Chinese Journal of Chemical Engineering 23 (2015) 1536–1541

Contents lists available at ScienceDirect

Chinese Journal of Chemical Engineering

journal homepage: www.elsevier.com/locate/CJChE

Process Systems Engineering and Process Safety

A procedure for design of hydrogen networks with multiple contaminants☆

Xuefei Wang [1], Zhe Wang [2], Huipeng Zhao [1], Zhiyong Liu [3,*]

[1] School of Chemical Engineering, Hebei University of Technology, Tianjin 300130, China
[2] The hospital of Hebei University of Technology, Tianjin 300130, China
[3] School of Marine Science and Engineering, Hebei University of Technology, Tianjin 300130, China

ARTICLE INFO

Article history:
Received 22 September 2014
Received in revised form 29 January 2015
Accepted 13 February 2015
Available online 10 April 2015

Keywords:
Multiple contaminants
Hydrogen network
Concentration potentials
Complementary sources

ABSTRACT

It is necessary to reduce hydrogen consumption to meet increasingly strict environmental and product-quality regulations for refinery plants. In this paper, the concentration potential concepts proposed for design of water-using networks are extended to synthesis of hydrogen networks with multiple contaminants. In the design procedure, the precedence of processes is determined by the values of concentration potential of demands. The usage of complementary source pair(s) to reduce utility consumption is investigated. Three case studies are presented to illustrate the effectiveness of the method. It is shown that the design procedure has clear engineering meaning.

1. Introduction

Hydrogen resources are widely used in hydrogenation process and desulfurization process to upgrade crude oil to light transportation fuels. Since crude oil is getting heavier and environmental regulations are becoming stricter, large amounts of hydrogen resources are required for hydro-treating processes. To reduce hydrogen consumption, one of the methods is synthesis of hydrogen networks.

A hydrogen network has several hydrogen consumers, such as hydrocracking and hydro-treating processes, and hydrogen producers, such as catalytic reforming process. The inlet streams are called as the demands (or sinks), the outlet streams as the internal sources, and the hydrogen stream from outside suppliers as the external source (or utility).

Two widely used techniques to synthesize hydrogen networks are pinch analysis and mathematical programming methods. The pinch-based methods present clear physical insight, but can deal with single impurity hydrogen system only. Alves and Towler [1] proposed a method for calculating the minimum flow rate of hydrogen utility required, in which purity profile and hydrogen surplus diagram were employed to identify hydrogen pinch and the minimum amount of hydrogen utility. Liu *et al.* [2] analyzed the characteristics of pinch point and the effect of purification to the hydrogen surplus diagram [1], with the flow rate of purification feed given, the pinch location of the hydrogen system can be identified qualitatively. El-Halwagi *et al.* [3] developed a non-iterative graphical technique for targeting the minimum utility consumption. Ding *et al.* [4] constructed average pressure profiles of sources and demands to design the hydrogen networks with pressure constraints. Zhao *et al.* [5] proposed a simple graphical method to identify the minimum utility consumption and pinch point. Based on ternary composition diagram [6] for three component systems, Wang *et al.* [7] proposed a graphical method for optimizing the match between multiple sources and one demand. Zhang *et al.* [8] proposed a graphical method for targeting and design of resource conservation networks with multiple contaminants, in which a triangle (polygon) rule was proposed to illustrate the match between multiple sources and a demand. Based on the ranked order of sources and demands, the material recovery pinch diagram for multiple contaminants was constructed. The resulting group of matching polygons gave the target and corresponding network.

The mathematical programming approaches are also important in the design of hydrogen networks. These methods can deal with complex system and achieve utility target, but the solving process is often complicated. Many mathematical models, including linear programming (LP), non-linear programming (NLP), mixed-integer linear programming (MILP) and mixed-integer non-linear programming (MINLP) models, have been developed to optimize hydrogen distribution systems [9–15]. Hallale and Liu [9] proposed a superstructure based approach for hydrogen networks accounting for pressure constraints and economic issues. By using the newly developed understanding of network interactions in refineries, Zhang *et al.* [10] proposed a method for overall refinery optimization through integration of hydrogen network and utility system with the material processing system. Khajehpour *et al.* [11] proposed heuristic rules to reduce the complexity of the superstructure of hydrogen network,

☆ Supported by the National Natural Science Foundation of China (21176057), the National Basic Research Program of China (2012CB720305), and the State Key Laboratory of Chemical Engineering (Open Research Project Skloche-K-2011-04).

* Corresponding author.
E-mail address: Liuzhiyong@hebut.edu.cn (Z. Liu).

http://dx.doi.org/10.1016/j.cjche.2015.04.004

and the reduced superstructure was used to optimize hydrogen system. Kumar *et al.* [12] employed mathematical modeling technique to optimize the hydrogen distribution network and analyzed the characteristics of LP, NLP, MILP and MINLP models. Based on the automated design approaches of Hallale and Liu [9] and Liu and Zhang [13], Ahmad *et al.* [14] proposed a method for multi-period design of hydrogen networks. Jiao *et al.* [15] proposed two mathematical methods based on two-step approach and simultaneous optimization approach to make efficient use of hydrogen streams. Liao *et al.* [16,17] proposed a method for hydrogen systems by combining pinch insight and rigorous mathematical optimization technique.

In this paper, the approach developed for water-using networks with multiple contaminants [18] is extended to hydrogen networks with multiple contaminants. The method proposed in this study considers constraints on flow rate and concentrations simultaneously. First, operation order is determined based on the values of concentration potential of the demands. Then, a few rules satisfying demands with sources are deduced. Based on the source–demand matches, utility consumption and corresponding network can be obtained.

2. The Concentration Potentials of the Source and Demand Streams

A water network with single contaminant can be designed by satisfying the demands in their ascending order of impurity concentrations, but it is difficult to determine the concentration order of the streams with multiple contaminants. In the design of water-using network with multiple contaminants, Liu *et al.* [18] proposed to use concentration potentials of demand streams (*CPDs*) and sources (*CPSs*) to determine the concentration order of the streams. Here we give a brief introduction about them.

The limiting quasi-allocation ratio of S_i for unit amount of D_j is

$$R_{i,j} = \frac{C^{\lim}_{Dj,KC}}{C_{Si,KC}} = \min_{m=1,2\ldots,NC}\left(\frac{C^{\lim}_{Dj,m}}{C_{Si,m}}\right) \tag{1}$$

where $C^{\lim}_{Dj,m}$ is the limiting concentration of contaminant m in demand D_j, $C_{Si,m}$ is the concentration of contaminant m in source S_i, and NC is the number of contaminants.

The contaminant(s) determining the value of $R_{i,j}$ is called as the reuse key contaminant(s) (*KCs*). The concentration of *KC* will reach its limiting value when D_j is satisfied by S_i. The concentration potential of demand D_j is the sum of the $R_{i,j}$ values for all the source streams:

$$CPD\left(D_j\right) = \sum_{i=1}^{NS} R_{i,j} = \sum_{i=1}^{NS} \min_{m=1,2\ldots,NC}\left(\frac{C^{\lim}_{Dj,m}}{C_{Si,m}}\right) \tag{2}$$

where NS is the number of source streams. The value of $CPD(D_j)$ reflects the overall possibility of demand D_j to reuse the source streams.

Similarly, the value of $CPS(S_i)$ reflects the overall possibility of source S_i to be reused by demand streams,

$$CPS(S_i) = \frac{1}{\sum_{j=1}^{ND} \min_{m=1,2\ldots,NC}\left(\frac{C^{\lim}_{Dj,m}}{C_{Si,m}}\right)} \tag{3}$$

where ND is the number of demand streams.

3. The Rules Satisfying a Demand with Complementary Source Pair(s)

3.1. The concept of complementary source pair

The concept of complementary sources [19] will be applied to hydrogen networks in this paper. When satisfying a demand, if the limiting quasi-allocation ratio for contaminant m of source S_i is larger than unity and that of the same contaminant of another source, say source S_k, is smaller than unity, the two sources are called as complementary source pair. If the complementary source pair is used to satisfy the corresponding demand, utility consumption may be reduced [19].

We will use an example to show its application with the limiting data in Table 1. In Table 1, the limiting impurity mole concentrations of demand D_2 are 0.1% and 8.57%, with those of source S_1 as 0 and 9.2 and S_2 as 0.21 and 6.18. The limiting quasi-allocation ratios of S_1 and S_2 for D_2 are $R_{1,2} = \min\{\infty, 0.93\} = 0.93$ and $R_{2,2} = \min\{0.48, 1.39\} = 0.48$, which are lower than unity, so that utility is needed. For contaminant H_2S, the limiting quasi-allocation ratio of S_1 for D_2 is infinity (∞), which is larger than unity, while that of S_2 for D_2 is 0.48, lower than unity. For contaminant *A*, the limiting quasi-allocation ratio of S_1 for D_2 is 0.93, which is lower than unity, while that of S_2 for D_2 is 1.39, larger than unity. For this case, if S_1 with an amount of 166.57 $mol\cdot s^{-1}$ and S_2 with an amount of 151.43 $mol\cdot s^{-1}$ are used to satisfy D_2, it is not necessary to use the utility, so that utility consumption can be reduced.

Table 1
Limiting data for case 1 [20]

		F/mol·s^{-1}	H_2/mol%	H_2S/mol%	A/mol%
Sources	Utility		99.99	0	0.01
	S_1	262	90.8	0	9.2
	S_2	295	93.61	0.21	6.18
	S_3	104	86.63	1.03	12.34
Demands	D_1	122	92.81	0	7.19
	D_2	318	91.33	0.1	8.57
	D_3	197	90	1	9

3.2. The rules satisfying a demand with complementary source pairs

When satisfying a demand with complementary source pairs, utility consumption may be reduced, as discussed above. If a few complementary source pairs are available, we should determine the one to be used. We will use the following rules to choose complementary source pair.

(1) When satisfying demand D_j, if a few complementary source pairs are available, arrange the pairs in the ascending order of $R_{h,j}$ values, where $R_{h,j}$ is the higher value of the quasi-allocation ratio of a complementary source pair; if a few complementary source pairs have the same $R_{h,j}$ value, arrange them in ascending order of $R_{l,j}$ values, where $R_{l,j}$ is the lower value of the quasi-allocation ratio of a complementary source pair.
(2) Consider the complementary source pairs in the above order. If one of the complementary source pairs can satisfy the demand without utility, this pair will be used to satisfy the demand. If none of the pairs can satisfy the demand without utility, choose the complementary source pair corresponding to the minimum amount of utility consumption to satisfy the demand.

The procedure of selecting complementary sources to satisfy a demand is shown in Fig. 1.

4. Design Procedure

We will use similar rules for design of water-using networks proposed by Liu *et al.* [18]. The design procedure proposed in this study is as follows.

(1) Calculate the values of *CPD* and *CPS* based on the limiting concentrations;
(2) The demand with the lowest *CPD* value will be satisfied first. If a few processes have the same *CPD* values, the process with the highest hydrogen purity will be satisfied first;
(3) If a source stream is used up, it will not be considered in the following steps;