

## Flowrate Targeting for Hydrogen Network with Intermediate Header

Chun Deng<sup>\*,a</sup>, Yuhang Zhou<sup>a</sup>, Xiao Feng<sup>b</sup>

<sup>a</sup>State Key Laboratory of Heavy Oil Processing, College of Chemical Engineering, China University of Petroleum, 18 Fuxue Rd., Changping, 102249, Beijing, China

<sup>b</sup>New Energy Institute, China University of Petroleum, Beijing, 102249, China  
 chundeng@cup.edu.cn

In this paper, Improved Problem Table (IPT) is utilized to locate the flow rate targets of hydrogen network with intermediate hydrogen header. The relationship between the purity and flow rate of hydrogen header is explored. One literature case is analysed to illustrate the applicability and effectiveness of the proposed approach. The results show that the flow rate of intermediate hydrogen header can be related to its purity via a piecewise function and the flow rate of the intermediate header increases with the reduction of its purity. The intermediate hydrogen header is fed by the mixture of hydrogen utility and process hydrogen sources. The flow rates of hydrogen utility and waste hydrogen streams that discharged into fuel system are kept unchanged with the variety of the purity of intermediate header.

### 1. Introduction

The current refineries have been facing the challenge of meeting the growing demand for cleaner fuels, i.e. European Standard CSN EN 228: 2008 and Chinese standard GB 17930: 2013 specify unleaded petrol with a maximum sulphur content of 0.001 %. The need to meet required end product specifications necessitate the increasing use of hydrogen in hydro-processing operations and the existing hydrogen production capacities often become the bottleneck. Hydrogen integration has been accepted as an effective tool to recover hydrogen and reduce the capacity of hydrogen plant. Generally, the methodologies for the synthesis of refinery hydrogen networks can be classified into Pinch analysis, such as, Hydrogen Surplus Diagram (Alves and Towler, 2002), Gas Cascade Analysis (Foo and Manan, 2006), improved Limiting Composite Curve and Composite Table Algorithm (Agrawal and Shenoy, 2006) and Improved Problem Table (Deng et al., 2014a) and optimization-based mathematical approached, such as, first superstructure model with pressure constraint (Hallale and Liu, 2001), systematic methodology for the selection of appropriate purifiers (Liu and Zhang, 2004), state-space superstructure (Liao et al., 2010), multi-component and integrated flash calculation (Jia and Zhang, 2011), hydrogen sulphide removal process embedded optimisation model (Zhou et al., 2012), total energy consumption of the hydrogen utility and compressor work (Wu et al., 2013), strategy for hydrogen integration in petroleum refining (Smith et al., 2012), key factor analysis (Deng et al., 2013) and comparative analysis for different scenarios (Deng et al., 2014b) for hydrogen integration, robust optimization of hydrogen network (Lou et al., 2014) and integrated hydroprocessor model (Umana et al., 2014).

However, in earlier works, hydrogen sources are directly connected to hydrogen sinks for reuse/recycle (with or without purification). The resulting network may thus be relatively complex, and any variations in hydrogen flow rate and Purity at an upstream hydrogen unit (hydrogen source) will affect the downstream hydrogen sinks. Intermediate hydrogen header is typically installed in order to simplify the network configuration and enhance the expandability and flexibility of the hydrogen network. Deng et al. (2014c) proposed a superstructure-based mathematical programming model for the synthesis of hydrogen network with intermediate hydrogen header.

In this paper, Improved Problem Table (IPT) is firstly utilized to determine the flow rate targets of hydrogen network with intermediate hydrogen header. It aims to explore the relationship between the Purity and flow rate of hydrogen header. One literature case is utilized to illustrate the feasibility of the proposed approach.

## 2. Problem statement

The problem can be expressed as follows. Given a refinery hydrogen network, there is a set of hydrogen-consuming processes. Their outlet streams are treated as a set of process (or internal) hydrogen sources ( $i \in NSR$ ) while inlet streams treated as a set of process hydrogen sinks ( $j \in NSK$ ). Each process hydrogen source is specified by its outlet flow rate ( $F_{SRi}$ ) and outlet hydrogen purity ( $y_{SRi}$ ). Each process hydrogen sink has inlet flow rate ( $F_{SKj}$ ) and the lower bound of inlet hydrogen purity ( $y_{SKj}$ ). And a set of hydrogen utilities, so called external hydrogen sources, are needed for supplementary. Hydrogen utilities can only be introduced to the intermediate hydrogen header directly. The demand of intermediate hydrogen header can be fulfilled by hydrogen utilities and/or internal hydrogen sources. Process hydrogen sources and hydrogen stream from intermediate hydrogen header are available for the utilization of process hydrogen sinks. The surplus hydrogen sources would be allocated to fuel system or purifiers (i.e. pressure swing absorption, membrane) for upgrading for further utilization. It aims to determine the flow rate targets for hydrogen network with intermediate hydrogen header and explore the relationship between the Purity and flow rate of hydrogen header.

## 3. Flowrate targeting for hydrogen network with intermediate header by IPT

In this section, IPT is referred to locate the minimum flow rates of hydrogen utility for hydrogen network with intermediate header. The limiting data shown in Table 1 for the case study is extracted from the literature (Alves and Towler, 2002). The steps for the IPT are given below.

Table 1: Limiting data for refinery hydrogen network

Hydrogen Sources	Purity (1)	Flow rate (mol/s)	Hydrogen Sinks	Purity (1)	Flow rate (mol/s)
SRU	0.93	623.8	HCU	0.8061	2,495
CRU	0.8	415.8	NHT	0.7885	180.2
HCU	0.75	1,801.9	DHT	0.7757	720.7
NHT	0.75	138.6	CNHT	0.7514	554.4
DHT	0.73	346.5			
CNHT	0.7	457.4			
Fresh Supply	0.95	277.2 (current)			

Step 1: Tabulate all the purities of hydrogen sources and sinks in decreasing order in the first column (Table 2). Do not repeat the same purity that occurs more than once. Add one more arbitrary purity at the bottom of the column so that it is the smallest value. The arbitrary purity serves to provide an end point and facilitates the plotting of the last segment of the Limiting Composite Curve. The second column shows impurities that is 1-y.

Step 2: Tabulate the net flow rates in the third column (Table 2) by subtracting the sum of the flow rates of the hydrogen sources from the sum of the flow rates of hydrogen sinks in each purity interval. Besides, the net flow rate corresponds to the reciprocal of the slope of a segment on the Limiting Composite Curve. And the last value in the third column (Table 2) which is obtained by subtracting the sum of all flow rates of the hydrogen sources from the sum of all flow rates of the hydrogen sinks can be defined as net flow rate deficit for the network. It determines the minimum net flow rate of external hydrogen sources for the network. For a given hydrogen network, the net flow rate deficit is a constant.

Step 3: Tabulate the net mass loads in the fourth column (Table 2). The net mass loads for each purity interval are the products of the net flow rates and the purity differences of the corresponding intervals.

Step 4: Tabulate the cumulative mass loads in the fifth column (Table 2). The first row has no cumulative mass load so that it equals zero. The cumulative mass loads of other rows are accumulated by the net mass loads above the row. The impurity column can be plotted against the cumulative mass load column to obtain the Limiting Composite Curve and it is omitted for simplification.

Step 5: Tabulate the possible intermediate header flow rates for each purity ( $F_{header}^v$ ) in the sixth column using Eq(1). Note that the stream from intermediate header is considered as external hydrogen source. The purity of intermediate header is assumed to be 90 %.

$$F_{header}^v = \frac{\Delta M_{cum}^v}{y_{header} - y^v} \quad (1)$$

where  $\Delta M_{cum}^v$  and  $y^v$  denotes the cumulative mass load and purity concentration for  $v$ th purity level and  $y_{header}$  denotes the purity of intermediate header.

The maximum value in sixth column of Table 2 is 336.03 mol/s and it is marked in bold. It is bigger than the minimum net flow rate (166.3 mol/s) determined in Step 2 and the maximum value (336.03 mol/s) is considered to be the minimum flow rate of intermediate header, and the corresponding impurity concentration (0.3) is identified as the Pinch impurity concentration. Negative values in the fifth column indicate that internal hydrogen sources can meet the demand of hydrogen sinks without the supply of external hydrogen sources. Thus, there is no need to calculate the values in the sixth column. Besides, if the maximum value in the sixth column is smaller than the minimum flow rate determined in Step 2, the minimum net flow rate is considered as the minimum flow rate of intermediate header.

Table 2: Improved Problem Table (intermediate hydrogen header with the purity of 0.90)

Purity (fraction)	Impurity (fraction)	Net flow rate (mol/s)	Net load (mol/s)	Cumulative load (mol/s)	Flow rate for intermediate header (mol/s)	Flow rate above Impurity Pinch (mol/s)	Flow rate for waste hydrogen stream (mol/s)
0.93	0.07			0			
		-623.8	-77.29				
0.8061	0.1939			-77.29			
		1,871.2	11.41				
0.8	0.2			-65.87			
		1,455.4	16.74				
0.7885	0.2115			-49.14			
		1,635.6	20.94				
0.7757	0.2243			-28.20			
		2,190	53.22				
0.7514	0.2486			25.02	168.34		
		2,910.7	4.07				
0.75	0.25			29.09	193.94		
		970.2	19.40				
0.73	0.27			48.49	285.26		
		623.7	18.71				
0.7	0.3			67.21	<b>336.03</b>		169.73
		166.3	8.32				
0.65	0.35			75.52	302.08	166.3	

Step 6: Identify waste hydrogen streams. On the impurity Pinch (0.3), the accumulated hydrogen flow rate is 336.03 mol/s. It can be considered as an internal hydrogen source with the impurity of 0.3. Then for each impurity interval above 0.3, the required flow rates can be calculated via Eq(2) and all possible flow rates above impurity pinch are listed in the seventh column of Table 2 and the maximum value (166.3 mol/s) determines the target. Therefore, only 166.3 mol/s of hydrogen source at the impurity of 0.3 needs to be distributed to the system and the residual flow rate 169.73 mol/s (with impurity concentration of 0.3) is identified as the waste hydrogen stream.

$$F_{pinch} = \frac{\Delta M_{cum}^v - \Delta M_{cum}^{pinch}}{y_{pinch} - y^v} \quad \forall y^{arbitrary} \leq y^v < y_{pinch} \quad (2)$$

Step 7: Perform material balance equations to target the minimum flow rate of fresh hydrogen supply. The waste hydrogen streams identified in Step 6 and fresh hydrogen supply are considered to meet the

demand of intermediate hydrogen header. Thus, the material balance equations can be described as follows:

$$F_{WH} y_{WH} + F_{HU} y_{HU} = F_{header} y_{header} \quad (3)$$

$$F_{WH} + F_{HU} = F_{header} \quad (4)$$

As shown in Table 2,  $F_{header} = 336.03$  mol/s and  $y_{header} = 0.7$ , the purity of hydrogen supply ( $y_{HU}$ ) and waste hydrogen stream ( $y_{WH}$ ) are 0.95 and 0.7. Substituting values in Eq(3) and Eq(4), it makes  $F_{HU} = 268.82$  mol/s and  $F_{WH} = 67.21$  mol/s. The residual flow rate for the waste hydrogen stream  $102.52$  mol/s (=  $169.73$  mol/s -  $67.21$  mol/s) is discharged to the fuel system. The results ( $F_{HU} = 268.82$  mol/s,  $F_{purge} = 102.52$  mol/s) show that the flow rate targets of hydrogen network with intermediate header are identical with those without intermediate header (Alves and Towler, 2002).

Step 8: Utilize Nearest Neighbours Algorithm (NNA) (Prakash and Shenoy, 2005) to design the hydrogen network. An optimal hydrogen network with one intermediate header is shown in Figure 1.

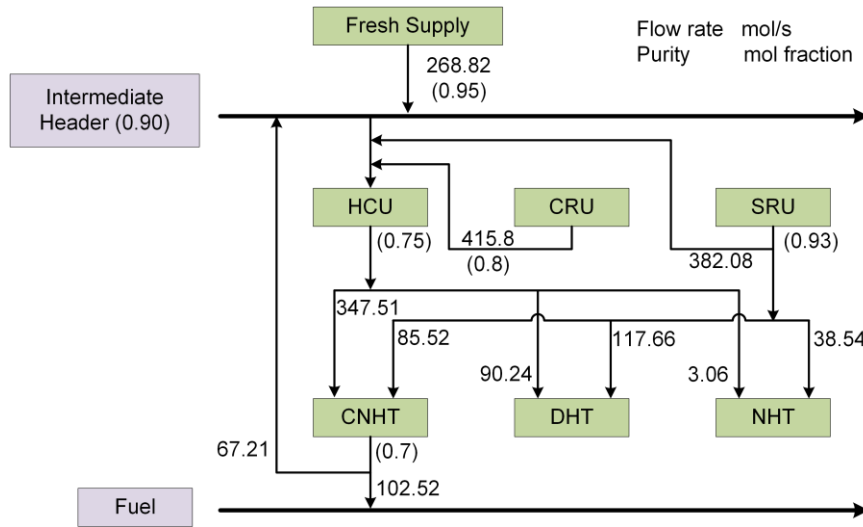


Figure 1: An optimal hydrogen network with one intermediate header (with the purity of 0.90)

#### 4. Discussion

Eq(1) indicates that the flow rate for intermediate header is inversely proportional to its purity. However, Pinch point would shift as the purity of intermediate header changes. In Step 5, if  $F_{header}^v$  equals  $F_{header}^{v\pm k}$ , it means that Double Pinch appears and any change of purity of intermediate header will cause the shifting of Pinch Point. The corresponding purity of intermediate header is defined as shifting purity.  $F_{header}^{v\pm k}$  can be calculated via solving Eq(5), which is similar with Eq(1).

$$F_{header}^{v\pm k} = \frac{\Delta M_{cum}^{v\pm k}}{y_{header} - y^{v\pm k}} \quad (5)$$

Combining Eq(1) and Eq(5), the shifting purity of intermediate header ( $y_{header}^{shifting}$ ) can be determined by solving Eq(6).

$$y_{header}^{shifting} = \frac{y^v \Delta M_{cum}^{v\pm k} - y^{v\pm k} \Delta M_{cum}^v}{\Delta M_{cum}^{v\pm k} - \Delta M_{cum}^v} \quad (6)$$

The first shifting purity of intermediate header ( $y_{header}^{shifting}$ ) is calculated as 0.808 via Eq(6) with the Pinch Purity is 0.7. Once the purity of intermediate header is lower than 0.808, the Pinch Purity is shifted from

0.7 to 0.73 and the second shifting purity of intermediate header is determined as 0.78 by solving Eq(6). If the purity of intermediate header is lower than 0.78, the Pinch Purity will be shifted from 0.73 to 0.75. If the purity of intermediate header is lower than 0.76, the Pinch Purity will be shifted from 0.75 to 0.7514. Additionally, the purity of intermediate header cannot be higher than the purity of hydrogen utility (i.e. 0.95 for this case) and cannot be lower than the lowest purity of hydrogen sink (i.e., 0.7514 for this case). Next the optimal flow rate of intermediate header can be expressed as a piecewise function Eq(7).

$$F_{header} = \begin{cases} \frac{67.21}{y_{header} - 0.7} & 0.95 \geq y_{header} \geq 0.808 \\ \frac{48.49}{y_{header} - 0.73} & 0.808 > y_{header} \geq 0.78 \\ \frac{29.09}{y_{header} - 0.75} & 0.78 > y_{header} \geq 0.76 \\ \frac{25.02}{y_{header} - 0.7514} & 0.76 > y_{header} > 0.7514 \end{cases} \quad (7)$$

On the basis of Eq(7), the optimal flow rate of intermediate header ( $F_{header}$ ) can be plotted against the purity of intermediate header ( $y_{header}$ ) to obtain the curve as shown in Figure 2.

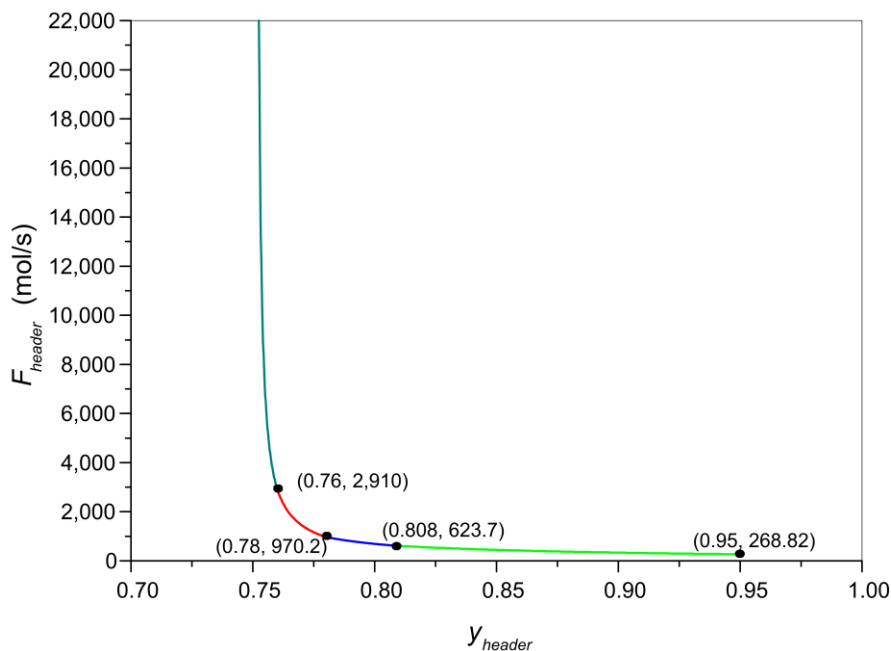


Figure 2: The relationship between optimal flow rate of intermediate header and its purity

Note that,  $F_{header}$  equals 268.82 mol/s with its purity of 0.95. Once its purity is decreased from 0.95 to 0.808,  $F_{header}$  increases gradually from 268.82 mol/s to 623.7 mol/s. If the purity is reduced from 0.808 to 0.78,  $F_{header}$  will increase accordingly from 623.7 mol/s to 970.2 mol/s. If the purity is reduced from 0.78 to 0.76,  $F_{header}$  will increase dramatically from 970.2 mol/s to 2,910.7 mol/s. Once the purity is lower than 0.76,  $F_{header}$  will increase sharply. The flow rate of intermediate header indicates the capacity of hydrogen pipeline. The lower flow rate leads to the smaller diameter of intermediate hydrogen pipeline. Therefore there is a trade-off between the flow rate of the intermediate header and its purity.

## 5. Conclusions

In this paper, the Improved Problem Table (IPT) is utilized to target the hydrogen network with intermediate hydrogen header. The results show that the flow rate of intermediate header can be related to its purity via piecewise function and the flow rate of the intermediate header increases with the reduction of its purity. The intermediate hydrogen header can be fulfilled by hydrogen utility and process hydrogen sources. Additionally, whatever the purity of intermediate header is, the flow rates of hydrogen utility and waste hydrogen streams that discharged into fuel system are kept unchanged.

## Acknowledgements

Financial support provided by the National Basic Research Program of China (No. 2012CB720500), National Natural Science Foundation of China (No. U1162121, 21276204) and Science Foundation of China University of Petroleum, Beijing No. 2462015YQ0305. are gratefully acknowledge.

## References

- Agrawal V., Shenoy U. V., 2006. Unified conceptual approach to targeting and design of water and hydrogen networks, *AIChE Journal*, 52, 1071-1082.
- Alves J. J., Towler G. P., 2002. Analysis of refinery hydrogen distribution systems, *Industrial & Engineering Chemistry Research*, 41, 5759-5769.
- CSN EN 228:2008, Automotive fuels - Unleaded petrol - Requirements and test methods. Brussels, Belgium: European Committee for Standardization
- Deng C., Li W., Feng X., 2013. Refinery Hydrogen Network Management with Key Factor Analysis, *Chemical Engineering Transactions*, 35, 61-66.
- Deng C., Zhou Y., Li Y., Feng X., 2014a. Flowrate Targeting for Interplant Hydrogen Networks, *Chemical Engineering Transactions*, 39, 19-24.
- Deng C., Pan H., Li Y., Zhou Y., Feng X., 2014b. Comparative analysis of different scenarios for the synthesis of refinery hydrogen network, *Applied Thermal Engineering*, 70, 1162-1179.
- Deng C., Pan H., Lee J. Y., Foo D. C. Y., Feng X., 2014c. Synthesis of hydrogen network with hydrogen header of intermediate purity, *International Journal of Hydrogen Energy*, 39, 13049-13062.
- Foo D. C. Y., Manan Z. A., 2006. Setting the minimum utility gas flowrate targets using cascade analysis technique, *Industrial & Engineering Chemistry Research*, 45, 5986-5995.
- GB 17930: 2013, Gasoline for motor vehicles. Beijing, China: China Standards Press.
- Hallale N., Liu F., 2001. Refinery hydrogen management for clean fuels production, *Advances in Environmental Research*, 6, 81-98.
- Jia N., Zhang N., 2011. Multi-component optimisation for refinery hydrogen networks, *Energy*, 36, 4663-4670.
- Liao Z., Wang J., Yang Y., Rong G., 2010. Integrating purifiers in refinery hydrogen networks: a retrofit case study, *Journal of Cleaner Production*, 18, 233-241.
- Liu F., Zhang N., 2004. Strategy of purifier selection and integration in hydrogen networks, *Chemical Engineering Research & Design*, 82, 1315-1330.
- Lou J., Liao Z., Jiang B., Wang J., Yang Y., 2014. Robust optimization of hydrogen network, *International Journal of Hydrogen Energy*, 39, 1210-1219.
- Prakash R., Shenoy U. V., 2005. Targeting and design of water networks for fixed flowrate and fixed contaminant load operations, *Chemical Engineering Science*, 60, 255-268.
- Smith R., Zhang N., Zhao J., 2012. Hydrogen Integration in Petroleum Refining, *Chemical Engineering Transactions*, 29, 1099-1104.
- Umana B., Shoaib A., Zhang N., Smith R., 2014. Integrating hydroprocessors in refinery hydrogen network optimisation, *Applied Energy*, 133, 169-182.
- Wu S., Yu Z., Feng X., Liu G., Deng C., Chu K. H., 2013. Optimization of refinery hydrogen distribution systems considering the number of compressors, *Energy*, 62, 185-195.
- Zhou L., Liao Z., Wang J., Jiang B., Yang Y., 2012. Hydrogen sulfide removal process embedded optimization of hydrogen network, *International Journal of Hydrogen Energy*, 37, 18163-18174.