



# Comprehensive Modeling of Hydrogen Network in Petrochemical Complexes

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Hydrogen is an important utility gas, which is used in various operations in petroleum refineries and petrochemical complexes. Although hydrogen is produced as by-product in petrochemical complexes, however it is not efficiently used and mostly sent to fuel. Most current works have applied hydrogen optimization approach for refineries. Therefore, this study is aimed to propose a new optimization mathematical model for hydrogen management in petrochemical complexes based on setting a comprehensive superstructure model. This superstructure including purifier and compressor of hydrogen plant or catalytic reformer unit offers more improvements. Having applied the proposed superstructure in two industrial petrochemical complexes, the results indicated that about 16.7 % reduction in hydrogen consumption could be achieved with a payback of 2 years.

## 1. Introduction

Nowadays, it is very important to efficiently utilize the hydrogen in chemical processes. Hallale et al. (2001) first developed an optimization approach using a hydrogen network superstructure. Liu and Zhang (2004) developed a systematic method to select purification processes and integrate them into hydrogen networks. In similar way, a superstructure was created for options of purifiers, and then an MINLP optimization procedure was performed to find the optimal solution. Liao et al. (2010) introduced a technique for refinery hydrogen network retrofit design. Their MINLP hydrogen network model was based on Hallale et al. (2001) hydrogen network superstructure. Ahmad et al. (2010) extended a new approach for multi-period operation. The optimization methodology focused on placement of hydrogen purifiers and compressors during retrofit design. The common objective in these methods was set to be the total annual cost by taking into account H<sub>2</sub> production cost, utility cost, and piping costs.

## 2. Comprehensive superstructure

A comprehensive superstructure is developed in order to consider hydrogen plant as a part of the hydrogen network. As shown in Figure 1, this superstructure consists of all hydrogen sources and sinks and connections between them. The modification in this superstructure compared to conventional ones is incorporating the hydrogen plant into the superstructure. Most reformers are followed by compressors and purifiers in refineries and petrochemical plants. This inclusion brings the whole network some benefits. First, a compressor is added into the network and it is possible to use the capacity of this compressor for low-pressure hydrogen sources. Furthermore, it allows applying extra capacity of purifier to enhance the purity of low-purity sources. Thus, it is observed that the comprehensive superstructure can take into account all parts of hydrogen network in a real process.

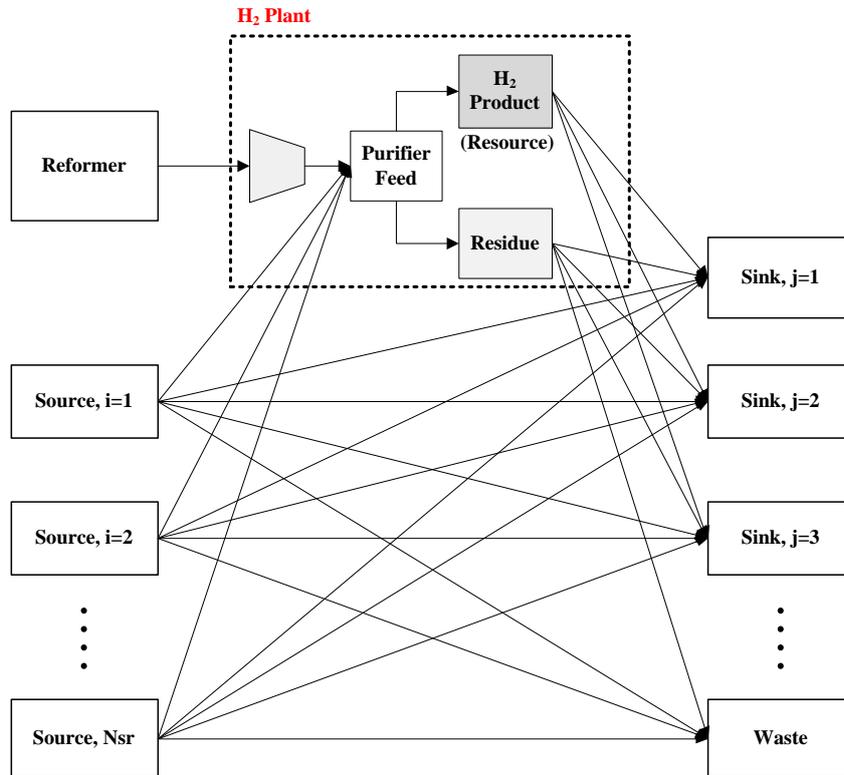


Figure 1: Hydrogen network superstructure for mathematical model

The superstructure presented here consists of purifier and compressor, which are next to the reformers. This leads to a beneficial usage of the facilities of the whole plant. In this way, these equipments could be applied for enhance quality of sources in terms of quality and pressure without adding new equipment. In addition, the residue stream of purifier can be considered in this way. After setting the superstructure, some important points should be noted. Being a compressor in the network, two sources and one sink are added into superstructure. The Pressure Swing Adsorption (PSA) product is regarded as fresh resource. As hydrogen consumption is changing during optimization, the other sink and source vary. Therefore, the relationship between these source and sink should be defined.

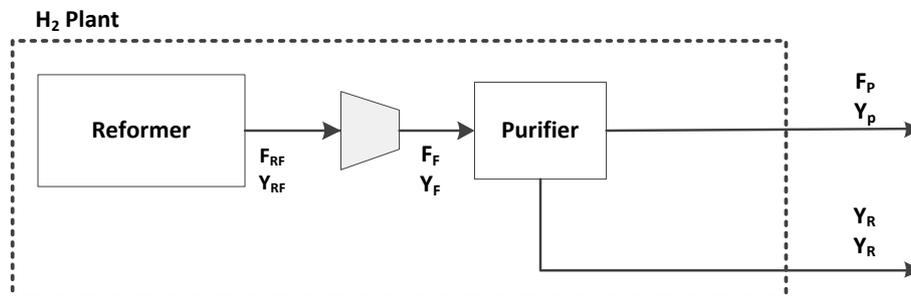


Figure 2: Hydrogen plant and its associated purification unit

As shown in Figure 2, the overall flow rate balance of the purification unit is as follows:

$$F_F = F_P + F_R \quad (1)$$

Where  $F_F$ ,  $F_P$ , and  $F_R$  are PSA feed, product and residue flowrates.

The relation between feed flow rate and residue flow rate is shown as

$$F_F = F_P (Y_P / Y_F \times R) \quad (2)$$

Where  $R$  is PSA recovery and  $Y_P$  and  $Y_F$  are PSA product and feed purities.

It is assumed that  $Y_P / Y_F \times R = \alpha = \text{constant}$ , Thus:

$$F_F = \alpha \times F_P \quad (3)$$

Using (3), the overall balance across purification unit (1) can be simplified as

$$F_R = (\alpha - 1) \times F_P \quad (4)$$

The other constraints are as follows:

$$\text{Sink flow rate} \quad \sum_{i=1}^{N_{sr}} F_{i,j} = F_{sk,j} \quad (5)$$

$$\text{Sink purity} \quad \sum_{i=1}^{N_{sr}} F_{i,j} y_i = F_{sk,j} y_j \quad (6)$$

$$\text{Source flow rate} \quad \sum_{j=1}^{N_{sk}} F_{i,j} + F_{i,w} = F_{sr,i} \quad (7)$$

$$\text{Compressor flow rate} \quad \sum_j F_{comp,j} = \sum_i F_{i,comp} \quad (8)$$

$$\text{Compressor purity} \quad \sum_j F_{comp,j} y_{comp} = \sum_i F_{i,comp} y_i \quad (9)$$

$$\text{Capacity limit} \quad \sum_i F_{i,comp} \leq F_{max,comp} \quad (10)$$

### 3. Case studies

To highlight the importance of hydrogen management in petrochemical complexes and also present the applicability of the comprehensive superstructure, two industrial case studies are investigated. Case A is an aromatic petrochemical complex and Case B is an integrated network of the aromatic complex with an ammonia complex.

#### 3.1 Case A

Aromatic complexes have several units, which consume hydrogen. To supply the required hydrogen usually a catalytic reformer is used. The existing hydrogen network of an industrial aromatic complex is shown in Figure 3, which have seven units that consume hydrogen such as hydrotreating (HT), hydrogenation (HG), arofining (AF), isomerization (IS), regeneration (RG), transalkylation (TA) and disproportionation (DP). It should be noted that the purge stream of regeneration unit is not used owing to the process constraints. The outlet stream of reformer is sent to the PSA unit using a compressor. As mentioned previously these compressor and purifier are incorporated into the superstructure. Table 1 summarizes stream data for the existing network including all hydrogen sinks and sources. Also, Table 2 shows the cost data.



Table 2: Cost data

Operating Cost	
Hydrogen cost	2000 \$ / MMscfd
Electricity cost	0.03 \$/KWh
Fuel costs	2.5 \$/MMBtu
Capital Cost	
Compressor costs	$115 + 1.91 \times \text{Power (kWh)}$ (k\$)
Piping cost	$0.15 \times \text{Capital cost}$

Now, the hydrogen petrochemical complex is formulated using the mathematical model. Minimizing total annual cost subject to constraints Eqs. (1)-(10) forms a NLP programming solved by GAMS (General Algebraic Modeling System), Brook et al. (2006). The optimized results of NLP model is presented in Table 3. As shown in Table 3, the hydrogen consumption reduced from 231.1 to 192.45 mol/s showing 16.7 % reduction in fresh hydrogen consumption. In addition, the operating cost is reduced by 9.6 %. In addition, a new compressor is added to the network on PSA residue stream to enhance its pressure.

Table 3: Results of optimized network for Case A

Case	Hydrogen Consumption (mol/s)	Operating Cost (M\$/year)	Capital Cost (M\$)	Payback (year)
Existing network	231.1	17.810	---	---
Optimized network	192.45	16.099	3.558	2.08

### 3.2 Case B

In case B the hydrogen integration of the aromatic complex (case A) with an ammonia complex is investigated. Figure 4 shows the hydrogen network flowsheet extracted from this ammonia petrochemical complex.

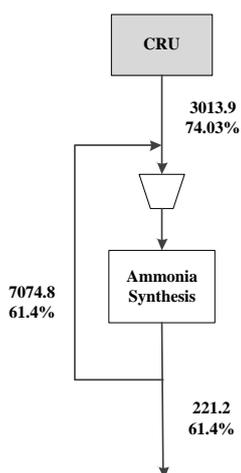


Figure 4: The existing hydrogen network of ammonia complex

The optimized results of NLP model and the associated network are presented in Table 4. As shown in Table 4, the hydrogen consumption reduced from 231.1 to 192 mol/s. Moreover, the operating cost is reduced by 4.9 %.

*Table 4: Results of optimized network for Case B*

Case	Hydrogen Consumption (mol/s)	Operating Cost (M\$/y)	Capital Cost (M\$)	Payback (y)
Existing network	231.1	35.766	---	---
Optimized network	192	34.025	3.55	2.04

The comparison between two case results is presented in Table 5. The results show a negligible reduction in hydrogen consumption in case B compared to those achieved in case A. In fact, the integration of two petrochemical complexes has not influenced the hydrogen consumption and costs significantly due to pressure constraints through the network.

*Table 5: Results of optimized network for Case A and Case B*

Case	Hydrogen Consumption (mol/s)	Operating Cost Reduction (M\$/y)	Capital Cost (M\$)	Payback (y)
Case A	192.45	1.711	3.558	2.08
Case B	192	1.741	3.55	2.04

#### 4. Conclusion

Hydrogen management through the petrochemical complexes is so important as well as refinery plants. As most of previously reported methodologies have considered the hydrogen plant as external utility, a new superstructure and mathematical approach developed in this work to consider the compressor and purification unit embedded on reformer. In this way, an optimized hydrogen network is achieved which reduces hydrogen consumption with a reasonable payback.

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