Modelling of a Vacuum Distillation Column at Sines Refinery

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ABSTRACT

This work addresses the modeling of a vacuum distillation unit at Sines refinery, the vacuum distillation unit II (VDU II), using Petro-SIM as process simulator. To accomplish this task, two distinct models were built: a DISTOP model, which is a simplified model, and a tray-to-tray rigorous model.

From the DISTOP model developed in this work it is possible to conclude that it leads to an improvement in the unit representation, and thus in the prediction of the properties of its products, when compared with the current model used by Galp. On the other hand, the tray-to-tray model built is able to satisfactorily predict the VDU II performance, although due to the low fractionation found between the light vacuum gasoil and the heavy vacuum gas oil it was necessary to manipulate the Murphree efficiency, which led to some deviations from the plant data. Thus, further studies are necessary to identify the causes of this low efficiency. Nevertheless, the tray-to-tray model developed is a good starting simulation tool for this distillation unit.

Keywords: Refining, Vacuum distillation columns, Modelling, Petro-SIM, DISTOP model, Tray-to-tray model.

1. Introduction

In the Petroleum refining industry, one of the most important, competitive and challenging on the world, it is crucial to minimize overall operational costs. To reach this goal models are developed to help select feedstock, evaluate the obtained products and troubleshoot and optimize the performance of individual refinery processes.

The distillation processes have a determinant role in the refining process as it separates the crude oil into fractions, which are subsequently processed in other units or sent to storage. This is an intensive energy operation and as such the economic benefits of an improvement can be substantial. Furthermore, the growing necessity of crude oil heavy fraction valorization makes the vacuum distillation a process that should be studied and optimized.

1.1. Objectives

The objective of this work was to model the vacuum unit II of Sines refinery (VDU II) using the process simulator [TM]Petro-SIM to develop two distinct models: a simplified model designated by [TM]DISTOP and a tray-to-tray rigorous model. The DISTOP model is used by Galp to generate data to feed the linear program model, used to select feedstock and to plan the refinery process. So, it becomes essential to have a constant monitoring and update of these models. On the other hand,

REGISTERED TRADEMARK REFERENCE: Petro-SIM and DISTOP are trademarks of KBC Advanced Technologies plc

the rigorous tray-to-tray model goal is to be used by process engineers as a troubleshooting tool in order to improve the unit performance.

2. Bibliographic review

2.1. Evaluation of petroleum fraction quality: Distillation test

Due to the complexity of its composition, the physical and chemical properties of a crude oil or petroleum fraction are usually evaluated by a set of laboratory tests called crude assay.

The distillation test is one of the most relevant tests and it is used to obtain the distribution of boiling points in order to characterize a sample's volatility. The results of this test are normally presented as a distillation curve showing the boiling temperature as a function of the distilled percentage.

2.1.1 True boiling point distillation

A true boiling point distillation (TBP) is obtained through a batch distillation test (ASTM 2892), in which the apparatus has 15–18 theoretical trays and operates with a 5:1 reflux ratio.

2.1.2 ASTM distillation

ASTM distillation is essentially a batch distillation with one equilibrium stage and no reflux and so with a minimum fractionation.

For light cuts (gasoline, kerosene and diesel) the distillation is run at atmospheric pressure under ASTM D86 test. For heavier fractions, the distillation is carried out under vacuum and using the ASTM D1160 test [2].

2.1.3 Distillation simulated by gas chromatography

The ASTM distillation is a quick test but is not a consistent one so it has often been replaced by the distillation simulated by gas chromatography (Dsim), which is a simple but accurate method.

The boiling point distribution of a crude oil or fraction can be determined by an injection of a sample in a gas chromatograph, which separates the hydrocarbons in boiling point order. Then the retention time is related to the boiling point through a calibration curve. The results of this test are comparable to the TBP distillation test [1].

In this work this type of distillation was conducted under the test ASTM D7169, in which is possible to determinate the distribution of boiling points up to temperatures of 720°C.

2.2. The Vacuum Distillation Unit II of Sines refinery

The Sine's refinery vacuum distillation unit II (VDU II) processes atmospheric residue in order to obtain distillate, light gas oil (LVGO), heavy gas oil (HVGO) and vacuum residue (RV). This unit is equipped with five packing beds – distillate bed, fractionation bed, LVGO bed, HVGO bed and wash section – and with 9 trays in the stripping section.

The feed of the VDU II is preheated in a heat exchanger train and then partially vaporized in a furnace before entering the column flash zone. The furnace effluent enters the flash zone through a transfer line with a large diameter, where a substantial amount of vaporization occurs due to big changes in pressure, resulting in a temperature decrease of 10°C [3].

It's relevant to mention that refinery distillation columns usually operate with pumparound streams, which is a liquid fraction that is withdrawn from the column, cooled and re-injected a few trays above. Pumparound streams increase the internal reflux, improve the thermal efficiency of the column and consequently decrease the duty required in the furnace.

Moreover, there are some important VDU II operation details that are worth to mention [3]:

• In the stripping section, due to the high temperatures (±400°C) and the long residence time (±15 min) which lead to cracking reactions, the residue from the vacuum unit I is used as quench fluid.

• The vapours from the flash zone pass through a wash and fractionation zone where the heavy materials that are entrained by the vapours are removed using HVGO as wash fluid (wash-oil). The wash-oil removed from the unit is recirculated to the furnace in order to avoid product losses.

• The column operates with three pumparounds that correspond to the withdrawal of distillate, LVGO and HVGO.

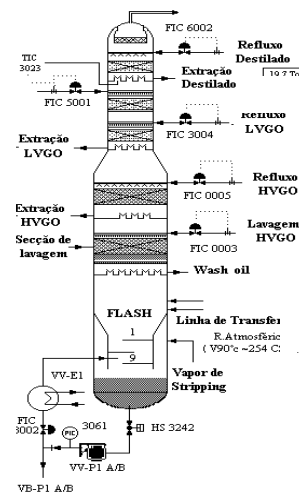Figure 1 presents a simplified representation of the VDU II.

Figure 1 – VDU II schematic [3].

2.2.1 Fractionation

The degree of fractionation in a distillation column is defined as the difference between the ASTM 5% boiling point of the product and the 95% point of the lighter product. When this difference is positive, we have a gap indicating good fractionation, while a negative difference is called an overlap indication that some light product is still in the heavier product and vice versa, creating tails in the distillation curves [1].

3. VDU II modelling: overview

In order to achieve the objectives proposed for this thesis it was used the process simulator Petro-SIM (PS), a KBC Advanced Technologies plc's software.

As previously referred, for the VDU II modelling process two distinct methods were

considered for the column resolution – the DISTOP and the tray-to-tray. To feed these models data from products analysis and operating conditions were used, synthetizing the feed from the products stream in a process called Back Blending.

The models development, as shown in figure 2, involved two distinct steps: calibration and prediction. In the calibration mode, information from the feed, products and operating conditions is known and the calibration factors are calculated in order to achieve an adequately representation of the unit under study. In prediction mode, the operating conditions and the calibrations factors (calculated in calibration mode) are known and the model is able to predict the quality of the products for different scenarios.
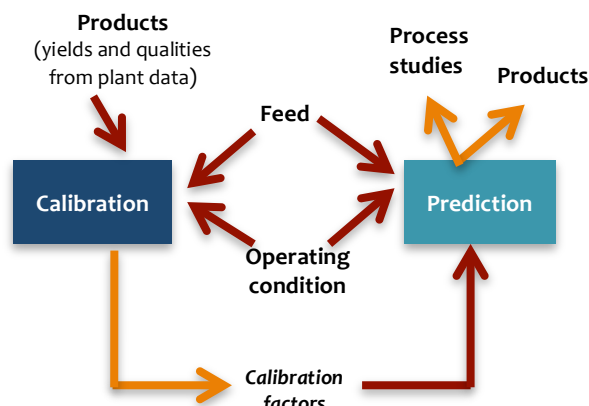

Figure 2 – Calibration and prediction

4. DISTOP model

DISTOP is a section-by-section[2] column solving method. This is a robust method with a quick convergence and an automatic calibration option therefore is very used in refineries simulation.

4.1 Automatic calibration

The automatic calibration option of a DISTOP column allows the model to easily adjust its calibration factors in order to match the observed performance.

There are four calibration factors used to adjust the fractionation performance in these models: section efficiency or base interchange parameter (BIP), stripper efficiency, front shape factor and back shape factor.

• **Section efficiency or BIP:** The section efficiency is the average efficiency of trays in the product section and affects the quality of the fractionation between two contiguous cuts and therefore the shape of the distillation curves. On the other hand the BIP is a multiplicative factor

that tune the quality of the fractionation in a column section. The BIP and the section efficiency are related and therefore fixing one of theme the other one is calculated.

• **Stripper efficiency:** The stripper efficiency is the average efficiency of trays into the product stripper and affects the strip-out of light boiling material into the product and the temperature drop across the stripper.

• **Shape factors:** In general, the front shape factor affects the 1% and 5% points of the product, while the back shape factor affects the 95% and 99% points of the next lighter product.

An increase in the front shape factor of a product reduces the amount of its light components and increases front-end distillation temperatures. On the other hand, an increase in the back shape factor reduces the amount of heavy components in the adjacent lighter cut and decreases its back-end distillation temperatures.

4.2 VDU II modelling

4.2.1 Required data

It was necessary to collet and analyse sets of operating and analysis data in order to build the DISTOP model. Data required to run DISTOP model are presented in table 1.

Table 1 – Required data for DISTOP model development.

Flow rate	• Feed • Products • Pumparounds • Stripping steam
Pressure	• Top of column • Bottom of column • Flash zone
Temperatures	• Top of column • Bottom of column • Flash zone • Products • Pumparounds • Stripping steam
Analysis	• Products distillation curves • Products gravity • RV viscosity

Distillation curves used in the DISTOP model calibration were obtained by the ASTM test - D86 for the distillation and D1160 for LVGO and HVGO, while the RV's quality was estimated by Petro-SIM since its distillation curve was not performed in the laboratory.

4.2.2 Model development

The model was initially implemented with the number of theoretical trays of each bed as well as the correspondents to the stripping section and considering a combined feed stream of

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[2] In petro-SIM the sections are defined by the draw locations.

atmospheric residue and wash-oil, a stripping steam stream, 5 product streams – overhead product, distillate, LVGO, HVGO and RV – and 3 pumparounds. The quench process, accomplished by the residue from the vacuum distillation unit I, was represented outside the column. Since the feed is synthetized through data of its products, the effect of the quench vacuum residue in the quality of the RV produced in VDU II is already being accounted, as well as its contribution to the gas oil recovery.

As previously mentioned in a DISTOP model the calibration is done automatically by the model, which calculates the calibration factors in order to adjust the fractionation. So, to obtain representative values for these factors it was necessary to use several data sets to calibrate the unit.

In order to choose the best configuration for the model it was evaluated the effect that the number of trays in a section has on the products properties and yields. From this evaluation it was possible to conclude that in general the effect is not very significant and quite compensatory, since DISTOP is a section-by-section solver. Thus, the final configuration is the one that leads to the best compromise found between the calculated key distillation points (5, 10, 50, 90 e 95%), density, viscosity and yields of the products. Figure 3 presents the chosen configuration.
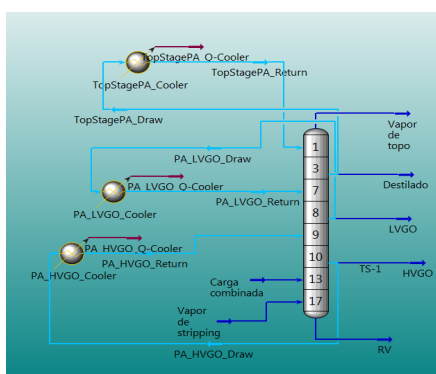

Figure 3 – DISTOP model configuration.

The obtained results were analysed, discarding the days that did not guarantee a mass balance closure with an error lower than 5% or an acceptable absolute deviation in the properties of the products. Then, several sets of calibration factors (FC), that result from the average of the FC obtained in each used data set, were considered in order to choose the one that leads to the best fit between the model and the plant data.

Finally, the chosen FC were the ones that guarantee the lowest deviation from the plant data in the key distillation points, usually not

higher than 10°C[3], while ensuring a deviation lower than 0.01 g/cm³ [4] for the densities and lower than 2 wt.%[4] for the yields and at the same time the lowest deviation possible for the viscosity of RV.

After the FC set that best represent the VDU II had been chosen the performance of the model build with these FC was compared with the model currently used by Galp. This comparison is presented in the next section.

4.2.3 Results and discussion

By analysing the fitting to the plant data of the properties and yields predicted with the current calibration (current FC) and with the new calibration (chosen FC) over the time period selected for the calibration it was possible to conclude that the model built along with the new calibration factors leads to a better representation of the VDU II.

Figure 4 exemplifies the improvement obtained in the distillation curves with new calibration for the data sets collected during one labour day. In this figure is represented the real distillation curves along with the ones predicted by the current calibration and the new calibration. As it easily observed, the new calibration eliminates the deviations found between the real and predicted values on the distillate key points 90-95%, decreasing the deviation[4] from 14°C to 5°C and to 1°C respectively. For the HVGO distillation curve the new calibration reduces the deviation found in the beginning of the curve from 19°C to 2°C at the point $T_{5\%}$ and from 12°C to 2°C at the point $T_{10\%}$. Regarding the LVGO curve both calibration result in a good adjust between real and predicted data.
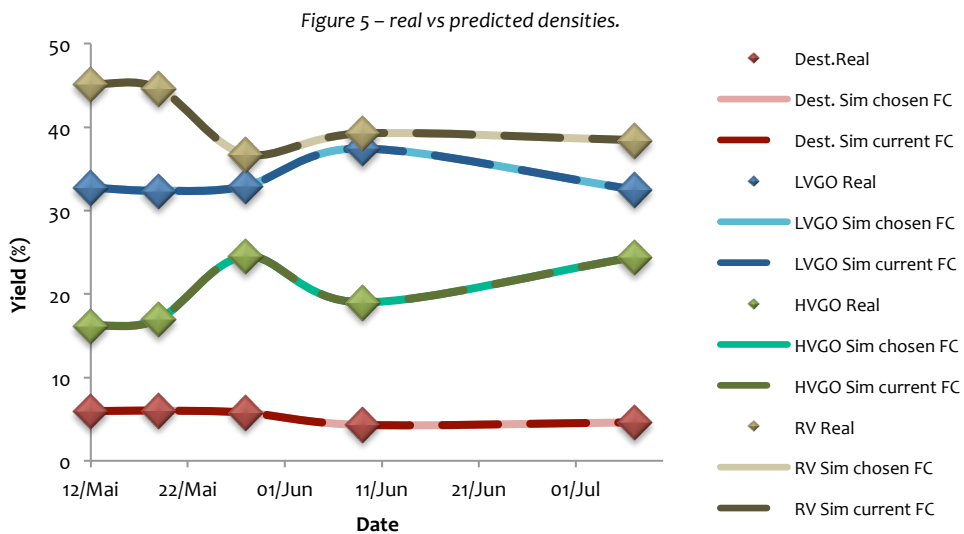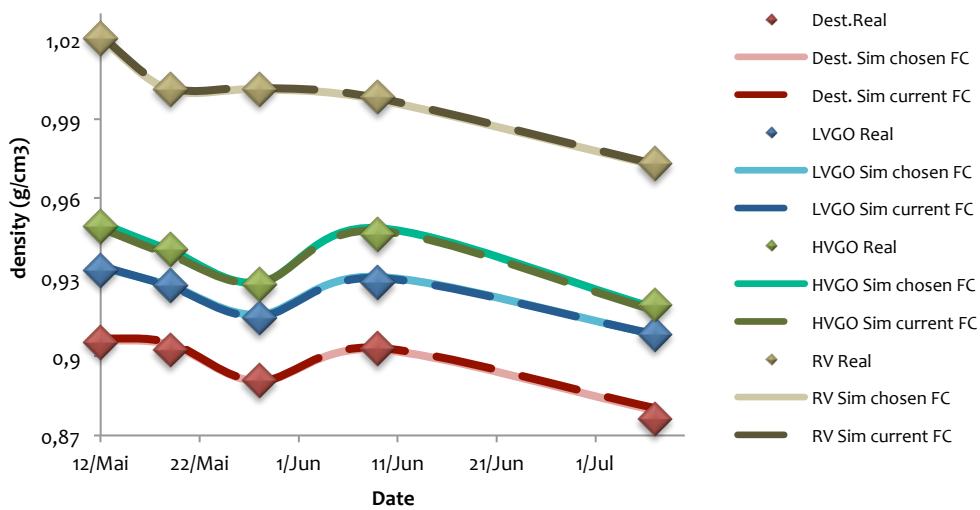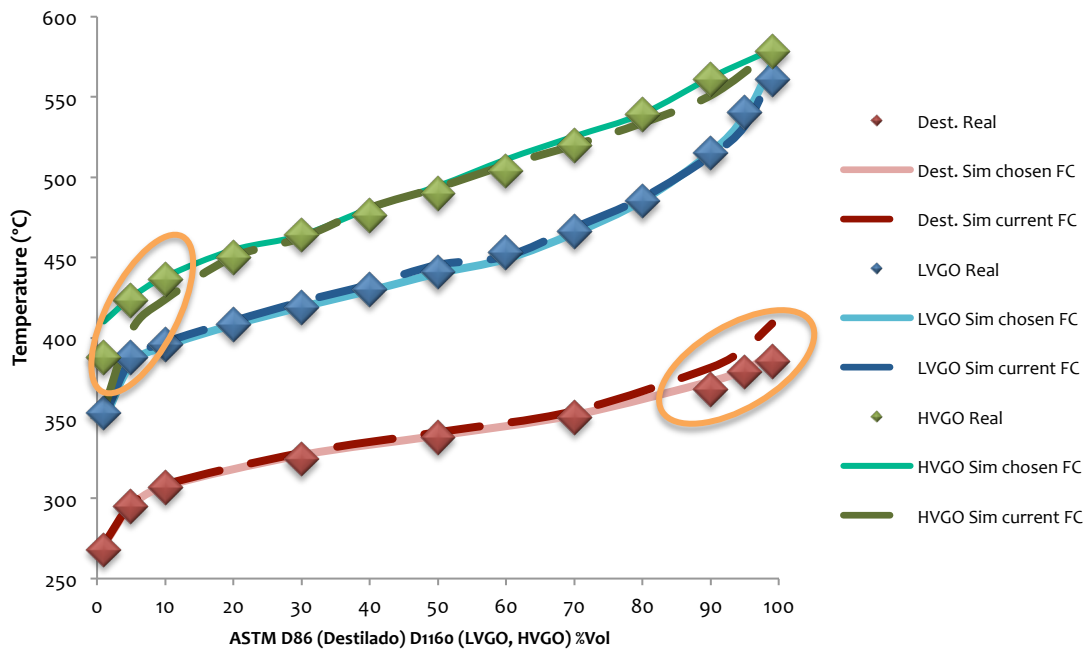
Regarding the density and yields of the products, both calibrations results in a good adhesion to the real data, as shown in figure 5 and 6 respectively, leading to a deviation lower than 0.01 g/cm³ on the densities and lower than 2 wt.% on the yields.

Finally, for the viscosity of RV, as shown in figure 7, the new calibration allows a slightly approximation to the plant data, resulting in an average deviation[5] that is about half the one obtained with the current calibration (AAD = 52 cSt *vs* 147 cSt). It should be noticed that the viscosities of the heavier fractions are very difficult to simulate, leading in general to inaccurate results due its dependence on the chemical composition [4].

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[3] Values considered acceptable by Galp.

[4] $AD = |real - predicted|$

[5] $AAD = \frac{1}{n}\sum|real - predicted|$

Figure 4 – Real vs predicted distillation curves correspondent to the data of 12th of May 2014.

Figure 5 – real vs predicted densities.

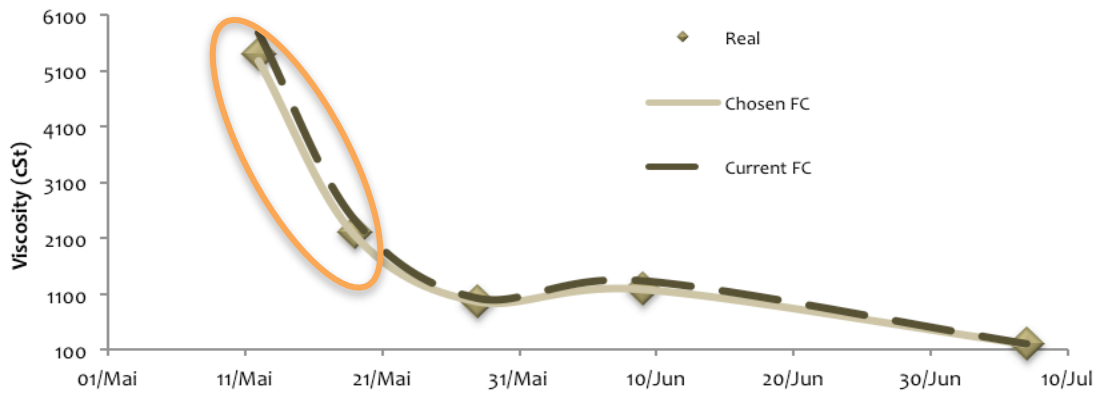*Figure 6 – real vs predicted yields.*

Figure 7 – Real vs predicted RV viscosity.

5. Tray-to-tray rigorous model

The tray-to-tray model (T2T) is used for the rigorous simulation of the column operation thus being a good tool for troubleshooting and optimisation.

5.1 Calibration

T2T models are implemented using ideal stages, however in a real column the liquid and vapour leaving the tray are not in equilibrium. Thus, to fit the model to plant data it is necessary to adjust either the number of ideal stages in each column section or the Murphree efficiencies. In practice, adjustments in Murphree efficiency should be avoided because usually liquid composition on the tray is not uniform[6], especially for large diameter columns. Its use should then be restricted to cases in which the section can be represented by one stage (or less) or when the only acceptable correspondence to the fractionation is found between two adjacent trays [6]. Efficiencies lower than one can lead to the entrainment of some heavy material through the column as well as the presence of some vapour in the products streams.

5.2 Model structure: Transfer line

The transfer line has a large diameter before entrance in the flash zone, which leads to a separation between the liquid and vapour phases. The liquid and vapour entering the flash zone of the column are not in equilibrium and the high velocities attained in this line leads to a substantial amount of liquid particles entrained in the vapour entering the flash zone. Furthermore, the transfer line vapour becomes superheated due to pressure reduction as the vapour approaches the flash zone which increases the wash-oil flow rate needed to prevent coking in the wash section,

since the superheated vapour tends to vaporize the wash-oil flowing through the bed [7].

So the process simulation needs to account for phase separation in the transfer line and the associated non-idealities. A model without this representation can over-predict vacuum gas oil product yield by 3-6 wt.% on whole crude and under-predict the wash-oil flow rate needed to prevent coking by as much as 300%[7].

5.3 VDU II modelling

5.3.1 Required data

Galp works with a wide variety of crudes with different characteristics. This variety is associated to different operating conditions, which in the case of VDU II may lead to the use or not of the residue from the vacuum distillation unit I as a quench stream.

Therefore it was build a T2T model for each situation using two data sets obtained in two different labour day. For those days the distillation curves were performed under the Dsim test in order to obtain the RV curve as well (with the exception of the distillate that remained under ASTM D86 test). The first data set was used to build a model in which the cooling of the RV is represented outside the column (case 1), while the second data set was used to build a model in which the quench stream is represented as a second feed (case 2). To build these models, in addition to the data previously required for the DISTOP model, it was necessary to collect information about the furnace inlet temperature and pressure (to simulate the transfer line), as well as the flow rates of the reflux to the fractionation bed, of the HVGO used as wash fluid and of the recirculated wash-oil.

5.3.2 Case 1: quench represented outside the column

5.3.2.1 Model development

The high vapour velocities low liquid levels of vacuum columns stages deviate the performance

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[6] Murphree efficiency assumes that the vapour between trays has uniform composition as well as the liquid on the tray, which has the same composition that the liquid leaving the tray.

of a real VDU from that predicted considering an ideal vapor-liquid-equilibrium. So, in the development of T2T models the first step was to adapt the DISTOP configuration. This adaptation is based on the recommended number of trays for each section of a vacuum column [6].

Then, in order to achieve a solution for the column (converged column) it was necessary to choose the variables that the model should use in their calculations.

With the converged column the transfer line was simulated, representing the pressure drop and the phase separation associated with this line. Since the model was predicting a better fractionation then really happens in the VDU II (see figure 9), especially for LVGO/HVGO fractionation, it was necessary to tune the model. The calibration of a T2T column is a long iterative process. For each column section it was necessary to change the number of ideal stages in order to achieve the fractionation observed in the unit. However, to fit the shape of the HVGO curve it was necessary to adjust the Murphree efficiency in its section, since even with one theoretical tray the key points of the calculated curve still did not fit the plant data.

It should be noticed that during the calibration process it was also necessary to consider the stripping section as a separated unit, as shown in figure 8, in order to adjust the RV properties and the fractionation between RV/HVGO.
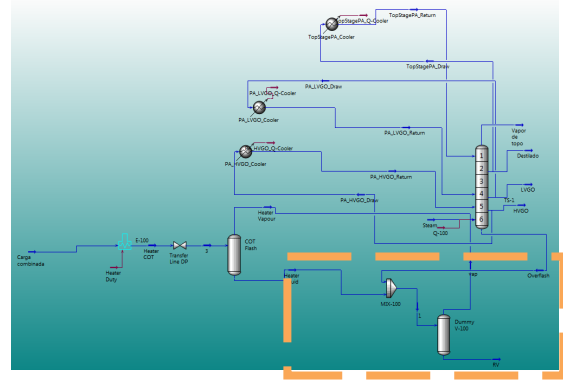

Figure 8 – Final configuration of the model.

5.3.2.2 Results and discussion

The final configuration of the model corresponds to the best compromise found between the operating conditions and product qualities.

The real and simulated distillation curves, before and after the calibration (Sim vs Sim tuning) are represented in Figure 9, where it is possible to notice a clear improvement in the fit to the plant data namely in the back-end of the distillate and LVGO curves, in the HVGO curve and even (although slight) in the first points of the RV curve. For the end of the distillate and LVGO curves an average deviation reduction of 13°C and 34°C were obtained respectively, while the begging of the RV curve shows a reduction of 26°C. The HVGO curve, on the other hand, shows an average deviation of 16°C.
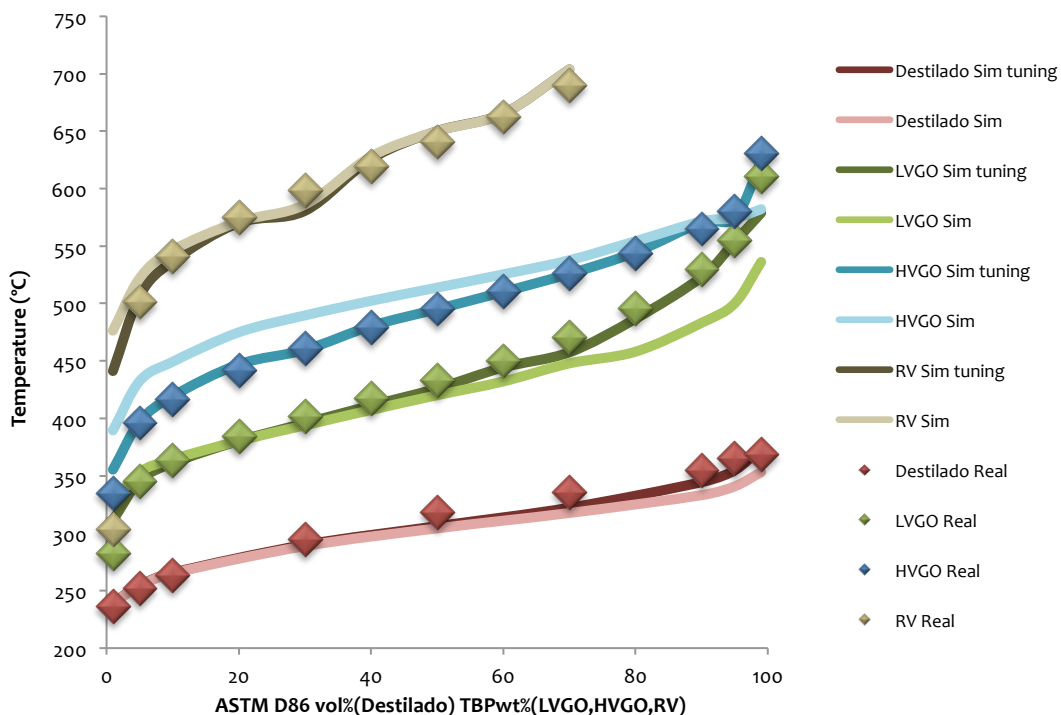

Figure 9 – Real vs predicted distillation curves.

In table 2 it is possible to observe a reduction in the deviation of the LVGO/HVGO fractionation from 92°C to 2°C with the model after tuning. There is also an approximation on the predicted temperatures resulting in a reduction in the distillate temperature deviation from 47°C to 25°C and in the RV temperature from 102°C to 58°C. It should be remembered that the RV cooling is represented outside the column in this case. It is worth enhancing that the deviations found between the calculated values and the plant data are result of the compensations made by the model so that it can reach the values of the variables chosen to solve the column (fixed specs).

Table 2 – Main results.

		Real	1st solution	Deviation	Model after tuning	Deviation
Product flow rate (ton/h)	**Distillate**	21.07	21.07	0.00	21.08	0.01
	LVGO	91.25	91.25	0.00	91.29	0.04
	HVGO	55.33	55.33	0.00	55.36	0.03
	RV	160.18	160.07	0.11	159.92	0.26
Temperatures (°C)	**Distillate**	178	131	**47**	133	**25**
	LVGO	244	243	2	239	6
	HVGO	306	320	14	283	22
	RV	325	223	**102**	383	**58**
Gap/Overlap (°C)	**T$_{5\%}$ HVGO–T$_{95\%}$ LVGO**	-159	-67	**92**	-157	**2**
	T$_{5\%}$ RV–T$_{95\%}$ HVGO	-88	-65	**23**	-68	**20**

5.3.3 Case 2: quench as second feed stream

5.3.3.1 Model development

It was used the final configuration of case 1 along with the data set corresponding to the second labour day. For this day analysis for the quench residue were performed as well, making possible to simulate this stream as a second feed.

Due to the introduction of this stream it was necessary to increase the number of ideal stages in the distillate section in order to adjust its fractionation and also consider the entrained heavy material present in the recirculated wash-oil, to match its flow rate, as shown in Figure 10.
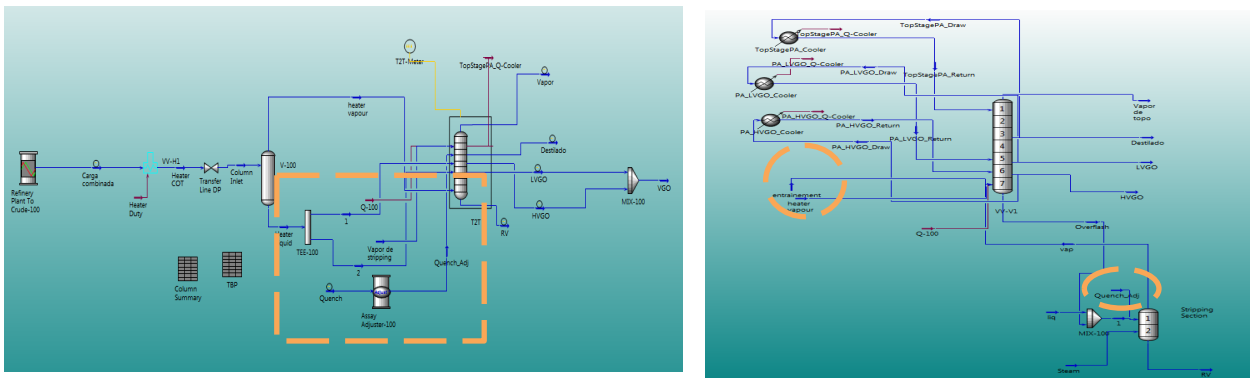

Figure 10 – Model configuration.

5.3.3.2 Results and discussion

The distillation curves represented in figure 11 shows a good fit between the model and the plant data. Even in the zones where there are less effective adhesion - the beginning of the RV curve, the end of the LVGO curve and the middle of the distillate curve – the deviations in the key distillation points are below 12°C. Figure 11 also shows the difference in predicted curves with and without adjusting the Murphree efficiency of HVGO section (Sim vs Sim ef.Murphree=1) and from that it is possible to conclude that this efficiency leads to a good fit in the HVGO and LVGO curves.
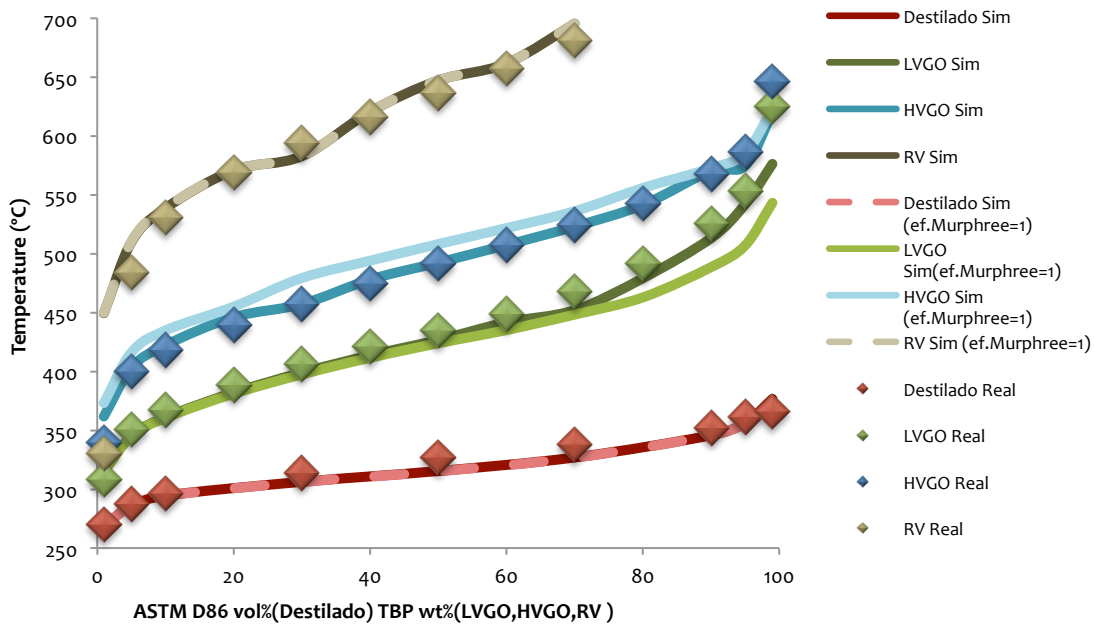
Figure 11 – Real vs predicted distillation curves.

Table 3 shows that the predicted degrees of fractionation between LVGO/HVGO and HVGO/RV have values close to real data (AD of 13°C and 14°C respectively), which enhances the good representation of the VDU II fractionation achieved. The calculated temperatures show acceptable deviations as well and it can be noticed that the deviation of RV temperature (20°C) is much lower than the one found in case 1 (quench outside the column).

From the T2T models developed it is possible to conclude that, in general, a good representation was achieved for the VDU II fractionation. Despite some encountered deviations, satisfactory results for the operating conditions of the column were obtained as well resulting in a good initial simulation tool for the unit.

It should be noticed that, according to KBC, converged T2T columns normally require little tuning to give acceptable results. However in the VDU II case the tuning was more complex, as it was necessary to adjust the Murphree efficiency in order to match the LVGO/HVGO fractionation, for which a quite pronounced overlap was found. Therefore, it would be important to ascertain whether this fractionation corresponds to the column normal operation, since LVGO and HVGO is mixed before entering another unit, or if this low efficiency is related to mechanical problems.

Table 3 – Main results.

		Real	Model	Deviation
Product flow rate (ton/h)	**Distillate**	13.09	13.09	0.00
	LVGO	110.95	110.95	0.00
	HVGO	65.81	65.81	0.00
	RV	160.88	160.82	0.06
Temperatures (°C)	**Distillate**	177	162	14
	LVGO	252	241	11
	HVGO	314	288	**25**
	RV	334	314	20
Gap/Overlap (°C)	**$T_{5\%}$ HVGO–$T_{95\%}$ LVGO**	-153	-139	13
	$T_{5\%}$ RV–$T_{95\%}$ HVGO	-103	-79	**24**

6. Conclusions and future perspective

In this work two models were developed for the VDU II, which are two important tools for simulation and optimisation of the unit.

As to the DISTOP model developed, it was found a good fit between the predicted results and the plant data thus improving prediction of the products properties when compared with the DISTOP model currently used in Galp.

For the T2T models it can be said that the models built in this work offer a good basis for the detailed simulation of the column.

However, it was necessary to decrease the HVGO section's efficiency resulting in a lower value than the expected for a normal operation in a vacuum column (typically 2 theoretical trays) [4,6]. This reduction in the efficiency can be related with the extremely poor fractionation found between the LVGO and the HVGO (overlaps of -155°C) or may be a sign of the existence of dry sections, coke formation, preferred flow paths or some damage in the distributors.

Thus, it would be interesting to evaluate the results of the model when replacing the LVGO and HVGO streams for the vacuum gas oil stream (VGO). This will allow the removal of more trays in order to adjust the model fractionation leading perhaps to the use of the standard value for the Murphree efficiency. On the other hand, it would be important to assess if the variables used for the model convergence are in fact the most suitable ones because, for example, one variable can be measured with less precision than other, thereby ensuring that the specs used in the column are the most reliable and relevant ones for the column operation. A day-to-day operation view would be crucial to the improvement of the model.

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