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Rigorous algorithmic targeting methods for hydrogen networks—Part II: Systems with one hydrogen purification unit

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A B S T R A C T

A new systematic targeting methodology has been developed to minimize the use of hydrogen utility in hydrogen networks that also feature purification of hydrogen. Sufficient and necessary conditions of optimality have been proved to extend the pinch based approach to this nonlinear problem. The proposed targeting procedure involves two steps: identification of purifier location and calculation of minimum hydrogen consumption. Examples from the literature are discussed.

1. Introduction

In the previous article, rigorous algorithmic targeting methods for hydrogen networks—Part I, a systematic targeting methodology has been established for hydrogen management problem (HMP), in which the purification was not allowed. An algebraic approach has been adopted to provide the accurate target in the hydrogen network design with simplified manipulating steps. This method is based on the rigorous mathematical simplification and deduction. However, the purification of hydrogen from refinery hydrogen sources was not considered in Part I. The hydrogen utility consumption could be further reduced by using a purifier. In this article (abbreviated as Part II), the methods established in Part I will be extended to systems with one purification unit.

The purification processes, which make possible to clarify the flow of hydrogen sources to quality of fresh hydrogen sources, include pressure swing adsorption (PSA), membrane and cryogenic process. These purification processes rely on different separation theories and they have different operating characteristics. Besides, the economic performance of these purifiers also depends on their placement in the context of an overall network. Superstructure based mathematical methods have been introduced to design the overall optimal hydrogen networks by minimizing the total annual cost (Hallale and Liu, 2001; Liao et al., 2010; Liu and Zhang, 2004). However, the overall optimal solution cannot be guaranteed due to the combinatorial and nonlinear nature of the complicated system model. Moreover the computational results are largely affected by the initial points and variable bounds. On the other hand, conceptual analysis before the structure design can provide good initial "guess" and valuable variable bounds. In addition, the conceptual analysis can also provide insightful understandings to the system. Therefore, evaluating the optimal placement of purifier by the conceptual analysis is necessary and important.

It should also be pointed that the conceptual analysis problem of the purifier placement is quite different from the regeneration placement problem in the water networks, although these two areas are very similar. In the widely reported regeneration problems of water networks (Agrawal and Shenoy, 2006; Bai et al., 2007; Bandyopadhyay and Cormos, 2008; Deng et al., 2008; Feng et al., 2007; Foo et al., 2006; Kuo and Smith, 1998; Wang and Smith, 1994), the regeneration units have only one inlet stream and one outlet stream. While in the hydrogen networks, the purifiers such as the membrane separation and the PSA unit usually have one inlet stream and two outlet streams. Therefore, the techniques developed in the regeneration case of water networks cannot be directly applied to the purification case of hydrogen networks.

In this specific case of HMP with purification, Alves (Alves, 1999; Liu and Zhang, 2004) analyzed three possible placement of the purifier (above the pinch, across the pinch and below the pinch), and reported that placing the purifier across the pinch is the best choice. However, this qualitative conclusion cannot give quantitative hydrogen utility target. Latter, Agrawal and Shenoy (2006) addressed the purification problem based on their limiting

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hydrogen profile. They illustrated that the system has two degrees of freedom and calculated the hydrogen utility consumption by fixing these two freedoms. Foo and Manan (2006) evaluated two different purification processes with given feed concentration via the GCA technique. Ng et al. (2009) employed an automated targeting approach to address this kind of purification problem. Although these works provide reasonable comparisons between purifiers, they did not release the two degrees of freedom simultaneously. None of the resulting target is sufficient to provide the overall optimal target. This is because releasing the two degrees of freedom leads to the nonlinearity of the purification model, which is difficult to be handled by the pinch based methods. In order to achieve the overall optimal target, we will extend the method from Part I to treat the nonlinear problem of HMP with purification.

This paper presents a systematic algebraic approach for setting the real targets for a hydrogen network with one purifier. The obtained results include the minimum hydrogen utility consumption as well as the purifier feed concentration. These targets will jointly provide solution to the general problem of the purifier optimal placement within the hydrogen network. The methodology is mathematically rigorous.

2. Purifier model

As described earlier in Part I, purifiers such as the membrane units and the PSA units, may be modeled as one demand (inlet stream of flow F_{in} and concentration C_{in}) and two sources (the product stream of flow F_{reg} and concentration C_{reg}, along with the residue stream of flow F_r and concentration C_r). In addition, the flow balance and impurity load balance for the purifier are given by

$$F_{in} = F_{reg} + F_r \tag{1}$$

$$F_{in}C_{in} = F_{reg}C_{reg} + F_rC_r \tag{2}$$

Moreover the hydrogen recovery ratio R and the product concentration C_{reg} are usually specified for the purifier (Agrawal and Shenoy, 2006), where R is defined by the following equation:

$$R = \frac{F_{reg}(1-C_{reg})}{F_{in}(1-C_{in})} \tag{3}$$

Since the purifier model consists three Eqs. (1), (2) and (3), in five unknowns (F_{reg}, F_{in}, F_r, C_{in} and C_r), the degree of freedom is two. In this work, F_{in} and C_{in} are chosen to be the two independent operating variables. For ease of representation, let $F_{reg,F_{in},C_{in}}$ and $F_{r,F_{in},C_{in}}$ denote the flow of F_{reg} and F_r under given F_{in} and C_{in}, respectively, also let $C_{r,C_{in}}$ denote the concentration of C_r under given C_{in}. Further manipulations on Eqs. (1)–(3) will give us representations of these dependent variables.

Rearranging Eq. (3)

$$F_{reg,F_{in},C_{in}} = \frac{F_{in}R(1-C_{in})}{(1-C_{reg})} \tag{4}$$

Substituting Eq. (4) into Eq. (1) and rewriting

$$F_{r,\,F_{in},\,C_{in}} = F_{in} - \frac{F_{in}R(1-C_{in})}{(1-C_{reg})} \tag{5}$$

Substituting Eqs. (4) and (5) into Eq. (2) and rearranging

$$C_{r,\,C_{in}} = \frac{(1-C_{reg})(1-R)}{R-\frac{(1-C_{reg})}{(1-C_{in})}} + 1 \tag{6}$$

Moreover the following constraint should be applied to the purifier

$$C_{r,\,C_{in}} > C_{in} > C_{reg}, \quad F_{r,\,F_{in},\,C_{in}}, \quad F_{reg,\,F_{in},\,C_{in}} > 0 \tag{7}$$

In this article, we assume that both the purifier product and residual are not allowed to reenter the purifier. In other words, we only address problems without purifier recycling. In addition, the hydrogen utility also not to be fed into the purifier. Consequently, the upper bound of F_{in} is constrained only by the flow of process hydrogen sources, and it depends on the feed concentration C_{in}. According to Theorem 1 of Part I, the HMP is now concentrated on the pinch problems in the hydrogen network, namely, problems with both F_{hs} and F_{fuel} positive.

3. Optimization formulation

In Part I, we obtained the hydrogen utility target using the following equations:

$$F_{hs,\,k'} = \sum_{C_j \le C_{k'}} F_j \frac{(C_{k'}-C_j)}{(C_{k'}-C_{hs})} - \sum_{C_i \le C_{k'}} F_i \frac{(C_{k'}-C_i)}{(C_{k'}-C_{hs})}, \quad k' = 1, 2, \ldots, K' \tag{8}$$

$$F_{hs,\,\min} = \max_{k'=1,\,2,\,\ldots,\,K'} [F_{hs,\,k'}] \tag{9}$$

where $C_{k'}$, C_i and C_j are constants. However, when the purification unit is taken into consideration, some of the $C_{k'}$ are not constants. Therefore, the representation of minimum hydrogen utility consumption needs to be reformulated.

When the purification unit is introduced, the hydrogen sources involve several fixed concentration levels and one variable concentration. The fixed concentration levels correspond to the concentration of process hydrogen sources and the purifier product, while the variable source concentration level is the purifier residual concentration $C_{r,C_{in}}$. Assume the fixed concentration levels are arranged in ascending order, and the highest level is denoted by $k=K$. Then, Eq. (8) can be evolved as follows:

$$F_{hs,\,k}(C_k-C_{hs}) + \sum_{i \in S,\; C_i \le C_k} F_i(C_k-C_i) = \sum_{j \in D,\; C_j \le C_k} F_j(C_k-C_j), \quad \forall k = 1, 2, \ldots, K \tag{10}$$

$$F_{hs,\,r}(C_{r,\,C_{in}}-C_{hs}) + \sum_{i \in S,\; C_i \le C_{r,\,C_{in}}} F_i(C_{r,\,C_{in}}-C_i) = \sum_{j \in D,\; C_j \le C_{r,\,C_{in}}} F_j(C_{r,\,C_{in}}-C_j) \tag{11}$$

where $F_{hs,k}$ and $F_{hs,r}$ denote the minimum hydrogen utility consumption that satisfies the hydrogen demands, whose concentration are below or equal to C_k and C_r, respectively. It should be noted that both $F_{hs,k}$ and $F_{hs,r}$ in Eqs. (10) and (11) vary with the independent variables F_{in} and C_{in}. Let $F_{hs,k,F_{in},C_{in}}$ and $F_{hs,r,F_{in},C_{in}}$ denote $F_{hs,k}$ and $F_{hs,r}$ under given F_{in} and C_{in}, respectively. Since only the process hydrogen sources are allowed to feed the purifier, then the purifier feed concentration C_{in} lies in the interval of $[C_{1'}, C_K]$, where $C_K = C_{K'}$. Therefore, Eqs. (10) and (11) can be rearranged as follows:

$$F_{hs,\,k,\,F_{in},\,C_{in}}(C_k-C_{hs}) + \sum_{C_i \le C_k} F_i(C_k-C_i) = \sum_{C_j \le C_k} F_j(C_k-C_j)$$
$$\forall k = 1, \ldots, K, \quad C_{in} \in [C_{1'}, C_K], \quad F_{in} \in [0, F_{in,\,C_{in},\,\max}] \tag{12}$$

$$F_{hs,\,r,\,F_{in},\,C_{in}}(C_{r,\,C_{in}}-C_{hs}) + \sum_{C_i \le C_{r,\,C_{in}}} F_i(C_{r,\,C_{in}}-C_i) = \sum_{C_j \le C_{r,\,C_{in}}} F_j(C_{r,\,C_{in}}-C_j)$$
$$\forall C_{in} \in [C_{1'}, C_K], \quad F_{in} \in [0, F_{in,\,C_{in},\,\max}] \tag{13}$$

where $F_{in,\,C_{in},\,\max}$ is the upper bound of F_{in} under given C_{in}.

It is worth to point out that the detailed expressions of Eqs. (12) and (13) depend on the location of the purifier. To illustrate the purifier location, let k_{reg} denote the concentration level of C_{reg}, also let k_{hs}, k_{in} and $k_{r,C_{in}}$ denote the highest concentration level that are below or equal to C_{hs}, C_{in} and $C_{r,C_{in}}$, respectively

$$C_{k_{hs}} \le C_{hs} < C_{k_{hs}+1}, \quad C_{k_{in}} \le C_{in} < C_{k_{in}+1}, \quad C_{k_{r,\,C_{in}}} \le C_{r,\,C_{in}} < C_{k_{r,\,C_{in}}+1} \tag{14}$$