

Pinch Location of the Hydrogen Network with Purification Reuse^{*}

LIU Guilian (刘桂莲)^{1,**}, LI Hao (黎浩)², FENG Xiao (冯霄)³ and DENG Chun (邓春)³

¹ Department of Chemical Engineering, School of Chemical Engineering and Technology, Xi'an Jiaotong University, Xi'an 710049, China

² WISDRI Engineering & Research Incorporation Limited, Wuhan 430223, China

³ State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing 102249, China

Abstract In the hydrogen network with the minimum hydrogen utility flow rate, the pinch appears at the point with zero hydrogen surplus, while the hydrogen surpluses of all the other points are positive. In the hydrogen purity profiles, the pinch can only lie at the sink-tie-line intersecting the source purity profile. According to the alternative distribution of the negative and positive regions, the effect of the purification to the hydrogen surplus is analyzed. The results show that when the purification is applied, the pinch point will appear neither above the purification feed nor between the initial pinch point and the purification feed, no matter the purification feed lies above or below the initial pinch point. This is validated by two case studies.

Keywords purification, pinch, hydrogen network, hydrogen surplus, hydrogen utility flow rate

1 INTRODUCTION

Nowadays, the hydrogen demand of refineries increases significantly because of the combination of low-sulphur fuel specifications, markets shifting toward lighter fuels, and the desire to process heavier, sourer crudes. Reducing the hydrogen consumption is the critical problem of many refineries. The hydrogen network integration optimizes the hydrogen network with all the hydrogen demands and hydrogen supplies considered as a whole, and hence can significantly increase the reuse of the process hydrogen and minimize the hydrogen utility consumption.

Alves and Towler [1] introduced a graphical method for the analysis of hydrogen distribution systems. Through the iterative calculation of the purity profiles and hydrogen surplus diagrams, the pinch and the minimum hydrogen utility consumption can be identified. To avoid the cumbersome iteration, El-Halwagi *et al.* [2] developed a graphic method with the source and sink composite curves plotted in the impurity load *versus* flow rate diagram. This method can be used to mass exchange networks with pure fresh resources. Later, the general graphic methods were proposed by Kazantzi and El-Halwagi [3] and Zhao *et al.* [4]. In these methods, the pinch point can be identified by shifting the composite curve. A unified conceptual approach was proposed for water and hydrogen networks by Agrawal and Shenoy [5]. In this approach, the composite curve was constructed in the contaminant concentration *versus* contaminant mass load diagram. Bandyopadhyay [6] proposed the source composite curve method to reduce the waste generation through maximizing the on-site reuse/recycling. Alwi *et al.* [7] developed the network allocation diagram to identify the minimum gas targets.

Manan and Foo [8] developed a numerical alternative

to the graphical targeting technique, the water cascade analysis (WCA). This method can quickly target the accurate minimum water targets and pinch point without the tedious iteration. Later, it was generalized to the property cascade analysis (PCA) technique, which is used to target the property-based material reuse network [9].

In a hydrogen network, only the hydrogen surplus with higher purity can be used to supplement the hydrogen deficient with lower purity [1], while the hydrogen transfer in the reverse direction is infeasible. To increase the hydrogen utilization, the purity of the hydrogen sources with lower purity can be increased through purification. Purification reuse is a good choice to reduce the hydrogen utility consumption and is widely used in practice. Since the purification will modify the hydrogen purity and the flow rate of source streams, it will affect the pinch point location and the minimum hydrogen utility consumption simultaneously. For the given purification equipment and feed purity, the pinch location changes with the purification feed flow rate (PFFR). To identify the pinch point of system with purification reuse quickly, it is necessary to make a quantitative analysis about the pinch point location.

Alves [10] and Liu *et al.* [11] analyzed the three possible placement of the purifier (above the pinch, across the pinch and below the pinch), and concluded that the purifier across the pinch is the best choice. Agrawal and Shenoy [5] analyzed the purification problem and calculated the hydrogen utility consumption. Foo and Manan [8] further generalized PCA to gas cascade analysis (GCA) for targeting the utility gas network. The selection of gas purification techniques was systematically studied *via* the GCA. Ng *et al.* [12–14] proposed the automated targeting technique to optimize the hydrogen networks with regeneration/

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^{**} To whom correspondence should be addressed. E-mail: liuguilian@yahoo.com

purification reuse. Nelson and Liu [15] developed an Excel spreadsheet to solve the problems of multiple-pinch systems with purification. Bandyopadhyay [6] and Tan *et al.* [16] presented the similar methods to identify the minimum utility target for the hydrogen network with purification reuse. Zhang *et al.* [17] proposed the triangle representation of the hydrogen purification process and developed a graphic method to identify the pinch point location and the minimum hydrogen utility consumption of the hydrogen system with purification reuse.

In addition to the graphic method, the mathematical optimization method can also be used to synthesize the hydrogen systems with purification reuse. Liu and Zhang [11] proposed a systematic methodology to identify the appropriate purification. In this method, superstructure was built with the shortcut models of different purification units and all possible purification scenarios included. The optimal solution can be obtained through the trade-offs among the hydrogen saving, the compression costs and the capital investment. Liao *et al.* [18] presented a systematic approach for the integration of hydrogen networks with purifiers. Later, they developed a mathematically rigorous targeting approach with the pinch insight combined [19]. And, this method was extended to the hydrogen networks with purification reuse [20]. Compared with the graphic methods, mathematical programming methods can deal with more complicated problems, but cannot give clear insights into the process operations.

For the hydrogen network with purification reuse, all the graphic and mathematical programming methods mentioned above did not analyze the characteristics of the pinch point. Based on the hydrogen profiles and hydrogen surplus diagram, the location of the pinch point will be qualitatively analyzed in this work, and the rules for identifying the pinch point will be proposed.

2 GRAPHIC METHOD OF ALVES AND TOWLER [1]

In a hydrogen network, the flow rates of most sources and sinks are determined by the product

requirement and production technology, and only the flow rates of fresh hydrogen (utility) is flexible. Based on the concept of hydrogen surplus, Alves and Towler proposed a systematic method for targeting the minimum hydrogen utility consumption of hydrogen distribution networks [1]. Given the initial hydrogen utility flow rate, the sink and source purity profiles can be plotted (in the decreasing order of hydrogen purity) in the hydrogen purity *versus* flow rate diagram, as shown in Fig. 1 (a).

In the hydrogen purity profile, every horizontal section represents a sink or source. Every vertical section is the tie-line connecting the two adjacent sources (or sinks) and does not have physical meaning, and it is termed as the source-tie-line (or sink-tie-line) in this work. For example, in Fig. 1 (a), $A'A''$ and $B'B''$ are source-tie-lines, $C'C''$ and $D'D''$ are sink-tie-lines. The two purity profiles intersect at some of the sink-tie-lines and source-tie-lines, and these tie-lines divide the two purity profiles into different regions. In each region, there might include several sources or sinks, and the source purity profile might lie above or below the sink purity profile. If the source purity profile lies above the sink purity profile, as denoted by “+” in Fig. 1 (a), there is an excess of hydrogen that amounts to the area between the corresponding sink and source purity profiles. The excess hydrogen can compensate for a deficit in hydrogen supply at a lower purity. On the contrary, if the source purity profile lies below the sink purity profile, as denoted by “-” in Fig. 1 (a), there is a deficit of hydrogen. The amount of the deficit also equals to the area of the space between the two curves. Overall, the purity profiles can be divided into regions with alternating excess and deficit of hydrogen. Based on this, the net cumulative excess of hydrogen at a given flow rate (F) is termed as hydrogen surplus (H') and can be calculated according to Eq. (1).

$$H' = \int_0^F (y_{SR} - y_{SK}) dF \quad (1)$$

where F is the flow rate of the overlapped sink and source; y_{SR} and y_{SK} represent the hydrogen purity of the source and the sink, respectively.

According to the hydrogen purity profiles, the hydrogen surplus profile can be plotted in the hydrogen

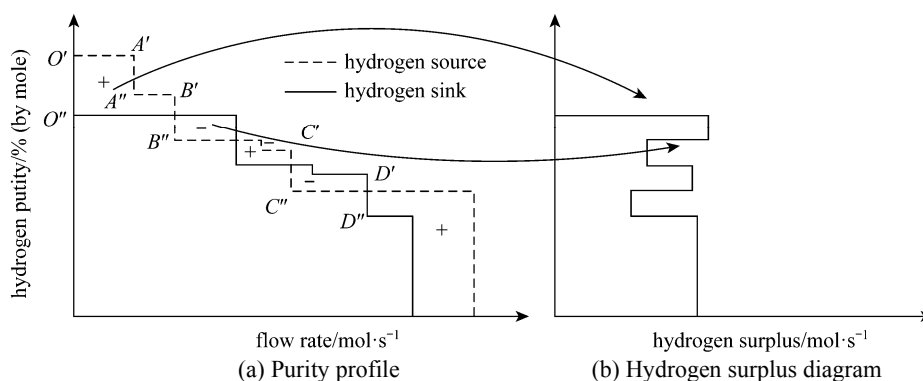


Figure 1 Purity profiles and the hydrogen surplus diagram of a hydrogen network

purity versus hydrogen surplus diagram, as shown in Fig. 1 (b). When the hydrogen surplus is positive throughout the diagram, there is the potential of saving hydrogen utility.

As the hydrogen utility flow rate decreases, the hydrogen surplus of this system will decrease. When the hydrogen surplus of a point is reduced to zero, while those of all the other points are larger than zero, the “hydrogen pinch” is identified, as shown in Fig. 2. The corresponding hydrogen utility flow rate is the minimum hydrogen utility consumption. The purity of the source where the pinch appears is taken as the pinch purity.

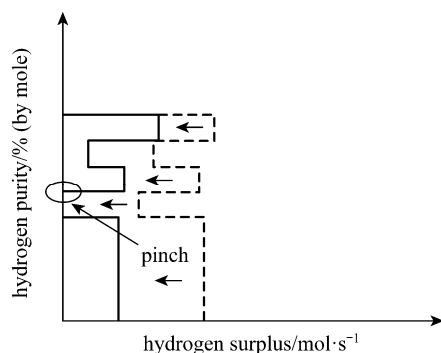


Figure 2 Hydrogen surplus diagram

3 PINCH POINT LOCATION OF THE SYSTEM WITH PURIFICATION REUSE

3.1 Location of the pinch point

In the hydrogen purity versus flow rate diagram, there are multiple intersections between the sink and source purity profiles. These intersections separate the whole purity profiles into different regions, and the relative position of the sink and source profiles alters at each intersection point. Because of this, the positive and negative regions appear alternatively. As stated earlier, there might be one or more sources (or sinks) in each region. For simplicity and clarity, the system with one source and one sink in each region is used to analyze the characteristic of the pinch point, as shown in Fig. 3. In this system, each sink-tie-line intersects a source and each source-tie-line intersects a sink.

For two neighboring regions with the positive one on the left and the negative one on the right, their dividing line must be a source-tie-line, such as LL' and II' in Fig. 3. On the contrary, if the negative region lies on the left and the positive one on the right, their dividing line must be a sink-tie-line, such as AA' , BB' and CC' in Fig. 3. In other words, there is a positive region on the right of the sink-tie-line intersecting with the source purity profile or a negative region on the right of a source-tie-line intersecting with the sink purity profile.

According to the pinch principle, the hydrogen surplus at the pinch point should be zero, while that at any other points should be larger than zero. If the

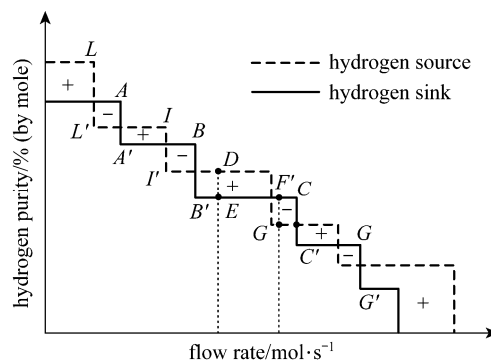


Figure 3 Purity profiles with one source and one sink in each region

pinch point appears at a source-tie-line, the hydrogen surplus at its right adjacent sink-tie-line must be negative, and this is infeasible. Take Fig. 3 as an example, if the pinch point locates at source-tie-line II' , its hydrogen surplus should be zero. Since the negative region between II' and BB' has hydrogen deficient, the hydrogen surplus at BB' must be negative, and this is infeasible. Therefore, the pinch point can never appear at a source-tie-line. Similarly, it can be derived that the pinch point can neither appear inside a positive region, nor appear inside a negative region, such as point D and point F' in Fig. 3. Thus, the pinch point can only appear at the sink-tie-line, such as BB' and CC' in Fig. 3. Hence, the hydrogen surplus at the sink-tie-line is the emphasis of analysis.

For the hydrogen networks with irregular distribution, not all sink-tie-lines intersect the source purity profile. The necessary condition for a sink-tie-line to intersect the source purity profile is that there is at least one source whose purity lies between the two sinks connected by this sink-tie-line. Furthermore, whether a sink-tie-line intersects the source purity profile or not is affected by the hydrogen utility flow rate, as shown by AA' in Fig. 4.

The pinch point will never appear at the sink-tie-line, which cannot intersect with the source purity profile. For example, if the pinch point appears at sink-tie-line AA' shown in Fig. 4 (a), its hydrogen surplus must be zero. Since the hydrogen surplus between AA' and BB' is positive, it can be derived that the hydrogen surplus at BB' should be negative. This does not meet the pinch principle. Similarly, the pinch point will not appear at sink-tie-line AA' in Fig. 4 (b). Therefore, the pinch point can only appear at the sink-tie-line intersecting with the source purity profile.

3.2 Pinch point of the hydrogen network with purification reuse

The purifier can separate the feed stream (with purity y_{pur}) into two streams, the purified product (with purity y_g) and the tail gas (with purity y_w), as shown in Fig. 5. Since the tail gas contains hydrogen

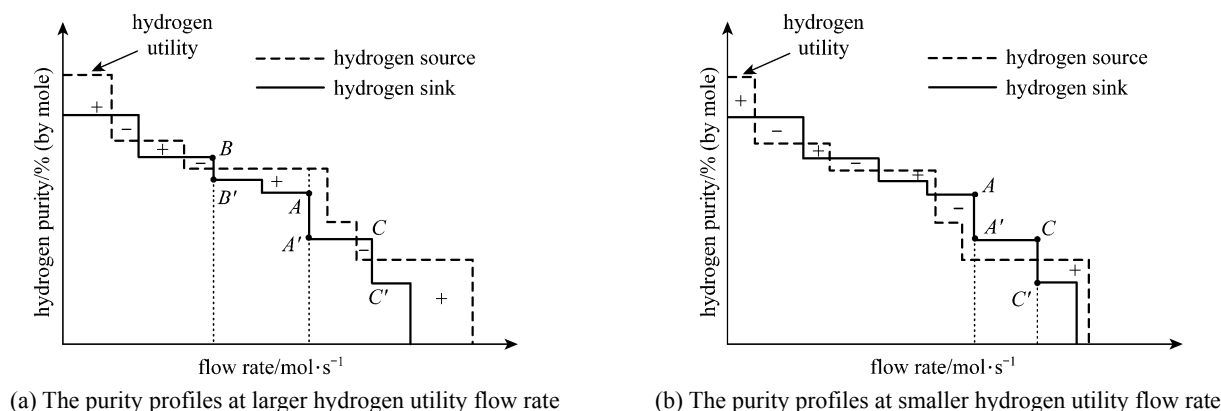


Figure 4 Purity profiles of the hydrogen network with irregular source and sink distribution

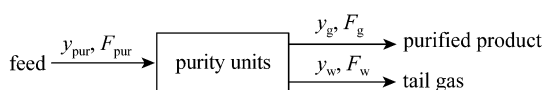


Figure 5 General process of purification

and is generally sent to the fuel system, there is hydrogen loss. For a hydrogen purification process with given y_{pur} , F_{pur} , y_g and the hydrogen recovery R , y_w , F_g and F_w can be calculated according to the material balance of this process, as shown by Eqs. (2), (3) and (4).

$$F_g = F_{\text{pur}} y_{\text{pur}} \frac{R}{y_g} \quad (2)$$

$$F_w = F_{\text{pur}} \left(1 - y_{\text{pur}} \frac{R}{y_g} \right) \quad (3)$$

$$y_w = \frac{1 - R}{\frac{1}{y_{\text{pur}}} - \frac{R}{y_g}} \quad (4)$$

With the purification applied, the purity of the purification feed will be increased, and hence the hydrogen utility flow rate can be reduced. However, as there is hydrogen loss in the tail gas and the purification will modify the distribution of the hydrogen sources, the initial pinch point might change. The pinch of the system with purification reuse cannot locate at all place. This will be analyzed quantitatively in the following.

For easy understanding, the system shown in Fig. 6 is used to illustrate the analysis. When the purification reuse is not considered, the pinch point appears at the sink-tie-line, PP' , as shown in Fig. 6 (a). AB represents the hydrogen utility and its purity equals to that of the purified product. For simplification, the minimum hydrogen utility flow rate of the system without purification reuse is taken as the initial utility flow rate, and the corresponding pinch is taken as the initial pinch. When the purification is applied, the purified product with flow rate F_g can be represented by CD (point C overlaps with point B), as shown in Fig. 6

(b). If the hydrogen utility flow rate is unchanged, the hydrogen surplus at PP' together with that at any other sink-tie-lines will be higher than zero. Decreasing the flow rate of the hydrogen utility can reduce the hydrogen surplus below the hydrogen utility. If the amount of the decreased hydrogen utility flow rate is greater than F_g , the distribution of the source curves is shown in Fig. 6 (c). Obviously, the hydrogen surplus between PP' and EE' is less than that when the purification reuse is not applied. Considering that the hydrogen sinks and sources above EE' are unchanged, the hydrogen surplus at EE' does not change either. Hence, the hydrogen surplus at PP' will decrease to negative value. Obviously, this is infeasible. Therefore, when the purity of the purified product equals to that of the hydrogen utility, the amount of the decreased hydrogen utility flow rate can never be higher than the purified product flow rate.

If the purification feed lies above the initial pinch, the pinch point when the purification reuse is applied cannot appear above the purification feed. The reason is that at the initial hydrogen utility flow rate, the hydrogen surplus of each sink-tie-line above the purification feed is higher than zero when the purification is not applied. When the purification is applied, the purification product with flow rate F_g should be added to the source purity profile. Hence, the source composite curve between the purified product and the purification feed will shift to the right by flow rate F_g , and the hydrogen surplus of the sink-tie-line lying between the purified product and purification feed will increase. Only when the hydrogen utility is decreased by a flow rate greater than F_g , the hydrogen surplus of a sink-tie-line above the purification feed can decrease to zero. But this is against the conclusion that the amount of the decreased hydrogen utility flow rate cannot be higher than the purified product flow rate (F_g), and thus, the pinch point of the system with purification reuse cannot appear above the purification feed. This conclusion is feasible for the system that the purified product has the same purity with the hydrogen utility.

Similarly, the pinch point cannot appear at the sink-tie-line between the purification feed and the initial

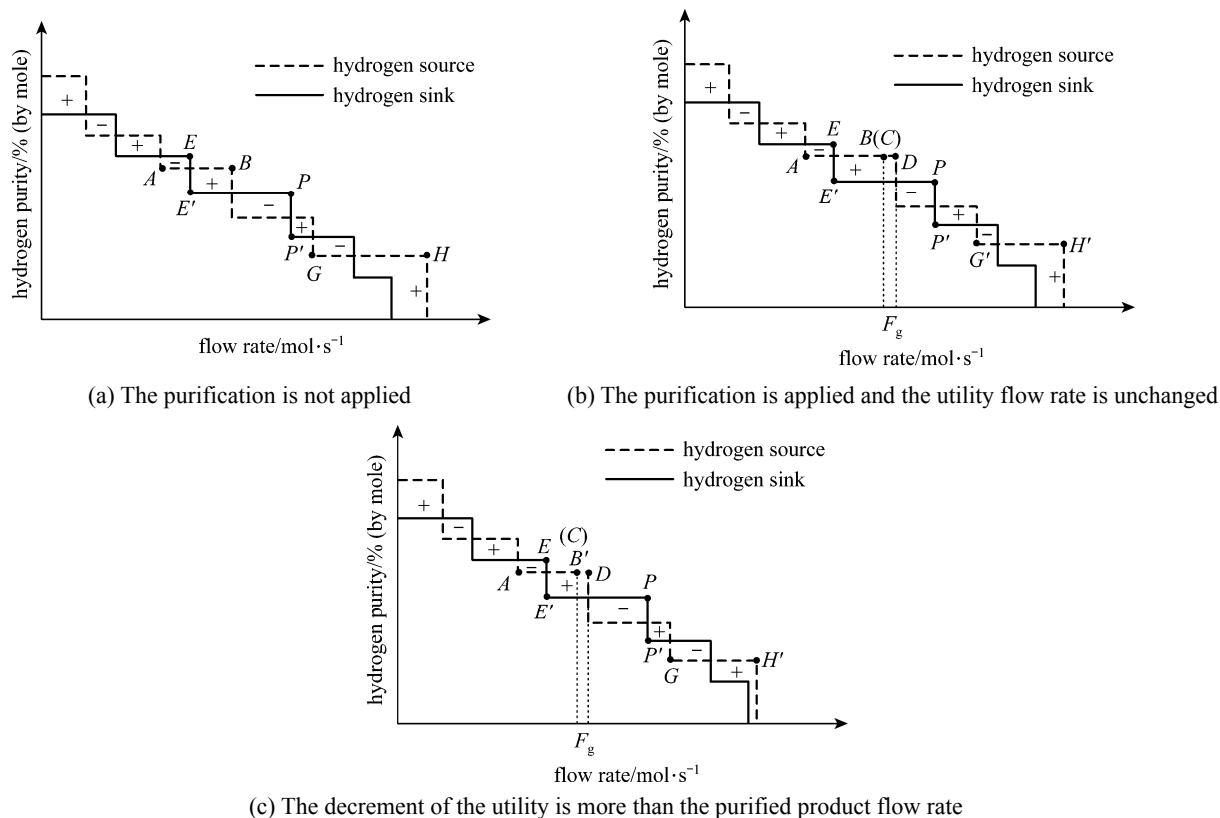


Figure 6 Hydrogen purity profiles

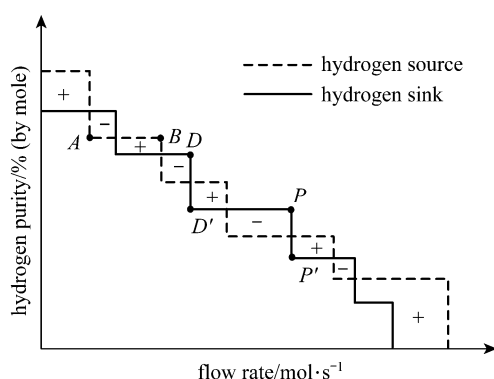


Figure 7 Hydrogen purity profiles with purification feed above the initial pinch point

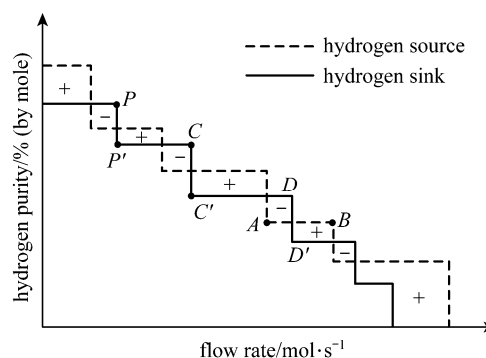


Figure 8 Hydrogen purity profiles with purification feed below the initial pinch

pinch. This can be explained by the system shown in Fig. 7. In this figure, PP' is the sink-tie-line where the initial pinch appears, AB is the purification feed, and DD' is a sink-tie-line lying between PP' and AB . Before the purification is applied, the hydrogen surplus between the sink-tie-lines DD' and PP' is less than zero. When the purification is applied, the source composite curve on the right of the purification feed, AB , will shift to the left, because of the pure hydrogen and flow rate loss in the tail gas. Therefore, the sources between DD' and PP' will be partly substituted by that with lower purity, and the hydrogen surplus between these two sink-tie-lines will decrease. If the new pinch point appears at DD' , its hydrogen surplus should be

zero. Then, the hydrogen surplus at PP' must be negative. This does not satisfy the pinch theory which requires that the hydrogen surplus at each sink-tie-line must not be less than zero. Therefore, the pinch point cannot appear between the purification feed and the initial pinch.

If the purification feed lies below the initial pinch point, the new pinch point cannot appear between the initial pinch point and the purification feed either. Take the system shown in Fig. 8 as an example, PP' is the sink-tie-line where the initial pinch point appears, AB represents the purification feed, CC' is the sink-tie-line lying between PP' and AB , DD' is the sink-tie-line intersecting the source AB . Before the

purification is applied, the hydrogen surplus between PP' and DD' is higher than zero. When the purification is applied, the source composite curve between the purified product and the purification feed will shift to the right by F_g . Therefore, the hydrogen surplus of the sink-tie-lines lying between PP' and DD' will increase. When the hydrogen utility flow rate is decreased, the source composite curve below the purified product will shift to the left. If the new pinch point appears at CC' , the hydrogen surplus at this sink-tie-line must be zero. This happens only when the decrement of the hydrogen utility flow rate is higher than F_g . However, this is against the conclusion that the amount of the decreased hydrogen utility flow rate can never be higher than the purified product flow rate (F_g). Thus, the new pinch point cannot appear between the initial pinch point and the purification feed.

Furthermore, the new pinch point cannot appear above the initial pinch point as the hydrogen sinks and the hydrogen sources above the initial pinch point do not change.

Based on the above analysis, it can be seen that the pinch point of the hydrogen network with purification reuse cannot appear above the initial pinch point and that between the initial pinch point and the purification feed (when the purification feed is below the initial pinch point).

4 CASE STUDIES

4.1 Case 1

In a hydrogen network, there are 10 hydrogen sources (excluding the hydrogen utility) and 9 hydrogen sinks, as shown in Table 1. The purity of hydrogen utility is 98%.

The hydrogen utility consumption is assumed to be $60 \text{ mol} \cdot \text{s}^{-1}$ firstly. In the decreasing order of hydrogen purity, the sink and source purity profiles can be plotted in the hydrogen purity versus flow rate diagram, as shown in Fig. 9. According to Eq. (1), the hydrogen surplus can be calculated, and then the hydrogen surplus diagram of this system can be constructed, as shown in Fig. 10. From this figure, it can be seen that some of the hydrogen surpluses are negative. Therefore, there is no pinch point and the hydrogen utility flow rate should be increased.

Increasing the hydrogen utility flow rate will result in the new purity profiles and new hydrogen surplus diagrams. The hydrogen utility flow rates are assumed to be $65 \text{ mol} \cdot \text{s}^{-1}$, $70 \text{ mol} \cdot \text{s}^{-1}$, $75 \text{ mol} \cdot \text{s}^{-1}$ and $76 \text{ mol} \cdot \text{s}^{-1}$, respectively. All the hydrogen surpluses are positive when the hydrogen utility flow rate equals to $76 \text{ mol} \cdot \text{s}^{-1}$, while there are some negative hydrogen surpluses when the utility flow rate equals to $75 \text{ mol} \cdot \text{s}^{-1}$ or less. It means that the minimum hydrogen utility flow rate lies between $75 \text{ mol} \cdot \text{s}^{-1}$ and $76 \text{ mol} \cdot \text{s}^{-1}$. According to this, the hydrogen utility flow rates are assumed to be $75.1 \text{ mol} \cdot \text{s}^{-1}$, $75.3 \text{ mol} \cdot \text{s}^{-1}$, $75.5 \text{ mol} \cdot \text{s}^{-1}$ and $75.7 \text{ mol} \cdot \text{s}^{-1}$, respectively. When the

Table 1 Data of hydrogen source and hydrogen sink streams (Case 1)

Streams		Hydrogen purity/% (by mole)	Flow rate $/\text{mol} \cdot \text{s}^{-1}$	Hydrogen load $/\text{mol} \cdot \text{s}^{-1}$
hydrogen source	hydrogen utility	98	unknown	
	SR ₁	87	90	78.3
	SR ₂	85	40	34
	SR ₃	80	135	108
	SR ₄	73	180	131.4
	SR ₅	62	160	99.2
	SR ₆	56	135	75.6
	SR ₇	53	35	18.55
	SR ₈	45	136	61.2
	SR ₉	38	96.5	36.67
	SR ₁₀	35	142	49.7
hydrogen sink	SK ₁	90	130	117
	SK ₂	83	140	116.2
	SK ₃	77	155	119.35
	SK ₄	70	115	80.5
	SK ₅	64	110	70.4
	SK ₆	58	135	78.3
	SK ₇	52	110	57.2
	SK ₈	40	130	52
	SK ₉	30	90	27

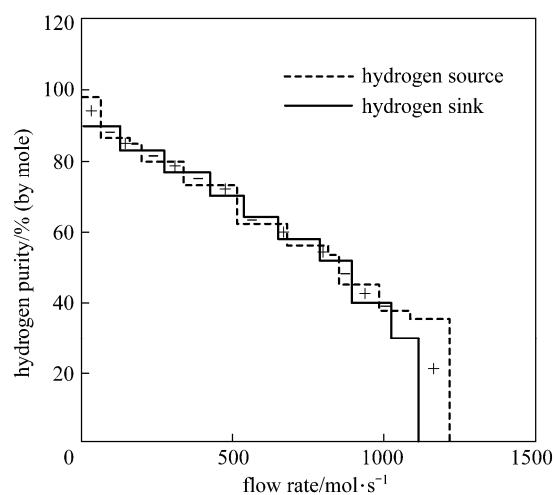


Figure 9 Hydrogen purity profiles of Case 1 (the utility flow rate is $60 \text{ mol} \cdot \text{s}^{-1}$)

flow rate of the hydrogen utility equals to $75.3 \text{ mol} \cdot \text{s}^{-1}$, the hydrogen surplus curve in the hydrogen surplus diagram touches the vertical axis. The corresponding intersection point is the pinch point, as shown in Fig. 11. Therefore, the purity of the pinch point is 45% and the minimum hydrogen utility target is $75.3 \text{ mol} \cdot \text{s}^{-1}$.

Source SR₆ (with purity 56%) locates above the

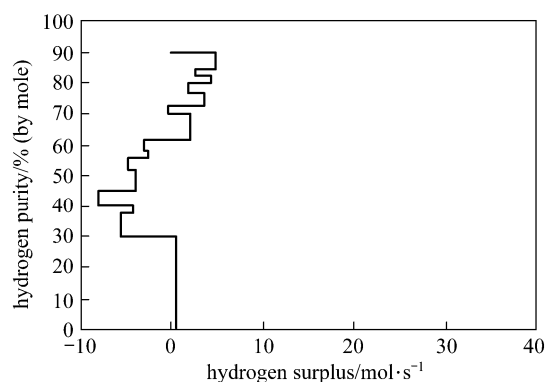


Figure 10 Hydrogen surplus diagram of Case 1 (the utility flow rate is $60 \text{ mol} \cdot \text{s}^{-1}$)

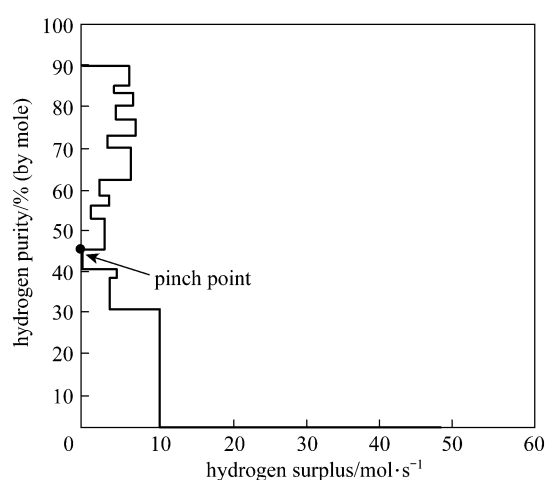


Figure 11 Hydrogen surplus diagram of Case 1 when the pinch point appears

initial pinch point. If it is taken as the purification feed, and the purity of the purified product and the hydrogen recovery are set to be 73% (same with that of SR_4) and 0.8, respectively, the purified product flow rate at different PFFR can be calculated according to the mass balance, as shown in Table 2. Through the same procedure of identifying the initial pinch point, the new pinch purity and the corresponding minimum hydrogen utility target under different PFFR can be obtained, as listed in Table 2. The PFFR listed in Table 2 changes between 0 and the total flow rate of SR_6 , $135 \text{ mol} \cdot \text{s}^{-1}$. From this table, it can be seen that when the PFFR equals to $107.6 \text{ mol} \cdot \text{s}^{-1}$, $115.8 \text{ mol} \cdot \text{s}^{-1}$ and $128 \text{ mol} \cdot \text{s}^{-1}$, respectively, there are two pinch points. At different PFFR, the pinch purity can only be 45%, 38% and 73%, and none of them lies between the purification feed (with purity 56%) and the initial pinch point (with purity 45%). This is consistent with the conclusion presented above that the pinch point cannot form between the purification feed and the initial pinch point. When the PFFR equals to $128 \text{ mol} \cdot \text{s}^{-1}$, $130 \text{ mol} \cdot \text{s}^{-1}$ and $135 \text{ mol} \cdot \text{s}^{-1}$, respectively, the pinch point appears at the source (SR_6) with purity 73%, above the purification feed. The reason is that, the

Table 2 Locations of the pinch point at different PFFR (Case 1)

PFFR/ $\text{mol} \cdot \text{s}^{-1}$	Remained flow rate of SR_6 $\text{mol} \cdot \text{s}^{-1}$	Flow rate of the purified product $\text{mol} \cdot \text{s}^{-1}$	Pinch purity/% (by mole)	Hydrogen utility target $\text{mol} \cdot \text{s}^{-1}$
0	135	0	45	75.3
10	125	6.1	45	74.1
60	75	36.8	45	68.3
100	35	61.4	45	63.6
107.6	27.4	66	45, 38	62.7
110	25	67.5	38	62.6
115.8	19.2	71.1	38, 35	62.2
120	15	73.6	35	62.1
128	7	78.8	35, 73	61.8
130	5	79.8	73	61.8
135	0	82.8	73	61.8

purified product purity does not equal to the hydrogen utility purity in this case.

4.2 Case 2

In this case, a hydrogen network with 10 hydrogen sources (excluding the hydrogen utility) and 8 hydrogen sinks will be studied. The corresponding data are shown in Table 3. The purity of hydrogen utility is 98%.

Table 3 Data of hydrogen source and hydrogen sink streams (Case 2)

Streams		Hydrogen purity/% (by mole)	Flow rate $\text{mol} \cdot \text{s}^{-1}$	Hydrogen load $\text{mol} \cdot \text{s}^{-1}$
hydrogen source	hydrogen utility	98	unknown	
	SR_1	86	80	68.8
	SR_2	82	50	41
	SR_3	73	100	73
	SR_4	69	135	93.15
	SR_5	65	190	123.5
	SR_6	60	100	60
	SR_7	57	90	51.3
	SR_8	45	136	61.2
	SR_9	33	51	16.83
	SR_{10}	30	180	54
hydrogen sink	SK_1	90	130	117
	SK_2	78	125	97.5
	SK_3	71	150	106.5
	SK_4	67	123	82.41
	SK_5	63	145	91.35
	SK_6	54	185	99.9
	SK_7	40	110	44
	SK_8	28	130	36.4

With the hydrogen utility consumption assumed to be $56 \text{ mol} \cdot \text{s}^{-1}$, the purity profiles diagram and the hydrogen surplus diagram can be plotted, as shown in Figs. 12 and 13, respectively. From Fig. 13, it can be seen that the initial hydrogen utility consumption is deficient. Increasing the flow rate of the hydrogen utility until it reaches $65.2 \text{ mol} \cdot \text{s}^{-1}$, the pinch point appears. The purity of the pinch point is 65% and the minimum hydrogen utility target is $65.2 \text{ mol} \cdot \text{s}^{-1}$. The corresponding hydrogen surplus diagram is shown in Fig. 14.

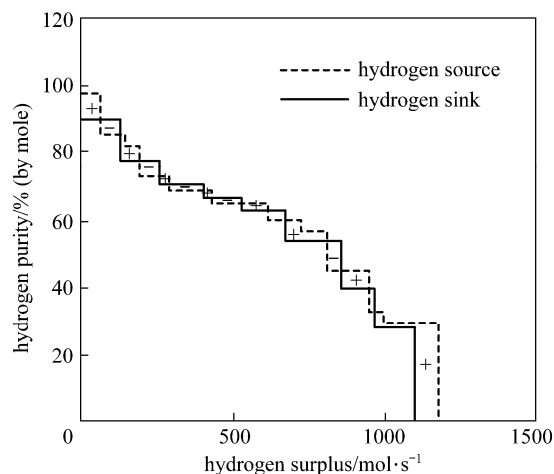


Figure 12 Hydrogen purity profiles of Case 2 (the utility flow rate is $56 \text{ mol} \cdot \text{s}^{-1}$)

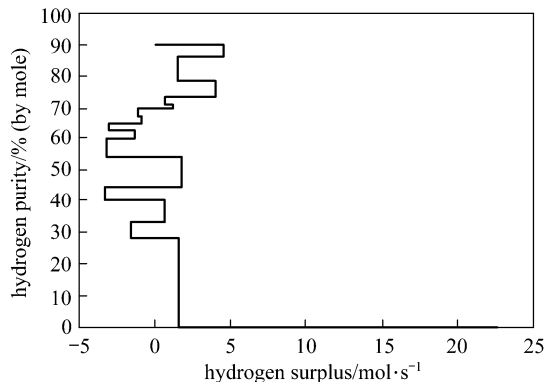


Figure 13 Initial hydrogen surplus diagram of Case 2 (the utility flow rate is $56 \text{ mol} \cdot \text{s}^{-1}$)

With source SR_7 (with purity 57%), which locates below the initial pinch point, taken as the purification feed, and the purity of the purified product and the hydrogen recovery are set to be 73% (SR_3) and 0.75, respectively; the corresponding flow rate of the purified product can be calculated according to the mass balance for different PFFR, as shown in Table 4. According to the hydrogen surplus diagram proposed by Alves *et al.* [1], the pinch purity and the corresponding minimum hydrogen utility target under different PFFR can be calculated, as shown by Table 4.

Similarly, for this case, it can be known that none of the new pinch points locate between the purification feed (with purity 57%) and the initial pinch point

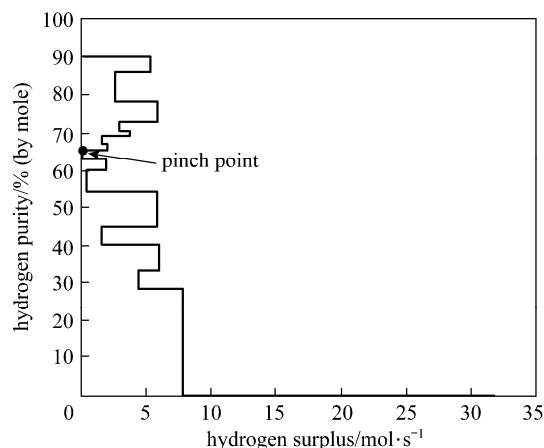


Figure 14 Hydrogen surplus diagram of Case 2 when the initial pinch point exists

Table 4 Locations of the pinch point at different PFFR (Case 2)

PFFR $/\text{mol} \cdot \text{s}^{-1}$	Remained flow rate of $\text{SR}_7/\text{mol} \cdot \text{s}^{-1}$	Flow rate of the purified product $/\text{mol} \cdot \text{s}^{-1}$	Pinch purity/% (by mole)	Hydrogen utility target $/\text{mol} \cdot \text{s}^{-1}$
0	90	0	65	65.2
10	80	5.8	65	63.8
20	70	11.7	65	62.3
30	60	17.6	65	60.9
40	50	23.4	65	59.5
44.5	45.5	26.1	65, 33	58.8
50	40	29.3	33	58.9
55.4	34.6	32.4	33, 30	58.9
70	20	41.0	30	59.3
80	10	46.8	30	59.6
90	0	52.7	30	59.9

(with purity 65%). This is consistent with the conclusion presented above.

5 CONCLUSIONS

Based on the alternative distribution of the negative and positive regions, the definition of the pinch point and the concept of the hydrogen surplus, the characteristics of the pinch point and the effect of the purification to the hydrogen surplus are analyzed. The following results are obtained: (1) The pinch point can only appear at the sink-tie-lines which can intersect the source purity profile; (2) When the purity of the purified product equals to that of the hydrogen utility, the pinch point will not appear above the purification feed; (3) The pinch point will not appear between the initial pinch point and the purification feed. This is validated by the study of two different cases.

The results obtained in this work can be used to qualitatively identify the pinch location of the hydrogen

system with purification at a given purification feed flow rate. However, it cannot identify the exact location of the pinch. To achieve this, the qualitative relationship between the purification feed flow rate and the hydrogen utility flow rate should be analyzed. This will be studied in the future work.

NOMENCLATURE

F	flow rate of overlapped sink and source, $\text{mol} \cdot \text{s}^{-1}$
F_g	flow rate of purification product, $\text{mol} \cdot \text{s}^{-1}$
F_{pur}	flow rate of purification feed, $\text{mol} \cdot \text{s}^{-1}$
F_w	flow rate of tail gas, $\text{mol} \cdot \text{s}^{-1}$
H'	hydrogen surplus, $\text{mol} \cdot \text{s}^{-1}$
R	hydrogen recovery
y_g	purity (mole fraction) of purification product
y_{pur}	purity (mole fraction) of purification feed
y_{SK}	hydrogen purity (mole fraction) of sink
y_{SR}	hydrogen purity (mole fraction) of source
y_w	purity (mole fraction) of tail gas

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