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Optimization Model for Refinery Hydrogen Networks Part I

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ABSTRACT
Petroleum refineries have many process units that consume hydrogen.These process units are distributed in different places everywhere in the refinery.In order to feed them, it is necessary to have sources capable of supplying, in amount and quality, the hydrogen that every consuming unit needs.It is also needed to have a distribution network that it is correctly designed and which operation is adjusted in an optimal manner to the changing conditions of the refinery.This involves the minimization of the cost of installation and operation of the hydrogen network.The installation cost is dominated by the amount of pipelines, compressors and purifying units; while the cost of operation is dominated by the amount of fresh hydrogen that the plant consumes.In this work a mathematical model is developed for a hydrogen network,which is adapted to the different information levels available in the different stages of design of that system.The model is currently in use in the YPFLuján de Cuyo refinery (Mendoza, Argentina). In this first part, the basic model is presented; whereas in a second part, the model is enlarged to accommodate the incorporation of purifying units and new compressors.

Keywords–Integration in Hydrogen Networks, LINGO, Optimization, Refinery Hydrogen Management,Refinery Hydrogen Networks, RefineryHydrogen Pinch.

I. INTRODUCTION

In the petroleum refineries and the petrochemical complexes, a great amount of units consuming hydrogen exist, such as hydrotreaters, hydrocrackers, isomerization units and lube refining units.Hydrogen production units also exist, such as the catalytic naphtha reformers and the hydrogen plants.In order to take the hydrogen from the source points to the point where hydrogen is consumed, it is necessary to have a distribution network.This distribution network must be adequately designed and must also be adequately operated in order to supply the amount and quality of hydrogen required by every consuming unit.An optimally designed and operated network will demand a minimum amount of fresh hydrogen (make-up). With this purpose, it will minimize the amount of hydrogen leaving the network (off-gas) and it will maximize the amount of recycled hydrogen.

Any optimization study of a hydrogen network must begin with an analysis of the hydrogen pinch.Through the systematic analysis of offer (sources) and demand (sinks), the hydrogen pinch analysis tries to minimize the flowrates of the make-up of fresh hydrogen and the discharges of off-gas.For this purpose, the study maximizes the amount of recovered and reused hydrogen, though the recovery might demand the purification of off-gas hydrogen.

The first step in the determination of the hydrogen pinch is the calculation of the mass balance of the hydrogen sinks and sources of the network. The hydrogen sources comprise the sources of fresh hydrogen (make-up), recycle streams, streams issuing from hydrogen produces (e.g. the naphtha reformer), product and residue streams of hydrogen purifiers (e.g. membrane separators and PSA units), off-gas streams of low and high pressure separators and off-gas streams of consuming units (e.g. hydrotreaters and hydrocrackers). The hydrogen demand comprises the streams entering the hydrogen consuming units and the purifying units.For each stream the flowrate and purity are indicated.Molar or STP flowrates must be used for unambiguous calculations.

Basically, the hydrogen pinch is the purity at which the hydrogen network has no surplus nor deficit of hydrogen.The pinch represents the bottleneck of the network or how much hydrogen can be recovered and reused.The traditional approach to the hydrogen pinch is graphic, and does not consider the pressure of each current [1]-[4]. For this reason the theoretical hydrogen consumption determined by this pinch analysis is the theoretical minimum consumption, whichcan be used to take decisions at an early stage of the design.The changes needed in the real network for achieving this minimum can be as simple as the opening and closing of some valves, or as costly as the installation of a multistage compressor for connecting a low pressure source to a high pressure sink.An intermediate change can be the implementation of cascaded connections between the purge of one unit and the make-up of other one [5].

In order to take into account the pressure in the management of the hydrogen network, optimization techniques can be applied, which minimize the costs of installation as well as the costs of operation [6]-[8].

A model of optimization has the objective of finding the best solution for a given problem.The model of optimization is composed of decision variables, an objective function and the restrictions.The decision variables are the variables that can be changed in order to find the best solution.In this search, the decision variables must respect the conditions imposed by the restrictions of the problem.The goodness of the explored alternatives is measured by the objective function.The best alternative will be the one that minimizes or maximizes the objective function.

In this work, a mathematical model is presented for a hydrogen network. This model is adapted to the different levels of information available as a progress is made during the design of a hydrogen network.The model is currently being used by the YPFLuján de Cuyo refinery (Mendoza, Argentina).The optimization model was implementedby using Excel and LINGO.The Excel spreadsheet enables entering the data in an easy way and also shows the results obtained.The mathematical model is solved by using LINGO, a commercial optimization software package.

II. MODEL TO MINIMIZE THE DEMAND OF HYDROGEN

2.1 Formulation of the model

In this first model, called Min *Fg*, the objective function is the demand of hydrogen service (amount of fresh or make-uphydrogen), and the restrictions take into account the pressure levels and the capacities of the compressors in order to determine the feasibility of the flows in the network. The model determines the connections to be made, together with the flowrates and the purities of the streams of the network that make minimum the demand of hydrogen. In favorable conditions, the demand can be reduced to the minimum level determined by the pinch analysis.

The formulation of the model demands the definition of the following sets of elements:

- *N*: set of source and sink nodes that belong to the network.

Fig. 1 shows a simplified scheme of a hydrogen consuming unit. In this diagram the right location of the sink and source nodes is defined.

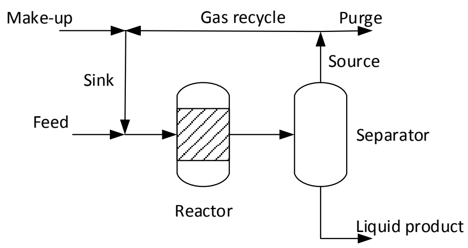

Figure 1. Simplified scheme of a hydrogen consuming unit showing the correct location of the source and sink nodes.

Each source of the *N* set has a process nucleusand an output splitter (Fig. 2), whereaseach sink of the *N* set is formed by an input mixer and a process nucleus (Fig. 3). Each node thus defined has the following attributes:

- *Type:*
  - FUE: source
  - SUM: sink
- *Unit:* identifying code of the piece of equipment to which the node belongs.
- *Class:* defines the type of unitto which the node belongs, such as:
  - UP: process unit.
  - COM: compressor. It is model as a combination of a sink and a source with only one input stream and only one output stream.
  - SEP: separator.
  - GEN: pure generator, only has source nodes.
  - CON: pure consumer, only has sink nodes.
- *Pn:* absolute pressure of the nucleus (kgf/cm^2).
- *Fn:* flowrate of the stream connected to the nucleus (Nm^3/h).
- *yn:* hydrogen purity of the stream connected to the nucleus (molar fraction).
- *Femax:* maximum input flowrate (maximum compatible with the capacity of the piece of equipment or the unit). This attribute is only valid for sinks of units with COM class.

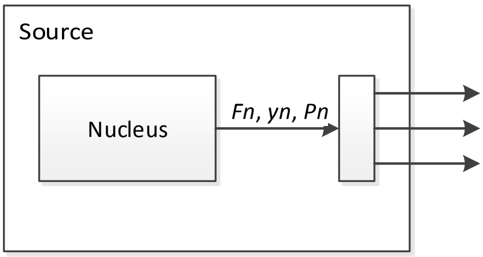

Figure 2. Structure of a source node.

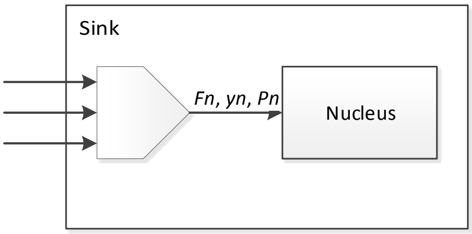

Figure 3. Structure of sink node.

From the *N* set, the following subsets are defined:

- *CF:* set of source nodes.
- *CS:* set of sink nodes.

The data required by the sources are the following:

- From UP class units: *Pn, Fn, yn*
- From COM class units: *Pn*
- From SEP class units: *Pn, Fn, yn*
- From GEN class units: *Pn, yn*

The data required by the sinks are the following:

- From UP class units: *Pn, Fn, yn*
- From COM class units: *Pn, Femax*
- From SEP class units: *Pn, Fn, yn*
- From CON class units: *Pn*

For convenience, the derived set *FxS* is defined with elements (*i*, *j*), which are ordered pairs of the source-sink type:

$$(i, j) \in FxS \Leftrightarrow i \in CF, j \in CS \tag{1}$$

The elements of this set have the following attributes:

- *F:* flowrate of the stream that goes from the source*i* to the sink*j* (Nm^3/h).
- *y:* hydrogen purity of the stream that goes from the source*i* to the sink*j* (molar fraction).

The derived *FxSP* set is also defined. Its elements are the elements of the *FxS* set that represent connections between nodes that do not belong to a same unit and that are feasible due to the pressure difference between the origin and the end of the connection:

$$(i, j) \in FxSP \Leftrightarrow (i, j) \in FxS \mid \left(Unit_i \neq Unit_j\right) \wedge \left(Pn_i \geq Pn_j\right) \tag{2}$$

That is, ordered pairs are defined of the source-sink type, where the first condition prevents the connection of the source of one units with the sink of the same units. The last condition selects the connections that are feasible from the point of view of the pressures of the connected nodes.

The objective function is the total demand of hydrogen service, *Fg*. The optimization problem is written for the minimization of the objective function by varying the hydrogen flowrates of the existing streams among the nodes of the network. The corresponding mathematical model is written below:

$$\underset{F_{i,j}, y_{i,j}, Fn_k, Fn_l, yn_l, Fg}{\mathrm{Min}} \quad Fg$$

$$(i, j) \in FxSP, k \in N \mid Class_k = \mathrm{GEN}, \quad l \in N \mid \left(Class_l = \mathrm{CON}\right) \vee \left(Class_l = \mathrm{COM}\right) \tag{3}$$

The objective function is defined as:

$$Fg = \sum_{i \in CF \mid Class_i = \mathrm{GEN}} Fn_i \; yn_i \tag{4}$$

On the other side, mass balances must be written forthe splitter of each source *k* and for the mixer of each sink *l*:

$$\sum_{(i,j) \in FxSP \mid i = k} F_{i,j} = Fn_k \quad k \in CF \tag{5}$$

$$\sum_{(i,j) \in FxSP \mid j = l} F_{i,j} = Fn_l \quad l \in CS \tag{6}$$

The purities of the streams must comply with the following restriction:

- Definition of the molar fraction:

$$0 \leq y_{i,j} \leq 1 \quad (i, j) \in FxSP \tag{7}$$

- Hydrogen balance in the source splitters:

$$yn_i = y_{i,j} \quad (i, j) \in FxSP \tag{8}$$

- Balance of hydrogen in the mixers of the sinks:

$$\sum_{(i,j) \in FxSP \mid j = l} F_{i,j} \; y_{i,j} = Fn_l \; yn_l \quad l \in CS \tag{9}$$

For the compressors these additional restrictions are written:

$$Fn_i = Fn_j \quad (i, j) \in FxS \mid \left(Unit_i = Unit_j\right) \wedge \left(Class_i = \mathrm{COM}\right) \tag{10}$$

$$yn_i = yn_j \quad (i, j) \in FxS \mid \left(Unit_i = Unit_j\right) \wedge \left(Class_i = \mathrm{COM}\right) \tag{11}$$

$$Fn_j \leq Femax_j \quad j \in CS \mid Class_j = \mathrm{COM} \tag{12}$$

Also, all the unfeasible connections must be eliminated:

$$F_{i,j} \leftarrow 0 \quad (i, j) \in FxS \mid (i, j) \notin FxSP \tag{13}$$

$$y_{i,j} \leftarrow 0 \quad (i, j) \in FxS \mid (i, j) \notin FxSP \tag{14}$$

For the same reason, for all nodes that are not entries of compressors, *Femax* must be annulled:

$$Femax_k \leftarrow 0 \quad k \in N \mid \left(k \notin CS\right) \vee \left(Class_k \neq \mathrm{COM}\right) \tag{15}$$

Finally, the purities of the streams that begin in sources of constant purity must be fixed:

$$y_{i,j} \leftarrow yn_i \quad (i,j) \in FxSP \mid \left(Class_i \neq \mathrm{COM}\right) \tag{16}$$

2.2 Implementation

The model thus described was implemented in the LINGO software environment. In order to ease the data input and the reading of the results, an Excel spreadsheet was developed that used many sheets and a color coding. Blue sheets were restricted to data input, whereas the sheet with salmon color where used by LINGO to output the optimization results.

2.3 Example I

Fig. 4 presents the initial configuration of the plant to be analyzed in this example. The example was taken from a work of Hallale and Liu [6]. The pinch analysis for this plant reports that the minimum production of the hydrogen plant is 182.8 MMscfd. This means a potential saving of 8.6 % with respect to the initial 200 MMscfd. However, the employed method only considers the flowrates and the purities, leaving aside the pressures. Therefore, the obtained result can be considered as an inferior limit for the production of the hydrogen required by the plant. Fig. 5 shows an implementation of the solution reported by the pinch method. This solution is not feasible because it suggests the connection between the output of A and the input of B, which is not possible due to the existing pressure difference.

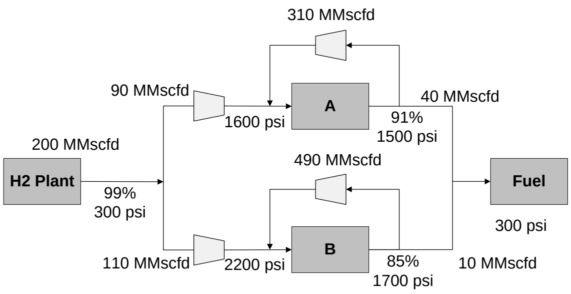

Figure 4. Initial configuration of the plant of Example I.

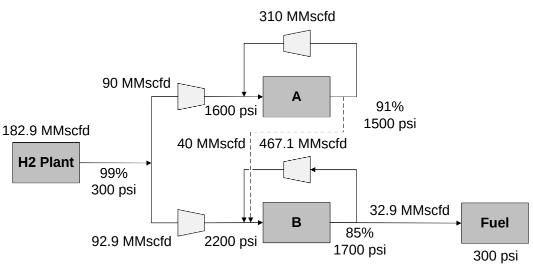

Figure 5. Scheme that implements the non-feasible solution obtained by the pinch method (Example I).

Fig. 6 shows the superstructure to be implemented in the optimization model presented in this work. In this superstructure, the plant has been decomposed into source nodes and sink nodes, and all feasible connections between them are drawn. The maximum flowrate *Femax* of each compressor is supposed to be a 5 % superior to the operation flowrate. The first solution obtained has a consumption of 195.9 MMscfd. However, it involves streams that have no practical meaning (e.g., the connection between the output of the make-up compressor and the inlet of the recycle compressor). Those streams would be automatically eliminated if the objective function considered the cost of compressor and pipelines. An alternative to eliminate those streams is to minimize the amount of connections of the network. This alternative will be presented in the following section.

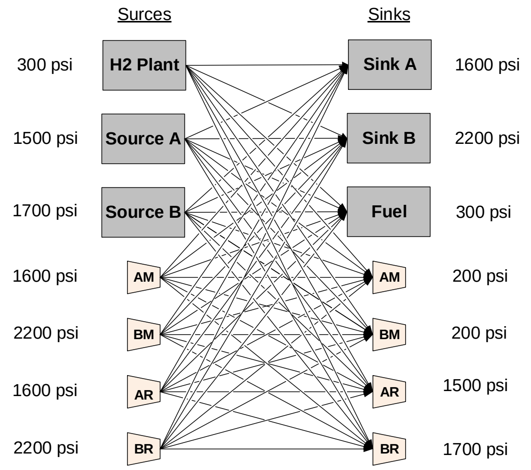

Figure 6. Superstructure for Example I.
M: make-up compressor; R: recycle compressor.

III. MODEL TO MINIMIZE CONNECTIONS

As explained in the previous section, the minimization of the hydrogen demand can lead to the posing of streams withoutpractical sense. One alternative for eliminating those streams is solving again the optimization model of the previous section, but this time adopting the following objective function and additional restriction:

$$\underset{F_{i,j},\, y_{i,j},\, Fn_k,\, Fn_l,\, yn_l,\, Fg}{\mathrm{Min}} \sum_{(i,j)\in FxSP} \mathrm{sign}\left(F_{i,j}\right)$$

$$(i,j) \in FxSP,\; k \in N \mid Class_k = \mathrm{GEN}, \tag{17}$$

$$l \in N \mid \left(Class_l = \mathrm{CON}\right) \vee \left(Class_l = \mathrm{COM}\right)$$

$$Fg \leq Fg_{\min} \tag{18}$$

Where $Fg_{\min}$ is the minimum demand of hydrogen determined by the model of the previous section, and sign(x) is the sign function of x. As all $F_{i,j}$ flowrates are not negative, the objective function represent the amount of streams employed by the solution. The goal is to minimize this amount, while keeping the minimum consumption obtained in the first solution. For this reason, the additional restriction is used. The new objective function tries to minimize the amount of pipelines required by the network. Although, it is does not account for the length of the pipelines, it is a good approximation to be used in an early stage of the design of the hydrogen network. This new model is called Min F.

3.1 Example II

Continuing with the example of the previous section,$Fg_{\min}$ takes the following value 195.9×0.99 MMscfd of H_2. Fig. 7 shows the optimal structure obtained with the model that considers the pressures of the nodes, and that employs a minimum amount of streams. This time, no spurious streams exist.

Analyzing the solution, it can be concluded that the B make-up compressor is the limiting one for the recovery of hydrogen. This can be verified by a study of sensitivity in which the minimum consumption of hydrogen is determined for a given range of capacities of the compressors. This study demonstrates that the hydrogen consumption reported by the pinch method (182.8 MMscdf) can be reached if an increase of 21 % of the flowrate of the B make-up compressor is performed.

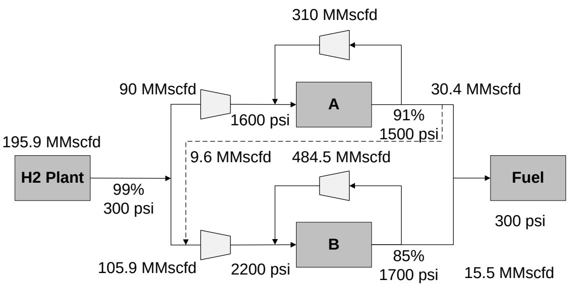

Figure 7. Plant of Example II optimized for minimizing the consumption of the service of hydrogen considering the pressures of the nodes and minimizing the amount of connections.

IV. CONCLUSIONS

In this first part of the work,an optimization model was presented, which was developed for the design of hydrogen networks of refineries. The model has many variants that can be adjusted to the levels of information available at the different stages of the design or evaluation of a network. The basic variant, the Min Fg model, minimizes the hydrogen consumption considering the pressures of the nodes of the network. The second variant, the model Min F,minimizes the number of connections of the network, keeping the minimum hydrogen consumption determined by the first model.

The model was implemented in the LINGO software environment. For data input and results output an Excel spreadsheet was implemented that was interfaced to LINGO.

In the second part of this work, the model will be enhanced to take into account the length of the pipelines, the addition of purifying units and the installation of new compressors.

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