Production of Light Naphtha by Flash Distillation of Crude Oil

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Abstract:
The escalating global demand for sustainable, renewable energy sources has catalyzed research into advanced refining processes, particularly focusing on the generation of essential raw materials like light naphtha. This paper delves into the production of naphtha via the flash distillation of crude oil, underlining its critical role in fulfilling the petrochemical industry's requirements. The research delineates the fundamentals of flash distillation, incorporating both physical and mathematical models, with a specific emphasis on Raoult's Law, to demystify the hydrocarbon separation process in crude oil. The mathematical framework encompasses material and energy balances, coupled with the application of liquid-vapor equilibrium equations, thereby shedding light on the thermodynamic principles steering this procedure. The progression of this study involved analyzing the distillation curve of the referenced crude oil and identifying the pseudo-components representative of the involved hydrocarbons. Utilizing the DWSIM commercial simulator, the flash distillation process of Namba crude oil was simulated, taking into account diverse operational conditions and thermodynamic models. The outcomes were juxtaposed with industrial datasets, demonstrating a significant alignment and affirming the simulation's predictive efficacy. A parametric sensitivity analysis was conducted to refine light naphtha yield, elucidating the effect of variables like the temperature of crude oil feed and naphtha separator feed on the process efficiency. The response surface methodology underscored the feasibility of augmenting naphtha production under certain conditions. Furthermore, this study assessed the impacts of employing two distinct thermodynamic models – the Soave-Redlich-Kwong (SRK) and Peng-Robinson (PR) equations of state. This analysis revealed minimal discrepancies in physical parameters, confirming the simulation's robustness and the reliability of both models. The findings of this paper validate the efficacy of flash distillation in light naphtha production, with numerical simulation emerging as a potent tool for enhancing process optimization and predictive analysis. These insights not only contribute to a deeper understanding of environmental sustainability but also offer strategies for maximizing light naphtha production in the oil industry. In conclusion, the results from this investigation significantly advance our comprehension of phase equilibrium profiles and their relationship with the applied thermodynamic state equations, thereby enriching the quality of the results.

Keywords:
Light Naphtha, Flash Distillation, Crude Oil, Simulation, DWSIM.

1. Introduction

From the perspective of energy production, the quest for cleaner and more sustainable fuels has remained a persistent challenge for governments and researchers worldwide. This endeavor stems from a dual concern: firstly, the pursuit of alternative energy sources is driven by the imperative to address global warming, reduce the carbon footprint, and mitigate environmental pollution associated with the utilization of fossil fuels. Secondly, there is a recognition of petroleum as a finite and non-renewable resource (Handogo, 2021; Noriler et al, 2009, Wolf-Maciel et al, 2001).

Another pivotal facet of this endeavor lies in the identification of exceptionally valuable raw materials that facilitate the development of novel industrial processes. In this context, the transformation of crude oil into naphtha meets the exigencies of the petrochemical sector assumes paramount significance in fostering and sustaining a diverse array of industrial activities.

Naphtha, as a constituent of crude oil, predominantly comprises hydrocarbons featuring carbon chains ranging from 6 to 12 carbons in length. It serves as a foundational feedstock for the production of an extensive spectrum of chemical products, including plastics, most notably polyethylene and polypropylene, which are prominent commodities in the global market. Naphtha is procured through a direct distillation process and encompasses hydrocarbons with boiling points within the temperature range of 38°C to 200°C. Its versatility extends to its use in gasoline production and as a fundamental raw material for the petrochemical industry. The latter application involves its conversion into ethylene, propene, butadiene, benzene, toluene, and xylene through processes such as thermal cracking and catalytic reforming. The specific classification of
naphtha into light or heavy variants in refineries is contingent upon the cut-off point determined within the atmospheric distillation column (ABIQUIM, 2007).

This dynamic landscape has spurred investments in scientific research geared towards developing processes that render naphtha a viable source for the production of butadiene and aromatics. Consequently, the quality of naphtha is predicated upon its hydrocarbon composition, boiling point characteristics, and the presence of impurities. As delineated by Rahimpour et al (2013) and Prauchner et al (2022), the distribution of paraffins, olefins, naphthenes, and aromatics serves as a decisive determinant of naphtha quality. This is particularly pertinent in the context of catalytic reforming processes, where naphthenes undergo selective transformation into aromatics.

Numerous research efforts are being directed towards finding sustainable solutions for liquid fuels, with a significant focus on renewable feedstock-based alternatives. Among these, the development of biodiesel has a well-established history, as evidenced by studies from Lulic et al. (1998), Alahmer et al. (2022), and Jeyakumar et al. (2022). Another major area of investigation is the potential use of alcohols as diesel substitutes, which has been intensively researched (e.g., Tutak et al., 2015). Additionally, waste-based fuels, including pyrolytic feedstocks, have garnered attention for their potential in sustainable fuel production (Kondor et al., 2022).

While exploring alternatives to traditional fossil fuels, researchers have also examined options like OME (oxymethylene ethers), which, despite their fossil origin, present as viable alternative liquid fuels (Virt and Arnuld, 2022). Beyond liquid fuels, there's a growing interest in gaseous fuels like CNG (compressed natural gas), as highlighted in the work of Matijosius et al. (2022).

A notable contribution in this field is the research by Goldbach et al. (2022) and Da Silva Mateus et al (2022), which demonstrates that fast pyrolysis can be an effective method for large-scale biofuel production from waste fish oil, yielding products with properties akin to conventional petroleum fuels. While there have been practices of blending diesel oil with vegetable or waste oil as an alternative, these blended fuels often fail to meet the stringent fuel quality standards set by governments and engine manufacturers. Issues such as corrosion and polymerization are common medium-term consequences of using these blends. However, biofuels produced through pyrolysis show promise due to their compatibility with current engine standards, addressing these concerns.

Furthermore, naphtha has emerged as a precursor in the synthesis of an extensive spectrum of chemical products, with notable applications in the realm of resins, solvents, and pharmaceuticals. Additionally, it assumes a pivotal role as a key constituent in the formulation of high-octane gasoline formulations.

1.1. Principle of Flash Distillation

Flash distillation of petroleum represents a widely employed and intricate separation process conducted within flash tanks, amenable to description through both physical and mathematical models, as illustrated in Figure 1:

![Flowchart of a flash distillation unit](image)

The flash tank, a single-stage distillation unit, plays a pivotal role in the separation of hydrocarbons within petroleum. It operates by receiving a preheated liquid hydrocarbon stream that passes through an expansion valve before entering the flash tank. Within this tank, a sudden pressure drop occurs, leading to the separation of the liquid and vapor phases. Given the diverse range of hydrocarbons present in the incoming crude oil, the vapor stream emerging from the top of the flash tank predominantly consists of lighter hydrocarbons, falling within the category of light naphtha. In contrast, the descending
liquid stream contains hydrocarbons with higher carbon structures, necessitating further fractionation within an atmospheric distillation column (Pasquini and Bueno, 2007).

For the elucidation of this separation process, the physical model relies on Raoult's Law. This law expounds upon the principles of liquid-vapor equilibrium within ideal liquid mixtures, with a primary focus on vapor pressure and mole fraction of constituent components as the principal process variables. Raoult's Law affords insights into the phase equilibrium governing the various components of crude oil at varying temperatures, a fundamental aspect of flash distillation.

In this context, a comprehensive grasp of phase equilibrium principles underpins the predictability of vaporization rates during the depressurization process within flash distillation columns. This entails a profound understanding of the key physical properties of crude oil components, encompassing boiling temperatures and vapor pressures. Establishing a robust relationship between these properties and the principles of phase equilibrium is instrumental in enhancing vaporization rates and facilitating the recovery of lighter components.

Moreover, the physical model encompasses the tenets of heat and mass transfer, particularly concerning the preheating of crude oil and the ensuing vaporization. This entails the application of mass and energy balances, intertwined with the thermal exchanges inherent to the process.

Consequently, the mathematical model associated with this process emerges from material balances as the foundational framework for modeling component flow within a flash distillation process. These equations enable the determination of mass flow rates for both the distillate (vapor) and the bottom product streams (as represented by Equation 1) (Luyben, 2006):

(1) \[ F = V + L \]

Where F, V and L are the feed, top product and bottom product flow rates, respectively, in kmol/h.

For a given component, mass balances can be drawn up using Equation (2).

(2) \[ Fx_F = Vy + Lx \]

Where \( x_F, y \) and \( x \) are the fractions of the components in the feed, at the top and at the bottom of the flash distillation column, respectively.

Energies balances are used to calculate the heat transfer rate and temperature changes in the distillation process and are essential for determining energy requirements and ensuring separation efficiency (Equation 3).

(3) \[ Fh_F + Q = Lh_L + VH_v \]

Where \( h_F, h_L \) and \( H_v \) are the feed, bottom product and top product enthalpies, respectively, in kJ/h, and \( Q \), in kJ/h, is the energy added to the system that results in the heating of the crude oil stream to ensure phase separation in the flash tank.

On the other hand, liquid-vapor equilibrium equations, based on Raoult's Law or other phase equilibrium models, are used to predict the composition of the vapor phase at a given temperature and pressure. These equations make it possible to understand the distribution of the different components between the liquid and vapor phases during flash distillation (Equation 4) (Reis et al, 2006 and Barros (2022)):

(4) \[ y_i = \frac{x_i p_{sat}^i}{\phi_i} \]

Where \( P_{sat} \) is the vapor pressure calculated based on the equation proposed by Antoine (Equation 5) and \( \gamma_i \) and \( \phi_i \) are, respectively, the activity and fugacity coefficients associated with phase equilibrium in the liquid and vapor phases:

(5) \[ \ln P_{vap}^{sat}(KPa) = A_i - \frac{B_i}{T(C+C_i)} \]

Characterized as a separation technique based on the principles of phase equilibrium, this process guarantees the effective recovery of the light components contained in oil, especially light naphtha. In addition to the equilibrium principles described by Raoult's law, the equilibrium equation (Equation (6)) proposed by Lewis can be used (Perry, 2018; Kalvelage et al, 2017).

(6) \[ y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n} \]

Where \( \alpha \) is the relative volatility that relates the vapor pressures of the light and heavy key components.
Flash distillation calculations serve as a crucial tool for determining the requisite thermal (temperature) and mechanical (pressure) conditions necessary to achieve phase equilibrium between the exiting streams from the flash tank. These calculations are inherently iterative in nature and involve the simultaneous resolution of mass and energy balances, in conjunction with phase equilibrium equations. This integrated approach is indispensable for solving a system of differential equations, which is pivotal in evaluating the behavior of the flash distillation column (Shuncheng and Bagajewicz, 2002).

The resolution of flash distillation problems can be executed through the utilization of commercial simulators or the development of algorithms grounded in mathematical modeling, which rely on the formulation of mass and energy balances. Numerous computational tools are available for this purpose, including Aspen HYSYS, CHEMSEP, DWSIM, and others (Leite et al, 2005). These tools enable the simulation of flash distillation processes, as well as more complex separation processes, providing valuable insights into the separation of crude oil into various fractions, including naphtha. Additionally, alternative thermodynamic models may be explored to enhance process performance in terms of separation capacity for specific crude oil fractions. Within this context, Kister (1992) and Fraga (2010) noted that flash distillation offers notable advantages such as reduced energy consumption, lowered capital costs, and heightened process sustainability when compared to conventional distillation methods.

Handogo (2021) has conducted studies demonstrating the widespread utilization of flash distillation in refineries and oil processing plants to segregate light components, such as naphtha, from the heavier constituents of crude oil. According to the author, flash distillation effectively achieves the swift separation of light naphtha from the heavier components by capitalizing on differences in relative volatility and vapor pressure. It is noteworthy, however, that the precise composition of the light naphtha can vary contingent upon the type of crude oil being processed and the operational conditions of the flash distillation column. Subsequent to the separation of streams within the flash tank, the light naphtha can undergo additional processing stages, particularly sulfur recovery and other refining processes, to meet the requisite quality specifications and fulfill the demands of the chemical and petrochemical industries that rely on this essential raw material.

In this specific context, a flash distillation study was undertaken on Nemba crude oil for the production of light naphtha, employing the support of the commercial simulator DWSIM. This investigation involved the exploration of optimal operating conditions and thermodynamic models to ensure peak process performance, with the resulting data subjected to comparison with existing literature data.

2. Data and methods
2.1 Software
The research conducted in this study facilitated a parametric evaluation of the light naphtha production process via flash distillation of Nemba crude oil. The study harnessed the capabilities of the commercial simulator DWSIM, version 8.6.1. The primary focus of this investigation was to systematically analyze the process parameters, with a specific emphasis on assessing operating conditions and thermodynamic models that could enhance process performance.

The utilization of process simulation provides a powerful means to gauge the sensitivity of various parameters in separation operations and other industrial processes. As elucidated by Leite et al. (2005), who employed a commercial simulator to investigate physical and chemical gas absorption processes, the flexibility afforded by commercial simulators greatly expands the analytical capacity for industrial processes. It enables the identification of critical parameters that exert the most significant influence on the outcomes of these processes, thereby facilitating informed decision-making and optimization efforts.

2.2. Characteristics of Simulated Oil
The oil used in this simulation study was extracted in Angola, and is coded as Nemba. Its characteristics are as follows:
Density @ 15°C: 0.8394 g/cm³; API gravity @ 60°C: 37.0 degrees API (American Petroleum Institute); Viscosity @ 10°C: 13.3 cSt and Acidity: 0.24 mg KOH/g.

On the other hand, the distillation curve for Nemba crude oil is shown in Figure 2. For this configuration, Prauchner et al. (2022) point out that the constituent compounds of petroleum cover very wide boiling temperature ranges, as illustrated in the distillation curve in Figure 2, which describes the main way of characterizing a petroleum sample. Generally, paraffinic compounds are concentrated mainly in the low and medium boiling point fractions, while naphthenic and aromatic compounds are present in the heavier fractions, with the usual concomitant occurrence of two or more of the aforementioned classes of compounds, as illustrated in Figure 2:
The naphtha from Namba Crude Oil was characterized by cutting it in two temperature ranges, i.e. 15-65°C and 15-80°C, respectively. Once the cuts had been made, the physicochemical characterization was carried out in TOTAL Energy's laboratory, the results of which are shown in Table 1:

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Unity</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cutting temperature range</td>
<td>°C</td>
<td>15-65</td>
</tr>
<tr>
<td>Yield</td>
<td>wt %</td>
<td>4.95</td>
</tr>
<tr>
<td></td>
<td>vol %</td>
<td>6.40</td>
</tr>
<tr>
<td>Density at 15°C</td>
<td>kg/m³</td>
<td>648.00</td>
</tr>
<tr>
<td>Sulphur content</td>
<td>wt %</td>
<td>0.0001</td>
</tr>
<tr>
<td>Mercaptans content (RSH)</td>
<td>mg/kg</td>
<td>0.00</td>
</tr>
<tr>
<td>Naphthenic compound content</td>
<td>vol %</td>
<td>7.90</td>
</tr>
<tr>
<td>Aromatic compounds content</td>
<td>vol %</td>
<td>0.70</td>
</tr>
<tr>
<td>RON</td>
<td>-</td>
<td>74.20</td>
</tr>
<tr>
<td>MON</td>
<td>-</td>
<td>72.70</td>
</tr>
</tbody>
</table>

Where RON and MON stand for Research Octane Number and Motor Octane Number respectively. The data in Table 1 was compared with simulation data, based on the use of two cubic equations of state, which made it possible to assess the consistency of these models in analyzing the behavior of flash distillation columns.

2.3 Procedures Used for the Simulation
This work was carried out at the Instituto Superior Politécnico de Tecnologias e Ciências (ISPTEC), with the support of the physical and operational parameters of Nemba crude oil shown in Table 1. The simulation studies involved the following sequence of procedures:

i. **Definition of the operating variables:** the critical operating variables were established, covering parameters such as flow rates, temperatures, pressures and compositions. These variables play a fundamental role in configuring the simulation model.
ii. **Pseudo-component selection:** in the simulation process, the initial steps involved using the distillation curve to define the pseudo-components of the crude oil mixture, the results of which were used in the simulation to represent the multi-component nature of the feedstock used in flash distillation.

iii. **Selection of the thermodynamic model:** the Peng Robinson model was selected for this process, as it enables the phase equilibrium behavior of substances in high pressure and temperature systems to be described.

iv. **Drawing up the flowchart:** DWSIM software was used to describe the process flowchart, which describes the sequence of equipment and respective operations in the flash distillation of crude oil for the production of light naphtha.

v. **Definition of operating conditions:** the feed conditions were then defined, with emphasis on the flow rate, temperature and pressure. Once these conditions had been established, the simulation was carried out, which essentially consisted of closing the mass and energy balances in order to meet the specifications previously established.

vi. **Evaluation of the results:** the results obtained in the simulation were evaluated to check the consistency and validation of the thermodynamic model and to identify any discrepancies or needs for improvement.

Therefore, the simulation reproduces the industrial processes of flash distillation of crude oil to produce light naphtha, the results of which can be evaluated in terms of consistency and performance by comparing the simulated data with industrial data.

### 2.4. Experimental planning

Flash distillation involves the intensive use of energy, a factor that affects operating costs in these industrial units. To this end, parametric sensitivity analysis makes it possible to explore the behavior of the operations involved in flash distillation columns. This condition resulted in the elaboration of the 22 factorial experimental design, used to evaluate the effect of two independent factors on a response variable. For this case, each factor has two configuration levels.

For this study, two independent variables were used (crude oil feed temperature – \( X_1 \) and naphtha separator feed temperature – \( X_2 \)) and one dependent or response variable (flow rate of the light naphtha produced), a condition that guarantees the optimization of light naphtha production. Table 2 shows the experimental planning used in this study, based on the descriptions of the variables described above.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>( X_1 )</th>
<th>( X_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>3</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

In this way, 5 experiments were carried out to evaluate the variables described in this work and the responses evaluated in terms of comparative consistency with the experimental data.

### 3. Results and Discussion

The simulation first involved using experimental data from the distillation curve and API of the Nemba crude oil as input data for the DWSIM simulator and then choosing the operating conditions and thermodynamic model. Once this stage was completed, the characteristic pseudo-components of the crude were generated and used to carry out the numerical simulation study carried out in this work.
Table 2 Pseudo-components generated from Nemba crude oil

<table>
<thead>
<tr>
<th>Pseudo-components</th>
<th>Mass Fraction</th>
<th>Boiling Temp. (K)</th>
<th>SG</th>
<th>Molar weight (Kg/Kmol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_5181_NBP_-51</td>
<td>0.0846</td>
<td>222.444</td>
<td>0.5732</td>
<td>37.90</td>
</tr>
<tr>
<td>C_5181_NBP_18</td>
<td>0.0941</td>
<td>291.278</td>
<td>0.6691</td>
<td>62.24</td>
</tr>
<tr>
<td>C_5181_NBP_92</td>
<td>0.1771</td>
<td>364.875</td>
<td>0.7410</td>
<td>96.64</td>
</tr>
<tr>
<td>C_5181_NBP_141</td>
<td>0.2347</td>
<td>414.628</td>
<td>0.7787</td>
<td>125.00</td>
</tr>
<tr>
<td>C_5181_NBP_213</td>
<td>0.1217</td>
<td>486.550</td>
<td>0.8234</td>
<td>173.53</td>
</tr>
<tr>
<td>C_5181_NBP_282</td>
<td>0.1016</td>
<td>555.138</td>
<td>0.8583</td>
<td>228.39</td>
</tr>
<tr>
<td>C_5181_NBP_346</td>
<td>0.0800</td>
<td>618.848</td>
<td>0.8860</td>
<td>287.04</td>
</tr>
<tr>
<td>C_5181_NBP_412</td>
<td>0.0477</td>
<td>685.163</td>
<td>0.9112</td>
<td>356.12</td>
</tr>
<tr>
<td>C_5181_NBP_481</td>
<td>0.0315</td>
<td>753.674</td>
<td>0.9347</td>
<td>436.19</td>
</tr>
<tr>
<td>C_5181_NBP_550</td>
<td>0.0271</td>
<td>823.477</td>
<td>0.9567</td>
<td>526.86</td>
</tr>
</tbody>
</table>

Pseudo-components represent a complex mixture of hydrocarbons with a boiling temperature within an established temperature range. For this case, the pseudocomponents individually represent a discrete component, with an average boiling point temperature and average properties throughout the mixture (Quirino, 2009). In this way, the sum of the fractions of all the pseudocomponents constitutes the total sample of crude oil from the referenced crude.

3.1. Simulation
In this study, the mass and energy balances were carried out using numerical simulation, supported by the DWSIM simulator, whose procedure followed the one described in the methodology of this work and involved preheating, pre-flash distillation, stabilization and fractionation of the naphtha, in order to produce products with a quality similar to that produced in the industrial unit, referred to here in this work.

The operating conditions involved a feed flow rate of 1000 Kg/s of crude oil, with the Peng Robinson cubic equation of state used as the thermodynamic model for the gas phase. In this way, the crude oil was heated to 274°C (548.15 K) and a pressure of 4.2 bar, a condition that guarantees the total vaporization of the components associated with light naphtha and, partially, the components of heavy naphtha. Thus, in this operating condition, the stream enters the flash distillation column when there is a sudden reduction in pressure to approximately 1.2 bar, resulting in the separation of the descending liquid and ascending vapor phases in this industrial equipment.

Also in this process, the ascending vapour stream is cooled in a heat exchanger to 80°C (353.15 K), and then feeds the second flash distillation column, a condition that guarantees the separation of LPG as ascending top vapour and descending liquid naphtha in this industrial equipment. The second flash distillation column is therefore characterised as a stabilisation tower and is used to produce light naphtha (C4-C6), the results of which are shown in Table 3.

Based on the data in Table 3, it can be seen that it is possible to produce up to 231.72 tonnes/day of light naphtha, a condition that could increase the rate of petrol production through catalytic reforming or the use of light naphtha as a raw material for the petrochemical industry. On the other hand, the efficiency of light naphtha production from this simulation study is on a par with TOTAL ENERGY’s experimental data (Table 3), with an average deviation of 3.06%.

Numerical simulation is therefore a fundamental tool for analysing the performance of industrial processes, capable of predicting the behaviour of separation equipment, with deviations obtained within the range established in the literature. For these cases, Fernandes (2018) states in his studies that deviations between experimental data of up to 5% are admissible because they are related to the characteristics of the mathematical and thermodynamic models used in these processes.
Table 3: Results of the mass flow of products obtained in the simulation.

<table>
<thead>
<tr>
<th>Product</th>
<th>Boiling Temperature (°C)</th>
<th>Mass Flow</th>
<th>Recovery Percentage (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Feed (Kg/s)</td>
<td>Output (Kg/s)</td>
</tr>
<tr>
<td>Crude oil</td>
<td>---</td>
<td>1000</td>
<td>---</td>
</tr>
<tr>
<td>LPG</td>
<td>15 – 80</td>
<td>---</td>
<td>6.473</td>
</tr>
<tr>
<td>Light Naphtha</td>
<td>15 – 80</td>
<td>---</td>
<td>64.366</td>
</tr>
<tr>
<td>Heavy Naphtha</td>
<td>80 – 175</td>
<td>---</td>
<td>390.075</td>
</tr>
<tr>
<td>Atmospheric Current</td>
<td>175 – 370</td>
<td>---</td>
<td>539.086</td>
</tr>
<tr>
<td>Balance (Input = Output)</td>
<td>1000 Kg/s = 1000 Kg/s</td>
<td>100%</td>
<td></td>
</tr>
</tbody>
</table>

The parametric simulation analysis based on the experimental planning made it possible to evaluate the effects of the crude oil feed temperature and the naphtha heating temperature before the flash separator or distiller. The results obtained were plotted on a response surface graph (Figure 5) and show that the increase in naphtha production rates is related to the maximisation of the experimental planning parameters mentioned here. Unlike the results in Table 3, Figure 5 defines the best parametric operating conditions and, as mentioned above, it can be seen that temperatures close to the maximum admissible boiling temperatures of the light naphtha components (C4-C6) guarantee higher yields in terms of flow rates or light naphtha production.

3.1.1 Analysis of thermodynamic parameters

To better understand the influence of the thermodynamic model in terms of response quality, the flash distillation was simulated using two cubic equations of state, Soave-Redlich-Kwong (SRK) and Peng-Robinson (PR) respectively. In order to analyse the data obtained, the physical parameters of the products of the ascending vapour stream of the stabilised flash distillation were compared, according to the results shown in Table 4. Overall, it can be seen that there is a numerical similarity between the parameters derived from the two equations of state, with minimal deviation between them, even considering that the LPG produced involves a multicomponent mixture, which interferes differently, based on the molecular interaction forces, characterised by repulsion and attraction of the molecules making up the mixture. For this analysis,
thermal conductivity showed the greatest deviation, followed by specific mass, volumetric flow, internal energy and molar internal energy. This behaviour is due to the mathematical similarity between the two thermodynamic models, and because they consider the acentric factor which relates the size of the molecules when evaluating the molecular forces involved in the process.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Unity</th>
<th>SRK</th>
<th>PR</th>
<th>Variation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Conductivity</td>
<td>W/[m.K]</td>
<td>0.01949</td>
<td>0.01947</td>
<td>0.15%</td>
</tr>
<tr>
<td>Specific Mass</td>
<td>kg/m³</td>
<td>2.41777</td>
<td>2.41957</td>
<td>0.07%</td>
</tr>
<tr>
<td>Internal Energy</td>
<td>kJ/kg</td>
<td>67,28390</td>
<td>67,31500</td>
<td>0.05%</td>
</tr>
<tr>
<td>Molar Internal Energy</td>
<td>kJ/kmol</td>
<td>4874.56000</td>
<td>4876.82000</td>
<td>0.05%</td>
</tr>
<tr>
<td>Helmholtz Free Energy</td>
<td>kJ/kg</td>
<td>-120,65000</td>
<td>-120,65100</td>
<td>0.00%</td>
</tr>
<tr>
<td>Molar Gibbs Free Energy</td>
<td>kJ/kmol</td>
<td>-5704.68000</td>
<td>-5707.01000</td>
<td>0.04%</td>
</tr>
<tr>
<td>Specific Enthalpy</td>
<td>kJ/kg</td>
<td>109,19200</td>
<td>109,19200</td>
<td>0.00%</td>
</tr>
<tr>
<td>Molar Enthalpy</td>
<td>kJ/kmol</td>
<td>7910.72000</td>
<td>7910.72000</td>
<td>0.00%</td>
</tr>
<tr>
<td>Specific Entropy</td>
<td>kJ/[kg.K]</td>
<td>50.5359</td>
<td>50.3733</td>
<td>0.03%</td>
</tr>
<tr>
<td>Molar Entropy</td>
<td>kJ/[kmol.K]</td>
<td>36.48360</td>
<td>36.49390</td>
<td>0.03%</td>
</tr>
<tr>
<td>Gibbs Free Energy</td>
<td>kJ/kg</td>
<td>-78.74210</td>
<td>-78.77420</td>
<td>0.04%</td>
</tr>
<tr>
<td>Molar Helmholtz Free Energy</td>
<td>kJ/kmol</td>
<td>-8740.84000</td>
<td>-8740.91000</td>
<td>0.00%</td>
</tr>
<tr>
<td>Volumetric Flow @ T, P</td>
<td>m³/s</td>
<td>26.62220</td>
<td>26.60240</td>
<td>0.07%</td>
</tr>
</tbody>
</table>

On the other hand, the analysis of light naphtha from the second stabilised flash distillation column requires the use of thermodynamic models for the liquid phase, which makes it possible to determine the physical parameters of this phase and consequently compare the data obtained with industry data, a condition that can favour an understanding of the phase equilibrium principles involved in this study.

4. Conclusion
Based on the results obtained from this work, it can be concluded that:

a) Flash distillation is an effective operation capable of predicting the operational performance of processes for producing light naphtha from crude oil, whose separation capacity depends on the boiling points of the constituent components of the mixture;

b) Process simulation makes it possible to predict the behaviour of each operation and to know the energy content involved, conditions that make it possible to evaluate various mathematical and thermodynamic models that fit the experimental data;

c) The simulation carried out using the DWSIM simulator made it possible to predict naphtha production rates and the results were compared with those of TOTAL ENERGY’s industrial processes, with an average deviation of 3.06%;

d) Flash distillation, based on the principles of phase equilibrium, can be numerically optimised to guarantee knowledge of environmental sustainability, which is necessary for the national oil industry, maximising light naphtha production rates.

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