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# **Optimization Model for Refinery Hydrogen Networks** Part II

# Enrique E. Tarifa<sup>1\*</sup>, Carlos R. Vera<sup>2</sup>, Samuel FrancoDomínguez<sup>3</sup>, Leonel A. Benite $z^4$

<sup>(1)\*</sup>Consejo Nacional de InvestigacionesCientíficas y Técnicas (CONICET), Facultad de Ingeniería, Universidad Nacional de Jujuy (UNJu). ÍtaloPalancaN°10 - San Salvador de Jujuy (4600), Argentina.

<sup>(2)</sup>Consejo Nacional de InvestigacionesCientíficas y Técnicas (CONICET). INCAPE, Facultad de Ingeniería *Química, Universidad Nacional delLitoral (UNL). Santa Fe*(3000), Argentina. <sup>(3)</sup>Facultad de Ingeniería, Universidad Nacional de Jujuy (UNJu). ÍtaloPalancaN°10 - San Salvador de Jujuy

(4600), Argentina. <sup>(4)</sup>Instituto de Investigaciones para la IndustriaQuímica - INIQUI (CONICET-UNSa), Facultad de Ingeniería

Universidad Nacional de Salta (UNSa). Avda. Bolivia Nº 5150 - Salta (4400), Argentina.

#### ABSTRACT

In the first part of this work, a model of optimization was presented that minimizes the consumption of the hydrogen of a refinery. In this second part, the model will be augmented to take into account the length of the pipelines, the addition of purification units and the installation of new compressors, all features of industrial real networks. The model developed was implemented in the LINGO software environment. For data input and results output, an Excel spreadsheet was developed that interfaces with LINGO. The model is currently being used in YPFLuján de Cuyo refinery (Mendoza, Argentina).

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

#### I. INTRODUCTION

As it was explained in the first part of this work, in the petroleum refineries and the petrochemical complexes a great number of units exist that consume hydrogen. These are hydrotreaters, hydrocrackers, and hydrogenation units. There also exist hydrogen production units such as the hydrogen plants and the catalytic naphtha reformers. To take the hydrogen from the points where it is produced to the places where it is consumed, it is necessary to have a distribution network. This network must be correctly designed and operated in order to supply the required amount and quality of hydrogen to the demanding units. A network optimally designed and operated will demand a minimum amount of fresh hydrogen (make-up). For this, it will minimize the amount of hydrogen leaving the network (off-gas) and will maximize the amount of hydrogen that is recycled.

A model of optimization has the objective of finding the best solution to a given problem. The model of optimization is composed of decision variables, an objective function and restrictions. The decision variables are the variables of the problem that can be varied with the aim of finding the best solution. In this search, the decisionvariables must respect the restrictions of the problem. The goodness of the explored alternatives is measured by the objective function. The best alternative will be that

one minimizing or maximizing the objective function.

In the first part of this work, a mathematical model was presented that was adapted to the different information levels available at different stages in the hydrogen network design effort. The developed model of optimization minimized the hydrogen consumption of a refinery. In this second part, the model will be enhanced to consider the length of the pipelines, the addition of purification units and the installation of new compressors, all features of real refinery hydrogen networks.

The model of optimization was implemented in an Excel spreadsheet. This spreadsheet eases the data input and output; and it is interfaced to LINGO, an optimization software. LINGO solves the mathematical model and yields a solution. The developed model is currently in use in the YPFLuján de Cuyo refinery (Mendoza, Argentina).

#### **II. MODEL TO MINIMIZE OF THE** LENGTH OF THE CONNECTING **PIPELINES**

The two models presented in the first part of this work did not consider the length of the pipelines required for implementing the solution, leaving aside an important component of the cost of operation and the cost of installation of the network. In a design stage in which the physical location of the

equipment is already known, it is possible to use this information to estimate the length of the required pipelines. Doing so, the model Min Fg (the first model defined in the first part of this work to minimize the hydrogen consumption) can be modified, adopting the following objective function and additional restriction:

$$\begin{array}{l} \underset{F_{i,j}, y_{i,j}, Lt_{i,j}, Fn_{k}, Fn_{i}, yn_{i}, Fg}{\text{Min}} \sum_{(i,j) \in FxSP} \operatorname{sign}\left(F_{i,j}\right) Lt_{i,j} \\ (i,j) \in FxSP, k \in N \mid Class_{k} = \operatorname{GEN}, \end{array}$$
(1)

$$l \in N \mid (Class_{l} = CON) \lor (Class_{l} = COM)$$

$$Fg \leq Fg_{\min}$$
(2)

In these equations,  $Lt_{i,j}$  is the estimated length of the pipeline connecting node *i* with node *j*,  $Fg_{min}$  is the minimum demand of hydrogen determined by the model Min Fg, and sign(x) is the sign function of *x*. As all the  $F_{i,j}$  flows are not negative, the objective function represents the total length of the pipelines employed by the solution. It is desired to minimize this total length while keeping the minimum consumption achieved in the first solution. For this reason, the additional restriction is written. This new model is called Min Lt.

The lengths  $Lt_{ij}$  can be estimated by means of the following expression (Manhattan distance):

$$L = \left| \Delta x \right| + \left| \Delta y \right| + \left| \Delta z \right| \tag{3}$$

in which,  $\Delta x$  is the distance in the coordinatex between the final and initial points of the pipeline,  $\Delta y$  is the distance in the coordinatey between the final and initial points of the pipeline, and  $\Delta z$  is the distance in the coordinatez between the final and initial points of the pipeline.

In this way, to estimate  $Lt_{i,j}$ , it is necessary to know the coordinates of the nodes. Formally, to enhance the model, the following actions should be performed:

- 1. Define *Lt* as an additional attribute of the elements of the set*FxS*.
- 2. Define cx (x coordinate of the node) and cy (y coordinate of the node) as additional attributes of the set N. To simplify the problem, the coordinate z is not considered (height).

The length of each path is then calculated in the following way (Manhattan distance):

$$Lt_{i,j} = \left| cx_i - cx_j \right| + \left| cy_i - cy_j \right| \quad (i, j) \in FxS$$
(4)

#### **III. LT-FG PARETO FRONTIER**

As it can be deduced from the discussion of the previous sections, the model that considers the cost of hydrogen production and the cost of the pipelines is complex, and requires a great amount of data that is not always available. For this reason before beginning its development it is convenient to analyze if the possible improvements justify the additional effort. In order to determine the improvements that could be got, one possible method is that of calculating the Pareto frontier for Lt-Fg.

For the case being studied, the Pareto frontier is a curve in the plane Lt-Fg [1]. For any point of this curve, it happens that Fg is the minimum demand for the network with a total pipeline length Lt, and Lt is the minimum pipeline length for the network with a demand Fg.

In order to Fg having an effect on Lt, it is necessary to relax the restriction of purity in the sink nodes so that they can accept a feed of purity equal or higher than the purity demanded by them. This is done by replacing in the model Min Fg eq. (9) by the following:

$$\sum_{(i,j)\in F \times SP \mid j=l} F_{i,j} y_{i,j} \ge F n_i y n_i \quad l \in CS$$
(5)

It can be remarked that after making this modification, the process units can receive a feed of higher purity than the one they demand. However, the model does not consider the effect that this higher purity has on the unit throughput or the properties of the output stream. It neither considers the effect of this higher purity on the capacity of the compressors.

For obtaining each point on the Pareto frontier the following procedure is followed:

- 1. The optimization problem Min Fg is solved to minimize the hydrogen demand. The value  $Fg_{min}$  is thus obtained.
- 2. A value of hydrogen demand  $Fg_{\text{test}}$ , higher than  $Fg_{\min}$ , is proposed.
- 3. The model Min Lt is solved to get the minimum total pipeline length  $Lt_{Pareto}$ , subjected to the condition of not surpassing the demand  $Fg_{test}$  proposed in step 2.
- 4. The optimization problem Min Fg is solved again, with the additional restriction:

$$\sum_{(i,j)\in FxSP} \operatorname{sign}\left(F_{i,j}\right) Lt_{i,j} \leq Lt_{\operatorname{Pareto}}$$
(6)

The minimum consumption obtained as a result of solving this problem is  $Fg_{Pareto}$ .

5. The point ( $Fg_{Pareto}$ ,  $Lt_{Pareto}$ ) is added to the graph of the Pareto frontier.

The study of the Pareto frontier allows to determine if the decrease of the total pipeline length produced by the increase in the hydrogen demand justifies an economic analysis. If this were the case, an economic analysis can be performed using the point of interest on the Pareto frontier. Finally, and only if it is advisable, an enhancement of the model of optimization —adding costs of installation and operation— can be undertaken.

#### IV. ADDITION OF PURIFICATION UNITS

#### 4.1 PSA units

The process of cyclic adsorption with pressure swing (PSA, pressure swing adsorption) is a variant of the processes of cyclic adsorption. The processes of cyclic adsorption are widely used in the process industry, and are based on the differential adsorption of one component of a mixture in relation to the other components. The process equipment is a set of columns packed with adsorbent. The units have at least two columns. During the cycle of adsorption or production the stream that needs to be purified or concentrated is passed through the fresh or regenerated bed where the adsorption of the determined compounds occurs (gases other than hydrogen). Once the capacity of adsorption of the bed has decreased, or the mass front of the adsorbed compounds reaches the exit, the valves are actuated, and desorption of the bed is initiated. During regeneration of this bed, another already regenerated bed is used to keep a continuous production. For this reason the minimum amount of beds is two, though it can be higher if the adsorption cycle is shorter than the regeneration one. When the regeneration step is shorter than the adsorption one, an additional idle cycle with no activity must be set up.

#### 4.2 Membrane units

The membrane separators operate with the principle of selective permeation of gases. Each gas that enters in the membrane separator has characteristic rate of permeation that is a function of the capacity of entering the membrane, diffusing through it and desorbing. Membrane separators use the relative differences in permeation rates of different gases for the separation of "fast" gases (hydrogen, helium, water vapor) from "slow" ones (methane, argon, nitrogen). Carbon dioxide has an intermediate permeation rate.

The driving force for the separation of the gas is the difference in partial pressure of each component on one side and the other side of the membrane. The typical polymeric membrane separators comprise a compact bunch of hollow fibers that are sealed in one end and open in the other. The fibers are encapsulated inside a vessel. The feed is pressurized in the gas state and enters and flows through the separator on the outer side of the fibers (shell side). The fast gases permeate selectively through the membrane inside the hollow fibers (tube side) where a lower pressure can be found. The permeate stream is collected in a manifold in one end of the separator. The retentate gas exists from the other end of the separator, at essentially the same pressure than the entrance. Each separating element employs hundreds of thousands of these hollow fibers of small diameter for

supplying the highest possible area of separation in compact modules of easy handling (up to 5000  $m^2 m^{-3}$  in the case of the bundles of polymeric hollow fiber). For obtaining the desired performance, the final equipment employs many of these separation modules in series, parallel and cascaded arrangements finally mounted on skids.

#### 4.3 Modeling of purification units

This section presents the modifications performed to the optimization model in order to incorporate the addition of purification units. Two kinds of purification units are considered:PSA and membrane units. For this reason two new classes of units are defined: PSA and MEM. These equipment are modelled as the combination of a sink and two sources, i.e. they have a unique inlet (the feed) and two outlets (the purified product and the residue). The model does not consider the incorporation of compressors associated to these units. new Therefore, the purification units must be installed in a way that can work with the pressure levels available in the process units or those provided by the already installed compressors.

The modelling of the purification units requires the incorporation of sink and source nodes to the sets CF and CS, respectively. It is also necessary to incorporate these nodes to the sets FxS and FxSP;however, the incorporation to this last set is not straightforward as it will be explained later. The modifications to the original Min Fg model are detailed below.

In the first place, the following additional sets are defined:

- *NI:* set of nodes belonging to intermediate equipment, like compressors and purification units. It is a set derived from *N*. The main feature of the intermediate units is that they require equations linking their inlets to their outlets.
- *CFI:* set of sources of intermediate equipment that represents the outlet streams of compressors and purification units. It is a subset of *NI*.
- *CFP*: set of purification sources. It is a subset of *CFI*. It has the following additional attribute:
  - *Output:* indicates the kind of outlet,PRO for the outlet that is a product of the equipment. RES for the outlet that is a residue of the unit.
- *CSI:* set of sinks of intermediate equipment that represent the streams feeding compressors and purification units. It is a subset of *NI*. This sinks have the following additional attribute:
  - *Femax:*maximum inlet flowrate.
- *CSPA:* set of sinks of purification units that represent the streams feeding *PSA* or membrane purification units. It is a subset of *CSI*. This sinks have the following additional attributes:

- *R*:recovery of the unit, expressed as a fraction of one (value between 0 and 1).
- *Pnmin:* minimum absolute pressure of the feed required by the unit.
- *Pnmax:* maximum absolute pressure admitted by the unit.
- *DPmax:* maximum pressure difference admitted by the unit.
- *Theta:* is the selectivity of the adsorbent (value between 0 and 1) for PSA units. For membranes, however, is the ratio between the average permeability of the feed gases, without considering hydrogen, divided by the permeability of hydrogen. A typical value is 4/500 = 0.008.
- O *ynmin:* minimum purity of the feed.
- *CFPP:* set of sources that represent the streams of product of purification units. It is a subset of *CFP.* These sources have the following additional attribute:
- *ynmax:* maximum purity that can be achieved by the product.
- *CFPR:* set of sources that represent the streams of residue of purification units. It is a subset of *CFP*.

The required data for the nodes of purification units are the following:

- Feed nodes: *Femax, R, Pnmin, Pnmax, DPmax, Theta, ynmin.*
- Product nodes:*ymax*.

The derived set FxSE is also defined, whose elements are elements of FxS that represent connections between nodes with known pressures(i.e., it does not involve purification units because they have unknown pressures):

$$(i, j) \in FxSE \Leftrightarrow (i, j) \in FxS | (i \notin CFPP) \land (i \notin CFPR) \land (j \notin CSPA)$$
 (7)

From this set, the set FxSEP is derived, whose elements are elements of FxSE that represent connections between nodes with known pressures and that are possible because of the pressure difference existing between the origin and the destination of the connection. It is also required that the nodes do not belong to the same unit:

$$(i, j) \in FxSEP \Leftrightarrow (i, j) \in FxSE | (Unit_i \neq Unit_i) \land (Pn_i \ge Pn_i)$$
(8)

Then, from the set 
$$FxS$$
 the set  $FxSI$  is derived, whose  
elements represent connections that involve nodes with unknown pressures (i.e., it involves the purification units):

$$(i, j) \in FxSI \Leftrightarrow (i, j) \in FxS | (i \in CFPP) \lor (i \in CFPR) \lor (j \in CSPA)$$

$$(9)$$

From this last set, the set *FxSIP* is derived, whose elements represent connections that involve

nodes with unknown pressures. The connected nodes do not belong to the same unit.

$$(i, j) \in FxSIP \Leftrightarrow (i, j) \in FxSI |$$
  
 $Unit \neq Unit$ 
(10)

Finally, the *FxSP* set is redefined —it had been defined by eq. (2) in the first part of this work—. Its elements are now those elements of *FxS* that contain connections that are possible or potentially possible, either because of the pressure difference or because equipment with unknown pressures are involved.

$$(i, j) \in FxSP \Leftrightarrow (i, j) \in FxS | ((i, j) \in FxSEP) \lor ((i, j) \in FxSIP)$$
 (11)

The equations that must be added to the optimization model in order to consider a purification unit are the material balance, the hydrogen balance and the limitation of the feed flowrate, i.e.:

$$Fn_{j} = \sum_{i \in CFI \mid (Unit_{i} = Unit_{j})} Fn_{i} \quad j \in CSI$$
(12)

$$Fn_{j}yn_{j} = \sum_{i \in CFI \mid (Unit_{i} = Unit_{j})} Fn_{i}yn_{i} \quad j \in CSI$$
(13)

$$Fn_{j} \le Femax_{j} \quad j \in CSI \tag{14}$$

These equations eliminate the need to have the equations previously written for compressors in the first part of this work:(10)-(12).

For a correct operation of the unit, the feed must have a purity higher than the minimum required, while the purity of the product should not surpass the established maximum:

$$yn_j \ge ynmin_j \quad j \in CSPA$$
 (15)

$$yn_i \le ynmax_i \quad i \in CFPP$$
 (16)

An equation for the performance of the piece of equipment is also added to the previous ones. This equation uses the recovery R that is equal to the ratio of the product hydrogen flowrate to the feed hydrogen flowrate, i.e.:

$$R_{i} F n_{i} y n_{i} = F n_{i} y n_{i}$$

$$i \in CFPP, j \in CSPA \mid (Unit_i = Unit_j)$$

$$(17)$$

The recovery R is tightly linked to the size and features of the purification unit. Hence, it is also related to the cost of the piece of equipment. For this reason, in some cases is convenient to fix the desired recovery while in others it convenient to let it vary freely so that the optimizer can determine the recovery in accord with the chosen objective function. In this last, case the following restriction must be added:

$$0 \le R_{j} \le 1 \quad j \in CSPA \tag{18}$$

The model is completed with the equations that involve the pressures of the piece of equipment. The inlet pressure is a decision variable of the model. This inlet pressure will be equal or lower than the lowest pressure of the streams of the feed. If there are many streams feeding the purification unit, the streams with a pressure higher than the feed pressure will have to reduce it somehow, e.g. by passing through a valve. Therefore, calculating the entrance pressure in a purification unit requires the addition of the following restrictions to the model:

$$\left(Pn_{i}-Pn_{j}\right)F_{i,j}\geq0$$
(19)

$$(i, j) \in FxSP \mid j \in CSPA$$

$$Pn_{j} \le Pnmax_{j} \quad j \in CSPA \tag{20}$$

$$Pn_{j} \ge Pnmin_{j} \quad j \in CSPA \tag{21}$$

The pressure of the product and the pressure of the residue are also variables, and they are determined by the intrinsic features of the purification unit. It is in the way that R and these two pressures are calculated that PSA and membrane models are different. However, for both types of purifiers, the product pressure and the residue pressure must be higher than the pressure of the destination nodes:

$$\left(Pn_{i}-Pn_{j}\right)F_{i,j}\geq0$$
(22)

$$(i, j) \in FxSP \mid i \in CFPP$$

$$(Pn_k - Pn_j)F_{k,j} \ge 0$$

$$(k, j) \in FxSP \mid k \in CFPR$$

$$(23)$$

#### 4.4 Model of PSA units

As detailed in the end of the previous section, in order to complete the model of PSA units, equations must be added that determine the pressure of the product and the pressure of the residue. In PSA units, the product pressure can be considered equal to the feed pressure:

$$Pn_{i} = Pn_{j}$$

$$i \in CFPP, j \in CSPA \mid$$

$$(Unit_{i} = Unit_{j}) \land (Class_{j} = PSA)$$

$$(24)$$

The pressure of the residue is calculated by means of the following equation [2]-[3]:

$$Pn_{k} = Pn_{i} yn_{j} \left( 1 - \frac{R_{j}}{1 - Theta_{j}} \right)$$

$$i \in CFPP, j \in CSPA, k \in CFPR \mid$$

$$\left( Unit_{i} = Unit_{j} \right)$$

$$\wedge \left( Unit_{i} = Unit_{k} \right)$$

$$\left( (25) \right)$$

 $\wedge (C lass_{j} = PSA)$ 

Finally, a restriction for the maximum allowable pressure differencethat can resist the PSA must be written:

$$Pn_{j} - Pn_{k} \leq DPmax_{j}$$

$$j \in CSPA, k \in CFPR \mid$$

$$(Unit_{j} = Unit_{k}) \land (Class_{j} = PSA)$$

$$(26)$$

#### 4.5 Model of membrane units

In a similar way to what was done for a PSA unit, the model for a membrane unit involves additional equations to determine the pressure of the product and the pressure of the residue. In the case of membranes, the pressure of the residue can be supposed to be equal to the pressure of the feed:

$$Pn_k = Pn_j$$

$$j \in CSPA, k \in CFPR \mid$$
(27)

 $(Unit_i = Unit_k) \wedge (Class_i = M EM)$ 

The pressure of the product is determined by means of the following equation [3]-[4]:

$$Theta_{j} yn_{i} (Pn_{j} - Pn_{i} - Pn_{j} yn_{j} + Pn_{i} yn_{i})$$

$$= (1 - yn_{i}) (Pn_{j} yn_{j} - Pn_{i} y_{i})$$

$$i \in CFPP, j \in CSPA \mid$$

$$(Unit_{i} = Unit_{j}) \land (Class_{j} = MEM)$$

$$(28)$$

In order to make sure that a positive permeation exists, the partial pressure of hydrogen in the residual stream should be equal or higher than the partial product of hydrogen in the product:

$$Pn_{k} yn_{k} \ge Pn_{i} yn_{i}$$

$$i \in CFPP, k \in CFPR \mid$$
(29)

 $(Unit_i = Unit_k) \land (Class_i = M EM)$ 

Finally, a restriction for the maximum allowable pressure difference that can resist the membrane must be written:

$$Pn_{j} - Pn_{i} \leq DPmax_{j}$$

$$i \in CFPP, j \in CSPA \mid$$

$$(Unit_{i} = Unit_{j}) \land (Class_{j} = MEM)$$

$$(30)$$

#### V. INCORPORATION OF BYPASS AND COMPRESSORS

The model of optimization presented in this work can be enlarged to include the following aspects:

- Compressors with unknown pressures:although the optimization model described until here already takes compressors into account, both the inlet and outlet pressure must be entered as data. The enlarged model considers compressors with pressure levels managed by the optimizer.
- Mixers: remarkable savings in lengths of pipelines can be made when many streams that have the same destination can be mixed in only one pipeline. As it is not known which are the streams that will be mixed and which is the

destination node, the pressure of one unit of this kind is a decision variable.

- Splitters:another savings in pipeline lengths can be made when only one pipe is used to carry a stream that will feed many destination nodes. For this purpose it is necessary to have a splitting unit at the end of the pipe. This splitter will distribute the streams to the destination nodes. Again, as the destinations and origins are not known a priori, the pressure of this kind of equipment is a decision variable.
- Bypass in purification units:in analyzed examples the optimizer was forced to make multiple connections in one destination node to get the desired purity. This can be done in a simpler way by using a bypass of the feed to mix it in the product reaching the desired purity without the use of multiple connections.

To implement the new commented aspects, a new class of equipment was defined: COMP. One unit of the COMP class is a compressor in which the inlet and outlet pressures are decision variables. This class of equipmentis also employed for modeling mixers and splitters. A bypass can be modeled by using a splitter before the purification unit and a mixer after it. For these reason it is only necessary to build the model for the equipment of class COMP. This is done in the next section.

# 5.1 Model for compressors with unknown pressures

This sectionpresents the modifications needed to enlarge the model of section 4 so that it can consider the installation of compressors with unknown pressures. These equipment are modeled as the combination of a sink and a source, with unknown suction and discharge pressures, but establishing upper limits for the feed flowrate and the compression ratio.

The modeling of these compressors requires their nodes to be added to the sets *N* and *NI*. The following new sets are also defined:

- *CFC*: set of sources of compressors of the COMPclass. This is a subset of *NI*.
- *CSC:* set of sinks of compressors of the class COMP. This is a subset of *NI*. These sinks have the following additional attribute:
- *RCmax:* maximum compression ratio (ratio to the discharge pressure to the suction pressure). Typically, it has a value close to 2. To model one mixer or a splitter, the compression ratio should be equal to 1.

The data required for the nodes of the equipment of the COMP class are the following:

• Feed nodes: *Femax, RCmax.* 

The derived set FxSE is also redefined. Its elements are the elements of FxS that represent

connections between nodes with known pressures (i.e., not involving purification units nor the new compressorsbecause they have unknown pressures):

$$(i, j) \in FxSE \Leftrightarrow (i, j) \in FxS |$$

$$(i \notin CFPP) \land (i \notin CFPR) \land (j \notin CSPA)$$
(31)
$$\land (i \notin CFC) \land (j \notin CSC)$$

Then, the set FxSI is redefined. Its elements represented those connections involving nodes with unknown pressures (i.e., including both the purification units and the new compressors):

$$(i, j) \in FxSI \Leftrightarrow (i, j) \in FxS |$$

$$(i \in CFPP) \lor (i \in CFPR) \lor (j \in CSPA)$$

$$(i \in CFC) \lor (j \in CSC)$$

$$(32)$$

To complete the model of equipment of the COMP class, equations are added that control the streams that enter the suction of a compressor so that they respect the existing pressure differences:

$$\left(Pn_{i}-Pn_{j}\right)F_{i,j}\geq0$$
(33)

$$(i, j) \in FxSP \mid j \in CSC$$

Also the stream that exit the discharge of a compressor must respect the existing pressure differences:

$$\left(Pn_{i}-Pn_{j}\right)F_{i,j}\geq0$$
(34)

$$(i, j) \in FxSP \mid i \in CFC$$

And finally, the maximum allowable compression ratio of a compressor must be respected:

$$Pn_{i} \leq RCmax_{j}Pn_{j}$$

$$i \in CFC, j \in CSC \mid Unit_{i} = Unit_{j}$$
(35)

## VI. CONCLUSIONS

In this second part of the work, the presentation of a model of optimization for refinery hydrogen networks was made. The model has many variants that accommodate to the different degrees of information available during the refinery hydrogen network design or evaluation. The basic model variant, the Min Fg model, minimizes the hydrogen consumption considering the pressures of the network nodes. The second variant, the model MinF, further minimizes the number of connections of the network.

The model was implemented in the LINGO software environment, an optimization software package. For the data input and results output, an Excel spreadsheet that interfaced with LINGO was programmed and used.

In the second part, the model was augmented to consider the length of the pipelines —model Min Lt—, the installation of purification units (PSA and membrane units) and the installation of new compressors, mixers, splitters and bypasses.

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