogen production was achieved. Liao et al.[9] introduced a state-space superstructure to further evaluate the possibility of integrating purifiers and successfully demonstrated the application of a superstructure-based approach for the retrofit design of an existing refinery. Kumar et al.[10] utilized a mathematical modeling technique for the optimization design of the hydrogen distribution network and analyzed the characteristics of a linear programming (LP) model, a nonlinear programming (NLP) model, a mixed-integer linear programming (MILP), and a mixed-integer nonlinear programming (MINLP) model of optimization problem. Ahmad et al.[11] developed an improved approach for the design of flexible hydrogen networks under multiple periods operation. Jiao et al.[12] decomposed the optimization problem into two subproblems, and a sequential two-step method is employed to retrofit the existing hydrogen network. Jiao et al.[13] presented a novel multiobjective optimization approach to optimize the hydrogen distribution network, and the relationship between the operating cost and investment cost is explored based on the obtained Pareto curve of the optimization problem. Fonseca et al.[14] and Salary et al.[15] employed graphical and mathematical methods simultaneously in the retrofit design problem of the hydrogen distribution network in a refinery.

All the reported research works mentioned above mainly concentrated on the design optimization of the hydrogen network. However, few research works currently considered the hydrogen system scheduling problem in a refinery. Van Den Heever and Grossmann[16] discussed the integration of production planning and reactive scheduling for the optimization of a hydrogen supply network. The network described in their paper consists of five hydrogen production plants, four interconnected pipelines, and 20 customers. They proposed a heuristic method for this level, based on Lagrangean decomposition to solve the multiperiod MINLP models for both the planning and scheduling levels.

Similar to crude oil scheduling problem, bilinear terms exist in the hydrogen system scheduling problem. A bilinear term brings difficulty for solving the hydrogen system scheduling. With this feature, the scheduling problem must be described as an MINLP model, and thus making it difficult to find a feasible solution. In this work, a discrete-time MINLP model that considers the penalties for abnormal situations in the HPN, compressors start−stop, and changes in the hydrogen sources for hydrogen consumers is proposed for the optimal scheduling of the hydrogen system under multiperiod operation. Given T time periods with varying demands of the hydrogen consumers, the aim of scheduling is to determine the scheme of optimal scheduling that meets the demands at the lowest total cost. However, solving the MINLP model directly may results in inconsistency in solution quality and time. Based on the work of Li et al.,[17] an improved MILP−NLP iterative method is proposed to address the optimization problem, avoiding the solution of the problem as a MINLP problem but still keeping the consistency of the solution, resulting in better quality, stability, and efficiency than that obtained by solving the MINLP model directly.

The remainder of the paper is organized as follows. The hydrogen system scheduling problem is introduced first in Section 2. In Section 3, the mathematical formulation of the scheduling problem is described in detail. This is followed by the proposed iterative solution strategy for solving the hydrogen system optimal scheduling problem in Section 4. Section 5 performs a case study to illustrate the effectiveness and feasibility of the proposed method. Section 6 summarizes the work and provides some concluding remarks.

2. PROBLEM STATEMENTS

There are many processes for hydrogen production and consumption in the refining industry. The interactions among these processes comprise a hydrogen system. Hydrogen producers supply hydrogen for the hydrogen system, such as the hydrogen plant, which employs steam reforming or partial oxidation for the production of high-purity hydrogen, and catalytic reforming unit, which produces hydrogen as a byproduct of cyclization and dehydrogenation reactions of hydrocarbon molecules.[4] The hydrogen consumers are mainly these conversion processes, such as the hydrocracking process (which breaks down large hydrocarbons into smaller and higher-value molecules), hydrotreating processes (which is used to remove impurities such as sulfur from streams and to hydrogenate aromatics and olefins to satisfy cleaner fuel specifications), lubricant plants, and the isomerization process. These processes consume hydrogen as a reactant to upgrade the quality of the refinery products. Hydrocracking and hydrotreating processes are the major hydrogen consumers in refineries. Figure 1 shows a flow diagram of a high-conversion refinery in which the hydrogen-consuming processes are highlighted.[1]

Besides the above-mentioned hydrogen production and consumption processes, purifiers and compressors are also parts of the refinery hydrogen system. Purifiers are usually employed to recover hydrogen from off-gases from hydrogen consumers and the residue from the purifiers. Compared to

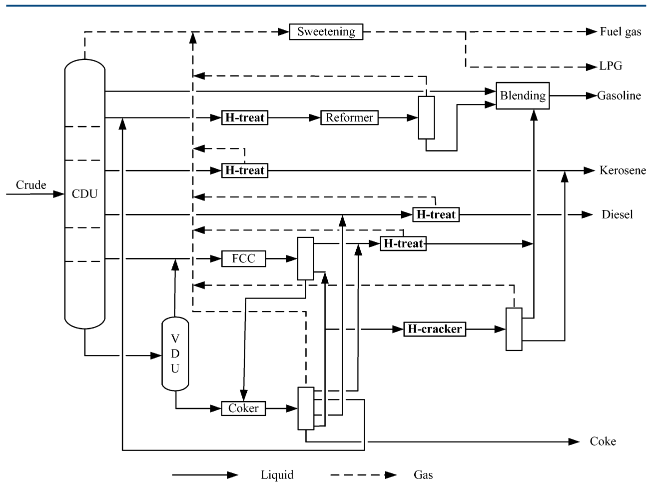

Figure 1. Simplified flow diagram of a high-conversion refinery.

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other processes of hydrogen production, the hydrogen purification process has the advantages of lower investment cost and operating cost and higher hydrogen purity, thus purifiers have been used more and more widely in refineries. Compressors are often used to increase the pressure of hydrogen from hydrogen producers to meet the inlet pressure requirement for hydrogen consumers. Purifiers and compressors make hydrogen more acceptable for hydrogen consumers; therefore, they are indispensable equipment for the refinery.

Hydrogen system scheduling is a decision-making process used to determine the hydrogen production, purification, transmission, and feed routes of hydrogen consumers to achieve the lowest total cost. In this paper, the optimal scheduling problem of a hydrogen system in a refinery is addressed based on the simplified workflow. Figure 2 is a schematic of a hydrogen system in a refinery, involving hydrogen producers (such as the hydrogen plant, catalytic reforming units, and purifiers), hydrogen consumers (such as hydrotreating units, hydrocracking units, and isomerization units), compressors, and the HPN used for the storage and transmission of hydrogen. Hydrogen from hydrogen producers is transported into HPN, and the hydrogen from HPN is utilized by hydrogen consumers. Each hydrogen consumer has purity requirement and pressure requirement for hydrogen feed stream, thus the hydrogen which can not meet the requirements can improve its purity and pressure by purifiers and compressors so as to make it more acceptable for hydrogen consumers. The off-gases from the hydrogen consumers can be purified by purifiers for further utilization after desulfurization. The off-gases from purifiers whose purity is much lower than that from hydrogen consumers are often sent to the fuel gas system. HPN also has a requirement on pressure and capacity in which HPN can supply hydrogen for hydrogen consumers successfully. If the hydrogen supplies of hydrogen producers are larger than the demands of hydrogen consumers, it will make the HPN exceed its capacity, lead to the hydrogen emission into the flare and bring economic loss for the refinery.

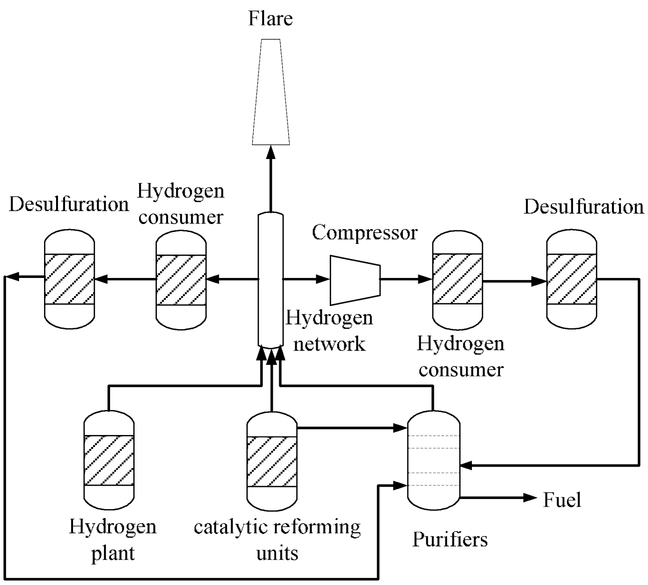

Figure 2. Schematic of a hydrogen system in refinery.

The hydrogen system scheduling process can be described as follows. Hydrogen from hydrogen producers is first transported into HPN, the hydrogen from the HPN directly is transported into the hydrogen consumers, whose required inlet pressure is smaller than or equal to the pressure of the HPN, and the pressure of hydrogen from the HPN must be increased by compressors to be transported into the hydrogen consumers when the required inlet pressure of hydrogen consumers is greater than the pressure of HPN. The schedulers should adjust the supplies of hydrogen producers in time, to match them to fluctuating hydrogen demands. When the hydrogen demands are smaller than that of normal demand, the schedulers should decrease the supplies of the hydrogen producers to meet the decreasing hydrogen demands. When the hydrogen demands are larger than that of normal demand, the schedulers should increase the supplies of hydrogen producers to meet the increasing hydrogen demands.

However, in most cases, under intense time pressure and low inventory flexibility, hydrogen imbalance occurs frequently in the refinery process and causes the excess or shortage of hydrogen in the hydrogen system. On the one hand, larger hydrogen supplies than the demands make the HPN exceed its capacity and lead to hydrogen emission into the flare, which means an economic loss for the refinery. On the other hand, a shortage of hydrogen will bring mechanical troubles and create an unstable production process. Furthermore, the compressors may be started or stopped because of the changing hydrogen demand of hydrogen consumers, which may bring unstable operation and mechanical trouble for the compressors. Moreover, the hydrogen sources of some hydrogen consumers may be changed due to the changing hydrogen demand of hydrogen consumers, which will bring unstable operation for hydrogen consumers, unstable production for hydrogen producers, and large labor intensity for operators during the production process.

These above-mentioned consequences arising from the poor scheduling can be compensated by optimizing the scheduling of the hydrogen system. The optimal scheduling of the hydrogen system should keep the amount of hydrogen in HPN within the operation range to avoid unfavorable hydrogen emission and hydrogen shortage and, at the same time, maximize the operation stability of the hydrogen producers, consumers, and compressors.

With the above brief introduction, the hydrogen scheduling problem is addressed as described below.

Given the following:

(1) Configuration details (numbers of hydrogen plants, purifiers, hydrogen consumers, compressors and their interconnections) of the refinery.
(2) Information about the minimum and maximum supply, purity, outlet pressure of hydrogen producers.
(3) Information about the minimum and maximum consumption, minimum feed purity, inlet pressure, and hydrogen demands during the scheduling period of the hydrogen consumers.
(4) Information about the normal inventory and capacity of HPN.
(5) Information about the efficiency and capacity of each compressor.
(6) Economic data, such as unit costs of hydrogen and electricity, the penalty costs for the compressor start–stop, changes in the hydrogen sources, the capacity overrun and shortage of HPN, and so forth.

(7) Limits on interconnections from hydrogen producers to hydrogen consumers, from hydrogen producers to HPN, from HPN to hydrogen consumers, and from off-gas suppliers to purifiers.

The scheduling procedure needs to determine the following:

(1) The hydrogen yield of hydrogen producers during each period.
(2) Detailed start−stop profiles for compressors during each period.
(3) Inventory and composition profiles of HPN during each period.
(4) The distribution of hydrogen from the hydrogen producers to HPN, from the hydrogen producers to consumers and from the HPN to hydrogen consumers during each period.

Finally, the following assumptions of the hydrogen system scheduling in refinery are made:

(1) Hydrogen streams are represented by a binary mixture of hydrogen and methane
(2) Hydrogen is mixed perfectly in the HPN; therefore, the hydrogen concentration in the HPN is uniform.
(3) The time for the change of hydrogen sources is neglected.
(4) None of the hydrogen consumers were ever shut down during operations.
(5) The purity of each hydrogen producer is considered to be constant during the scheduling periods.
(6) The inlet and outlet pressures of the compressors and inlet temperature are set to their operating value.
(7) The efficiency of each compressor is considered to be constant.
(8) Hydrogen does not leak during the transmission process.
(9) Hydrogen yield for some hydrogen producers and the hydrogen consumption for hydrogen consumers can be predicted precisely.

The optimal scheduling of the hydrogen system must satisfy the following conditions:

(1) The amount of hydrogen in HPN should be maintained within the operation range to avoid unfavorable hydrogen emission and hydrogen shortage.
(2) Minimum deviation from the normal capacity of the HPN.
(3) Maximization of operation stability of the hydrogen producers, consumers, and compressors, i.e., a minimal number of hydrogen source changes for hydrogen consumers, a minimal number of compressor start−stop.

3. OPTIMIZATION MODEL

According to the above analysis, an optimization strategy is proposed to address the optimal scheduling problem of hydrogen system. In this paper, a MINLP model is proposed for the optimal scheduling problem of a hydrogen system. The model mainly includes the mass balance constraints, operational constraints, HPN constraints, purifier constraints, compressor constraints, and hydrogen demand satisfaction constraints.

3.1. Objective Function. The objective of the optimal scheduling problem is to achieve the minimum operation cost of the hydrogen system based on the prediction of hydrogen demand during all periods. The operation cost of the hydrogen system includes the energy costs, the value created by fuel gas, and the penalty costs. The energy costs are composed of hydrogen cost and electricity cost, while the penalty costs consist of the penalty for compressor start−stop, the penalty for capacity overrun and deviation of the HPN, and the penalty for changing the hydrogen source of the hydrogen consumers. Consequently, the objective function of the optimal scheduling problem is

$$\text{Min} = \text{CH} + \text{CE} - \text{CF} + \text{CN} + \text{CP}_1 + \text{CP}_2 \quad (1)$$

The first term of the objective function (CH) is the hydrogen cost of hydrogen producers. The minimization of hydrogen cost is employed to guarantee that the hydrogen production of the hydrogen producers should be as small as possible on the premise of satisfying the hydrogen demands of the hydrogen consumers. The hydrogen cost of hydrogen producers is given as

$$\text{CH} = \sum_{t\in T}\sum_{u\in U} F_{u,t}t_{u,t}C_u \quad (1a)$$

In a refinery, compressors are used to increase the pressure of hydrogen from hydrogen producers or the HPN and make it more acceptable for hydrogen consumers. During the scheduling operations, it is necessary for schedulers to avoid the excessive operation of compressors, to save electricity costs by making good use of higher-pressure hydrogen sources, such as the hydrogen from a fertilizer plant; thus, a minimization of electricity cost (CE) should be imposed.

$$\text{CE} = C_e\sum_{t\in T}\sum_{\text{comp}\in C} \text{Power}_{\text{comp},t}t_{\text{comp},t} \quad (1b)$$

where $\text{Power}_{\text{comp},t}$ is the power of compressor during period t, as illustrated in eq 1c.[4]

$$\text{Power}_{\text{comp},t} = \frac{C_pT_{\text{comp},t}}{\eta}\left[\left(\frac{P^{\text{out}}_{\text{comp},t}}{P^{in}_{\text{comp},t}}\right)^{(\gamma-1)/\gamma} - 1\right]\frac{\rho_0}{\rho}F_{\text{comp},t} \quad (1c)$$

Petroleum refining processes represent one of the most energy-intensive industries, whose energy cost is another large cost component of all the costs. Among all the types of consumed energy sources, fuel gas, which is continuously generated from the production process, contributes most of the primary energy source to the energy needs of the refinery. Furthermore, fuel gas can be converted to other forms of energy, such as steam, electricity, and heat. Therefore, the fuel gas generated from the hydrocracking and hydrotreating process is also an important energy source for the refinery during the scheduling. The benefit created by the fuel gas sent to the fuel system can be obtained through the following heat value calculation:

$$\text{CF} = F_{\text{fuel},t}(y_{\text{fuel},t}\Delta H^{\circ}_{\text{c},\text{H}_2} + (1 - y_{\text{fuel},t})\Delta H^{\circ}_{\text{c},\text{CH}_4})C_{\text{heat}}t_{\text{fuel},t} \quad \forall\, t \in T \quad (1d)$$

The production scheme of hydrogen consumers often changes based on the sulfur content and nitrogen content of crude oil and product demand; therefore, the hydrogen demand of hydrogen consumers also changes with the production scheme. When the hydrogen demand changes, the operating state of the compressors supplying the hydrogen for the hydrogen consumers may change and the compressors may be started or stopped during scheduling operations. It may bring unstable operation and mechanical trouble for compressors; therefore, a penalty term (CN) will be imposed to avoid the occurrence of compressor start–stop.

$$CN = \sum_{t \in T} \sum_{\mathrm{comp} \in C} P_{\mathrm{comp}}(z_{\mathrm{comp},t} + zs_{\mathrm{comp},t}) \tag{1e}$$

The capacity of the HPN must be maintained in the normal range, to prevent the occurrence of hydrogen capacity overrun and a shortage of hydrogen amount in the HPN. These abnormal phenomena should be avoided, because they will bring large economic loss and unsafe factors for the refinery. A penalty term (CP_1) is imposed to avoid the hydrogen capacity overrun and shortage of hydrogen amount in the HPN.

$$CP_1 = \sum_{t \in T} (V^{+}_{\mathrm{HV},t} P^{+}_{\mathrm{HV}} + V^{-}_{\mathrm{HV},t} P^{-}_{\mathrm{HV}} + \Delta V^{+}_{\mathrm{HV},t} P^{\Delta +}_{\mathrm{HV}} + \Delta V^{-}_{\mathrm{HV},t} P^{\Delta -}_{\mathrm{HV}}) \tag{1f}$$

In the refinery, the hydrogen sources of some hydrogen consumers may be changed because of the changing hydrogen demand of hydrogen consumers during scheduling periods, which will bring unstable operation for hydrogen consumers, unstable production for hydrogen producers, and large labor intensity for operators during the production process. Therefore, another penalty term (CP_2) is imposed when the change of hydrogen sources happens to some hydrogen consumption units between two scheduling periods.

$$CP_2 = \sum_{t \in T} \sum_{uc \in UC} \alpha_{uc,t} P^{\mathrm{hex}}_{uc} \tag{1g}$$

3.2. Constraints. *3.2.1. General Constraints.* *(1). Mass Balance Constraints.* The scheduling optimization of a hydrogen system under multiple period operations requires mass balance constraints to be satisfied for all the units of the hydrogen system for all the operating periods under consideration. Mass balance constraints ensure that each of the hydrogen consumers is supplied by a hydrogen source that has a sufficient flow rate and hydrogen purity in each scheduling period. To make the scheduling model more suitable for the real system, the flow rate and purity of hydrogen consumers are considered to be variables.

The flow rate balance for each hydrogen consumer is given by

$$F_{uc,t} = \sum_{u \in ES_{uc}} F_{u,uc,t} \qquad \forall\ uc \in UC,\ \forall\ t \in T \tag{2}$$

In previous studies,[4,8−11,14,15] the hydrogen flow rate and purity of each sink have been assumed to be constants; although the optimization model is relatively easier, it cannot achieve an optimal combination of flow rate and purity. To make the proposed approach more practical for the real system, the flow rate and purity of each hydrogen consumer are considered as variables to achieve an optimal combination of flow rate and purity. The hydrogen balance for each hydrogen consumer is illustrated by eq 3.

$$F_{uc,t} y_{uc,t} = \sum_{u \in ES_{uc}} F_{u,uc,t} y_u \qquad \forall\ uc \in UC, \forall\ t \in T \tag{3}$$

The range of the purity of hydrogen consumers is shown as follows:

$$y^{\min}_{uc} \le y_{uc,t} < y^{\max}_{uc} \qquad \forall\ uc \in UC,\ \forall\ t \in T \tag{4}$$

Similarly, the amount of hydrogen sent to all the hydrogen consumers must be equal to the amount available from each hydrogen source.

$$F_{u,t} = \sum_{uc \in EC_u} F_{u,uc,t} \qquad \forall\ u \in U,\ \forall\ t \in T \tag{5}$$

(2). Operation Constraints of Equipments. To determine the state of feed routes from hydrogen producers to hydrogen consumers, binary variable $Y_{u,uc,t}$ is presented as follows:

$$Y_{u,uc,t} = \begin{cases} 1 & \text{if hydrogen producer } u \text{ supplies hydrogen for} \\ & \text{the hydrogen consumer } uc \text{ during period } t \\ 0 & \text{otherwise} \end{cases}$$

Considering general binary variable $Y_{u,uc,t}$, the relationship between $Y_{u,uc,t}$ and $F_{u,uc,t}$ is stated as follows:

$$Y_{u,uc,t} = 1 \Leftrightarrow F_{u,uc,t} > 0 \tag{6}$$

$$Y_{u,uc,t} = 0 \Leftrightarrow F_{u,uc,t} = 0 \tag{7}$$

Consequently, the lower and upper bounds on the flow rate of hydrogen steam are enforced by eqs 8 and 9, while logical conditions in eqs 10 and 11 specify that the binary variables $\alpha_{\mathrm{u,uc,t}}$ will be equal to 1 if the change in hydrogen source happens for hydrogen consumer uc at the beginning of period t and 0 if there is no change. To make the hydrogen supply routes easier and more acceptable for the hydrogen system, the number of hydrogen sources of each hydrogen consumer is also limited by eq 12.

$$F^{\min}_{u} \le F_{u,t} \le F^{\max}_{u} \qquad \forall\ u \in U,\ \forall\ t \in T \tag{8}$$

$$F^{\min}_{uc} Y_{u,uc,t} \le F_{u,uc,t} \le F^{\max}_{uc} Y_{u,uc,t} \quad \forall\ u \in U,\ \forall\ uc \in UC,\ \forall\ t \in T \tag{9}$$

$$\alpha_{u,uc,t} \ge Y_{u,uc,t} - Y_{u,uc,t-1} \quad \forall\ u \in U,\ \forall\ uc \in UC,\ \forall\ t \in T \tag{10}$$

$$\alpha_{u,uc,t} \ge Y_{u,uc,t\text{-}1} - Y_{u,uc,t} \quad \forall\ u \in U,\ \forall\ uc \in UC,\ \forall\ t \in T \tag{11}$$

$$Y_{ui,uc,t} + Y_{uj,uc,t} \le N^{\max}_{u,uc} \quad \forall\ ui,\ uj \in U,\ \forall\ uc \in UC,\ \forall\ t \in T \tag{12}$$

Based on the binary variable $Y_{u,uc,t}$, the pressure constraints between hydrogen producer u and hydrogen consumer uc are expressed as follows:

$$P^{\mathrm{in}}_{uc} - U_{u,uc}(1 - Y_{u,uc,t}) \le P_u \quad \forall\ u \in U,\ \forall\ uc \in UC,\ \forall\ t \in T \tag{13}$$

3.2.2. HPN Constraints. *(1). Mass Balance.* The mass balance for HPN is represented by eq 14, where $V_{\mathrm{HV},t}$ is the hydrogen amount in the HPN in period t. The HPN receives the hydrogen from the hydrogen producers and supplies hydrogen for the hydrogen consumers at the same time. As a result, $V_{\mathrm{HV},t}$ is equal to the sum of the amount of hydrogen in period $t - 1$ and the difference between the input and output amount of hydrogen between the two scheduling periods.

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$$V_{\mathrm{HV},t} = V_{\mathrm{HV},t-1} + \left(\sum_{u \in ES_{HPN}} F_{u,t} - \sum_{uc \in EC_{HPN}} F_{uc,t} \right) \Delta t \quad \forall\ t \in T \tag{14}$$

Similarly, the hydrogen balance for HPN is stated as:

$$V_{\mathrm{HV},t} y_{\mathrm{HV},t} = V_{\mathrm{HV},t-1} y_{\mathrm{HV},t-1} + \left(\sum_{u \in \mathrm{ES}_{HPN}} F_{u,t} y_{u,t} - \sum_{uc \in \mathrm{EC}_{HPN}} F_{uc,t} y_{\mathrm{HV},t} \right) \Delta t \quad \forall\ t \in T \tag{15}$$

The range of the purity of HPN is represented as follows:

$$y_{\mathrm{HV}}^{\min} \le y_{\mathrm{HV},t} < y_{\mathrm{HV}}^{\max} \quad \forall\ t \in T \tag{16}$$

(2). Capacity Constraints. The amount of hydrogen in the HPN should be limited in the permitted capacity. However, the abnormal phenomena of hydrogen capacity overrun and shortage of hydrogen amount in the HPN may occur in emergency conditions. The slack variable $V_{\mathrm{HV},t}^{+}$ and $V_{\mathrm{HV},t}^{-}$ are introduced to define the overrun amount and shortage amount of HPN, respectively. The limitation for the HPN capacity is considered in the model, as indicated in eqs 17. Equation 18 corresponds to the deviation of hydrogen from the normal capacity. The slack variables $\Delta V_{\mathrm{HV},t}^{+}$ and $\Delta V_{\mathrm{HV},t}^{-}$ represent the hydrogen amount above and below the normal capacity of HPN, respectively.

$$V_{\mathrm{HV}}^{\min} - V_{\mathrm{HV},t}^{-} \le V_{\mathrm{HV},t} \le V_{\mathrm{HV}}^{\max} + V_{\mathrm{HV},t}^{+} \quad \forall\ t \in T \tag{17}$$

$$V_{\mathrm{HV},t} = V_{\mathrm{HV}}^{\mathrm{n}} + \Delta V_{\mathrm{HV},t}^{+} - \Delta V_{\mathrm{HV},t}^{-} \quad \forall\ t \in T \tag{18}$$

3.2.3. Purifier Constraints. *(1). Mass Balance.* Hydrogen from refinery off-gases and the catalytic reforming units is usually recovered by purifiers, to obtain the high-purity hydrogen. The most common unit operations used for purifying hydrogen are pressure-swing adsorption (PSA) and membranes. Compared to other process of hydrogen production, the hydrogen purifying technique has the lower recovery cost and higher hydrogen purity, thus it has been used more and more widely in refinery.

Purifiers such as PSA and membrane separation, can be considered as one sink (inlet stream) and two sources (the product stream and the residue stream).[5] The constraints for an existing purifier are expressed as

Flow rate balance:

$$\sum_{uc \in \mathrm{EC}_p} F_{uc,p,t} = F_{p,t}^{\mathrm{P}} + F_{p,t}^{\mathrm{R}} \quad \forall\ p \in P,\ \forall\ t \in T \tag{19}$$

Hydrogen balance:

$$\sum_{uc \in \mathrm{EC}_p} F_{uc,p,t} y_{uc,t}^{\mathrm{o}} = F_{p,t}^{\mathrm{P}} y_{p,t}^{\mathrm{P}} + F_{p,t}^{\mathrm{R}} y_{p,t}^{\mathrm{R}} \quad \forall\ p \in P,\ \forall\ t \in T \tag{20}$$

(2). Capacity Limit. An existing purifier is designed for a specific flow rate; therefore, is a flow rate constraint on each purifier.

$$F_p^{\min} \le \sum_{uc \in \mathrm{EC}_p} F_{uc,p,t} \le F_p^{\max} \quad \forall\ p \in P,\ \forall\ t \in T \tag{21}$$

(3). Logistic Restriction. Binary variable $Y_{uc,p,t}$ is presented to indicate the state of feed routes from off-gas to purifiers, which can be defined as

$$Y_{uc,p,t} = \begin{cases} 1 & \text{if hydrogen consumer } uc \text{ supplies the off-gas for purifier } p \text{ during period } t \\ 0 & \text{otherwise} \end{cases}$$

Considering the general binary variable $Y_{uc,p,t}$, the relationship between $Y_{uc,p,t}$ and $F_{uc,p,t}$ is stated as follows:

$$Y_{uc,p,t} = 1 \Leftrightarrow F_{uc,p,t} > 0 \tag{22}$$

$$Y_{uc,p,t} = 0 \Leftrightarrow F_{uc,p,t} = 0 \tag{23}$$

Therefore, based on the preceding binary variable $Y_{uc,p,t}$, the off-gas flow rate constraint from hydrogen consumers to purifiers is represented as follows:

$$Y_{uc,p,t} F_p^{\min} \le F_{uc,p,t} \le Y_{uc,p,t} F_p^{\max} \quad \forall\ uc \in \mathrm{UC},\ \forall\ p \in P,\ \forall\ t \in T \tag{24}$$

To make the off-gas supply routes easier and more acceptable for the hydrogen system, the number of hydrogen consumers that supply hydrogen off-gas for each purifier is also limited.

$$Y_{uci,p,t} + Y_{ucj,p,t} \le N_{uc,p}^{\max} \quad \forall\ uci,\ ucj \in \mathrm{UC},\ \forall\ p \in P,\ \forall\ t \in T \tag{25}$$

Based on the binary variable $Y_{uc,p,t}$, the pressure constraints between hydrogen consumers and hydrogen purifiers are given as

$$P_p - U_{uc,p}(1 - Y_{uc,p,t}) \le P_{uc}^{\mathrm{out}} \quad \forall\ p \in P,\ \forall\ uc \in \mathrm{UC},\ \forall\ t \in T \tag{26}$$

3.2.4. Compressor Constraints. *(1). Mass Balance.* In a refinery, compressors are used to increase the hydrogen pressure and make it more acceptable for hydrogen consumers. To make the proposed approach more suitable for the real system, just like other hydrogen consumers, here, both the flow rate and the purity of compressors are considered as variables. The constraints on the compressors can be described as follows.

The amount of hydrogen fed into the compressors must be equal to the exit amount.

Flow rate balance:

$$\sum_{u \in \mathrm{ES}_{\mathrm{comp}}} F_{u,\mathrm{comp},t} = \sum_{uc \in \mathrm{EC}_{\mathrm{comp}}} F_{\mathrm{comp},uc,t} \quad \forall\ \mathrm{comp} \in C,\ \forall\ t \in T \tag{27}$$

The amount of pure hydrogen entering the compressor must be equal to the amount leaving.

Hydrogen balance:

$$\sum_{u \in \mathrm{ES}_{\mathrm{comp}}} F_{u,\mathrm{comp},t} y_u = \sum_{uc \in \mathrm{EC}_{\mathrm{comp}}} F_{\mathrm{comp},uc,t} y_{\mathrm{comp},t} \quad \forall\ \mathrm{comp} \in C,\ \forall\ t \in T \tag{28}$$

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The outlet purity of the compressors should be between the purities of minimum and maximum of hydrogen sources into the compressors:

$$y_{u,\mathrm{comp}}^{\min} \le y_{\mathrm{comp},t} < y_{u,\mathrm{comp}}^{\max} \quad \forall\, u \in U,\ \forall\ \mathrm{comp} \in C,\ \forall\, t \in T \tag{29}$$

(2). Capacity Limit. The amount of gas fed into one compressor must never exceed its maximum capacity.

$$\sum_{u\in \mathrm{ES}_{\mathrm{comp}}} F_{u,\mathrm{comp},t} \le F_{\mathrm{comp}}^{\max} \qquad \forall\ \mathrm{comp} \in C,\ \forall\, t \in T \tag{30}$$

(3). Logistic Constraints. To determine the state of compressors operation, binary variable $Y_{\mathrm{comp},t}$ is defined as the following:

$$Y_{\mathrm{comp},t} = \begin{cases} 1 & \text{if compressor comp operates during period } t \\ 0 & \text{otherwise} \end{cases}$$

Considering the binary variable $Y_{\mathrm{comp},t}$, the relationship between $Y_{\mathrm{comp},t}$ and $F_{\mathrm{comp},t}$ is stated as follows:

$$Y_{\mathrm{comp},t} = 1 \Leftrightarrow F_{\mathrm{comp},t} > 0 \tag{31}$$

$$Y_{\mathrm{comp},t} = 0 \Leftrightarrow F_{\mathrm{comp},t} = 0 \tag{32}$$

Compressors also have their own operation ranges for stable operation. Based on the binary variable $Y_{\mathrm{comp},t}$, the hydrogen flow rate constraint from the compressors to the hydrogen consumers is illustrated as follows:

$$Y_{\mathrm{comp},t}F_{\mathrm{comp}}^{\min} \le F_{\mathrm{comp},t} \le Y_{\mathrm{comp},t}F_{\mathrm{comp}}^{\max} \quad \forall\ \mathrm{comp} \in C,\ \forall\, t \in T \tag{33}$$

Logical conditions in eq 34 specify that the binary variables $z_{\mathrm{comp},t}$ will be equal to 1 if a compressor start happens at the beginning of period t and 0 if there is no start. Logical conditions in eq 35 specify that the binary variables $zs_{\mathrm{comp},t}$ will be equal to 1 if a compressor stop happens at the end of period t and 0 if there is no start.

$$z_{\mathrm{comp},t} \ge Y_{\mathrm{comp},t} - Y_{\mathrm{comp},t-1} \qquad \forall\ \mathrm{comp} \in C,\ \forall\, t \in T \tag{34}$$

$$zs_{\mathrm{comp},t} \ge Y_{\mathrm{comp},t} - Y_{\mathrm{comp},t+1} \qquad \forall\ \mathrm{comp} \in C,\ \forall\, t \in T \tag{35}$$

3.2.5. Hydrogen Demand Satisfaction Constraints. The generated hydrogen from hydrogen plant, purifiers, and catalytic reforming units at each period must satisfy the hydrogen demand of hydrogen consumers.

$$\sum_{u\in \mathrm{ES}_{uc}} F_{u,uc,t} \ge F_{uc,t} \qquad \forall\, uc \in \mathrm{UC},\ \forall\, t \in T \tag{36}$$

$$\sum_{u\in \mathrm{ES}_{uc}} F_{u,uc,t}y_u \ge F_{uc,t}^{\mathrm{d}} \qquad \forall\, uc \in \mathrm{UC},\ \forall\, t \in T \tag{37}$$

The overall mathematical model with the aforementioned constraints (2)−(37), and the objective function (1), comprise a nonconvex MINLP problem that involves bilinear terms in (1d), (3), (15), (20), and (28). The next section will address how to solve the corresponding nonconvex MINLP problem.

4. SOLUTION STRATEGY

The nature of the hydrogen scheduling problem is a MINLP problem, because of bilinear constraints in the formulation. However, solving an MINLP model directly will result in inconsistency in solution quality and time. Thus, some methods are proposed in the literature to address the MINLP problem. In the crude oil scheduling problem, it is inevitable that bilinear terms that represent the amount of properties in tanks or flows like this problem exist. In some of the previous works,[18,19] the bilinear terms were linearized by applying the reformulation−linearization technique (RLT) and the original MINLP problems were converted to relaxed MILP problems. Lee et al.[18] used the RLT to reformulate bilinear terms in mass balance equations into linear equations. However, as noted by Li et al.,[17] this linearization approximation will lead to a discrepancy between the composition of crude delivered by a set of storage tanks to a CDU and that actually received by the CDU, which arises from the charging of crude blends. Li et al.,[17] recognizing this composition discrepancy, proposed an iterative MILP−NLP combination algorithm to solve the problem. Reddy et al.[20] proposed a rolling horizon solution algorithm, based on the composition-based blocks, which identifies the composition-known interval and solves the MILP problem in that time interval. However, their algorithm also failed to obtain feasible schedules and requires a long solution time to solve large, practical-sized problems. The methods are improved by adding a backtracking strategy proposed by Li et al.[21]

As noted by Li et al.,[17] if a unit, such as a mixer, has no mass accumulation inside, then its bilinear terms in mass balance constraints can be replaced by individual component flows and reformulated into exact linear constraints. Nonlinear constraints can thus be avoided. If mass accumulates in a unit, such as a charging tank, in some cases, using individual component flows and solving the model with MILP will give incorrect results. Similarly, in the hydrogen scheduling problem in a refinery, there is one unit, HPN, in which there is mass accumulation. Therefore, its bilinear terms in mass balance constraints of HPN cannot be replaced by individual component flows. Otherwise, it will lead to a discrepancy between the composition of hydrogen inside the HPN and from the HPN. In this paper, based on the work of Li et al.,[17] we propose an improved MILP−NLP iterative method that iteratively solves the MILP model and the NLP model and avoids the composition discrepancy, resulting in better quality, stability, and efficiency result than by solving the MINLP model directly.

The MILP model in this MILP−NLP iterative method is obtained by linearizing the bilinear terms in (1d), (3), (15), (20), and (28), based on the linearization technique proposed by Quesada and Grossmann.[22] The constraints linearized from the bilinear constraints using the linearization technique proposed by Quesada and Grossmann are tighter than the constraints obtained from the work of Li et al.[17] and also provide a valid lower bound on the optimum.

For the bilinear term Fy, it can be relaxed into the following linear constraints, based on the linearization technique proposed by Quesada and Grossmann:[22]

$$f \ge F^{\min}y + Fy^{\min} - F^{\min}y^{\min} \tag{38}$$

$$f \ge F^{\max}y + Fy^{\max} - F^{\max}y^{\max} \tag{39}$$

$$f \le F^{\min}y + Fy^{\max} - F^{\min}y^{\max} \tag{40}$$

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$$f \le F^{\max}y + Fy^{\min} - F^{\max}y^{\min} \tag{41}$$

where $f = Fy$.

Through similar procedures, the bilinear terms in (1d), (3), (15), (20), and (28) can be relaxed into linear terms, and the original MINLP model can be transformed to a MILP model.

Figure 3 shows the flow diagram of the solution procedure. In the algorithm, an initial MILP model is used to initialize the proposed iterative method. A feasibility check then is introduced to determine the composition discrepancy and an NLP model is used to remove the discrepancy. The description for each step of the algorithm is as follows:[17]

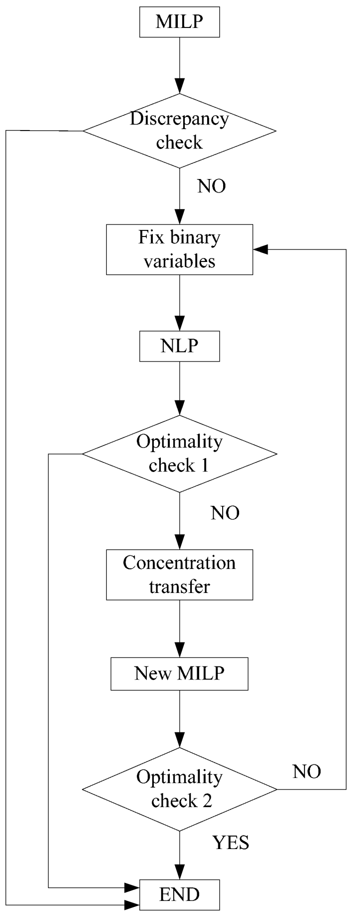

Figure 3. Flowchart for proposed algorithm.

(1) One of the critical methods to improve an optimization procedure is appropriate initialization of the problem. The initial MILP model is employed to initialize the proposed algorithm. In this model, all the bilinear terms are linearized as linear terms, and the initial MINLP model is transformed to a MILP model. Although the model does not guarantee a consistent hydrogen concentration inside the HPN and in the discharge from the HPN, it can generate a good starting point for the next calculations.

(2) In this procedure, the consistency of the concentration values from the initial MILP is checked. The consistency criteria are whether the concentration of hydrogen in the HPN is the same as that of the stream flowing out from the HPN. If the consistency criteria are satisfied, the optimum solution is found and the procedure is terminated.

(3) The values of binary variables determined by initial MILP are fixed to the corresponding parameters in the following NLP model.

(4) The constraints in the NLP model include all the constraints except the linearized constraints and those constraints including binary variables. All the binary variables in the initial MILP model become parameters for the NLP model. The NLP model is used to determine the accurate hydrogen concentration values based on rigorous bilinear constraints. These concentration data will be further used in the next step.

(5) If the difference between the objective values of the NLP and the previous MILP is bigger than an appropriate tolerance, then the procedure continues to iterate. Otherwise, the procedure is terminated. The tolerance used in this paper is 1.0×10^{-5}.

(6) If the previous optimality check is not satisfied, it can be determined that the hydrogen concentrations in the HPN have a strong effect on the objective function values, and they may even have an effect on the binary variables that were determined in the initial MILP. To verify this, the hydrogen concentrations of the HPN, consumers, compressors, and purifier residue are fixed at the values generated from the NLP, but the binary variables that were previously fixed will be free in the next step.

(7) A new MILP model is generated from the previous step by fixing the hydrogen concentration of the HPN, consumers, compressors, and purifier residue but allowing all the binary variables to vary.

(8) If the objective function value of the NLP is better than that of the new MILP model and all the values of binary variables calculated by the new MILP are the same to the corresponding parameters, then the procedure is terminated. Otherwise, the procedure continues to iterate.

At first, the proposed MILP−NLP iterative algorithm is used to solve the initial MILP problem. If the concentration values of the HPN determined by the initial MILP model are the same as that of the streams that flow out from the HPN, then the final solution has already been found. Otherwise, the iterative procedure goes to the next step, and the values of the binary variables determined by the initial MILP model are used as parameters for the NLP model. The NLP model then is solved to obtain the correct hydrogen concentrations. The procedure then decides whether the objective value of the MILP and the objective value of the NLP are close enough to satisfy the error requirements. If yes, no better solution to the problem can be expected, and the iteration is terminated. If no, these hydrogen concentration data from the calculation results of the NLP model are transferred to a new MILP as parameters. In the new MILP, the concentration values are set as fixed values from calculation results of the NLP model, but all of the other binary variables are calculated again. After the new MILP is solved, the optimality check criterion is employed to decide whether a better solution to the problem is possible. If yes, the values of binary variables determined by MILP are sent to the corresponding parameters in the next NLP model, and the next iteration is continued until the terminating condition of

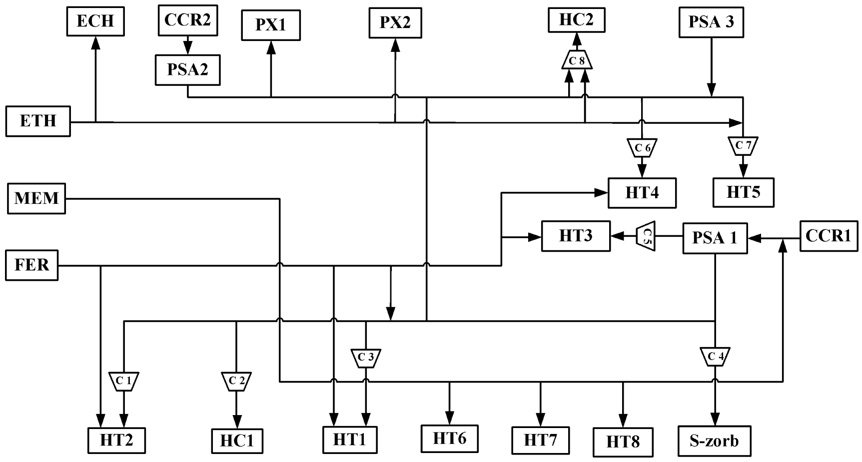

Figure 4. Flowchart of the hydrogen system in a refinery.

optimality check is satisfied. If no, the procedure is terminated, and the solution of the optimization problem is obtained.

Although the algorithm does not guarantee a global optimal solution, considering the fact that solving the MINLP is a challenging problem, the proposed approach is quite attractive, because it does not require solving a MINLP problem and gives near-optimal schedules within a reasonable time.

5. CASE STUDY

In this section, to illustrate the applicability and effectiveness of the proposed method, a case study is performed by using the hydrogen system model of a refinery shown in Figure 4. The refinery mainly processes both high-sulfur crude, to produce a full range of fuel products and other chemical products. Hydrogen producers include two continuous catalytic reforming units (CCR1 and CCR2), a fertilizer plant (FER), and an ethylene plant (ETH), which supply the most of hydrogen for hydrogen consumption devices. Two PSA plants are also used to purify the hydrogen product of CCR1 and CCR2 in the refinery, to obtain the higher-purity hydrogen. There are 14 hydrogen consumers: catalytic diesel hydrotreater (HT1), straight-run diesel hydrotreater (HT2), diesel hydrotreater (HT3), kerosene hydrotreater (HT4), wax oil hydrotreater (HT5), aviation kerosene hydrotreater (HT6), two non-aromatic hydrocarbon hydrotreaters (HT7 and HT8), two hydrocracking units (HC1 and HC2), *p*-xylene isomerization (PX1), *p*-xylene disproportionation (PX2), a gasoline adsorptive desulfurization unit (S-zorb), and a ethylene cracking hydrogenation unit (ECH).

The optimal scheduling strategy for the hydrogen system developed in the above-mentioned sections is applied to this case study. The scheduling horizon is composed of eight periods, and each period is 1 h. Table 1 shows the hydrogen producers data, which includes the range of hydrogen supply, hydrogen purity, outlet pressure, and price of the hydrogen producers. Table 2 gives hydrogen consumers data including the range of hydrogen consumption, minimum feed purity, and inlet pressure for the hydrogen consumers. Table 3 shows the capacity bound of the HPN. Table 4 shows the compressors data which includes efficiency of compressors and the range of capacity. Table 5 shows the penalty value for the objective function. In order to make good use of hydrogen in the refinery, on the one hand, hydrogen from CCR1, CCR2, and ETH is a byproduct of these hydrogen producers; thus, the hydrogen supplies from CCR1, CCR2, and ETH should be used up. On the other hand, hydrogen supplies from FER and the purifiers can change with the hydrogen demands of the hydrogen consumers; thus, hydrogen from FER and the purifiers are the optimization decision variables. The hydrogen

Table 1. Hydrogen Producers Data in the Case Study

hydrogen producer	minimum supply (Nm^3/h)	maximum supply (Nm^3/h)	purity (%)	outlet pressure (MPa)	price ($\$/Nm^3$)
CCR1	25000	52000	92	1.2	0.08
CCR2	40000	74000	93	1.3	0.08
FER	15000	90000	97.5	6.8	0.185
ETH	30000	48000	95	3	0.077
PSA1	24000	60000	97	1.2	0.11
PSA2	38400	80000	96.5	1.3	0.12
PSA3	8000	15000	96.7	0.46	0.07
MEM	3500	6000	92	1.33	0.093

Table 2. Hydrogen Consumers Data in the Case Study

hydrogen consumer	minimum consumption (Nm^3/h)	maximum consumption (Nm^3/h)	minimum feed purity (%)	inlet pressure (MPa)
HC1	31000	60000	95	17
HC2	42000	62000	95	15
HT1	5000	9000	85	6
HT2	8000	13000	85	4
HT3	7500	12000	92	5
HT4	21000	34000	92	6
HT5	12000	28000	95	12
PX1	5200	6500	95	2.5
PX2	12000	15000	95	3.1
HT6	1300	2100	91	2.5
HT7	150	800	89	2.3
HT8	610	1000	92	2.1
S-zorb	1500	3500	95	2.6
ECH	4300	8000	95	3

Table 3. Capacity Bound of the HPN

bound	capacity
lower bound	3000 Nm^3
normal	4000 Nm^3
upper bound	5000 Nm^3

Table 4. Compressor Data in the Case Study

	C1	C2	C3	C4	C5	C6	C7	C8
efficiency	0.92	0.88	0.92	0.93	0.92	0.9	0.9	0.88
minimum capacity (Nm^3/h)	0	0	0	0	0	0	0	0
maximum capacity (Nm^3/h)	12000	60000	12000	6000	15000	35000	30000	60000

Table 5. Penalty Value for Objective Function

penalty term	penalty value
penalty for changing the hydrogen sources for hydrogen consumers ($)	300
penalty for compressor start−stop ($)	200
penalty for deviation of HPN from normal capacity ($/($Nm^3$))	1
penalty for HPN from permitted capacity ($/($Nm^3$))	5

supplies from CCR1, CCR2, and ETH also change with different feed throughput and operating conditions. Table 6 shows the hydrogen yields of CCR1, CCR2, and ETH for each scheduling period. The prediction of hydrogen demands of hydrogen consumers is listed in Table 7. The unit costs of electricity and fuel are 0.091 $/kWh and 0.0045 $/MJ, respectively. It is assumed that the initial capacity of HPN is 3500 Nm^3.

This case study was formulated in Lingo 8.0 and solved using an Intel 2.4 GHz personal computer with 1 GB of memory. The MILP problem was solved using B-and-B, and the NLP problem was solved with the default nonlinear solver of Lingo.

The computational results for the case study are summarized in Table 8. When the problem is solved as a MINLP, no feasible solution was found within the iteration limit, even after imposing initial values of variables from the MILP solution. Using the proposed solution algorithm, the concentration values calculated by the initial MILP violate the consistency criteria of the concentration; thus, the algorithm continues to solve the NLP and new MILP models. The value of the objective function of NLP is better than that of the new MILP model and all the values of binary variables calculated by the new MILP are the same as the corresponding parameters; thus, the iteration procedure is terminated.

Concentration data calculated by the MILP model and new algorithm are listed in Tables 9 and 10. It can be seen from Table 9 that the concentration discrepancy exists between hydrogen in the HPN and the hydrogen streams that flow out from the HPN. As shown in Table 10, we can find that the calculation values of the hydrogen concentration in the HPN are exactly equal to the hydrogen stream concentration that flows out from the HPN by applying the proposed solution method.

Figure 5 shows the total hydrogen production for each scheduling period versus the total demand. It can be seen that the total production of producers closely follows the total demand of consumers. The proposed scheduling strategy can guarantee the hydrogen balance between the hydrogen producers and consumers. The frequent occurrence of an excess and shortage of hydrogen supply in the scheduling of hydrogen system in the refinery can be prevented; thus, economic loss due to hydrogen emission into the flare and the mechanical trouble and unstable production process of hydrogen producers can be avoided. However, the overproduction of 0.25% is found in period 1. That is because the hydrogen from the overproduction is stored in the HPN to maintain the hydrogen amount in HPN under normal conditions.

Figure 6 shows the hydrogen production of each plant as a part of the total production. This figure shows that the change of the hydrogen yield from each hydrogen producer is minor, the stable production of hydrogen producers is achieved, and the abnormal phenomenon of big hydrogen production fluctuation is avoided. The hydrogen from hydrogen producers under stable production is transported into the HPN safely, and the stable transportation of hydrogen will not bring big influence on the HPN, which can guarantee the stable and safe hydrogen supply from HPN to the consumers.

The running profile of each compressor for each scheduling period is shown in Figure 7. As the outlet pressure of hydrogen from FER is higher than some hydrogen producers, the hydrogen from the FER can supply hydrogen for HT1, HT2, HT3, HT4, and S-zorb units directly without compressors, it is necessary to make good use of the hydrogen from FER, to save the electricity cost of compressors. Compressors C1 and C6 are shut down during scheduling periods, because of the greater use of hydrogen from FER; therefore, great savings in electricity cost can be realized. Moreover, other compressors (other than C1 and C6) maintain stable operation during scheduling periods; thus, the abnormal phenomenon of compressor start−stop is avoided, which guarantee the stable operation and avoid the mechanical trouble for compressors.

Figure 8 shows the inventory profile of HPN for each scheduling period. In the process of hydrogen system scheduling, the inventory of HPN should be kept at a reasonable range, to guarantee the safe and stable operation of the hydrogen system. Large fluctuations in the inventory of HPN will bring unsafe influence on the hydrogen system. Because the hydrogen from producers is transported into HPN, suitably based on the changing demands of consumers during all the scheduling periods, hydrogen inventory in HPN is maintained at the safe and normal range, and the economic loss arising from the hydrogen emission into the flare and unstable production process of hydrogen consumers arising from the shortage of hydrogen can be avoided.

Table 11 shows the hydrogen supply strategy for hydrogen consumers during scheduling periods. Each hydrogen consumer is supplied by definite hydrogen producers or HPN. The

Table 6. Hydrogen Yield Data for Each Scheduling Period

period	1	2	3	4	5	6	7	8
CCR1 (Nm^3/h)	29498	28992	29295	28448	29061	28089	28545	29507
CCR2 (Nm^3/h)	56051	56404	56868	55871	57352	55626	54859	56818
ETH (Nm^3/h)	53157	50612	51080	53361	55040	54654	52417	52829

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Table 7. Hydrogen Demand Data for Each Scheduling Period

period	1	2	3	4	5	6	7	8
HC1 (Nm^3/h)	45456	45646	44168	47395	46768	47662	48727	49635
HC2 (Nm^3/h)	46000	47072	48780	48499	49375	49226	48742	49278
HT1 (Nm^3/h)	7541	7680	7697	7847	7962	8094	8653	7639
HT2 (Nm^3/h)	9876	9463	9550	9830	10403	9917	9907	9386
HT3 (Nm^3/h)	10264	9806	9844	9965	9726	9833	10721	10644
HT4 (Nm^3/h)	25732	25006	24819	26257	28282	28200	27991	26978
HT5 (Nm^3/h)	18266	18010	18388	19147	19369	19340	18633	17682
HT6 (Nm^3/h)	1420	1441	1404	1420	1435	1413	1364	1400
HT7 (Nm^3/h)	646	641	631	522	425	448	444	433
HT8 (Nm^3/h)	909	914	956	798	849	810	826	836
PX1 (Nm^3/h)	5719	5660	5649	5768	6001	5897	5927	5742
PX2 (Nm^3/h)	14795	14742	14854	14684	14781	14751	14758	14838
S-zorb (Nm^3/h)	2836	2840	2135	2569	2688	2925	2702	2536
ECH (Nm^3/h)	6853	6853	6923	6803	7116	7083	6755	6877

Table 8. Summary of Computational Results in the Case Study

	model	number of iterations	number of continuous variables	number of discrete variables	CPU time (s)	objective value
initialization	MILP	34324	740	136	2	195931
iteration 1	NLP	211	508	0	0.55	196054
iteration 1	new MILP	2543	476	136	0.45	196058
	MINLP		692	136		infeasible solution

Table 9. Concentration Data Calculated by the MILP Model in the Case Study

period	1	2	3	4	5	6	7	8
y_{HV}	0.975	0.965	0.975	0.975	0.975	0.965	0.965	0.965
$y_{HV,HC1}$	0.965	0.967	0.966	0.967	0.966	0.968	0.968	0.975
$y_{HV,HC2}$	0.965	0.965	0.965	0.965	0.965	0.965	0.965	0.969
$y_{HV,HT1}$	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975

Table 10. Concentration Data Calculated by the New Algorithm in the Case Study

period	1	2	3	4	5	6	7	8
y_{HV}	0.966	0.967	0.967	0.967	0.967	0.967	0.967	0.967
$y_{HV,HC1}$	0.966	0.967	0.967	0.967	0.967	0.967	0.967	0.967
$y_{HV,HC2}$	0.966	0.967	0.967	0.967	0.967	0.967	0.967	0.967
$y_{HV,HT1}$	0.966	0.967	0.967	0.967	0.967	0.967	0.967	0.967

hydrogen sources of each hydrogen consumer are kept the same during scheduling periods. The change of hydrogen sources for each consumer, which may happen in a refinery because of the changing hydrogen demand of hydrogen consumers, is avoided, which can bring stable operation for hydrogen consumers, stable production for hydrogen producers, and small labor intensity for operators during the production process.

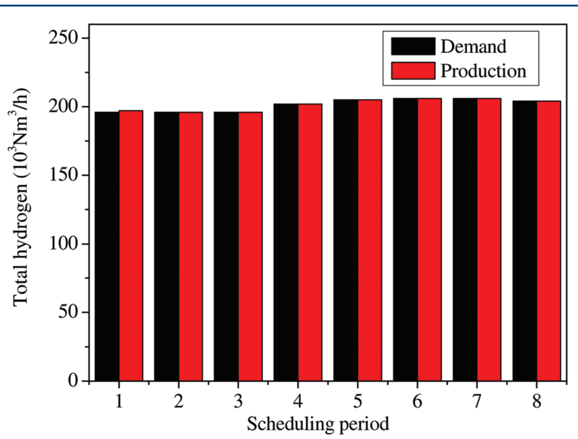

Figure 5. Demand versus production for each scheduling period.

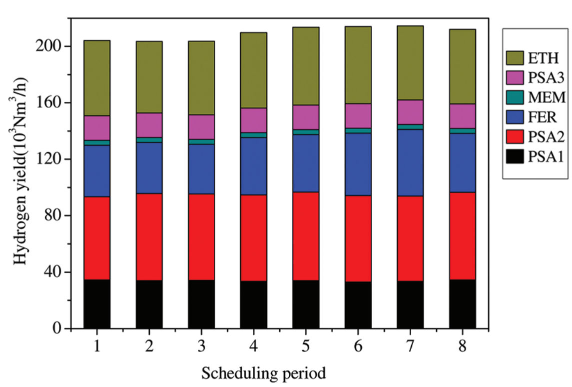

Figure 6. Hydrogen yield of producers for each scheduling period.

Table 12 shows a comparison of the operating cost between actual operation and optimized operation during eight scheduling periods. The optimized operation process, based

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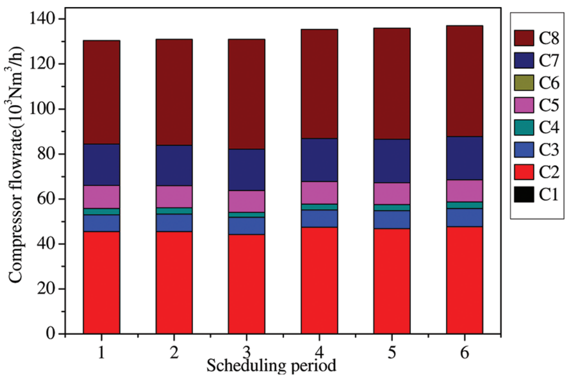

Figure 7. Flow rate of each compressor for every scheduling period.

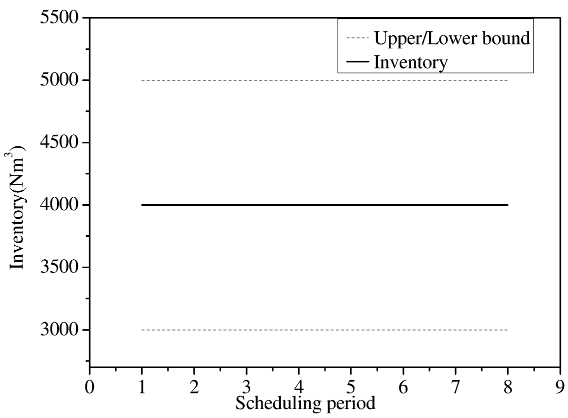

Figure 8. Inventory of HPN for each scheduling period.

on the proposed approach, has a total operation cost of \$196.054 × 10^3 during eight scheduling periods and results in a savings of \$3.73 × 10^6/yr, corresponding to a reduction of 1.71% in the total annual operating cost, compared to the actual operation.

6. CONCLUSION

With the increasing demand for hydrogen, hydrogen is now getting scarce and becoming a critical issue to refiners worldwide. Therefore, it is necessary for decision makers to consider the optimal scheduling problem of the hydrogen system in a refinery, to avoid suboptimal operations. In this work, a discrete-time multiperiod scheduling model for a hydrogen system is proposed to achieve the minimum operation cost of the hydrogen system. Because of the existence of bilinear constraints employed to denoting the hydrogen balance of the hydrogen system, the corresponding optimal scheduling problem of the hydrogen system is mathematically formulated into a MINLP problem. Furthermore, a MILP−NLP iterative algorithm is employed to address the optimal scheduling problem, avoiding the solving of the MINLP problem directly and the occurrence of composition discrepancy. Finally, a case study is presented to illustrate the effectiveness and feasibility of the proposed methodology. Results show that the optimized scheduling scheme is reliable and practical, the abnormal phenomenons of the hydrogen imbalance, compressor start−stop, and hydrogen source change could be avoided, and the economic loss and unstable operation arising from the abnormal phenomenons can be avoided. The proposed optimal scheduling strategy can reduce the operation cost, guarantee the stable and safe operation of the hydrogen system, and provide important management information of the hydrogen system for decision makers in refineries.

Table 12. Comparison of Operating Cost between Actual Operation and Optimized Operation

	actual operation	optimized operation
PSA1	30930	26600
PSA2	59132	63127
FER	59909	62424
MEM	2596	3396
PSA3	9691	9436
ETH	32766	32766
electricity	14729	16285
fuel	−14568	−13699
total	199466	196054

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Notes

The authors declare no competing financial interest.

Table 11. Hydrogen Supply Strategy of Hydrogen Consumers for Each Scheduling Period

period	1	2	3	4	5	6	7	8
HC1	HPN	HPN	HPN	HPN	HPN	HPN	HPN	HPN
HC2	HPN + ETH	HPN + ETH	HPN + ETH	HPN + ETH	HPN + ETH	HPN + ETH	HPN + ETH	HPN + ETH
HT1	HPN	HPN	HPN	HPN	HPN	HPN	HPN	HPN
HT2	FER	FER	FER	FER	FER	FER	FER	FER
HT3	PSA1	PSA1	PSA1	PSA1	PSA1	PSA1	PSA1	PSA1
HT4	FER	FER	FER	FER	FER	FER	FER	FER
HT5	ETH	ETH	ETH	ETH	ETH	ETH	ETH	ETH
HT6	MEM	MEM	MEM	MEM	MEM	MEM	MEM	MEM
HT7	MEM	MEM	MEM	MEM	MEM	MEM	MEM	MEM
HT8	MEM	MEM	MEM	MEM	MEM	MEM	MEM	MEM
PX1	PSA2	PSA2	PSA2	PSA2	PSA2	PSA2	PSA2	PSA2
PX2	ETH	ETH	ETH	ETH	ETH	ETH	ETH	ETH
S-zorb	PSA1	PSA1	PSA1	PSA1	PSA1	PSA1	PSA1	PSA1
ECH	ETH	ETH	ETH	ETH	ETH	ETH	ETH	ETH

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■ NOMENCLATURE

Sets

C = compressor
EC_{comp} = hydrogen consumers consuming hydrogen from compressor "comp"
EC_{HPN} = hydrogen consumers consuming hydrogen from HPN
EC_p = hydrogen consumers supplying off-gas for purifier p
EC_u = hydrogen consumers consuming hydrogen from hydrogen producer u
ES_{comp} = hydrogen producers supplying hydrogen for compressor "comp"
ES_{HPN} = hydrogen producers supplying hydrogen for HPN
ES_{uc} = hydrogen producers supplying hydrogen for hydrogen consumer uc
P = purifiers
T = time periods
U = hydrogen producers
UC = hydrogen consumers

Superscripts

in = inlet
max = maximum
min = minimum
out = outlet
P = product
R = residual

Subscripts

comp = compressor; comp $\in C$
p = purifier; $p \in P$
t = time period; $t \in T$
u = hydrogen producer; $u \in U$
uc = hydrogen consumer; $uc \in$ UC

Parameters

C_e = unit cost of electricity (\$ kWh^{-1})
C_p = heat capacity of the stream at constant pressure (J kg^{-1} K^{-1})
C_{heat} = unit cost of fuel gas (\$ J^{-1})
C_u = unit cost of hydrogen for hydrogen producer u (\$ Nm^{-3})
F_{comp}^{max} = upper bound of the capacity for compressor "comp" (Nm^3 h^{-1})
F_{comp}^{min} = lower bound of the capacity for compressor "comp" (Nm^3 h^{-1})
F_p^{max} = lower bound for the capacity of purifier p (Nm^3 h^{-1})
F_p^{min} = upper bound for the capacity of purifier p (Nm^3 h^{-1})
F_u^{max} = maximum flow rate of hydrogen producer u (Nm^3 h^{-1})
F_u^{min} = minimum flow rate of hydrogen producer u (Nm^3 h^{-1})
$F_{uc,t}^{d}$ = pure hydrogen demand of hydrogen consumer uc during period t (Nm^3 h^{-1})
F_{uc}^{max} = maximum flow rate consumed by hydrogen consumer uc (Nm^3 h^{-1})
F_{uc}^{min} = minimum flow rate consumed by hydrogen consumer uc (Nm^3 h^{-1})
$N_{u,uc}^{max}$ = maximum connection number between hydrogen producer u and hydrogen consumer uc
$N_{uc,p}^{max}$ = maximum connection number between hydrogen consumer uc and purifier p
P_{comp} = penalty of start−stop for compressors "comp"
$P_{comp,t}^{in}$ = inlet pressure of compressor "comp" (MPa)
P_p = inlet pressure of purifier p (MPa)
P_u = outlet pressure of hydrogen producer u (MPa)
P_{uc}^{in} = inlet pressure of hydrogen consumer uc (MPa)
P_{uc}^{out} = outlet pressure of hydrogen consumer uc (MPa)
P_{HV}^{+} = penalty for inventory of HPN above the maximum capacity of HPN
P_{HV}^{-} = penalty for inventory of HPN below the minimum capacity of HPN
$P_{HV}^{\Delta+}$ = penalty for inventory of HPN above the normal capacity of HPN
$P_{HV}^{\Delta-}$ = penalty for inventory of HPN below the normal capacity of HPN
P_{uc}^{hex} = penalty for change of hydrogen sources for hydrogen consumer uc
$t_{u,t}$ = working time of hydrogen producer u during period t (h)
$t_{fuel,t}$ = working time of fuel gas suppliers during period t (Nm^3 h^{-1})
$T_{comp,t}$ = gas temperature of compressor inlet during period t (K)
$U_{uc,u}$ = upper bound of pressure between hydrogen consumer uc and hydrogen producer u (MPa)
$U_{uc,p}$ = upper bound of pressure between hydrogen consumer uc and purifier p (MPa)
V_{HV}^{max} = upper bound for the capacity of HPN (Nm^3)
V_{HV}^{min} = lower bound for the capacity of HPN (Nm^3)
y_{HV}^{max} = maximum purity of hydrogen in HPN during period t (%)
y_{HV}^{min} = minimum purity of hydrogen in HPN during period t (%)
$y_{p,t}^{P}$ = purity of hydrogen product from purifier p during period t (%)
y_u = hydrogen purity of hydrogen producer u (%)
$y_{u,comp}^{max}$ = maximum hydrogen purity of hydrogen producer u into compressor "comp" (%)
$y_{u,comp}^{min}$ = minimum hydrogen purity of hydrogen producer u into compressor "comp" (%)
y_{uc}^{max} = maximum hydrogen purity of hydrogen consumer uc (%)
y_{uc}^{min} = minimum hydrogen purity of hydrogen consumer uc (%)
$y_{uc,t}^{\circ}$ = off-gas purity of hydrogen consumer uc (%)
ΔH_c° = standard heat of combustion (J Nm^{-3})
η = efficiency
γ = ratio of heat capacity at constant pressure to that at constant volume
ρ = gas density (kg m^{-3})
ρ_0 = gas density under standard conditions (kg m^{-3})

Variables

CE = electricity cost of compressors (\$)
CF = benefits created by fuel gas (\$)
CH = hydrogen cost of hydrogen producers (\$)
CN = start−stop cost of compressors (\$)
CP_1 = cost for HPN capacity overrun and shortage (\$)
CP_2 = cost for the change of hydrogen source (\$)

$F_{\text{comp},t}$ = flow rate of hydrogen from compressor "comp" during period t ($\text{Nm}^3\ \text{h}^{-1}$)
$F_{\text{comp},uc,t}$ = flow rate of hydrogen from compressor "comp" to hydrogen consumer uc during period t ($\text{Nm}^3\ \text{h}^{-1}$)
$F_{\text{fuel},t}$ = flow rate of fuel gas during period t ($\text{Nm}^3\ \text{h}^{-1}$)
$F^{\text{P}}_{p,t}$ = flow rate of hydrogen product from purifier p during period t ($\text{Nm}^3\ \text{h}^{-1}$)
$F^{\text{R}}_{p,t}$ = flow rate of hydrogen residual from purifier p during period t ($\text{Nm}^3\ \text{h}^{-1}$)
$F_{u,t}$ = flow rate of hydrogen from producer u during period t ($\text{Nm}^3\ \text{h}^{-1}$)
$F_{u,\text{comp},t}$ = flow rate of hydrogen from hydrogen producer u to compressor "comp" during period t ($\text{Nm}^3\ \text{h}^{-1}$)
$F_{u,uc,t}$ = flow rate of hydrogen from hydrogen producer u to hydrogen consumer uc during period t ($\text{Nm}^3\ \text{h}^{-1}$)
$F_{uc,t}$ = flow rate of hydrogen consumed by hydrogen consumer uc during period t ($\text{Nm}^3\ \text{h}^{-1}$)
$F_{uc,p,t}$ = flow rate of off-gas from hydrogen consumer uc to purifier p during period t ($\text{Nm}^3\ \text{h}^{-1}$)
Min = objective function
$P^{\text{out}}_{\text{comp},t}$ = outlet pressure of compressor "comp" (MPa)
$\text{Power}_{\text{comp}}$ = power of compressor "comp" (W)
$t_{\text{comp},t}$ = running time of compressor "comp" during period t (h)
V^{n}_{HV} = normal capacity of the HPN (Nm^3)
$V_{\text{HV},t}$ = hydrogen amount in the HPN during period t (Nm^3)
$V^{+}_{\text{HV},t}$ = hydrogen amount above the upper bound of HPN capacity during period t (Nm^3)
$V^{-}_{\text{HV},t}$ = hydrogen amount below the lower bound of HPN capacity during period t (Nm^3)
$\Delta V^{+}_{\text{HV},t}$ = hydrogen amount above the normal capacity of HPN during period t (Nm^3)
$\Delta V^{-}_{\text{HV},t}$ = hydrogen amount below the normal capacity of HPN during period t (Nm^3)
$Y_{\text{comp},t}$ = 0−1 variables that denotes whether compressor "comp" runs during period t
$Y_{u,uc,t}$ = 0−1 variables that denotes whether hydrogen producer u supplies hydrogen for hydrogen consumer uc during period t
$Y_{uc,p,t}$ = 0−1 variables that denotes whether hydrogen consumer uc supplies off-gas for purifier p during period t
$y_{\text{comp},t}$ = hydrogen purity from compressor "comp" during period t (%)
$y_{\text{fuel},t}$ = hydrogen purity of fuel gas during period t (%)
$y_{\text{HV},t}$ = hydrogen purity of HPN during period t (%)
$y_{\text{HV},uc}$ = purity of hydrogen from HPN to hydrogen consumer uc (%)
$y^{\text{R}}_{p,t}$ = purity of hydrogen residual from purifier p during period t (%)
$y_{uc,t}$ = purity of hydrogen consumed by hydrogen consumer uc during period t (%)
$Z_{\text{comp},t}$ = 0−1 variables that denotes whether compressor "comp" starts before and after period t
$ZS_{\text{comp},t}$ = 0−1 variables that denotes whether compressor "comp" stops before and after period t
$\alpha_{uc,t}$ = 0−1 variables that denotes whether changes in the hydrogen source for hydrogen consumer uc happen during period t

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