

Simulation of Catalytic Reforming Units and Construction of Linear Vectors to the Linear Programming Model of Galp Energia

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1. Abstract

The present work is focused on the construction of rigorous models to the Catalytic Reforming Units of the company Galp Energia, using the process simulator software Petro-SIM™. Two models were developed, one for Sines CCR (Continuous Catalytic Regeneration Reformer) (PP), and the other for Matosinhos CCR (Un.3300).

The PP model presents results very close to the reality, providing results for feedstocks with different characteristics and for different working conditions of the unit, becoming a better tool than the model nowadays used by Galp Energia. As for the Unit 3300, the construction of the model was far more challenging as this unit operates in more restrict conditions. Nevertheless the new model approaches reality in a very satisfactory way.

At last, the construction of Base-Delta vectors allows the creation of a linear match between feed properties and products, as the result of an analysis on the effect that a small variation in feed properties (Delta) has on the products. To evaluate an afterword performance of the base and deltas in the Linear Programming Model of Galp Energia (LP), a simpler Excel model was developed in order to compare the linear results with the reality (LRM – Linear Representation Model)

Keywords: Catalytic Reforming, Platforming™, CCR, Process Simulation, Petro-SIM™, Base-Delta vectors.

CCR – <i>Continuous Catalyst Regeneration</i> KBC – <i>KBC Advanced Technologies</i> LP – <i>Linear Programming Model</i> LPG – <i>Liquefied Petroleum Gas</i> LRM – <i>Linear Representation Model</i> PP – <i>Sines Refinery Platforming Unit</i> RON – <i>Research Octane Number</i> Un.3300 – <i>Matosinhos Refinery Platforming Unit</i> UOP – <i>Universal Oil Products</i> WAIT – <i>Weighted Average Inlet Temperature</i> %wt – <i>Weight percent</i>
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simulation models enables the prediction of treatments that certain types of oils can undergo.

The main purpose of the Catalytic Reforming Units is to produce High Octane gasolines from a Heavy Naphtha cut, being also important due to the production of hydrogen gas. So, the need of rigorous models for these units is essential to predict the treatment that is possible to achieve from a certain naphtha cut as well as the hydrogen production.

1. Introduction

Due to growing competitiveness of nowadays markets, the use of technical tools that allow the optimization of profits is very important. The petroleum industry is no exception as the feedstock may vary in many different ways, therefore the construction of computerized

1.1. Objectives

The main purpose of the present work was to create rigorous models to two Reforming units of the company Galp Energia.

After the conclusion of the complex models, the information obtained has to be linearized to be included in the existing Linear Programming Model of Galp Energia.

2. Catalytic Reforming

The Catalytic Reforming Units are used to convert naphtha molecules in high octane reformates, rich in aromatics and other cyclic compounds. Alongside with reformates, hydrogen gas is an important byproduct of the reforming units.^[1]

In a very simple way, this process re-arranges or re-structures the hydrocarbon molecules of the heavy naphtha cuts, and also breaks some of them in smaller molecules. The outcome is a reformat with more complex hydrocarbon structures with higher octane number.^[2]

Other important byproducts are de LPG and small amounts of methane and ethane.^[2]

The new reformers are called Continuous Catalyst Regeneration Reformers (CCR) that are characterized for a continuous regeneration of the catalyst in the unit, and continuous addition of regenerated catalyst to the reactors.^[1]

2.1. Platforming

Galp Energia uses the reforming technology licensed by UOP (Universal Oil Products) called Platforming.

The company has 3 Reforming units, one CCR in Sines Refinery and one CCR and one semi-regenerative unit in Matosinhos Refinery.

2.2. Platforming Chemical Reactions

Has said before, the purpose of this kind of units is to improve the quality of heavy naphtha cuts through the rearrangement of Paraffin and Naphthene molecules of the feed.^{[3],[4]}

The main chemical reactions are:

- Naphthene Dehydrogenation
- Naphthene Isomerization
- Paraffin Isomerization
- Paraffin Dehydrocyclization
- Hydrocracking

- Demethylation
- Aromatic Dealkylation

2.3. Catalyst

The Platforming catalyst is a bi-functional catalyst consisting in a metallic function (Platinum) and an acid function (Alumina + Chloride). It is necessary to find the right balance between the two functions. A more metallic catalyst promotes the Dealkylation reactions and a more acid catalyst promotes the cracking reactions.

The catalyst is a very expensive substance, so it is very important to prevent coke deposition (with a stream of recycled hydrogen gas) and contamination by heavy metals and sulfur (pre-treatment of the feed).^{[3],[4],[5]}

3. Modelling the Reforming Units of Galp Energia

The modelling and simulation of the Reforming units of Galp Energia uses a very rigorous simulator for petrochemical processes called Petro-SIM™, licensed by KBC Advanced Technologies. These models were developed on top of a base model of a reforming unit provided by KBC.

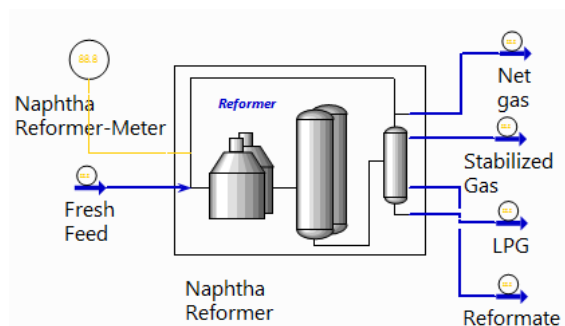


Figure 1 – KBC base model for Reforming Units

During the course of this work, two models were developed, one for Sines CCR (PP) and other for Matosinhos CCR (Un.3300).

The models were developed in two distinct phases: Calibration and Prediction.

In the first phase – Calibration – the model requires as input, the feed streams, the product streams and the operating conditions. With this information, the simulator calculates the calibration factors for the Reforming unit that allows the given feed to be transformed in the given products.

As for the second phase – Prediction – the input values are now, the feed streams, the calibrations factors and operating conditions. The simulator calculates the product streams.

The main purpose is to choose the best calibration for the unit that has the capability to predict the most accurate result for different kinds of feeds and operating conditions.

The calibration begins with the selection of complete data sets (days that have a complete analysis of feed and products composition), which are tested in calibration mode, each one providing a different set off calibration factors.

During the prediction phase, each one of the calibration factors sets will be tested, as they will be used to predict results for all data days, using only the information about the feeds and the calibration factors obtained in the previous mode.^{[6],[7],[8]}

By comparing the results of Prediction with the real values it is possible to determine which set of calibration factors yields results closest to the reality. This analysis is done considering several key properties of reforming units, being those:

- RON
- WAIT
- Reformate yield
- Benzene yield
- Toluene yield
- Xylenes + Eb yield
- Hydrogen yield
- Reformate Vapour Pressure

- Reformate Density

The set of calibration factors that best predicts these properties in the overall of all the data days will be choose has the final calibration for the unit, and become a tool for future predictions of the CCR units of Galp Energia.

In order for this choice to be accurate, an objective function was defined, which concerns the associated error for each set of calibration factors and is defined as the sum of the error of all data days predicted with the same set of calibration factors (Eq.3). The error of each day will be the sum of the error of each one of the key properties of that day (Eq.2). The error of each property will be the difference between the real value and the predicted value (Δx_i) divided by the real value (x_i) (Eq.1).

$$Error_{Property} = \left| \frac{\Delta x_i}{x_i} \right|_{Property} \quad (1)$$

$$\left| \frac{\Delta x}{x} \right|_{day} = \sum_i \left| \frac{\Delta x_i}{x_i} \right|_{Properties} \quad (2)$$

$$F_{obj} = \sum_{day} \left| \frac{\Delta x}{x} \right|_{day} \quad (3)$$

3.1. Sines CCR

The Sines CCR (PP) has the following configuration:^[9]

- 4 Reactors
- 2 Feeds (Nafta Pesada Tratada and Nafta de Hydrocracker)
- 4 product streams (Net Gas, Stabilized Gas, LPG and Reformate)
- Low Pressure Separator (model: Separator)
- High Pressure Separator (model: Recontactor)
- Recycled hydrogen stream

These configurations are all specified in the base model as shown below:

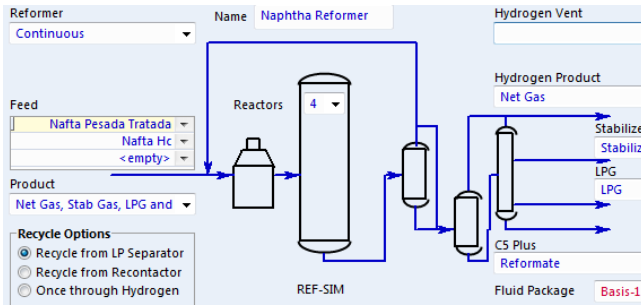


Figure 2 – Internal configuration of Sines CCR (PP)

Despite the fact that the KBC base model already contained a Separation Column (last vessel of Figure 2), it was verified that the results obtained for the product streams separation were not accurate. Because it is not possible to change its internal parameters, and to solve this problem it was added to the base model another separation unit, in which is now possible to define the separation points.

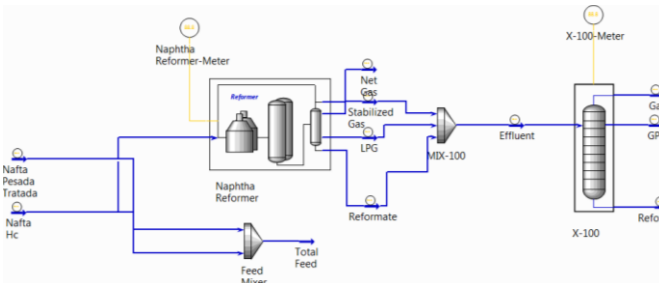


Figure 3 - Final configuration of PP Model

3.1.1. Selection of the best calibration set

With the simulation model defined it is now possible to run all the data days. As said before, each one of the data days will provide a set of calibration factors that will be analyzed in Prediction mode.

For the PP unit, 12 different days of data where tested.

The picture below demonstrates, as an example, the Prediction of the Reformate yield using the 12 calibration sets obtained in Calibration Mode, comparing their results with the real value. This representation was made for all the key properties.

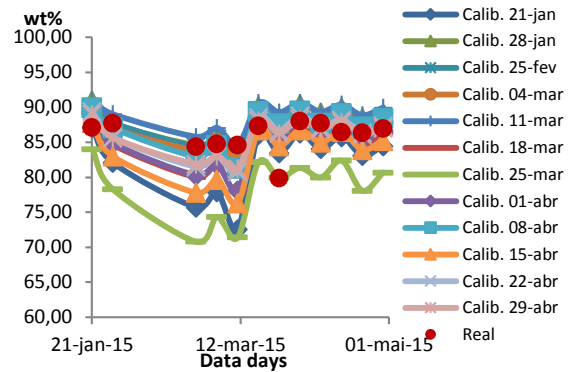


Figure 4 – Prediction with all calibration sets: Reformate yield

As it is easily seen in Figure 4, not all sets of calibrations factors provide a good result when in Prediction mode. Therefore, Prediction results were analyzed in comparison with the real value of the key properties above mentioned.

3.1.2. Best Calibration: Results and Analysis

The best set of calibration factors for the Sines PP Unit was the one provided by the 4th of March data.

Figures 5 to 12 show the comparison between the real value and the value calculated by the set of calibration factors from the 4th of March, for the key properties of the Unit.

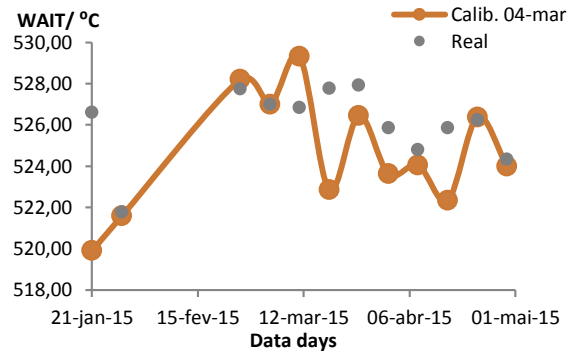


Figure 5 – Prediction with 4th of March Calibration: WAIT

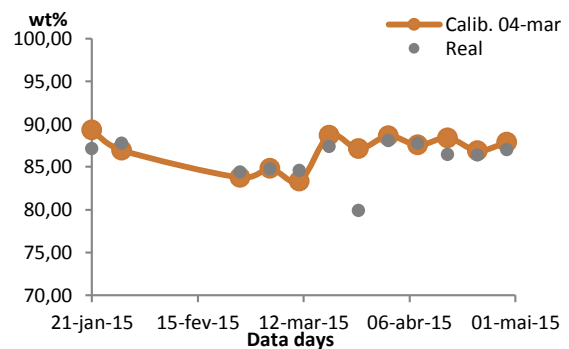


Figure 6 – Prediction with 4th of March Calibration: Reformate yield

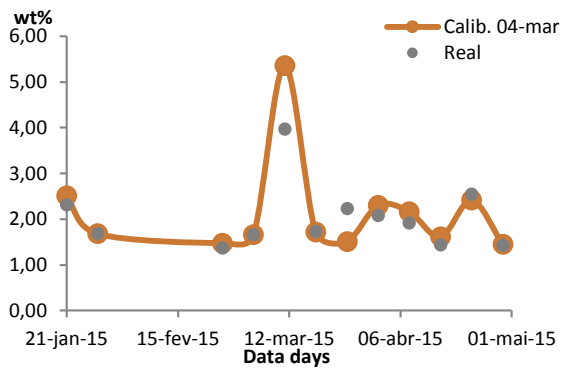


Figure 7 – Prediction with 4th of March Calibration: Benzene yield

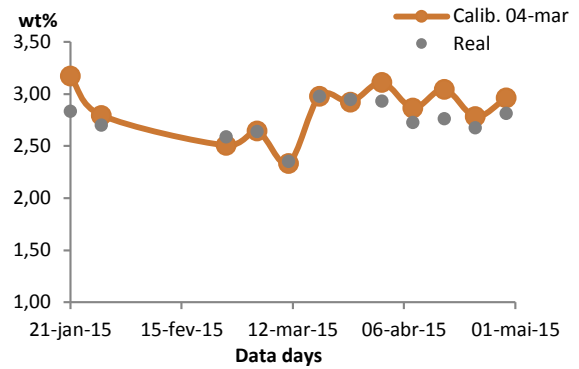


Figure 10 – Prediction with 4th of March Calibration: Hydrogen yield

The Hydrogen yield is also very well predicted with the 4th of March Calibration.

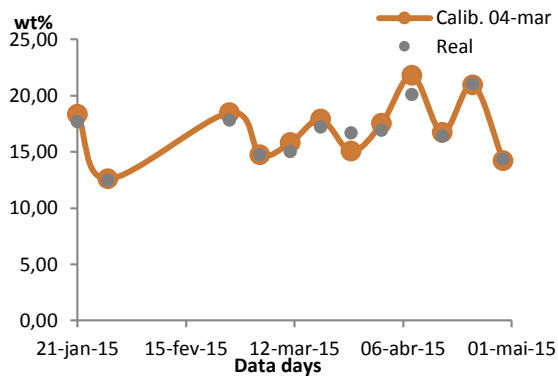


Figure 8 – Prediction with 4th of March Calibration: Toluene yield

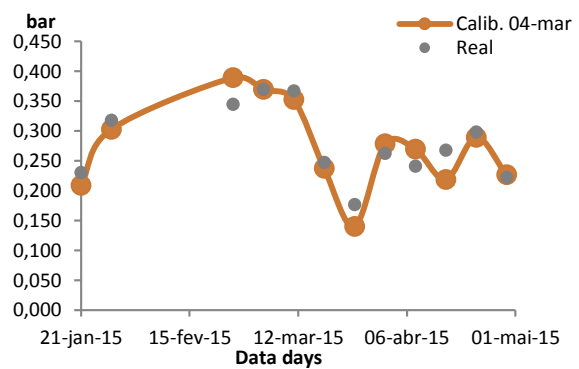


Figure 11 – Prediction with 4th of March Calibration: Reformate Vapour Pressure

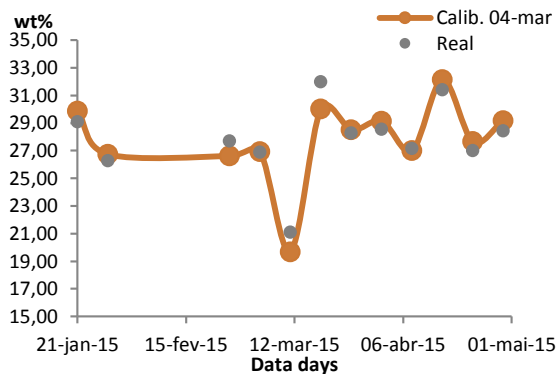


Figure 9 – Prediction with 4th of March Calibration: Xylenes and Ethylbenzene yield

In Figure 5 is possible to see that the reactors WAIT presents a considerable deviation for several days.

Figures 6 to 9 show the Reformate yield and Benzene, Toluene and Xylenes + Ethylbenzene yields when using the calibrations factors of the selected day in comparison with the real value. As it is easily seen, the several yields are very well predicted with the 4th of March calibration factors, showing only slight differences for the Reformate yield.

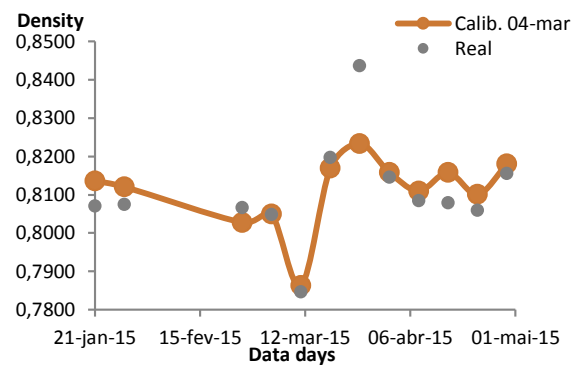


Figure 12 – Prediction with 4th of March Calibration: Reformate Density

As for the Reformate Vapour Pressure and Density, their predictions are adequate, with no significant deviation.

In an overall look, the property showing more differences between the 4th of March prediction and the reality is the Weighted Average Inlet Temperature (WAIT) of the reactors.

3.2. Matosinhos CCR: Un. 3300

The Matosinhos CCR has the following configuration:^[10]

- 4 Reactors
- 1 Feed (Gasolina Pesada Dessulfurada)
- 4 product streams (Net Gas, Stabilized Gas, LPG and Reformate)
- Low Pressure Separator (model: Separator)
- High Pressure Separator (model: Recontactor)
- Recycled hydrogen stream

These configurations are all specified in the base model in a similar way as shown before in point 3.1.

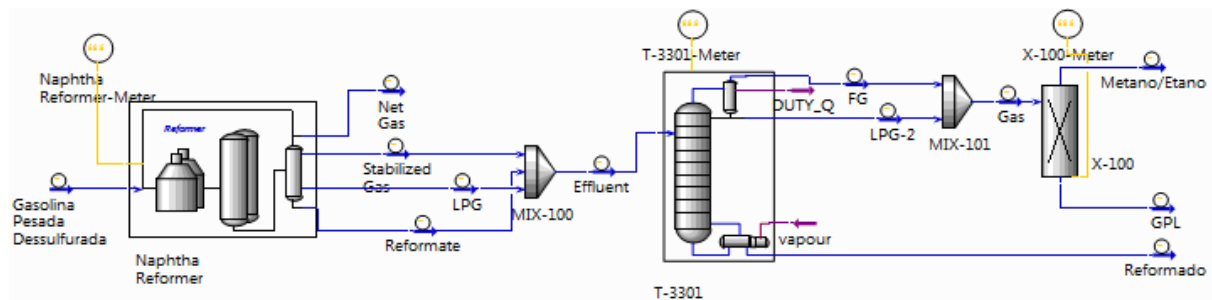


Figure 13 – Final Configuration of Matosinhos Un.3300 Model

3.2.1. Selection of the Best Calibration Set

Now that the model is capable of providing the right separation point for the product streams, is time to choose all days with complete data to run the model and obtain a series of calibration factors matching each day of complete data.

For the Un.3300 it was possible to obtain 13 days of complete data. Performing the calibration of these days, 13 sets of calibration factors were obtained.

As in the Sines PP case, all this sets were then tested in Prediction mode, and their results compared with the real values in order to choose the best calibration set to be used in futures predictions.

Figure 14 shows the outcome of all calibrations sets when predicting the Reformate yield, as an example. The same representation was made for all the other key properties.

Again, a new splitter was added after the Reformer model, to improve the components separation, but in this case a simple splitter was not enough because the separation was still far from the real values. So a more complex column was added instead. This new column is a very simple distillation column where it is now possible to define operating parameter as number of stages, reboiler and condenser pressure and temperature, feed entry and so on.

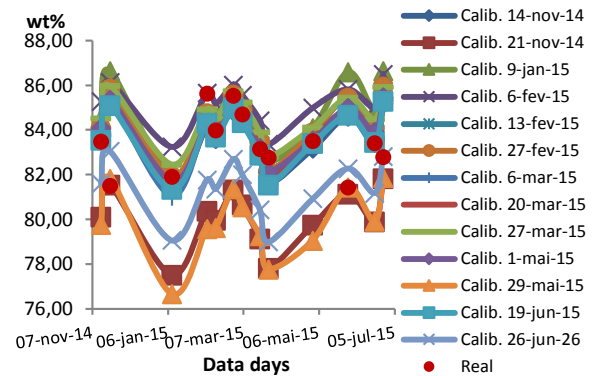


Figure 14 – Prediction with all calibration sets: Reformate yield

As it is easily observed in Figure 14, not all the calibration factors provide an accurate prediction of this property. By analyzing the Prediction results for the key parameters of the unit defined in the beginning of the current chapter it is possible to determine which set of calibration factors is the best to use in future predictions, being the best the one that provides results more accurate with the reality for all the key properties, as defined in the objective function.

3.2.2. Best Calibration: Results and Analysis

The best set of calibration factors for the Matosinhos Un.3300 was the one provided by the 20th of March data.

Figures 15 to 22 show the comparison between the real value and the value calculated by the set of calibration factors from the 20th of March, for the key properties of the Unit.

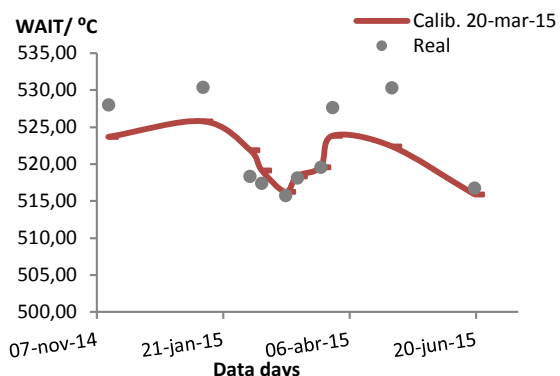


Figure 15 – Prediction with 20th of March Calibration: WAIT

The reactors WAIT presents several deviations in some of the data days, nevertheless this difference is not evident in more than half of the analyzed data.

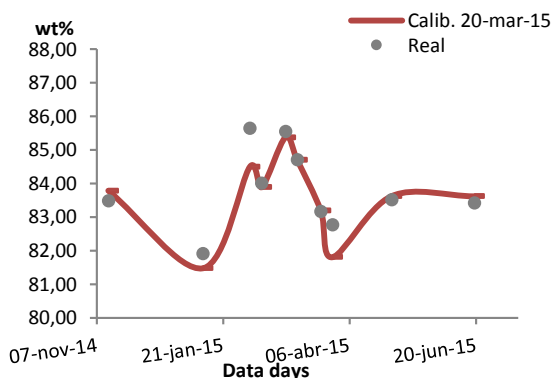


Figure 16 – Prediction with 20th of March Calibration: Reformate yield

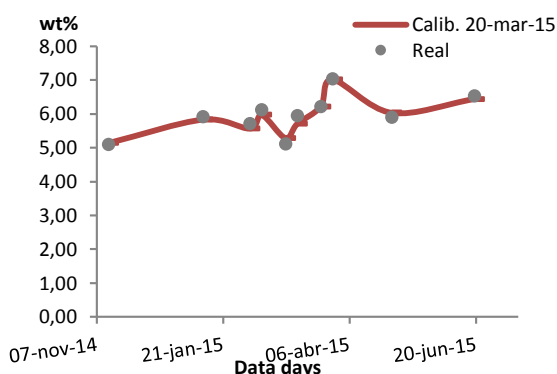


Figure 17 – Prediction with 20th of March Calibration: Benzene yield

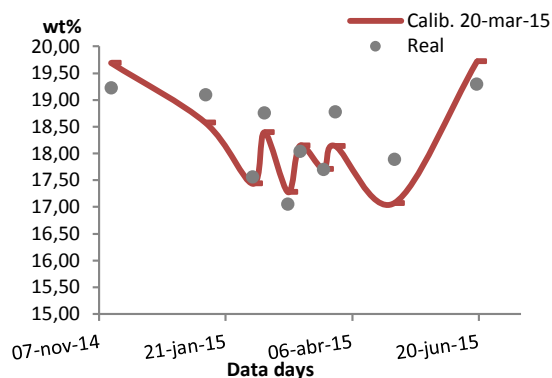


Figure 18 – Prediction with 20th of March Calibration: Toluene yield

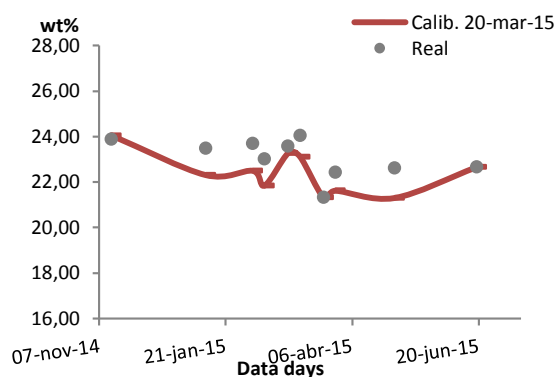


Figure 19 – Prediction with 20th of March Calibration: Xylenes + Ethylbenzene yield

From figure 16 to 19 it is shown the results for the Reformate yield and the yield of the most important aromatic compounds. Looking at these results it is verified that the prediction with the 20th of March calibration factors approaches in a very satisfactory way to the real values. The more significant error is verified for the Xylenes + Ethylbenzene yield.

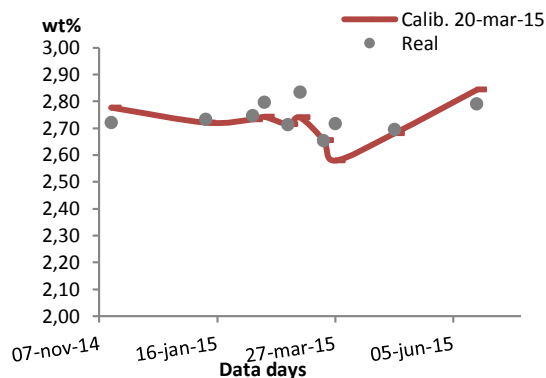


Figure 20 – Prediction with 20th of March Calibration: Hydrogen yield

The hydrogen yield is well predicted with the selected calibration set.

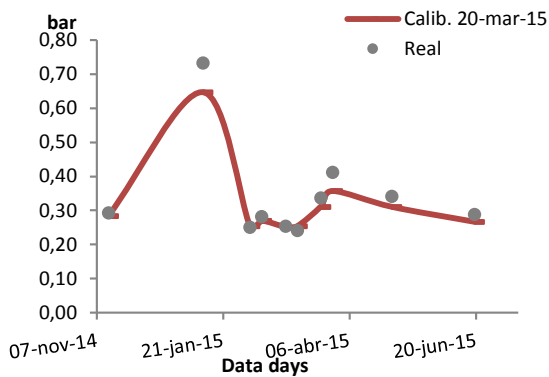


Figure 21 – Prediction with 20th of March Calibration: Reformat Vapour Pressure

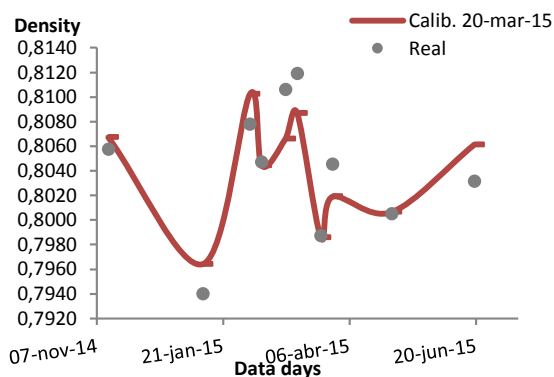


Figure 22 – Prediction with 20th of March Calibration: Reformat Density

At last, the Reformat Vapour Pressure and Density is adequate, showing minor deviation in 2 or 3 days of prediction.

So it is possible to conclude that the set of calibration factors coming from the 20th of March data presents a very good predictions of results to the key properties of the unit, registering the main differences in the WAIT and Xylenes + Ethylbenzene prediction.

4. Linear Programming Model

Nowadays is very common for the refining companies to use Linear Programming Models (LP) for optimization of their activity as well as choice of feedstock, production planning and economic analysis.

At this point the purpose is the development of a vectorial model for the Platforming using Base-Delta representation.

4.1. Linear Representation Model: Basis

Base-Delta representation consists on defining a Base with the most relevant properties

of the reforming units where a variation (Delta) will be applied, registering their effect on the product streams for each variation.

This representation is defined in 3 steps:

1. Chose the most influent parameters in the unit's performance (Feed Properties and Operating Conditions). These parameters will be defined as vectors.
2. Define their base values, that must be representative of the reforming unit;
3. Define which deltas to apply to each vector. (These deltas must be in a linear interval of response in the product streams)

The linear relation between a product property (x) and the feed properties (y) is defined in Equation 4:

$$x_j = x_{j0} + \sum_i \left[(y_i - y_{i0}) \times \frac{1}{\Delta_i} \times \Delta_{i,j} \right] \quad (4)$$

Where,

x_j – Product property by the Linear Model

x_{j0} – Product property in Base conditions

y_i – Feed properties current value

y_{i0} – Feed properties in Base conditions

Δ_i – interval of linearity of Deltas

$\Delta_{i,j}$ – Coefficient that reflects the impact that a Δ_i variation in variable y_i has on x_j .

The next step is to create a template file with data in base-delta representation to be read by the Linear Programming Model.

This template file will be generated with the Petro-SIM LPU (Linear Programming Utility).

To evaluate the template files before they are submitted to the LP Model a Linear Representation Model (LRM) was developed in Excel to test them.

4.2. Building Base-Delta template from LPU

To improve data manipulation in the LP Utility some changes were introduced to the initial simulation model in the form of a new feed, built in order to improve the manipulation of feed

compositions, because if a variation is made in the composition of one component, the remaining components need to be adjusted proportionally to maintain the total composition in 100%.

The manipulated variables will be:

- Feed Flow rate
- Feed C6 to C10 Naphthenic content
- Feed C6 to C9 Aromatics content
- RON

Each manipulated variable will be defined as vectors except for RON that will be defined as discrete bases, because of its non-linearity.

Each vector will have a base value and 3 discrete bases will be settled: RON=98 (base2), RON=100 (base1) and RON=102 (base3).

To generate data, only the RON=100 base was considered as this represents the typical working value of the units (Base 1 in fig. 23).

	Base 1	Base 2	Base 3
Mass Flow Modified Feed [tonne/hr]	114.7	114.7	114.7
C6A (Mass Fractions) Feeder-100	0.0015	0.0015	0.0015
C7A (Mass Fractions) Feeder-100	0.0270	0.0270	0.0270
C8A (Mass Fractions) Feeder-100	0.0620	0.0620	0.0620
C9A (Mass Fractions) Feeder-100	0.0230	0.0230	0.0230
C6N (Mass Fractions) Feeder-100	0.0140	0.0140	0.0140
C7N (Mass Fractions) Feeder-100	0.0930	0.0930	0.0930
C8N (Mass Fractions) Feeder-100	0.1380	0.1380	0.1380
C9N (Mass Fractions) Feeder-100	0.0830	0.0830	0.0830
C10N (Mass Fractions) Feeder-100	0.0140	0.0140	0.0140
Target C5 Plus RONC Naptha Reformer	100.0	98.00	102.0

Figure 23 – PL Model Bases

Additionally it is necessary to define which deltas to apply to the selected Base properties.

Property	Base Value	Up Delta	Down Delta
Mass Flow	114.7	24.0	17.0
Feed C6A	0.0015	0.0017	0.0002
Feed C7A	0.0270	0.0230	0.0060
Feed C8A	0.0620	0.0125	0.0125
Feed C9A	0.0230	0.0145	0.0145
Feed C6N	0.0140	0.0120	0.0030
Feed C7N	0.0930	0.0560	0.0080
Feed C8N	0.1380	0.0640	0.0240
Feed C9N	0.0830	0.0390	0.0100
Feed C10N	0.0140	0.0110	0.0110

Table 1 – PL Model Deltas (Mass Flow: tonne/h, following: mass fractions)

Petro-SIM™ LP Utility will now calculate the results for the previously selected streams, for each base and then for each delta using the RON=100 base, presenting the results in a

matrix of data, called base-delta matrix, that contains the values for the impact that a variation in a feed property has on a product property.

4.3. Development of the Linear Representation Model and Results

From the base-delta matrix it is now possible to build the Linear Representation Model (LRM) applying Equation 4 to all product properties wanted, predicting their value by the LRM.

Figures 24 to 27 present a comparison, for the main product properties, between the real value and prediction by the LRM and the simulation model for Sines Platforming Unit.

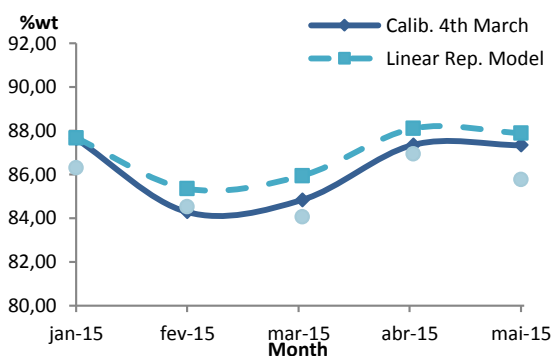


Figure 24 – Linear Representation Model: Reformate Yield

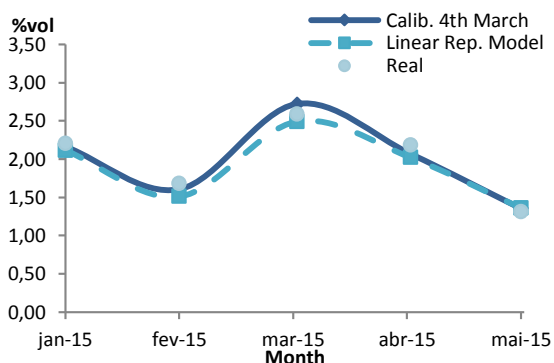


Figure 25 – Linear Representation Model: Benzene volume content in Reformate

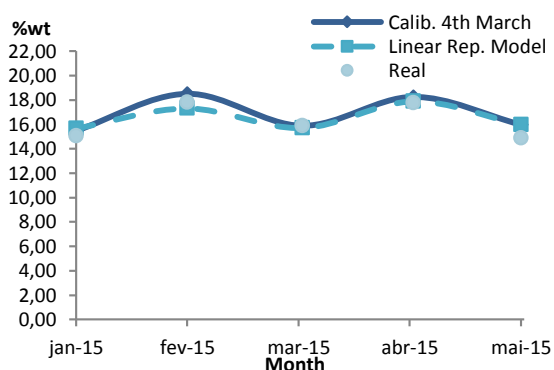


Figure 26 – Linear Representation Model: Toluene Yield

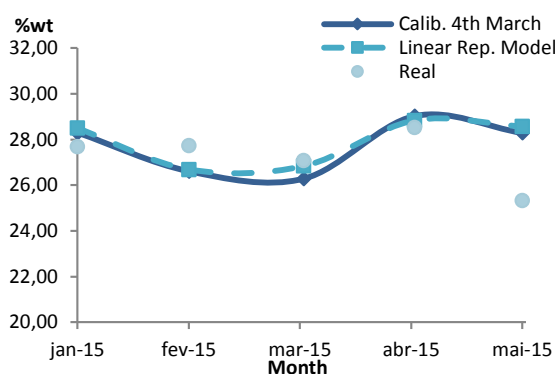


Figure 27 – Linear Representation Model: Xylenes + Ethylbenzene Yield

It is possible to see that the Linear Representation Model presents some deviations mainly when predicting the Reformate stream yield, giving however good results for the prediction of Benzene content and Toluene and Xylenes + Ethylbenzene yields.

5. Main Conclusions

In this work, two simulation models were developed for the CCR Platforming Units of Galp Energia. After that a Base-Delta representation was developed in order to integrate the Reforming Units in the Linear Programming Model of Galp Energia with this kind of representation.

The first one – Sines Unit (PP) – presented very good results when comparing the simulation predictions with the reality, becoming now a better tool for prediction and follow-up of the unit. The main differences appear when predicting the WAIT, nevertheless even for this property the developed model is an improvement.

The second one – Matosinhos Unit (Un.3300) – presents an adequate representation of the real unit, but shows some differences from the reality. Despite these differences the new model is an improvement to the one nowadays used.

At last the development of Linear Representation Models allows the study of the

impact that a base-delta representation for the Platforming Units will have in the Linear Programming Model (LP) of Galp Energia. The LRM for Sines unit presents good results in terms of result prediction, being solid enough to further implementation on the LP Model. As for Matosinhos LRM it is necessary to introduce some improvements in the model before its implementation, for instance in the ranges of linearity of the applied deltas.

The developed models main purpose is to update and improve the existing models for these units, being an essential tool to follow-up the unit and even be used for troubleshooting.

6. Main References

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