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Integration of the Hydrogen Network with Fresh Hydrogen and Purification Feed Optimized Simultaneously

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For hydrogen network, the Fresh Hydrogen Purity (FHP) and the purification affect its Hydrogen Utility (or fresh hydrogen) Consumption (HUC), and should be optimized simultaneously. Based on the quantitative relation among Hydrogen Utility Consumption (HUC), FHP and purification, a graphical method is developed to integrate the hydrogen network with the FHP and Purification Feed flow rate (PFFR) optimized simultaneously. Firstly, at given HUC, the relationship between PFFR and FHP is derived for sink-tie-lines with different locations. Then, the FHP versus PFFR diagram is plotted to analyse their relation. With the cost of fresh hydrogen and purification considered, the total cost (including the cost of fresh hydrogen and purification) versus FHP line is constructed to identify the optimal PFFR and FHP. The hydrogen network of a petrochemical enterprise is optimized by the proposed method with the optimal purification feed and fresh hydrogen purity identified.

1. Introduction

Hydrogen is an important material in refinery, and its consumption can be reduced through hydrogen network integration. In a hydrogen network, there are multiple hydrogen sources to provide hydrogen and multiple hydrogen sinks demanding hydrogen. Purification is widely applied to increase the purity of the source and hence the amount of its reuse. Besides, the Fresh Hydrogen Purity (FHP) also affects Hydrogen Utility Consumption (HUC). However, the cost of producing hydrogen increases as the FHP increases, and the cost of purification changes with the purification feed. Therefore, it is necessary to optimize the purification feed and the FHP simultaneously, with the cost of fresh hydrogen and purification considered.

Alves et al. (2002) identified that placing the purifier across the pinch is the best choice by comparing three possible placements of the purifier (above, across, and below the pinch). El-Halwagi et al. (2003) developed a graphic method with source and sink composite curves plotted in the impurity load verse flow rate diagram, but it is only applied to the situation resources are pure. Nelson and Liu (2008) developed an Excel spreadsheets used for multiple-pinch system with the purification considered. The method listed the same purity hydrogen streams respectively made it easily to detect the effects of changing the flowrate of an individual stream and to account for pressure and cost comparisons. Ng et al. (2009) proposed an automated procedure for resource conservation networks with single impurity and regeneration reuse. Borges (2012) introduced the hydrogen source diagram (HSD), an easy algorithmic method aimed at minimizing the HUC and identify the hydrogen network flowsheet simultaneously. Deng et al. (2014) proposed the improved problem table (IPT) to locate the flowrate targets of interplant hydrogen conservation networks, which is efficient and applicable. A graphical method was introduced by Zhang et al. (2014) for targeting the pinch point with the purification reuse considered. The hydrogen transformation from maximum hydrogen surplus to fresh hydrogen was described as the mass transfer triangle. Liu et al. (2013) and more recently (Liu et al., 2014) revealed the relationship between hydrogen utility savings and Purification Feed flow rate (PFFR), purification product purity (PPP) as well as purification feed purity (PFP). Through the quantitative relationships, the limiting and optimal values of the PFP, PPP, PFFR and the optimal hydrogen utility savings can be identified efficiently. Wang et al. (2016) developed a graphical method for optimizing the hydrogen recovery and purification feed simultaneously, and it can be applied to identify the limiting hydrogen recovery, optimal hydrogen recovery and optimal hydrogen utility savings. However, there are no studies considering the

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influence of FHP in the open literature. This work aims to develop a graphical method for integrating the hydrogen network with the FHP and PFFR optimized simultaneously. Based on the relationship between hydrogen utility savings and PFFR, the quantitative relation between HUC and PFFR is obtained. The HUC-FHP-PFFR diagram is built and applied to analyse their relation. Furthermore, the FHP and PFFR can be optimized simultaneously with the minimum HUC identified.

2. The quantitative relation among HUC, FHP and PFFR

For sink-tie-lines with different locations, relationships between HUC and PFFR are different and are derived by Liu et al. (2013). For sink-tie-lines lying above the purified product, between the purified product and purification feed and below the purification feed, the relationship between HUC and PFFR can be represented by Eq(1), Eq(2) and Eq(3).

$$\Delta F_{u,i}(c_u - c_i^*) = H_i \tag{1}$$

$$\Delta F_{u,i}(c_u - c_i^*) = H_i + F_{pur}c_{pur}R(1 - c_i^* / c_g) \tag{2}$$

$$\Delta F_{u,i}(c_u - c_i^*) = H_i + F_{pur}(1 - c_{pur}R / c_g)c_i^* - F_{pur}c_{pur}(1 - R) \tag{3}$$

Where, c_u denotes the FHP; c_i^* denotes the purity of the source intersecting sink-tie-line i ; H_i denotes the hydrogen surplus of sink-tie-line i , c_g , c_{pur} , F_{pur} and R denote the purified product purity, PFP, PFFR and hydrogen recovery of the purifier, $\Delta F_{u,i}$ is the hydrogen utility savings determined by the sink-tie-line i .

When the FHP changes from c_u to c_u' , the hydrogen surplus will change from H_i to $H_i + F_u(c_u' - c_u)$, as shown by Figure 1. Since $F_u' = F_u - \Delta F_u$, Eq(4) - Eq(6) can be derived from Eq(1) - Eq(3) to describe the relation between HUC and purification (when FHP is c_u').

$$F_{u,i}' = \frac{F_u(c_u - c_i^*) - H_i}{c_u' - c_i^*} \tag{4}$$

$$F_{u,i}' = \frac{F_u(c_u - c_i^*) - H_i - c_{pur}R(1 - c_i^* / c_g)F_{pur}}{c_u' - c_i^*} \tag{5}$$

$$F_{u,i}' = \frac{F_u(c_u' - c_u) - H_i - \left[(1 - c_{pur}R/c_g)c_i^* + c_{pur}(1 - R)\right]F_{pur}}{c_u' - c_i^*} \tag{6}$$

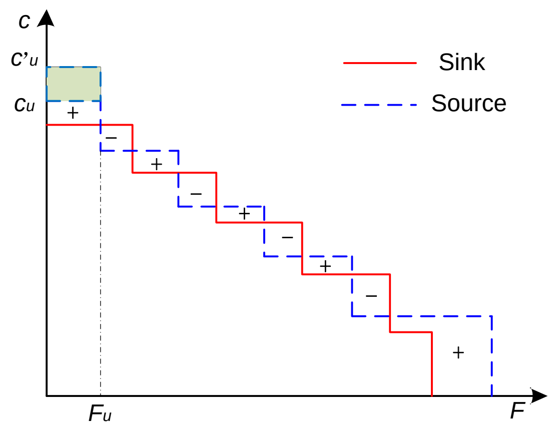

Figure 1: The effect of the fresh hydrogen concentration

3. Simultaneous optimization of the purification feed and fresh hydrogen

With the purified product purity and hydrogen recovery given, PFFR and FHP can be optimized simultaneously based on the equations derived in the previous section.

In a hydrogen network, there are multiple sink-tie-lines, and the PFFR-FHP-HUC relations corresponding to different sink-tie-lines are different. For the sink-tie-line lying above purification products, Eq(4) shows that HUC is only affected by the FHC, and has no relation with the PFFR. When the sink-tie-line lies between the purified product and purification feed ($c_g>c_i>c_{pur}$), Eq(5) shows that the coefficient of PFFR, $-c_{pur}R(1-c_i/c_g)$, is negative, and the HUC decreases as the PFFR increases. Eq(6) shows that for the sink-tie-line below the purification feed ($c_i<c_{pur}$), the coefficient of PFFR can be either negative or positive, and this depends on the concentration of the corresponding source. When the coefficient equals zero, the hydrogen source concentration can be calculated by Eq(7), and the HUC is irrelevant with the PFFR. When the concentration of the source is less than that determined by Eq(7), the coefficient of PFFR is positive and the HUC decreases as the PFFR decreases, and vice versa.

$$c_i=\frac{c_{pur}c_g(1-R)}{c_g-c_{pur}R} \tag{7}$$

In the PFFR-FHP-HUC diagram, each sink-tie-line corresponds a three dimensional surface, which can be plotted according to Eq(4), Eq(5) or Eq(6). Since each source can only intersect a sink-tie-line, the surface can be denoted by the source intersecting the studied sink-tie-line. For a hydrogen network, the surface corresponding to each source can be plotted in the same PFFR-FHP-HUC diagram, and they might intersect at different curves. In order to make the hydrogen network feasible, the HUC should be greater enough to make the hydrogen surplus of each sink-tie-line to be non-negative. Therefore, among all PFFR-FHP-HUC surfaces, the one corresponds to the maximum HUC determines the pinch and the minimum HUC of the hydrogen network. As the PFFR and/or FHP change, the minimum HUC will change correspondingly, and the variation trend is determined by the curved surface with the maximum HUC, which is generally composed by multiple surfaces corresponding different sources/sink-tie-lines and is termed as the limiting surface.

On the limiting surface, the minimum HUC is the optimal HUC of the hydrogen network. If the limiting surface is only determined by one source lying above the purified product, the optimal HUC is obtained when the FHP reaches maximal. If the source lying between the purified product and the purification feed, the optimal HUC is obtained when both PFFR and FHP are maximal. When the source lying below the purification feed, the location of the optimal HUC depends on the purity of the determining source, c_i. If c_i is greater than that determined by Eq(7), the optimal HUC is obtained when both PFFR and FHP are maximal. On the contrary, it is obtained when the PFFR is minimal and the FHP is maximal.

If the limiting surface is determined by multiple sources with different relative locations corresponding to the purification feed and purified product, the optimal HUC is usually corresponding to the maximal FHP and minimal PFFR. Only when the limiting surface includes part of which corresponds with the positive coefficient of PFFR, the optimal PFFR is on the intersecting line.

Besides, with Y_u' and Y_{pur} denote the fresh hydrogen cost and the purification cost minimizing the total cost of the fresh hydrogen and purification (Y , $Y=Y_u'+Y_{pur}$) can be taken as the optimization target, as shown by Eq(8).

$$Y=C_u'F_u'+C_{pur}F_{pur} \tag{8}$$

Where, C_u' is the fresh hydrogen price (when the FHP is c_u'), and C_{pur} is the purification price.

According to Eq(4) - Eq(6), it can be seen than they all can be written in the form of $F_{u,i}'=(a+bF_{pur})/(c_u'-c_i)$.

Then, the total cost Y can be calculated by Eq(9). In this equation, the coefficient of PFFR can be represented by k, which can be calculated by Eq(10). For a given FHP, when $k>0$, the total cost decreases as PFFR decreases; $k<0$, the total cost decrease as PFFR increases.

$$Y_{u.i}=C_u'\frac{a+bF_{pur}}{c_u'-c_i}+C_{pur}F_{pur}=\frac{C_{pur}(c'_u-c_i)+C_u'b}{c_u'-c_i}F_{pur}+\frac{aC_u'}{c_u'-c_i} \tag{9}$$

$$k=\frac{C_{pur}(c'_u-c_i)+C_u'b}{c_u'-c_i} \tag{10}$$

With the limiting surface identified, the relation between PFFR and FHP can be obtained, then the relation between total cost and FHP can be obtained. When the total cost reaches the minimum, the PFFR and FHP are optimal. In this case, the identified optimal HUC, PFFR and FHP are different from that identified with only the HUC as the optimization target, as will be illustrated by the case study.

4. Case study

For the hydrogen network of a refinery, the data of sinks and sources are shown in Table 1. SR0 is the fresh hydrogen. Based on the pinch method, it can be identified that the minimum HUC is 67.375mol/s, the initial pinch appears at the intersection point of sink-tie-line and SR5, its purity is 0.6, and the minimum fresh hydrogen cost is 7495.342 RMB/h.

Table 1: Data of the hydrogen sources and sinks

source	Hydrogen purity	Flow rate(mol/s)	sink	Hydrogen purity	Flow rate(mol/s)
SR0	0.92	80	SK1	0.9	100
SR1	0.86	80	SK2	0.8	160
SR2	0.82	80	SK3	0.71	148
SR3	0.73	75	SK4	0.67	95
SR4	0.69	133	SK5	0.63	170
SR5	0.65	167	SK6	0.54	175
SR6	0.6	110	SK7	0.38	130
SR7	0.58	105	SK8	0.28	120
SR8	0.45	93			
SR9	0.33	139			
SR10	0.3	130			

When the fresh hydrogen concentration changes and the purification is considered, the pinch might appear at the intersecting point of the sink-tie-line and SR1, SR3, SR4, SR5, SR6, SR8 or SR9. With R, c_{pur} and c_g taken as 0.75, 0.6 and 0.73 the PFFR-FHP-HUC relation is determined for these sources, and the resulted equation is shown by Eq(11) - Eq(17).

$$F_{u,\mathrm{SR1}}{}' = \frac{4}{c_u' - 0.86} \quad (11) \qquad F_{u,\mathrm{SR3}}{}' = \frac{10.6}{c_u' - 0.73} \quad (12)$$

$$F_{u,\mathrm{SR4}}{}' = \frac{14.56 - 0.02466F_{pur}}{c_u' - 0.69} \quad (13) \qquad F_{u,\mathrm{SR5}}{}' = \frac{18.06 - 0.04932F_{pur}}{c_u' - 0.65} \quad (14)$$

$$F_{u,\mathrm{SR6}}{}' = \frac{21.56 - 0.08014F_{pur}}{c_u' - 0.6} \quad (15) \qquad F_{u,\mathrm{SR8}}{}' = \frac{24.36 - 0.02260F_{pur}}{c_u' - 0.45} \quad (16)$$

$$F_{u,9}{}' = \frac{31.46 + 0.02343F_{pur}}{c_u' - 0.33} \quad (17)$$

According to these equations, the PFFR-FHP-HUC diagram can be constructed, as shown by Figure 2. It can be identified that the limiting surface includes four parts, as denoted by 1, 2, 3 and 4. These four parts correspond to source SR1, SR6, SR5 and SR9. SR9 lies below purification feed, and the coefficient of PFFR in Eq(17) is positive. According to the analysis in Section 3, the optimal PFFR lies on the intersecting line of the surfaces corresponding to SR5 and SR9. Combine Eq(14) with Eq(17), Eq(18) is obtained. Substitute Eq(18) into Eq(14), Eq(19) is obtained to determine the intersection line of the corresponding surfaces. Similarly, the equation corresponding to other intersecting lines can be obtained. According to these equations, the HUC versus FHP diagram can be plotted, as shown by Figure 3. From this diagram, the lower limit line of HUC, ABCD, can be determined directly (the optimal PFFR is the line BCD in Figure 4). It can be identified that the optimal HUC is 48.066 mol/s, the corresponding FHP is 0.999 (point D in Figure 3), and the PFFR is 29.720 mol/s.

$$F_{pur} = \frac{13.4c_u' - 14.4892}{-0.0727c_u' + 0.0315} \quad (18)$$

$$F_{u,SR5-SR9}' = \frac{1.974c_u' - 1.283}{(-0.0727c_u' + 0.0315)(c_u' - 0.65)} \quad (19)$$

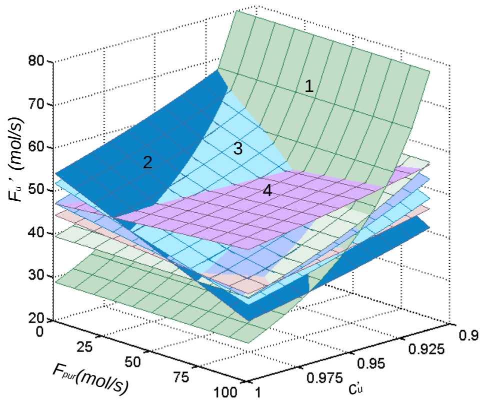

Figure 2: intersecting surfaces above other surfaces

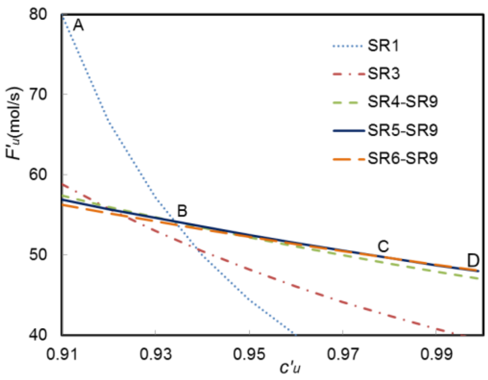

Figure 3: the HUC lower limit line

With the fresh hydrogen price and the purification price given by Eq(20) and Eq(21) the total cost can be taken as the optimization target (the fresh hydrogen price is based on the equation Liang and Liu (2017) proposed, and the purification price is the empirical formula from Towler et al. (1966)).

$$C_u' = 32.9417c_u' - 0.12955 \quad (20)$$

$$C_{pur} = \frac{2.306}{Rc_{pur}} + \frac{175.956}{F_{pur}} \quad (21)$$

Part 1 of the limiting surface can be ignored as it is not affected by purification. For part 2, 3 and 4, the corresponding total cost equations are shown by Eq(22), (23) and (24). Figure 4 reflects the relation of the intersecting surface and the location of intersecting line. According to Eq(22), when $2.485c_u'$-$3.064 \leq 0$, the total cost decreases as PFFR increases. Eq(23) shows that when $c_u' \geq 0.950$, $3.500c_u'$-$3.325 \geq 0$, the total cost decreases as the PFFR decreases; when $c_u' < 0.950$, it is opposite. From Eq(24) it can be seen that when $5.896c_u'$-$1.694 \geq 0$, the total cost decreases as the PFFR decreases. Based on this, the optimal PFFR is the line AEBF-GCD in Figure 4. Figure 5 shows the optimal total cost versus FHP curve, as well as the HUC versus FHP curve and the PFFR versus FHP curve. When the FHP reaches 0.999, the PFFR, HUC and minimal total cost are 29.720 mol/s, 48.066 mol/s and 6392.263 RMB/h. 1099.079 RMB/h can be saved compared with the initial integration.

$$Y_{SR6} = \frac{2.485c_u'\text{-}3.064}{c_u' - 0.6} F_{pur} + 21.56 \frac{32.9417c_u' - 0.12955}{c_u' - 0.6} + 175.956 \quad (22)$$

$$Y_{SR5} = \frac{3.500c_u'\text{-}3.325}{c_u' - 0.65} F_{pur} + 18.06 \frac{32.9417c_u' - 0.12955}{c_u' - 0.65} + 175.956 \quad (23)$$

$$Y_{SR9} = \frac{5.896c_u'\text{-}1.694}{c_u' - 0.33} F_{pur} + 31.46 \frac{32.9417c_u' - 0.12955}{c_u' - 0.33} + 175.956 \quad (24)$$

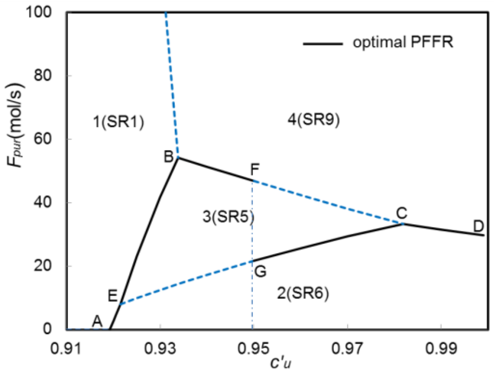

Figure 4: optimal PFFR with cost considered

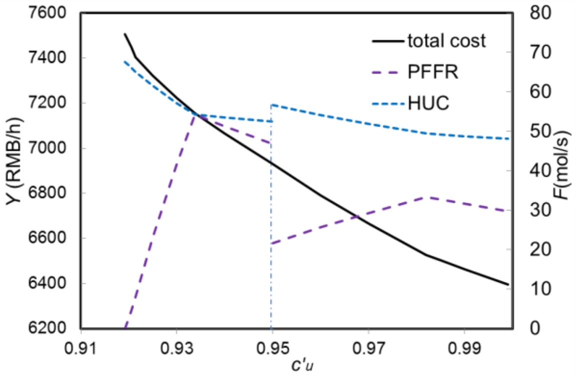

Figure 5: the optimal total cost line

5. Conclusions

A graphical method is proposed to optimize the FHP and PFFR together with the hydrogen network integration. By this method, the limiting surface is determined. With the relationship between PFFR and FHP derived first and substitute into the equation of HUC, the relation among the HUC, FHP and PFFR can be identified. And this relation can be easily extended with the total cost considered. For the studied case, the minimal HUC can reach 48.066 mol/s at the maximal FHP (0.999), reduced by 29.0 % compared with the initial integration. If the minimal total cost is the target, the optimal FHP, the optimal PFFR and the minimum HUC does not change, while the PFFR versus FHP curve is different. The total cost can be saved by 14.67% compared with the initial integration.

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