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Optimization of hydrogen networks with multiple impurities and impurity removal☆

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ABSTRACT

To explore the effect of removing different impurities to hydrogen networks, an MINLP model is proposed with all matching possibilities and the trade-off between operation cost and capital cost is considered. Furthermore, the impurity remover, hydrogen distribution, compressor and pipe setting are included in the model. Based on this model, the impurity and source(s) that are in higher priority for impurity removal, the optimal targeted concentration, and the hydrogen network with the minimum annual cost can be identified. The efficiency of the proposed model is verified by a case study.

1. Introduction

In recent years, on account of the increasing process of high-sulfur and heavier crude oil, refineries need to increase their capacity of hydrotreating and hydro-cracking to produce high-quality products to satisfy stricter environmental regulations. As a result, the hydrogen consumption is soaring rapidly. Therefore, the effective utilization of hydrogen and the optimization of hydrogen network have vital significance for refineries.

The fresh hydrogen consumption can be minimized with the match between sinks and sources, by integrating the hydrogen network as a whole. However, the amount of reuse is limited as the hydrogen purity of some sources is low or the impurity concentration is high. To overcome this problem and decrease the fresh hydrogen consumption, purifiers are often introduced.

Methods for hydrogen networks with purification reuse mainly include pinch-based conceptual ones and mathematical programming ones. In terms of conceptual methods, Agrawal and Shenoy [1] proposed a pinch-based approach, which can be used in hydrogen/water network with purification/recycle. Zhang *et al.* [2] proposed a triangle rule based on the mass balance of purification process to target the minimum fresh hydrogen consumption for hydrogen networks with purification reuse. Yang *et al.* [3,4] simplified and improved this method. Liu *et al.* [5,6] identified the optimal purification feed flowrate based on the concept of hydrogen surplus. These methods are for hydrogen networks with single impurity, and cannot be applied to that with multiple impurities.

As to mathematical methods, Liu and Zhang [7] proposed a model to select appropriate purifiers for hydrogen networks. Jiao *et al.* [8] and Jagannath and Almansoori [9] focused on the optimization of purification parameters. Deng *et al.* [10] and Kuo and Chang [11] compared and analyzed hydrogen networks without and with purification unit. Although the operation parameters and the cost of purification units are considered in these models, the effects to the whole network caused by the change of impurity concentrations are ignored.

For a hydrogen network with single impurity, all kinds of impurities in a hydrogen source are treated as a unified impurity. A hydrogen source can be reused directly if its hydrogen concentration or impurity concentration satisfies the demand of hydrogen sink. In such cases, impurity removal and hydrogen purification are the same, and both of them enhance the hydrogen concentration. However, for a hydrogen network with multiple impurities, besides the hydrogen concentration, the concentrations of impurities also restrict the hydrogen reuse. The removal of each impurity has different effects to the hydrogen network. It is necessary to analyze these effects on a hydrogen network with multiple impurities.

Zhou *et al.* [12] set a model to integrate hydrogen sulfide removal units into hydrogen networks. However, to the best of our knowledge, no report systematically considers the concentration changes of different impurities and their effects to the hydrogen networks.

In this work, an MINLP model is constructed to analyze the removal of different impurities and identify the impurity and source(s) that should be first considered for removal, the optimal targeted concentration, and the hydrogen network with the minimum annual cost.

2. Problem Statement

The hydrogen network has m sources (except fresh hydrogen) and n sinks [Fig. 1]. All the components, except hydrogen, are impurities, and the total number is n_c. Each sink SK_j ($j \in [1, n]$) requires a minimum flow rate F_{SK_j}. Its inlet impurity concentration should not be higher than the

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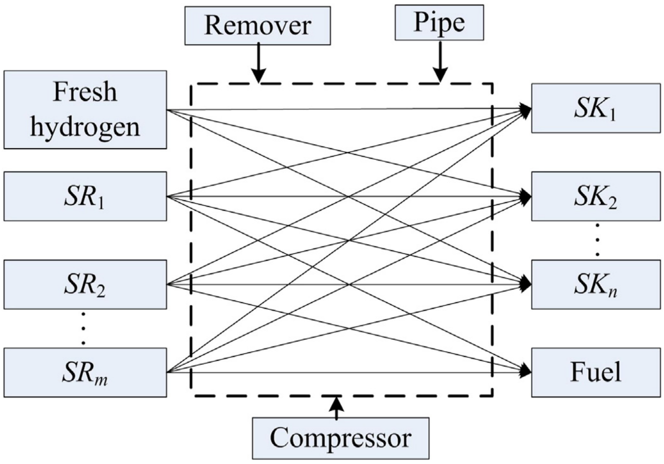

Fig. 1. Superstructure of a hydrogen network.

maximum allowable impurity concentration $C_{j,k}^{\max}$, and its operation pressure should not be lower than $P_j^{\min}$. The lower limit on hydrogen concentration can be transferred to the upper limit on the total concentration of impurities [13], so only concentrations of impurity are considered in this work.

Similarly, each source SR_i ($i \in [1, m]$) has a flow rate F_i and its pressure is P_i. Its impurity concentrations are $C_{i,k}$ ($k \in [1, n_c]$). Fresh hydrogen is purchased from other factories or specially produced, and its impurity concentrations and pressure are $C_{\text{fresh},k}$ and P_{fresh}, respectively.

In this work, impurity removers are integrated into the hydrogen network. If source SR_i is purified with impurity k partially removed, the flow rate and pressure of purified product are F_i^{RE} and P_i^{RE}, respectively, and the concentration of impurity k is decreased from $C_{i,k}$ to $C_{i,k}^{\text{RE}}$.

For matches between SR_i and SK_j, pipe is necessary to transport hydrogen to hydrogen sinks, and it is mainly determined by distance $L_{i,j}$ and flow rate $F_{i,j}$ between SR_i and SK_j. Furthermore, compressor is necessary if the pressure of SR_i is lower than that of SK_j.

For the hydrogen network, its total cost consists of operation cost and capital cost. The operation cost includes those for fresh hydrogen, electricity, and the operating cost of purifier or impurity remover, while the capital cost contains the investments of purifier or impurity remover, compressors and pipes. The objective of this work is to target the hydrogen network with the minimum total annual cost (TAC). This is an optimization problem with single objective, and the decision variables are the impurity and source to be removed first, and the match relation between each pair of sink and source.

3. Mathematical Models

For a multicomponent hydrogen network, the mathematical model consists four parts: (1) impurity remover section; (2) hydrogen distribution network section; (3) compressor section; (4) pipe section.

3.1. Impurity removal section

In this work, an impurity remover is pre-installed for each stream and can separate its inlet stream (inlet feed) into two outlet streams (product and waste gas). The mass balance in an impurity remover is

$$F_i^{\text{IN}} \cdot C_{i,k} = F_i^{\text{RE}} \cdot C_{i,k}^{\text{RE}} + F_i^{\text{D}} \cdot C_{i,k}^{\text{D}} \tag{1}$$

$$F_i^{\text{IN}} = F_i^{\text{RE}} + F_i^{\text{D}} \tag{2}$$

where superscripts IN, RE and D represent the inlet feed, removed product and discharge of waste gas, respectively. Eqs. (1) and (2) are also suitable for hydrogen purifiers.

The flow rate of feed should not be greater than that of the removed source,

$$F_i^{\text{IN}} \le F_i. \tag{3}$$

The impurity concentrations of removed product cannot be higher than that of the original source,

$$C_{i,k}^{\text{RE}} \le C_{i,k}. \tag{4}$$

Assuming that the removal process does not change the pressure of hydrogen sources, the pressure of the removed product equals that of the inlet feed,

$$P_i^{\text{RE}} = P_i. \tag{5}$$

The remover process can be either chemical absorption (absorbing H_2S by MDEA) or physical adsorption process (removing CO_2 by PSA). The operation costs and investments of these two processes are different.

For the chemical absorption, the operation cost can be calculated by

$$Cost_{\text{RE}} = Cost_{\text{ADS}} + Cost_{\text{REG}} \tag{6}$$

where $Cost_{\text{RE}}$ is the operation cost of the removal unit, $Cost_{\text{ADS}}$ is the consumption of energy, and $Cost_{\text{REG}}$ is the cost of adsorbent regeneration.

Since MDEA adsorbs H_2S as a ratio of 1:1, the cost of adsorbent regeneration is

$$Cost_{\text{REG}} = F_i^{\text{RE}} \cdot \left(C_{i,k} - C_{i,k}^{\text{RE}}\right) \cdot PR^{\text{MDEA}}. \tag{7}$$

For the removal unit (absorption column), the theoretical number of trays N can be calculated as [14]

$$N_i = \left(C_{i,k} - C_{i,k}^{\text{RE}}\right) / \left(C_{i,k}^{\text{RE}} - mx^{\text{IN}} - c\right) \tag{8}$$

where m is 1.45, x^{IN} is the concentration of absorbents, and c is 0. In this work, the absorption factor A is assumed to be 1.

When the diameter of removal tower is taken as 1 m, the investment can be calculated as [15]

$$I_{\text{RE}} = 4552 \cdot \sum_{i=1}^{m} N_i. \tag{9}$$

For the physical adsorption, its operation cost can be neglected compared with its vast investment. The investment is [16]

$$I_{\text{RE}} = a_{\text{PSA}} + b_{\text{PSA}} \cdot F_i^{\text{RE}}. \tag{10}$$

In order to understand the effects of removing different impurities on hydrogen networks, only one impurity is removed, but the number of removed source is not fixed, expressed as

$$\sum_{k=1}^{n_c} If_{i,k}^{\text{RE}} = 1 \tag{11}$$

where $If_{i,k}^{\text{RE}}$ is a binary variable representing whether impurity k in SR_i is removed or not.

3.2. Hydrogen distribution network

Any source can match with any sink, and a source can be interrupted and mixed to match a sink. For a sink, the total flow rate of all sources matched with it cannot be lower than that of the

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