MODELING, SIMULATION AND ANALYSIS APPLIED TO A NAPHTHA STABILIZER TOWER

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ABSTRACT

The use of simulation and analysis in the unit operation has the objective of checking the operation of an equipment under specified conditions and perform a possible operation optimization using many different tools. One of the objectives is to get the specification data of naphtha stabilizer tower and resorting Aspen HYSYS® commercial software. Applying this software it was possible to find the convergence of this process. The specified temperature of outlet stream in the heat exchanger was changed to have a possibility of getting the equipment convergence. Thus, the profile of the product streams was obtained for this operation, checking contamination of light chain by the presence of NBP 11, NBP 26, and NBP 40. Changing the temperature profile of the tower, could observed the decrease of contamination, which is already a desired result.

Keywords: Simulation, analysis, operation optimization, naphtha stabilizer tower.

1. INTRODUCTION

The Petroleum is used since ancient times for different purposes. The society started its application for simple purposes of medical use and building construction, and over time, their purposes has been expanded, mainly from the nineteenth century, with the advent of Petroleum wells.

Today, compounds obtained by purification have application in several areas, and he is best known for use as fuel, such as natural gas, gasoline and diesel.

Although these compounds have high recognition, naphtha is the most important. It has a composition similar to gasoline, but its energy use is not feasible, but due to their wide application, to obtain fuels, as well as compounds for the application in several process industries, has high value.

Because of this importance it is necessary a high control in their production, by performing the separation of the lightest compounds in its mixture through a distillation column known as naphtha stabilizer tower.

This control intended to keep the quality to ensure the maximum production, but this requires high costs, which makes modeling and simulation tools quite attractive.

Garcia (2009) defined a modeling being *the mathematic abstraction of a real process*. The statement of Chapra and Canale (2008) complements this theory, indicating that *modeling is a formulation that presents the essential features of a physical system or process in mathematic language*.

The major difficulties of these tools are the large number of environmental factors influences, as well as naphtha's infinite composite components number. These situations can be overcome with the use of commercial software, which are designed to simulate or simplify these problems, especially with the components creation based on the common characteristics of the substances in the mixture to be studied.

The operating systems evolution and the source codes simplification allow to obtain simpler and more accurate software, which made them very attractive in the industrial environment.

Despite to this facilitation, analysis of these simulations is still needed and is one of the more complex steps. This allows to define the success or failure of the experiment and requires extensive technical knowledge of the subject, and sometimes extreme attention to the smallest details.

The detailed analysis allows the identification of points in the process to be optimized, ensuring energy economy, raw material and process for low maintenance costs and equipment.

Publications related of modeling, simulation and analysis, as opposed up to the three decades ago, seek to optimize processes that exist today. Despite of this goal, few studies allow for a thorough analysis of the results obtained by the lack of information regarding the experiment.

The reason behind this information's absence is the treatment given to the process simulation as a secondary step, insignificant when compared to the study of a controller.

Today, mostly articles have as main objective obtaining or applying different controllers. As examples are the publications of Almeida Neto, Odloak and

Rodrigues (1999) and Ventin (2010), which seek to replace the employed controller for source codes with better response time and more robust results.

Few studies of simulation and analysis in chemical processes have been published in the last decade. Due to the expansion of this tool, the use of simulation in other areas is allowed, and a greater attention is generated to optimization studies of administrative systems and other scientific fields. The publication examples are the publication of Silva (2002), which deals the simulation for accelerated analysis of the air traffic, and Bleicher et al (2002), who seek a better learning method of the sound waves operation through mathematical and computational study, listing the frequencies of musical scales and different beats.

For industrial plants equipments simulation, has been seen more papers involving controller innovations, as the cited works and Marquini et al (2007), which demonstrate a simulation of a distillation system in a ethanol production. There are also works who seek study chemical treatments, escpecially recovery methods, as has Sadighi et al (2009), that seeks recovery of naphtha.

Maitelli et al (2006) presented at the 2006 *Rio Oil & Gas* Conference a naphtha stabilizer tower simulation and the application of a control that would provide greater profitability than that used in the Potiguar Clara Camarão Refinery, located in the Guamaré city, Brazil.

This Paper has the objective to propose a methodology for modeling and simulating a unit operation responsible for naphtha stabilization, obtaining parameters for use in future controller studies and analyzing possible procedure optimizations.

2. METODOLOGY

Due to the complexity of the mixture, it was decided to use commercial software. We adopted the software were whose operation is more acquainted, Aspen HYSYS®.

The simulation in these tools requests the knowledge of most appropriate thermodynamic model to the physical and chemical characteristics of the involved compound or mixture.

To define the best model, we used the model suggested by the Publication of Almeida et al (1999) and Ventin (2010), with the model of Peng-Robinson, and the procedure proposed by Carlson (1996), verifying a better fit for Grayson-Streed model, since it fits better to the physicochemical properties of the mixture.

The input current composition is based on the Paper presented by Ventin. This is listed in Table 1 as attached.

Table 1. Composition and physical properties of the compounds present in the Naphtha Stabilizer Tower input flow.

Components		NBP (ºC)	Molecular weight	% Volume liquid
Hydrogen	H_2	-252,60	2,02	0,0095
Nitrogen	N_2	-195,80	28,01	0,1149
Carbon Monoxide	CO	-191,45	28,01	0,0149
Methane	CH_4	-161,52	16,04	0,0088
Ethylene	C_2H_4	-103,75	28,05	0,1558
Ethane	C_2H_6	-88,60	30,07	0,1868
Propane	C_3H_8	-42,10	44,10	2,7790
Iso-Butane	C_4H_{10}	-11,73	58,12	1,9431
1-Butene	C_4H_8	-6,25	56,11	0,0409
n-Butane	C_4H_{10}	-0,50	58,12	5,4717
Iso-Pentane	C_5H_{12}	22,88	72,15	0,0450
NBP 11		11,03	60,61	1,6629
NBP 26		25,96	65,48	2,4385
NBP 40		40,37	72,37	4,2889
NBP 54		54,02	78,10	6,8701
NBP 67		67,32	83,86	7,1400
NBP 82		82,36	90,50	6,8055
NBP 97		96,58	97,45	7,9180
NBP 111		110,59	104,80	8,7766
NBP 125		124,80	112,38	8,2854
NBP 139		139,10	120,23	8,0347
NBP 153		153,25	128,47	8,0594
NBP 168		167,57	137,37	7,4376
NBP 181		181,09	145,28	4,3618
NBP 196		195,65	154,33	2,9562
NBP 210		209,98	163,78	2,2413
NBP 225		224,80	174,05	1,9526

Source: Ventin (2010)

The state variables were specified according to the article published by Almeida, as shown below:

1. Heat exchanged feed stream data (*Feed*):
   - Flow: 1445 m³/d;
   - Temperature: 40 ºC;
   - Pressure: 8 kgf/cm2;
   - Feeding in the heat exchanger shell;

2. Naphtha Stabilization Tower input stream data (*FeedHot*):
   - Vapour Fraction: 0.06;
   - Temperature: 136 ºC;

3. Heat exchanger parameters (TC-01):
   - Differential pressure in the tube (ΔP): 0,5 kgf/cm²;
   - Heat exchanger specification standardized by Tubular Exchanger Manufactures Association (TEMA): A-F-L, where "A" indicates removable lid and channel, "F" tells shell longitudinal deflector with two

steps, and "L" shows the bundle tube with fixed stationary head;

4. Naphtha stabilizer tower parameters (D-01):
   - Column with 30 actual stages, with increasing count from the top.;
   - Feed in stream FeedHot on stage 17;
   - Partial condenser;
   - Standard HYSYS® Reboiler;
   - Condenser pressure equivalent to 7 kgf/cm^2;
   - Pressure in the reboiler equal to 7.8 kgf/cm^2;

5. Temperature Profile Settings, on the *Parameters/Profiles* tab:
   - Top temperature: 54ºC
   - Bottom temperature: 163 ºC;

6. Murphree efficiency definition on the *Parameters/Efficiences* tab: 0.75 in all stages;

7. Heat exchange in the condenser: 1.0 MMcal/h.

The choice of a partial condenser is justified by the formation of a gas output stream (FG - Fuel Gas) and a liquid output stream (LPG - Liquefied Petroleum Gas).

The selection of the standard reboiler HYSYS® was done due to the process simplification, the lack of information regarding this simulation.

The process is defined in accordance with the software flowchart in Figure 1 as below.

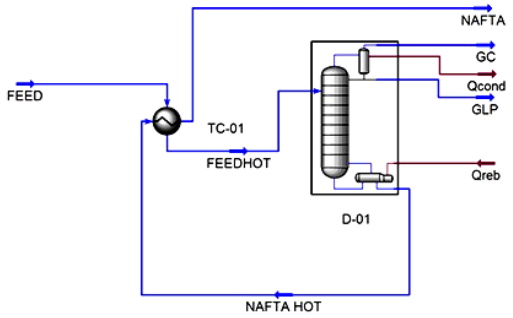


Figure 1: Flowchart of naphta stabilize unit operation.

In order to eliminate the freedom degrees, the design variables specifications are made on the tab *Design/ Specs*:

8. Distillate flow (constant): 108 m^3/d;
9. Temperature in stage 5 (state variable):
   - Minimum: 60 ºC;
   - Maximum: 92.5 ºC;
   - Fixed value obtained: 76.25 ºC.

To obtain a restriction results have been specified limits for the output variables:

10. Temperature in the LPG stream (output): 20 ºC;
11. Reboiler Heating:
    - Minimum: 1.2 MMcal/h;
    - Maximum: 3.5 MMcal/h;

The variable specified in item 10 allows to define the behavior of the LPG stream at the output in the top of the stabilizer tower, while the parameters established in item 11 allows an adjustment of the input stream of the same tower, in addition to ensure the production of naphtha with the desired characteristics, guaranteeing the absence or minimization of contamination by the light products.

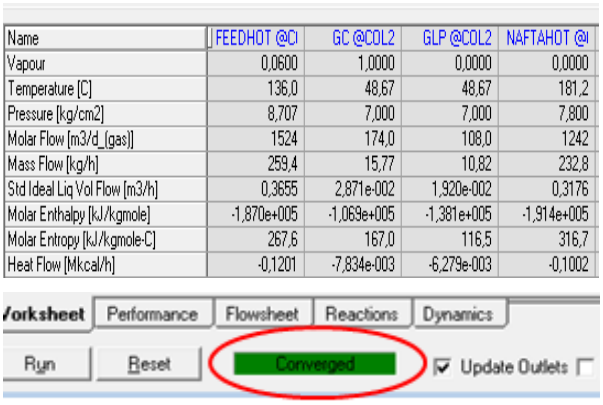
The variables manipulated are the temperature in the input stream in the stabilization tower and the temperature in stage 5 of the distillation tower. The selection of this stage should be generally defined as more sensitive stage for the temperature perturbations in this equipment.

The variables which affect these parameters are the temperature profile throughout the column and the temperature of the naphtha input stream in the heat exchanger, which will influence the FeedHot stream temperature. This enables to consider them as disturbance variables.

3. RESULTS

One of the commercial software problems is a partial analysis of the problem, identifying only the convergence mathematics. This causes certain illusion of the experiment's success.

Providing all data input, the convergence can be achieved, as shown in Figure 2.



Name	FEEDHOT @C	GC @COL2	GLP @COL2	NAFTAHOT @
Vapour	0,0600	1,0000	0,0000	0,0000
Temperature [C]	136,0	48,67	48,67	181,2
Pressure [kg/cm2]	8,707	7,000	7,000	7,800
Molar Flow [m3/d_[gas]]	1524	174,0	108,0	1242
Mass Flow [kg/h]	259,4	15,77	10,82	232,8
Std Ideal Liq Vol Flow [m3/h]	0,3655	2,871e-002	1,920e-002	0,3176
Molar Enthalpy [kJ/kgmole]	-1,870e+005	-1,069e+005	-1,381e+005	-1,914e+005
Molar Entropy [kJ/kgmole-C]	267,6	167,0	116,5	316,7
Heat Flow [Mkcal/h]	-0,1201	-7,834e-003	-6,279e-003	-0,1002

Figure 2: Example of convergence in a simulation, demonstrated in a results table.

With the same consideration, previously made to verify convergence, it is also possible to check the convergence of the physical states that are the output streams, which can be obtained by analyzing the total mass balance and the energy balance. The vapor fraction was found for the fuel gas was equivalent to 1 while for the other streams was equal to 0, which

indicates a certain agreement with the convergence and good phase separation.

The phase separation can also be observed through the net molar flow chart versus stage position in the distillation column, as shown in Figure 3.

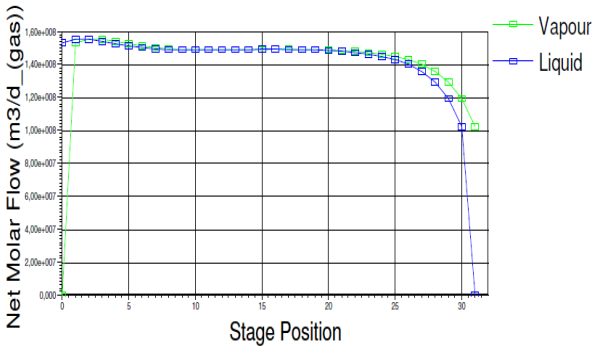


Figure 3: Net Molar Flow vs Stage Position

The higher molar flow observed at the highest position of the stabilizer tower is due to the greater volatility of lighter compounds. This allows having a greater molar flow. The heavier compounds have less volatility, therefore, a lower molar flow, as shown in the lower position of the column.

In despite of this result, the analysis should be done also considering the mass conservation per component, which will be discussed later.

By observing the temperature distribution of the equipment according to Figure 4, there is the expected behavior with sigmoidal curve, indicating good distribution of the trays, which ensures a good simulation of the equipment, but not the process simulation.

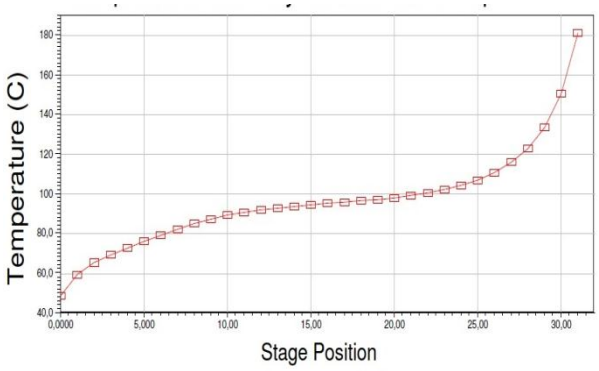


Figure 4: Temperature vs Stage position

Analyzing the composition obtained at the output, there is certain contamination in the overhead stream in the stabilizer tower with the presence of heavy compounds NBP11, and NBP26 NBP40, as shown in the Table 2.

Table 2: Stream out compositions (in molar fraction).

Components	Feed Hot	GC	GLP	Nafta Hot
Hydrogen	0,0040	0,0039	0,0000	0,0000
Nitrogen	0,0045	0,0390	0,0006	0,0000
Carbon Monoxide	0,0006	0,0050	0,0001	0,0000
Methane	0,0002	0,0019	0,0001	0,0000
Ethylene	0,0029	0,0239	0,0024	0,0000
Ethane	0,0030	0,0238	0,0040	0,0000
Propane	0,0434	0,2928	0,1415	0,0000
Iso-Butane	0,0256	0,1365	0,1410	0,0000
1-Butene	0,0006	0,0030	0,0035	0,0000
n-Butane	0,0747	0,3551	0,4824	0,0000
Iso-Pentane	0,0005	0,0001	0,0002	0,0006
NBP 11	0,0202	0,0861	0,1467	0,0000
NBP 26	0,0299	0,0288	0,0775	0,0259
NBP 40	0,0508	0,0000	0,0001	0,0623
NBP 54	0,0790	0,0000	0,0000	0,0969
NBP 67	0,0793	0,0000	0,0000	0,0973
NBP 82	0,0726	0,0000	0,0000	0,0890
NBP 97	0,0800	0,0000	0,0000	0,0982
NBP 111	0,0840	0,0000	0,0000	0,1030
NBP 125	0,0751	0,0000	0,0000	0,0922
NBP 139	0,0691	0,0000	0,0000	0,0848
NBP 153	0,0658	0,0000	0,0000	0,0807
NBP 168	0,0574	0,0000	0,0000	0,0705
NBP 181	0,0322	0,0000	0,0000	0,0395
NBP 196	0,0207	0,0000	0,0000	0,0255
NBP 210	0,0150	0,0000	0,0000	0,0184
NBP 225	0,0124	0,0000	0,0000	0,0152

Verifying the composition of the streams and the obtained temperature in the simulation, it is observed that the reason this contamination is due to the overhead stream temperature, which is higher than the boiling temperature of these three components.

This same contamination can be observed in the graphics obtained in this simulation, shown in Figures 5 to 7, with the high presence of these compounds in the top and intermediate stages.

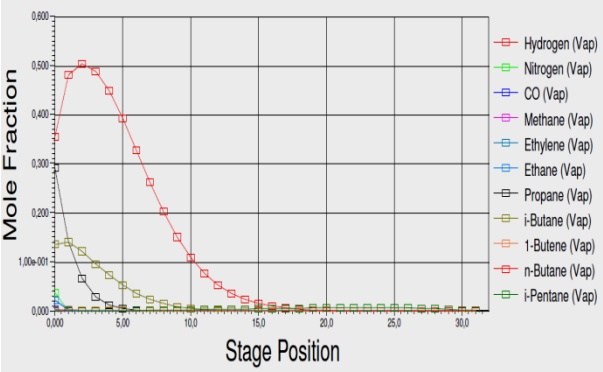


Figure 5: Light key (vapour) composition vs stage position

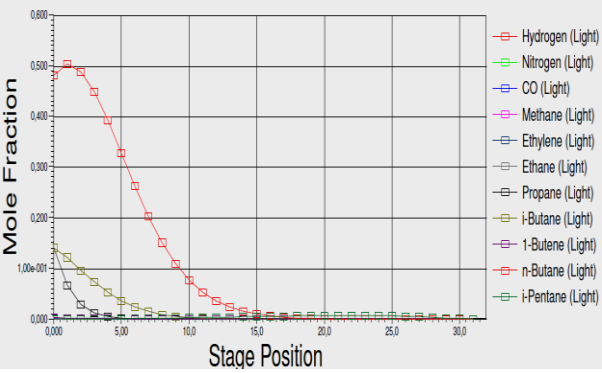


Figure 6: Light key (Liquid) composition vs stage position

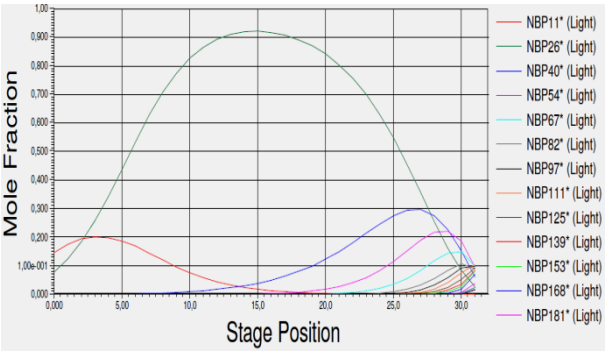


Figure 7: Heavy key composition vs stage position

To avoid this contamination, it is necessary to control the temperature of this stream below 11.03 °C, boiling point of NBP11, but it is more suitable to use a control to keep this temperature close to 2 °C as indicated by Almeida (1999).

This obstacle can have a second question which allows a better fit of the process. It was found that, in despite of the convergence, the occurrence of negative pressure (-0.51 kgf/cm²) in the shell side of the heat exchanger, which indicates a process malfunction.

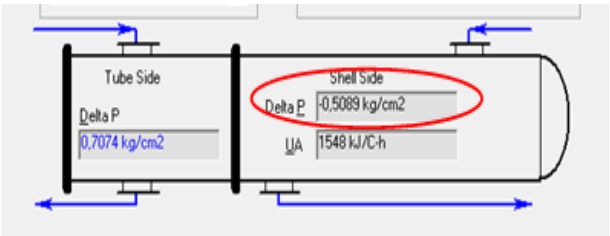


Figure 7: Presence of a negative pressure difference in a heat exchanger.

The simplest method to fix this problem is to decrease the temperature of the output stream present in the portion of the heat exchanger with negative differential pressure, since the temperature is an independent variable.

Changing the vapor fraction in this stream will affect the process of undesired manner, besides being dependent variable mentioned above.

Adopting the temperature to a value below the specified (130 °C) allows an increase in this pressure difference, allowing the flow of the feed stream in favor of the process feed (0,076 kgf/cm²) without a perceptible change in the output composition.

The temperature profile of the naphtha stabilizer tower has changed to observe the effect on the composition. The temperature was changed in stage 5 to 67.5 ° C by checking the change in composition as shown in Table 3, below.

There was a considerable contamination reduction of the compounds NBP26 and NBP40, with this measure.

Table 3: Stream out composition after temperature profile change.

Components	Feed Hot	GC	GLP	Nafta Hot
Hydrogen	0,0040	0,0039	0,0000	0,0000
Nitrogen	0,0045	0,0390	0,0006	0,0000
Carbon Monoxide	0,0006	0,0050	0,0001	0,0000
Methane	0,0002	0,0019	0,0001	0,0000
Ethylene	0,0029	0,0239	0,0024	0,0000
Ethane	0,0030	0,0238	0,0040	0,0000
Propane	0,0434	0,2929	0,1415	0,0000
Iso-Butane	0,0256	0,0030	0,1410	0,0000
1-Butene	0,0006	0,1365	0,0035	0,0000
n-Butane	0,0747	0,3551	0,4824	0,0000
Iso-Pentane	0,0005	0,0001	0,0002	0,0006
NBP 11	0,0202	0,0861	0,1467	0,0000
NBP 26	0,0299	0,0288	0,0775	0,0259
NBP 40	0,0508	0,0000	0,0001	0,0623
NBP 54	0,0790	0,0000	0,0000	0,0969

NBP 67	0,0793	0,0000	0,0000	0,0973
NBP 82	0,0726	0,0000	0,0000	0,0890
NBP 97	0,0800	0,0000	0,0000	0,0982
NBP 111	0,0840	0,0000	0,0000	0,1030
NBP 125	0,0751	0,0000	0,0000	0,0922
NBP 139	0,0691	0,0000	0,0000	0,0848
NBP 153	0,0658	0,0000	0,0000	0,0807
NBP 168	0,0574	0,0000	0,0000	0,0705
NBP 181	0,0322	0,0000	0,0000	0,0395
NBP 196	0,0207	0,0000	0,0000	0,0255
NBP 210	0,0150	0,0000	0,0000	0,0184
NBP 225	0,0124	0,0000	0,0000	0,0152

The thermodynamic package was changed for an appropriate package to the mixture (Grayson-Streed), obtaining a wide process improvement, with the elimination of the contamination by heavy component NBP40 and a minimal presence of NBP26, as shown in Table 4.

Table 4: Stream out composition after thermodynamic model change.

Components	Feed Hot	GC	GLP	Nafta Hot
Hydrogen	0,0040	0,0040	0,0000	0,0000
Nitrogen	0,0045	0,0394	0,0008	0,0000
Carbon Monoxide	0,0006	0,0051	0,0001	0,0000
Methane	0,0002	0,0019	0,0001	0,0000
Ethylene	0,0029	0,0237	0,0031	0,0000
Ethane	0,0030	0,0241	0,0042	0,0000
Propane	0,0434	0,2963	0,1417	0,0000
Iso-Butane	0,0256	0,0030	0,0036	0,0000
1-Butene	0,0006	0,1371	0,1427	0,0000
n-Butane	0,0747	0,3558	0,4883	0,0000
Iso-Pentane	0,0005	0,0001	0,0002	0,0006
NBP 11	0,0202	0,0858	0,1468	0,0000
NBP 26	0,0299	0,0238	0,0663	0,0276
NBP 40	0,0508	0,0000	0,0000	0,0622
NBP 54	0,0790	0,0000	0,0000	0,0968
NBP 67	0,0793	0,0000	0,0000	0,0972
NBP 82	0,0726	0,0000	0,0000	0,0889
NBP 97	0,0800	0,0000	0,0000	0,0980
NBP 111	0,0840	0,0000	0,0000	0,1029
NBP 125	0,0751	0,0000	0,0000	0,0920
NBP 139	0,0691	0,0000	0,0000	0,0847
NBP 153	0,0658	0,0000	0,0000	0,0805
NBP 168	0,0574	0,0000	0,0000	0,0703
NBP 181	0,0322	0,0000	0,0000	0,0394
NBP 196	0,0207	0,0000	0,0000	0,0254
NBP 210	0,0150	0,0000	0,0000	0,0183
NBP 225	0,0124	0,0000	0,0000	0,0152

4. CONCLUSION

The use of the methodology proposed in this work has enabled the convergence of both equipments in the studied unit operation.

Furthermore, makes possible to get parameters required for the experiment repeatability, as well as using it in other works and the procedure improvement with the adoption of milder temperatures and thermodynamic package more appropriate, achieving the proposed objective.

The small presence of contaminants was not completely solved, but the path to be used for obtaining better refined data has already been established.

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