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A thermodynamic irreversibility based design method for multi-contaminant hydrogen networks

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ABSTRACT

This paper presents a new method for the design of hydrogen networks with multiple contaminants. The proposed method is based on the principle that minimizing thermodynamic irreversibility of the satisfying process will result in minimum utility consumption of the hydrogen network. Therefore, the entropy change which indicates the thermodynamic irreversibility of the satisfying process is minimized for each sink to obtain the minimum utility consumption. A new concept, virtual concentration, which is drawn from the thermodynamic analysis of the satisfying process, is proposed to measure the purity of the hydrogen streams with multiple contaminants. Source streams with the nearest virtual concentration as the sink are used to satisfy the sink to reduce the entropy change of each satisfying process. The detailed design procedures are proposed to obtain the hydrogen network distribution. The exact flow rate of each source stream is achieved by solving the mass balance equations. Three literature examples are illustrated to show the effectiveness of the proposed approach.

Introduction

The rising cost of hydrogen and stricter environment regulations have motivated the management of hydrogen in refineries greatly. During the last decade, plenty of work has been done for the targeting and design of hydrogen networks. These methods can be classified into two categories: pinch-based conceptual methods and mathematical programming methods. Although the mathematical programming methods [1–12] are capable of solving large scale hydrogen networks with various practical considerations, they cannot provide insightful understandings to the results. In addition, it might be more efficient when insights of specific problems are added into the optimizing algorithm. To overcome this drawback, pinch based conceptual approaches are developed. They are easy to understand and interactive with the designers in the design procedure. Furthermore, the obtained design heuristics has the potential to help improving the efficiency of mathematical model or algorithm.

Typically, the pinch based conceptual methods include two stages: minimum hydrogen utility consumption target and network design. These approaches for hydrogen network are proposed by drawing analogy to the heat exchanger network [13] and water network [14–18] synthesis. The pinch based targeting approaches for hydrogen network were pioneered by introducing hydrogen surplus diagram [19,20]. Since then many pinch-based graphical methods such as material

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recovery pinch diagram [21,22] and limiting composite curves [23] have been proposed to target the hydrogen networks. Once the minimum utility consumption is targeted, a hydrogen network can be designed to achieve the established flow rate target. The nearest neighbor algorithm [23,24] (NNA) and network allocation diagram [17] were proposed to design both water and hydrogen networks. Recently, conceptual researches have made some breakthrough in targeting hydrogen networks with purification unit [25–29]. However, due to the limitations of the conventional pinch diagram, most of the methods are proposed with the assumption that only hydrogen and methane are taken into consideration in the streams. In other words, these networks are single-contaminant hydrogen networks (SCHNs) which is quite different from the actual industrial process.

To target and design multiple-contaminant hydrogen networks (MCHNs), Zhao et al. [30] proposed a multiple contaminant deficit method which is analogy to the hydrogen surplus diagram [20] for SCHNs. The contaminant profiles and contaminant deficit diagram of all contaminants are used to identify the pinch point of the hydrogen network. The minimum utility consumption can be achieved with iterative calculation. Wang et al. [31] took advantage of the unique features of ternary composition diagram to propose a new graphical procedure for minimizing utility consumption of multiple contaminants hydrogen networks. However, the main drawback is that a sink can only be matched with at most three sources in this method. Liu et al. [32] proposed an evolutionary method which employ several matrix tools to improve the source – sink satisfying procedure. This method took every match possibility and the complementary advantage of source streams into consideration. Other methods choose to rank the source and sink streams before the satisfying procedure, because good ranking can help achieving the utility target and accelerating the satisfying procedure. Zhang et al. [33] proposed an evolutionary graphical approach for simultaneous targeting and design of hydrogen networks with multiple contaminants. The nearest neighbor algorithm (NNA) for SCHNs is generalized to the MCHNs and a new ranking rule is established to rank those streams. Liu et al. [34,35] proposed the concentration potential concept for the ranking of source and sink streams. This concept is based on the overall allocation possibility of source to sink streams and is quite effective to simplify the design procedure.

It should be noted that the above ranking approaches are based on different insights of the system. In this paper, we will develop a ranking approach that is based on a new insight, the thermodynamic irreversibility. The thermodynamic irreversibility insight was first recognized by Agrawal and Shenoy [23] in the SCHN. They stated that a network should be designed toward minimizing the exergy losses or thermodynamic irreversibility. However, the thermodynamic irreversibility for MCHN is quite different from SCHN. To deal with MCHNs, a new concept, virtual concentration, is drawn from the entropy change of the satisfying process. Both source and sink streams are ranked according to the virtual concentration. Detailed procedures are also proposed to design hydrogen networks after ranking. Three literature examples are illustrated to show the effectiveness of this method.

Thermodynamic analysis of the satisfying process

For SCHNs, sinks can be satisfied sharply in the proposed targeting and design approaches to reduce the hydrogen utility consumption. The sharp match status means that both the flow rate and hydrogen load (or contaminant load for SCHNs) of the sink are exactly the same as the mixed source stream, which can be described as:

$$\sum F_i = F_j \quad \forall\ i \in \mathrm{SOURCE},\ j \in \mathrm{SINK} \tag{1}$$

$$\sum F_i y_i = F_j y_j \quad \forall\ i \in \mathrm{SOURCE},\ j \in \mathrm{SINK} \tag{2}$$

Prakash and Shenoy [24] proposed the nearest neighbors algorithm (NNA) to minimize the utility consumption of SCHN by minimizing the mixing irreversibility of the source streams. The mixing irreversibility is reduced by satisfying sinks with the nearest available source neighbors in terms of the hydrogen purity or the contaminant concentration.

However, the problem gets complicated for MCHNs. For example, sinks usually are not sharply satisfied by the sources in MCHNs, as the concentration of each contaminant of source stream is not proportional to that of the sink. Therefore, the mass balance of sinks in MCHNs is represented by equations (3)–(5):

$$\sum F_i = F_j \quad \forall\ i \in \mathrm{SOURCE},\ j \in \mathrm{SINK} \tag{3}$$

$$\sum F_i y_{i,k} \le F_j y_{j,k} \quad \forall\ i \in \mathrm{SOURCE},\ j \in \mathrm{SINK},\ k \in K \tag{4}$$

$$\sum F_i y_{i,H_2} \ge F_j y_{j,H_2} \quad \forall\ i \in \mathrm{SOURCE},\ j \in \mathrm{SINK} \tag{5}$$

When we know all the contaminants, as illustrated in the three examples, equations (3) and (4) are enough to represent the mass balance of sinks.

Let's take an extreme example that one sink with no hydrogen requirement is satisfied by pure hydrogen source. Although there is no mixing process in this scenario, this satisfying process also generates irreversibility which lies in the difference between the source stream and the sink requirement. The process that using the mixed source stream to satisfy the sink requirement is named matching process. The irreversibility of this process is generated by the difference between the mixed source stream and the sink requirement. Therefore, the thermodynamic irreversibility of the satisfying process of MCHNs is generated both in the mixing process and matching process.

In order to evaluate the irreversibility of each process, entropy change of each process is employed to represent the irreversibility. Suppose $n_1, n_2, \ldots, n_i$ are the flow rates of source streams $S_1, S_2, \ldots, S_i$ that are needed to satisfy the sink whose molar flow rate is n. $y_{l,i}$ represents the molar fraction of component l of source stream i and y_l represents the molar fraction of component l of the sink. The flow rate of the mixed source streams is specified identical to the sink, while the concentration of component l is represented by $y_{l,M}$. The satisfying process is shown in Fig. 1.