

Thermodynamic Modeling and Process Simulation of Kumkol Crude Oil Refining

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Abstract

The Crude Distillation Unit (CDU) mechanism is commonly regarded as the first stage in petroleum refining. In this study, Aspen Plus® is used to simulate the basic process of a CDU, which consists of an Atmospheric Distillation Column (ATC) and a Vacuum Distillation Column (VC). These columns are fed with two types of crude oil: KUMKOL from Kazakhstan and Soviet Export Blend, in the proportions of 0.75:0.25, 0.50:0.50, and 0.25:0.75, respectively. The goal was to do a parametric analysis and analyze the resultant streams of naphtha, kerosene, Atmospheric Gas Oil (AGO), Light Vacuum Gas Oil (LVGO), and Heavy Vacuum Gas Oil (HVGO). The simulation used the CHAO-SEA thermodynamic model, which included the Chao-Seader correlation, the Scatchard-Hildebrand model, the Redlich-Kwong equation of state, the Lee-Kesler equation of state, and the API gravity technique. Temperature, pressure, mass flow, enthalpy, vapor percentage, and average molecular weights of the streams at various phases within the CDU system were estimated. For both the ATC and VC columns, curves indicating Temperature-Pressure vs the number of stages, as well as ASTM D86 (temperature) versus stream volume % distillation, were developed. The results show that when compared to feed streams containing 0.25 and 0.50 StdVol of Kumkol Kazakhstan Oil, the feed stream with 0.75 StdVol produces more Heavy, Medium, and Light Vacuum Gas Oil (H-VGO, M-VGO, and L-VGO), as well as more Vacuum Gas (VG). These findings indicate that Kumkol Kazakhstan Oil is of high quality and has fewer contaminants, such as sulfur when compared to other accessible mixes throughout the world.

Abbreviation

CDU	Crude Distillation Unit
ATC	Atmospheric (distillation) Column
VC	Vacuum (Distillation) Column
AGO	Atmospheric Gas Oil
LVGO	Light Vacuum Gas Oil
HVGO	Heavy Vacuum Gas Oil
MVGO	Medium vacuum gas oil
TBP	True Boiling Point
EOS	Equations of State

NRTL	Non-Random Two-Liquid
RK	Redlich-Kwong
SRK	Soave-Redlich-Kwong
AT-Gas	Atmospheric Gas
SS1	Stripper 1
SS2	Stripper 2
CRD	Crude
VR	Vacuum Residue
ASTM-D86	American Society for Testing and Materials-Distillation 86
AT-GAS	Atmospheric Gas
LGO	Light gas oil
AT-V	Atmospheric To Vacuum Column
V-GAS	Vacuum Gas

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1. Introduction

Kazakhstan, a transcontinental landlocked country located in central Asia, is the world's 9th largest country by area having diverse terrain bearing abundant fossil fuel and mineral resources [1]. Natural gas, Petroleum and mineral exploitation have drawn the majority of the more than \$40 billion in foreign investment in Kazakhstan since 1993, accounting for around 57% of the nation's industrial production. Kazakhstan has the 11th biggest known reserves of both petroleum and natural gas, which is important for economic development [2]. There are 160 deposits totaling more than 2.7 billion tons of petroleum today. Kazakhstan's total oil reserves are estimated to be 6.1 billion tones [3]. The nation has only three refineries, which are located in Atyrau, Pavlodar, and Shymkent. Kazakhstan's oil exports grew to \$46.8 billion in 2022, with 65.0 million tons exported, up from \$31.0 billion and 65.5 million tons in 2021. Kumkol Oil Field is an oil field in Kyzylorda Province, 200 km from Kyzylorda town. The total proved reserves of the Kumkol oil field are estimated to be over 300 million barrels (4106 t), with a daily production capacity of 78,000 barrels per day (12,400 m³/d) [4].

Petroleum refineries are facilities that transform crude oil into petroleum products including fuel for cars and heating systems, asphalt for roads and power generation, as well as a feedstock for chemical synthesis. Crude oil is split down into parts during the refining process, where they are then carefully combined to create new products. The infrastructure of petroleum refineries is complicated and costly. The same three stages are followed by all refineries: As demonstrated in Fig. 1, separation, conversion, and treatment [5].

In addition to crude oil, petroleum also refers to any liquid, gaseous, and solid hydrocarbons. At surface pressure and temperature, lighter hydrocarbons like methane, ethane, propane, and butane exist as gases, whereas pentane and heavier hydro-

carbons exist as liquids or solids [6]. However, underground conditions as well as the phase diagram of the petroleum mixture dictate the ratios of gas, liquid, and solid in a subterranean oil resource [7]. Trace amounts of nitrogen, oxygen, and sulfur as well as the metals iron, nickel, copper, and vanadium as mentioned in Table 1 are also present [8-9]. As indicated in Table 2, the majority of the hydrocarbons in crude oil are alkanes, cycloalkanes, and aromatic hydrocarbons.

The hundreds of distinct hydrocarbon molecules in crude oil are separated by a refinery into constituents that may be utilized as fuels, lubricants, and feed stocks in petrochemical processes to make plastics, detergents, solvents, elastomers, and fibers like nylon and polyester [10]. Due to their various boiling temperatures, the hydrocarbons may be separated using distillation. A modern refinery will convert heavy hydrocarbons and lighter gaseous components into these higher-value products due to the significant demand for lighter liquid products for use in internal combustion engines [11]. Light distillates (LPG, gasoline, and naphtha), intermediate distillates (kerosene, jet fuel, and diesel), heavy distillates, and residuum (heavy fuel oil, lubricating oils, wax, and asphalt) are common categories for petroleum products [12]. An important step in the refinery process is blending different feed stocks and adding the appropriate additives. Additionally, this classification is dependent on how crude oil is fractionated and distilled [13].

Table 1. Composition of crude oil by weight percent [9]

Compound	Weight %
Carbon	85-90
Hydrogen	10-14
Sulphur	0.2-3
Nitrogen	0.1-2
Oxygen	1-1.5
Metals	<0.1

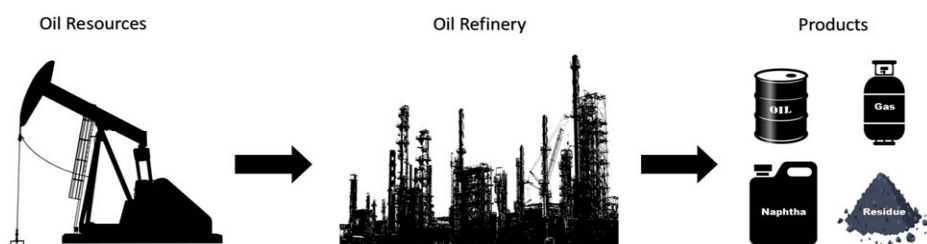


Fig. 1. Petroleum refinery process.

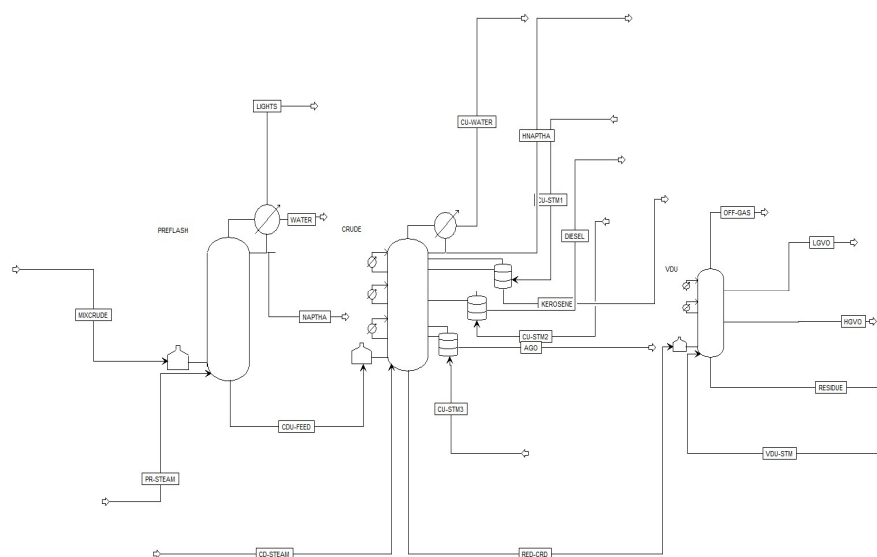


Fig. 2. Process flow sheet of Aspen Plus®.

Table 2. Molecular composition of crude oil [9]

Hydrocarbon	Average %	Range
Napthenes	49%	30-60%
Alkanes	30%	15-60%
Aromatics	15%	3-30%
Asphaltenes	6%	Residue

AspenTech is a software firm that focuses in sophisticated engineering solutions and process optimization for sectors including medicines, chemicals, and petroleum [14]. AspenTech's software portfolio includes Aspen HYSYS, Aspen Plus Dynamics, and Aspen DMC3. Aspen Plus is a popular program for modeling chemical processes [15]. It allows engineers and scientists to study and simulate processes such as heat transport, reaction kinetics, and distillation. Aspen Plus, with its mathematical models and algorithms, aids in the design, analysis, and optimization of complicated chemical processes, as demonstrated in the flow sheet generated by Aspen Plus in Fig. 2 [16].

Many unwanted contaminants are present in crude oil. These contaminants can cause a wide range of issues throughout the refining process. Desalting is used to eliminate unwanted contaminants from the crude oil stream prior to distillation [17]. These contaminants can cause several problems throughout the refining process. The main purpose of desalting is to eliminate these undesired contaminants from the crude oil feed before distillation. The most common impurities are sand and silt, corrosive by products from pipes like iron oxide and iron sul-

fide, crystalline and dissolved solids, drilling mud and polymers from well drilling, oil soluble and organic chloride compounds [18]. The crude oil also contains inorganic salts such as sodium chloride (NaCl), magnesium chloride ($MgCl_2$), and calcium chloride ($CaCl_2$) [19]. The typical byproducts of an atmospheric distillation column are LPG, naphtha, kerosene, diesel, light gas oil, heavy gas oil, and reduced crude oil, whereas the byproducts of a vacuum distillation unit are gas, light vacuum gas oil (LVGO), heavy vacuum gas oil (HVGO), medium vacuum gas oil (MVGO), and vacuum residue (VR) [20].

1.1 Thermodynamic model development

Aspen Plus uses estimation techniques as a component of a "Property Method." The term "property method" refers to a group of estimating methods that are used to estimate quantities like viscosity, thermal conductivity, diffusion coefficient, and surface tension that are important in the field of transport and thermodynamics [21]. The set of these properties along with the equations governing the changes in them are known as the thermodynamic models which enable the Aspen Plus to determine the behavior of the provided streams of pure and blends (mixtures) at given circumstances to generate the required results precisely. Common equations for the thermodynamic property method are the Equation of State, Redlich Kwong (RK) equation, Redlich Kwong Soave (RKS) equation, Benedict Webb Rubin (BWR) equation, Lee Kesler Plocker (LKP) equation, Chao-Seader (CS) equation, Grayson Stread (GS) equation and Brown K10 (BK10).

1.1.1 Thermodynamic Model Development

For petroleum refining process, CHAO-SEA property method is widely used for Aspen Plus simulations to determine the required data to optimize the production [22]. CHAO-SEA property method contains Chao-Seder correlation, the Scatchard-Hildebrand model, the Redlich-Kwong equation of state, the Lee-Kesler equation of state, and the API method [23]. It is applicable for both vacuum tower and crude distillation tower. It is not suitable for Hydrogen systems but can be used for Hydrocarbon and light gas systems such as carbon dioxide and hydrogen sulfide [24]. The Grayson Stread Equation (GS) was the addition to the CHAO-SEA method to be applicable for hydrogen rich mixtures with high temperature and pressure systems up to 4700 K and 200 bar respectively [25].

2. Experimental

The goal of this article is to simulate several aspects of crude distillation system that is frequently encountered in petroleum refineries. The building of a model of crude distillation in a petroleum refinery involves several steps as shown in Fig. 3. The process feed (CRUDE) is a mixture of two crude oils (assay) as mentioned in Table 3, Kumkol Kazakhstan and Soviet Export Blend, which is fed into the atmospheric distillation column furnace.

An atmospheric distillation unit (CDU) is made up of a crude unit furnace and an atmospheric tower. The bottoms of the crude are partially vaporized by the furnace, and then separated into five cuts by the atmospheric tower: heavy naphtha (HNAPHTHA),

kerosene (KEROSENE), diesel (DIESEL), atmospheric gas oil (AGO), and reduced crude (RED-CRD). The ATC column has a total of 25 stages and a condenser. No reboiler is required in the tower because steam is supplied from the bottom. The steam pressure and temperature in this column are 338 °F and 29.0075 psi, respectively. 350 000 kg/h of crude are fed to it. The ATC system is linked to three pump-around circuits and three side-strippers. In the 25th step, when the feed enters the column, the convention is taking place near the furnace. The convention is on stage when the tower's steam reaches the 25th stage. This stream has an average temperature and pressure of 752 °F and 43.5113 psi, respectively. H-Naphtha, the substance used in stage 1's stripper, is at stage 4, and stage 7's liquid draw is used. The lowest flow rate for the product is 29000 kg/h. Kerosene is the stripper product, stage 3 of stripper 2, liquid draw is from stage 14, and stage 13 is the overhead return. Steam is being stripped by SS2-ST. 34300 kg/h is the bottom product flow rate. Light Gas Oil (LGO) is the stripper product of Stripper 3, which is in Stage 3. Liquid draw is from Stage 19, and overhead return is from Stage 20. Steam is being stripped by SS3-ST. It operates at a bottom product flow rate of 76000 kg/h. The draw off type is partial, the standard flow is 387500 kg/h, the temperature is 224.6 °F, the first around draw stage (P-1) is 5, and the return draw stage is 4. The draw stage and return stage for the second pump around (P-2) are 12 and 11, respectively. The draw off type is partial, the standard flow is 235300 kg/h, and the temperature is 401 °F. The third pump around (P-3) draw stage is 18, the return stage is 18, the draw off type is partial, the standard flow is 2300 kg/h, and the temperature is 428 °F.

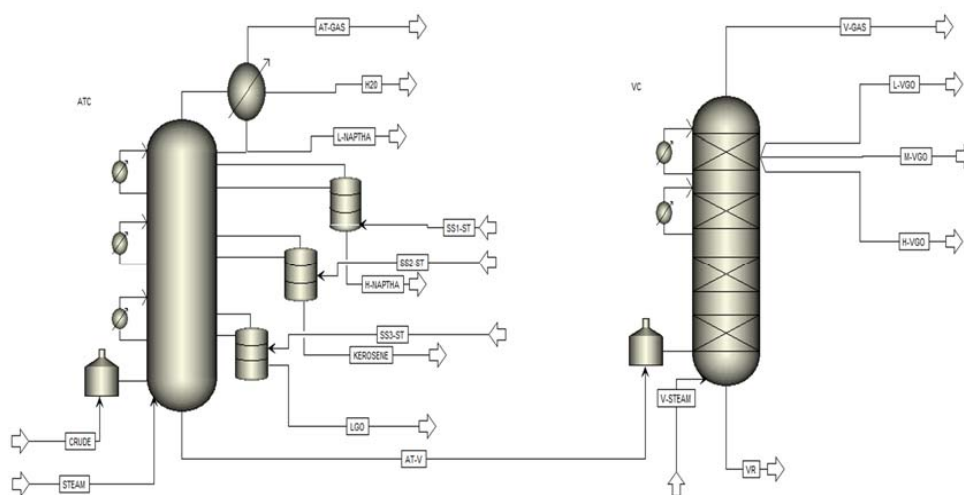


Fig. 3. Petroleum refinery flow sheet.

Table 3. Fractional composition of crude oils (in standard volume units)

Assay ID	Fraction (Stdvol %)		
Kumkol Kazakhstan	0.75	0.50	0.25
Soviet Export Blend	0.25	0.50	0.75

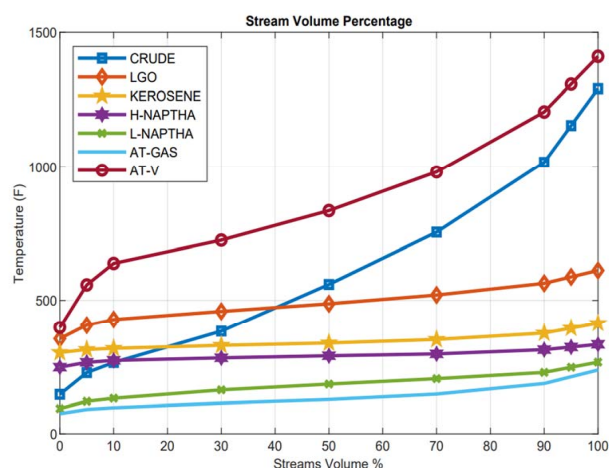
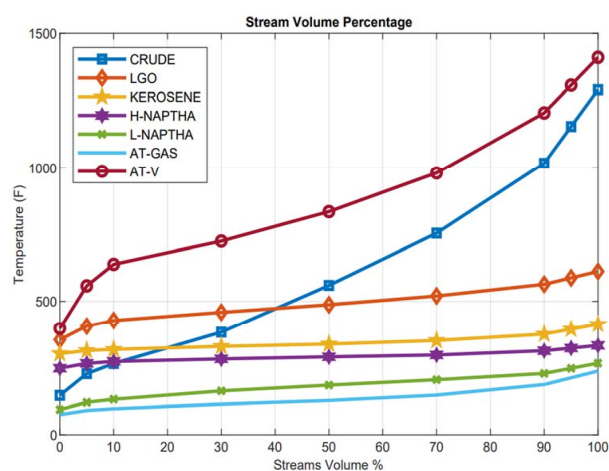
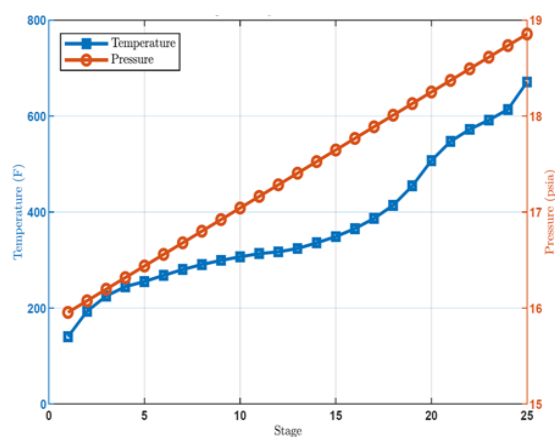
The vacuum distillation unit, which is supported by jet ejectors that enable the formation of a vacuum in the unit, is fed the bottom product of the atmospheric distillation unit at the temperature of 141.202464 °F and 1.45037738 psi a pressure. The atmospheric column bottom product is divided into V-Gas, light vacuum gas oil (LVGO), medium vacuum gas oil (MVGO), heavy vacuum gas oil (HVGO), and vacuum residue by the vacuum unit. All abbreviations for the units are listed in the abbreviations section.

3. Results and discussion

The tables (Table S1 – Table S15; see supplementary material) show the stream results of the Atmospheric distillation column (ATC) and Vacuum Distillation Column (VC), in which the properties of the different feed and product streams have been presented. Temperature, pressure, average molecular weight, mole, mass and volume flows, molar and mass enthalpy, molar and mass entropy, molar density, and enthalpy flow for three ratios of standard volumes of Kumkol Kazakhstan and Soviet Export Blend as mentioned in Table 3 to check the parametric results of different units of the refinery process using AspenPlus®.

Figure 4 shows the stream results of the atmospheric distillation column (ATC) including crude with a standard volume of Kumkol Kazakhstan 0.75 and Soviet Export Blend 0.25, stripper 1 (SS1-ST), stripper 2 (SS2-ST), stripper 3 (SS3-ST) and steam provided. Also, these tables demonstrate the results of the atmospheric gas (AT-GAS), water (H₂O), Heavy-NAPHTHA, KEROSENE, Light NAPHTHA, Light Gas Oil and the feed stream to the Vacuum Distillation Column (VC) which has been named AT-V.

Figure 5 shows the stream results of the Vacuum distillation Column (VC) in which AT-V comes from the atmospheric distillation column (ATC), feed steam (V-STEAM), Heavy Vacuum Gas oil (H-VGO) Light Vacuum Gas Oil (L-VGO), Medium Vacuum Gas Oil (M-VGO), Vacuum-Gas and Vacuum Residue (VR) with volume flow rate of 40441.56 bbl/day, 778461.465 bbl/day, 201.8720169 bbl/day, 10885.83873 bbl/day, 1080.4498 bbl/day,

**Fig. 4.** Stream results for ATC (StdVol 0.75:0.25).**Fig. 5.** Stream results for VC (StdVol 0.75:0.25).**Fig. 6.** Stage Vs temperature and pressure of ATC.

11973334.9 bbl/day, and 26964.03999 bbl/day respectively (see supplementary material).

Figure 6 shows the values of temperature and pressure at different stages of atmospheric tower having ratio of 75:0.25, ranging from 0 to 25 temperature profile remains straight while pressure drops between stage 15 and 20.

Figure 7 demonstrates the temperature and pressure profiles of the vacuum tower having ratio of 0.50:0.50 which shows that temperature increase with increase in number of stages, although pressure increase in starting stages but start decreasing at the mid of the stage number. Similarly, Fig. 8 shows the stream results of the atmospheric distillation column (ATC) with crude having a ration of 0.50:0.50 of both Kumkol Kazakhstan and Soviet Export blend. These tables have also detailed results of the streams as mentioned before for the previous ratio. Figure 9 shows the stream results of Vacuum distillation Column (VC) demonstrating H-VGO, L-VGO, M-VGO, V-GAS and VR having values of 198.5130932 bbl/day, 10731.31678 bbl/day, 1062.273345 bbl/day, 12029551.91 bbl/day and 26465.97908 bbl/day respectively as shown in Table S9 and Table S10 (see supplementary material).

For standard volume 0.25:0.75 of Kumkol Kazakhstan and Soviet Export Blend respectively as mentioned in Table 3, Fig. 10 and Fig. 11 demon-

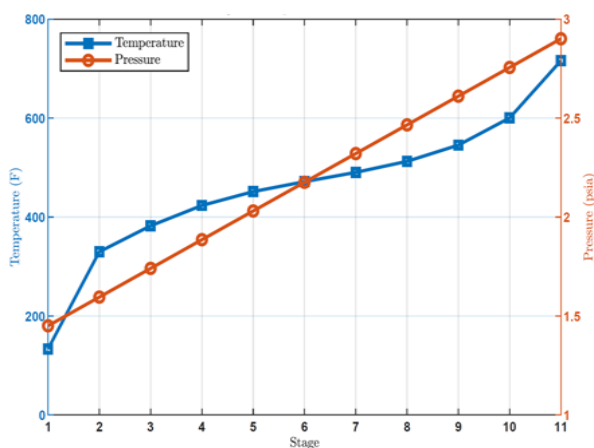


Fig. 7. Stage Vs temperature and pressure of VC.

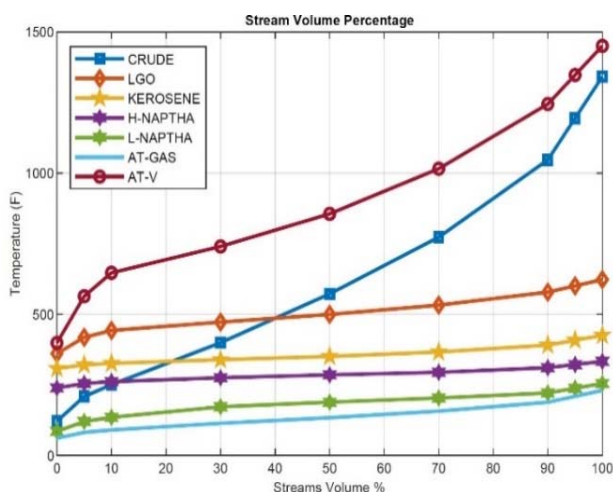


Fig. 8. Stream results of ATC (StdVol 0.50:0.50).

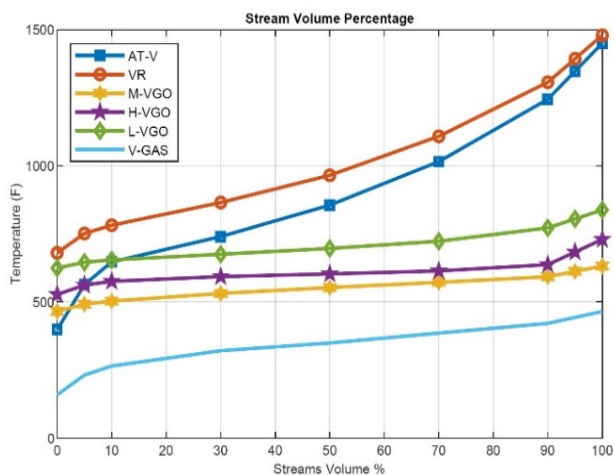


Fig. 9. Stream results of VC (StdVol 0.50:0.50).

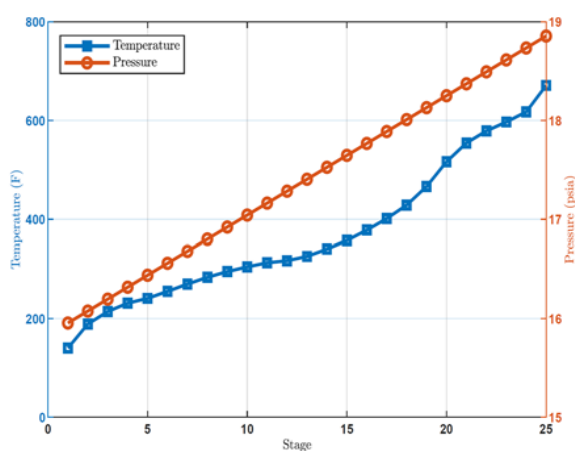


Fig. 10. Stage Vs temperature and pressure of ATC.

strate the temperature and pressure profiles of the atmospheric and vacuum towers with respect to number of stages in both towers, similar simulations were carried out using atmospheric distillation column (ATC) and Vacuum Distillation Column (VC), whose results are shown in Fig. 12 and Fig. 13 respectively for H-VGO, L-VGO, M-VGO, V-GAS and VR as 194.9814746 bbl/day, 10571.16664 bbl/day, 1045.456914 bbl/day, 12131495.51 bbl/day and 26026.20307 bbl/day respectively (see supplementary material).

Quantitative analyses of the results show that as we increase the standard volume of the Kumkol Kazakhstan Oil in the assay, the volume flow rate of required entities in production streams increases with remarkable values which can be proved by comparing the values of all three simulations.

In these graphs, a clear pattern of the products can be seen at different temperatures. Also, temperature and pressure vs. number of stages curves have been included in this paper to show the values of T and P

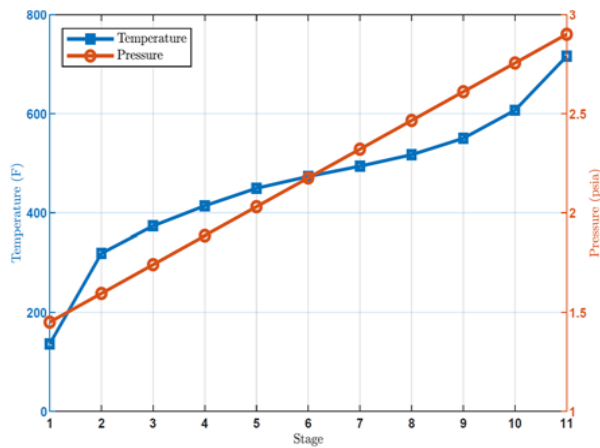


Fig. 11. Stage Vs temperature and pressure of VC.

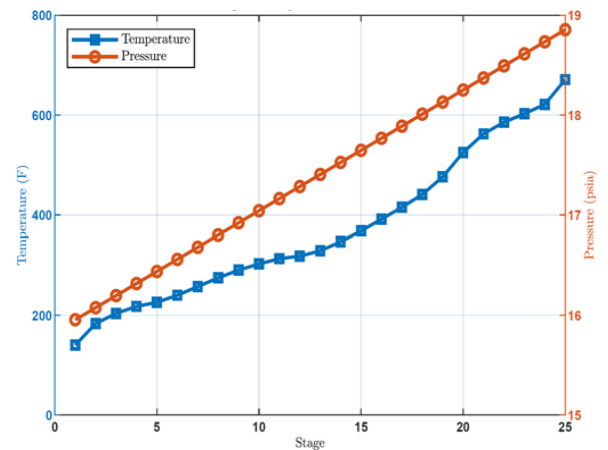


Fig. 14. Temperature and pressure of ATC (StdVol 0.25:0.75).

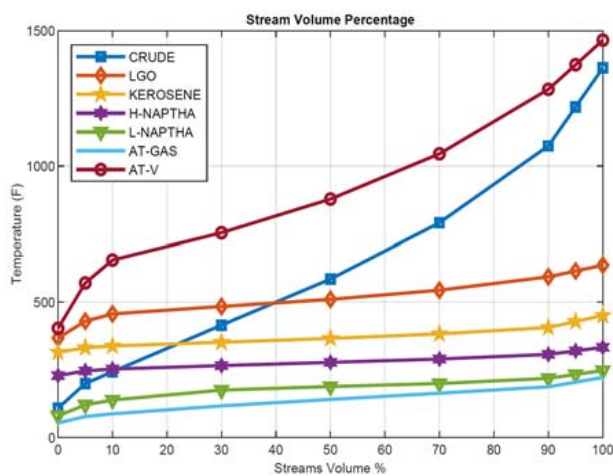


Fig. 12. Stream results of ATC (StdVol 0.25:0.75).

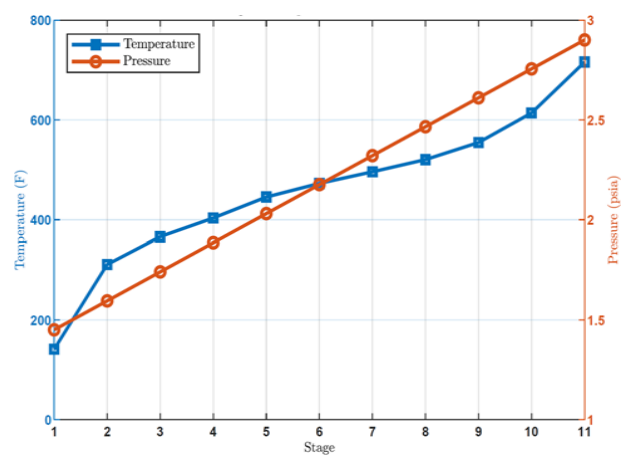


Fig. 15. Temperature and pressure of VC (StdVol 0.25:0.75).

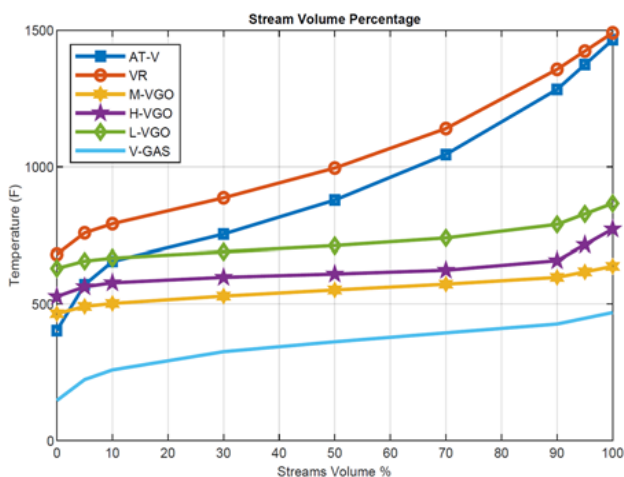


Fig. 13. Stream results of VC (StdVol 0.25:0.75).

at specified stages in Figs. 6 and 7. A similar approach was used for two other standard volumes of Kumkol Kazakhstan and Soviet Export Blend (0.50:50 and 0.25:0.75) which are shown in Figs. 10, 11, 14 and 15

respectively. These curves approximated the usual curves, proving that the simulation was correct. Estimates of Aspen Plus® product quality were found to be quite similar to published values [26].

The sulfur content of crude oil as mentioned in Table 4 generally ranges between 1-4%, it is allowed to have 500PPM in Heavy Naphtha but Kumkol Kazakhstan Oil is known as the low sulfur all over the world which has been endorsed by this simulation work which resulted in 277.355 PPM when the feed ratio was set up at 0.75:0.25 Kumkol and Soviet export blend respectively as shown in Fig. 9. In this work, three different ratios of the two crude oil feeds, one is from the Kumkol Oil Fields, Kazakhstan and other one is Soviet Export Blend (currently REBCO), have been used. Firstly, the ratio of 75% of Kumkol Oil Kazakhstan and 25% Soviet Export blend was used which showed impressive results in terms of the production of heavy naphtha which

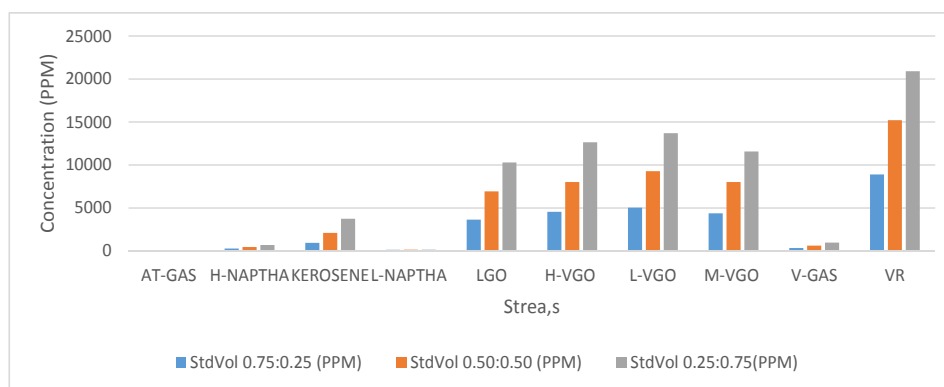


Fig. 16. Sulfur Content of the Streams.

Table 4. Stream Results for ATC (StdVol 0.75:0.25)

Stream	StdVol 0.75:0.25 (PPM)	StdVol 0.50:0.50 (PPM)	StdVol 0.25:0.75(PPM)
AT-GAS	82.731	84.199	85.119
H-NAPHTHA	277.355	461.722	686.518
KEROSENE	947.998	2096.953	3753.745
L-NAPHTHA	135.313	148.302	151.560
LGO	3646.508	6931.822	10298.255
H-VGO	4553.793	8017.843	12646.460
L-VGO	5044.295	9283.339	13705.640
M-VGO	4380.687	8017.843	11565.467
V-GAS	333.5688	622.846	965.210
VR	8899.877	15217.731	20911.825

amounts 6781.763 bbl/day in comparison with 6689.818 bbl/day and 6584.554 bbl/day from ratios 50:50 and 25:75 respectively. Similarly, the production of kerosene is higher in 75:25 ratio amounting 7692.914 bbl/day in contrast with the other two ratios which are 7616.307 bbl/day and 7527.581 bbl/day. Also, light naphtha is being produced more in 75:25 ratio ranging up to 7328.022 bbl/day, on the other hand, 50:50 and 25:75 ratios result in about 3789.138 and 1166.728 bbl/day respectively. The last stream of the ATC also shows some remarkable values in terms of light gas oil (LGO) 17842.140 bbl/day which is much higher than 17618.816 bbl/day and 17392.851 bbl/day for other ratios respectively. Ratio 75:25 produces 201.872 bbl/day of heavy vacuum gas oil in comparison with 198.513 bbl/day and 194.981 bbl/day for 50:50 and 25:75 ratios of both crude oil feeds respectively as shown in Fig. 5 and Table S4. Similarly, for medium vacuum gas oil, it results in 1080.449 bbl/day for ratio 75:25 ratio of Kumkol Oil and Soviet export blend in comparison with 1062.273 bbl/day and 1045.456

bbl/day for 50:50 and 25:75 ratios respectively as shown in Fig. 9 and Table S9. Also, results of light vacuum gas oil production in 75:25 ratio range more than 50:50 and 25:75 ratios respectively (see supplementary material). It results in 10885.838 bbl/day in comparison with the other two ratios 10731.316 bbl/day and 10571.166 bbl/day respectively. But when we compare the production of the vacuum gas, the phenomenon is different, the results show that the more the soviet export blend, more the vacuum gas as can be seen in Fig. 5 and Tables S4, S9, S14 in the supplementary material.

Figure 16 shows the concentration of the sulfur in the product streams of AT-Gas, H-Naptha, Kerosene, L-Naptha, LGO, H-VGO, L-VGO, M-VGO, V-Gas and VR.

In the Fig. 16, it can be observed that the ratio 0.75 of Kumkol and 0.25 of Soviet Export Blend has least concentration of sulfur in all the streams measured in part per million (PPM) which makes Kumkol Oil as least sulfur contaminated crude oil to be processed and used as fuel oil.

It shows that when we keep the ratio 75:25 for Kumkol and soviet export blend respectively, 11973334.79 bbl/day is the production of vacuum gas but when we increase the ratio in comparison with this to 50:50 and 25:75 respectively, the production of vacuum gas is 12029551.91 bbl/day and 12131495.51 bbl/day accordingly). There is no significant effect of changing the ratios of the feed oils on the number of stages vs. temperature and pressure, although, for 75:25 ratio, a slight drop in temperature can be seen at stages between 15 and 20. When we compare the ratios of 75:25 in terms of sulfur with the other two ratios, results show that the least amount of sulfur is traced in all the feeds as can be observed in Table 4.

4. Conclusions

The fundamental process of a crude distillation unit (CDU) system, which is a key stage in petroleum refining, was simulated using Aspen Plus® in this study. The major purpose was to do a parametric analysis and examine the streams produced during the distillation process. To validate the simulation results, temperature-pressure vs. stage and ASTM D86 (temperature) vs. volume percent distillation curves for the ATC column and VC column were developed. The findings show that the ratio of standard volume 0.75:0.25 of Kumkol Kazakhstan and Soviet Export Blend gives more prominent results in terms of the end products. These results show the potential to enhance process optimization and product quality control in the petroleum refining industry. By fully characterizing the material attributes and features of separate streams within the system, Aspen Plus® provides a detailed examination of composition, phase, temperature, pressure, fractions, enthalpy, entropy, density, flow rate, and average molecular weight. This study stresses the significance of simulation tools like Aspen Plus® in the petroleum refining industry. Modeling and estimating CDU system behavior increases process understanding, supports optimization efforts, and leads to improved product quality control. Future study might expand on these findings to look at further adjustments and increase the scope of simulation applications in the petroleum refining business.

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