Simulation of Fluid Catalytic Cracking Unit for Optimum Production of Gasoline Using Aspen HYSYS

1. Introduction

Refineries remain competitive in present markets due to the Fluid Catalytic Cracking (FCC) Unit which industry professionals refer to as the 'Heart of a Refinery.' This unit demonstrates direct importance for profitability because it allows refineries to remain competitive in terms of both economic conditions and environmental standards [1]. Due to its diverse capabilities the unit has been acknowledged as an efficient and economical conversion process in refineries and therefore will maintain its critical function in meeting reformulated fuel needs [1]. The gasoline production pool receives its primary source from the FCC unit that additionally provides feed materials and light olefins supply to the petrochemical industry [2]. The plant needs optimal operation to prevent equipment failures because it plays a direct role in creating the refineries' unreliable operational condition [3].

The Organization of Petroleum Exporting Countries (OPEC) together with the International Energy Agency (IEA) expect global oil demand will increase by 12% and 8% respectively from 2021 to 2030 [4]. Examining these projections demonstrates that fuel consumption will keep growing steadily into the future so Nigeria should strategically restart their refining operations for their crude oil resources. Stanley Macebuh President of Manufacturers Association of Nigeria (MAN) refers to Nigeria as the largest market in Africa because it possesses a young thriving dynamic demographic. Latest UN population projections show how Nigeria currently exceeds 211 million citizens who grow at a rate of 2.4% each year resulting in five million additional residents [5]. The increasing population creates higher demands for energy across the nation. Petroleum-derived fuels operate as energy suppliers and people refer to them as the "life-wire" of economic growth because they play a vital role in daily operations. The country's refineries run by the state only deliver mediocre results thus leading to a significant shortage of refined petroleum products [6].

The unit called Fluid Catalytic Cracking (FCC) functions as part of the refining industry by creating petroleum-fueled products. The unit achieves its main objective by processing high-boiling atmospheric gasoil and vacuum residues feedstocks into valuable output such as high-octane gasoline and olefins and liquefied petroleum gas in combination with catalyst participation. The FCC process functions as a singular operating system which combines the reaction section with fractionating section. The reactor-riser operates together with the regenerator within a two-part reaction section. All endothermic hydrocarbon feed cracking reactions along with catalyst coke formation activities take place in the riser component. The regenerator-reactor uses air to remove accumulated coke from catalyst after the riser reactor process. The heat needed for the endothermic cracking processes within the riser reactor comes from the catalyst regeneration stage [7].

The profitability of FCCUs depends on running operations for optimal gasoline output while reducing coke accumulation. Current market energy cost increases require operations within FCCU to optimize their processes for producing market-relevant products. There is no room for online FCCU optimization through "trial-and-error" because it results in expensive procedures with potential production losses that lead to reduced revenue. Process simulation stands as an optimal method of optimizing the FCCU by providing security against the risks inherent in trial-and-error operations because of advanced computer systems [8]. The modeling and simulation of catalytic crackers has been extensively discussed in the literature, and several scholars have proposed several process models to predict feed conversion. McFarlane et al. [9] dedicated their research to optimizing the Exxon model IV's Reactor/Regenerator section that contains most elements of a Fluid Catalytic Cracking Unit (FCCU). The research aimed to replicate complex interactions which produce difficult control situations within standard industrial FCCU systems. The description of combustion reactions is absent from the model while it uses a simplified cracking kinetic model. The author implemented the simulation code through the Advanced Continuous Simulation Language (ACSL) software system. A comprehensive kinetic model which controls a fluidized catalytic cracker during dynamic operation was developed by Arbel et al [10] both in the reactor and regenerator section. The paper extensively explains complete CO combustion kinetics which produces CO2 products in the regenerator zone using catalytic promoters. The reactor kinetics depend on the ten-lump model developed by Jacob et al. [11] allowing laboratory experiments to determine feed and catalyst properties.

Fernandes et al. [12] conducted research through their study where they investigated a simulation model of an industrial fluid catalytic cracking (FCC) UOP unit that included a high-efficiency regenerator. A six-lump kinetic scheme for gas-oil cracking and coke-on-catalyst function operated in the reactor section to simulate cracking kinetic and catalyst deactivation reactions. Scientists understood the need to model the freeboard zone of the regenerator vessel. The model developers coded the steady-state program in FORTRAN before performing validation tests with industrial data that was readily available. The behavior of industrial FCC unit riser and regenerator reactors was evaluated using a well-developed model presented by Dagde et al. [13]. A model based on five kinetic lumps represented all cracking reactions active within the riser reactor. Simulation results of this research showed that reactor performances were significantly affected by the ratio of catalyst to oil feed as well as regenerator inlet airflow speeds. Dasila et al. [14] unified the reactor kinetic models for riser and regenerator sections to recreate industrial operations of a Full Characterization Cracking plant. The main goal of this study involved predicting the cracking reaction temperature alongside feed conversion rates and product yield levels and coke formation on spent catalysts and regenerated material.

The proposed models enabled researchers to examine how sensitive FCC performance responses to changes in feed preheat temperature and feed flowrate and air flow rate parameters. Increasing catalyst circulation rate together with elevated air flow rate produces maximum conversion levels and product outputs when feed preheat temperature decreases. Former studies about the FCC unit depicted riser reactor kinetics through a simplified reaction framework (yield model) which explained the catalytic cracking unit operations. Models with three to six lump kinetic schemes serve well for simulations provided the model was developed for specific feed combined with specific catalyst [2]. Previous researchers analyzing the FCC unit used simplified reaction chemistry (yield model) to explain the catalytic cracking reactions in riser reactor systems. For specific simulations that use a particular feed with catalyst combination the kinetic model should contain three to six lump kinetic schemes. The typical refinery operations differ from this description because refinery feedstock compositions adjust based on what feedstocks are available.

Higher-order chemical lump models which consist of over ten components prove disadvantageous because they require additional differential equations in the mathematical model of an FCC unit. The estimation process becomes more complicated because more kinetic parameters require measurement alongside an increase in the complexity level of numerical solutions [2, 7]. The usage of such models remains restricted for monitoring FCC dynamics and control functions according to works [9] and [11]. The steady-state operation of gas oil cracking in a UOP type FCC process was predicted through the use of the Refining FCC model by Aspen Engineering Suite for detailed output yield predictions along with product property projections. An industrial optimization process for yield and throughput will be implemented in this model to enhance performance of the FCC unit.

2. Materials and Methods

2.1 Materials

This research work includes Tables 1 and 2 which present data on reacting species, catalysts, feedstock and products' physical characteristics. Table 3 displays the geometrical specifications for the fluid catalytic cracker's reactors.

Table 1. FCC feed and product properties [15]

Component	API Gravity	Specific Gravity	Flow Rate(kg/hr)
Gas oil feed	21.20	0.9270	244090
Fuel Gas	-	-	13180
C3(LPG)	-	-	15388
C4(LPG)	-	-	26118
Gasoline	60.00	0.7390	112037
Light cycle oil	14.00	0.9730	43448
Bottoms	0.50	1.0720	21480
Coke	-	-	12448

Table 2. Physical properties of reacting species and catalyst [15]

Parameter	Value
	9.520
Liquid density at 288°K (kg.m^{-3})	924.80
Specific heat (gas) (kj.kg^{-1}. K^{-1})	3.30
Specific heat (liquid) (kj.kg^{-1}. K^{-1})	2.670
Heat of vapourization (kj.kg^{-1})	156.00

Vapourization temperature(°K)	698.00
Catalyst Particle size(m)	75×10^{-6}
Specific heat capacity ((kj.kg^{-1}. K^{-1})	1.120
Mass flowrate from riser to regenerator (KJ.kg^{-1}K^{-1})	1,729,750
Bulk density (kg.m^{-3})	975.00
Fresh catalyst (kg.hr^{-1})	139.8
Hold in the regenerator(kg)	5000-70000

Table 3. FCC industrial riser reactor dimensions [15]

Parameters	**Value (m)**
Riser Length	22.900
Riser Diameter	2.900
Regenerator Length	35.450
Regenerator Diameter	9.800
Cyclone Height	14.240
Cyclone Diameter	1.500
Disengager Height	24.500

2.2 Simulation Methods.

The research utilizes Aspen HYSYS V10 as its industrial simulation software package. Aspen HYSYS Petroleum Refining utilizes the 21-lump kinetic model from Aspen Technology Inc for simulating intricate cracking kinetics in the riser-regenerator of this FCC unit [16]. The 21-lump model demonstrates capability to solve various types of feed oils and catalysts such as heavy feedstock (boiling point above 510°C) which the ten-lump model from Jacob et al. [11] fails to handle. Table 4 presents the representation of the 21-lump kinetic scheme. The visualization of FCC plant reaction regeneration and fractionation system performance appears in Fig. 1. The Aspen HYSYS Petroleum Refining FCC model runs through interconnected sub-models that both analyze operational units independently and maintain heat stability in riser sections and regenerators. The complete functional model incorporates the riser-reactor system together with feed supply and stripper and regenerator and feed vaporization valves and cyclones [17].

A configuration of FCC model utilizing plant data allowed researchers to validate product properties and yields by testing operational parameters. The simulation started with the intrinsic values of kinetic parameters while using operating parameter values collected from the industrial facility.

Table 4. Summary of 21-lump kinetics [18]

Boiling-point range	Lumps
<C5	Light gaseous aggregates
C5 – 221 °C	Gasoline
221-343°C (VGO)	Light paraffin (PL)
	Light naphthene (NL)
	Light aromatics with side chains (Als)
	One-ring light aromatics (ALr1)
	Two-ring heavy aromatics (ALr2)
343 -510 °C (Heavy VGO)	Heavy paraffin (PH)
	Heavy naphthene (NH)
	Heavy aromatics with side chains (AHs)
	One-ring heavy aromatics (Ahr1)
	Two-ring heavy aromatics (Ahr2)
	Three-ring heavy aromatics (Ahr3)
510+ °C (Residue)	Residue paraffin (PR)
	Residue naphthene (NR)
	Residue aromatics with side chains (ARs)
	One-ring Residue aromatics (ARr1)
	Two-ring Residue aromatics (ARr2)
	Three-ring Residue aromatics (ARr3)
Coke	Kinetic coke (produced by reaction scheme)

	Metal coke (produced by metal activity on catalyst)

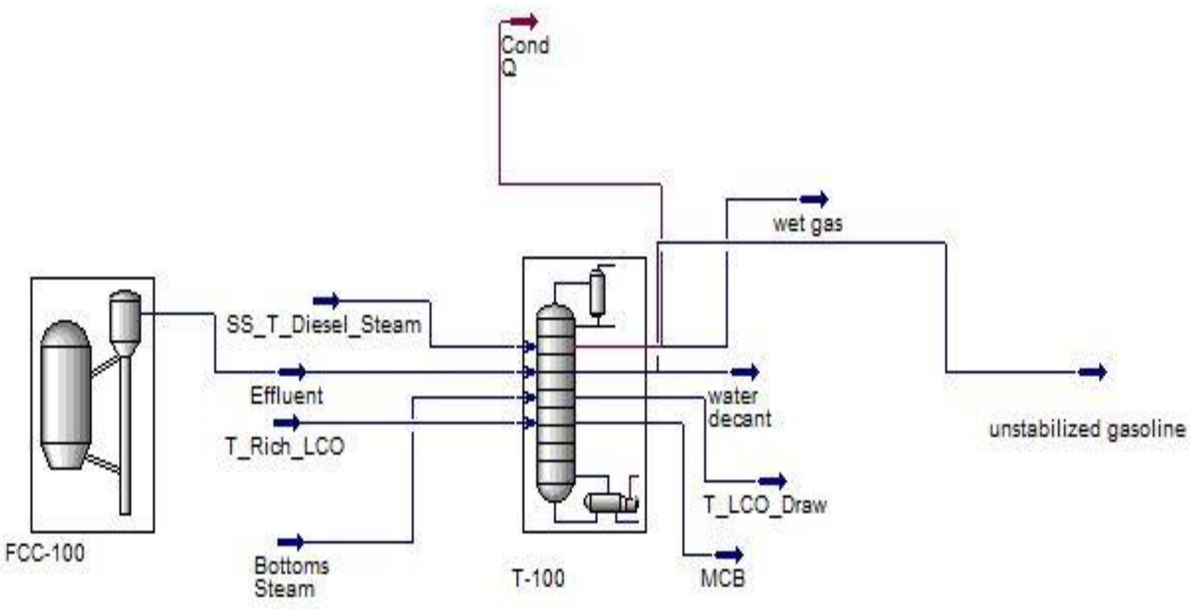

Fig. 1. Simulation diagram of Fluid Catalytic Cracking Unit**.**

3. Reactors Dimensions, Feedstock and Catalyst Properties

Tables 5 - 6 provide the New Port Harcourt Refinery Company's dimensions for the riser and regenerator reactors as well as the characteristics of the feedstock and end products.

Table 5. Distilled-off Gas-oil percentage and corresponding temperature-cuts [15]

Parameters	**Value**
Raw oil feed temp(°K)	505
Riser steam rate(kg.hr^{-1})	1,225
Bottom stripping steam rate(kg.hr^{-1})	2,915
Reactor pressure (kg.cm^{-2})	1.76
Regenerator pressure(kg.cm^{-2})	2.11

Table 6. Major operating conditions for reactor/regenerator

Percentage Distilled-off	**^{0}C**	**^{0}C**
Initial Point	271	544
10%	349	622
30%	421	694
50%	449	722
70%	483	756
90%	531	804
End Point	602	875

4. RESULTS AND DISCUSSION

Data obtained from the simulated study to examine gas-oil catalytic cracking kinetics using process kinetics appears in Tables 7 and 8. The model predictions for gas oil conversion and product yields align with the experimental values derived from an industrial riser reactor, as indicated in Table 7, while Table 8 illustrates the comparison between model predictions and plant data for the regenerator-reactor.

Table 7. Comparison of plant measured, and models predicted data in the riser- reactor

Parameters	**Plant Measured**	**Model Predicted**	**% Deviation**
Gas Oil (wt.%)	26.6	26.3	1.13
Gasoline (wt.%)	45.9	41.87	8.78
LPG (wt.%)	17.8	20.8	16.85
Dry Gas(wt.%)	5.4	4.8	11.11
Coke(wt.%)	5.1	5.65	10.78

Table 8. Comparison between model-predictions and plant data for the riser and regenerator

Parameters	**Plant Measured**	**Model Predicted**
Outlet Temperature of Riser (K)	797	797
Regenerator Temperature(K)	1017	1017

Gasoline RON	94	94
Conversion (%)	73.4	73.33
O_2(mol.%)	3	3
CO_2 (mol.%)	16	14.86
CO (mol.%)	0.00	0.070

The comparisons shown in each Table validate that predicted values match plant measurements accurately. The validated model serves various case analysis to examine flexibility capabilities.

4.1 Sensitivity Analysis

The sensitivity analysis section identifies how particular process variables affect the process output behavior patterns. The procedure serves crucial purposes for optimizing and controlling processes. Mass yields received examination when riser outlet temperature and feed flow rate experienced modification.

4.1.1 *Effect of Riser Outlet Temperature (ROT) on key product slates*

The ROT represents an essential functional aspect for FCC riser models because it governs reactor performance. The Case Studies tool within HYSYS was employed for carrying out this analysis. The Figure 2 shows the variation of the ROT with different species.

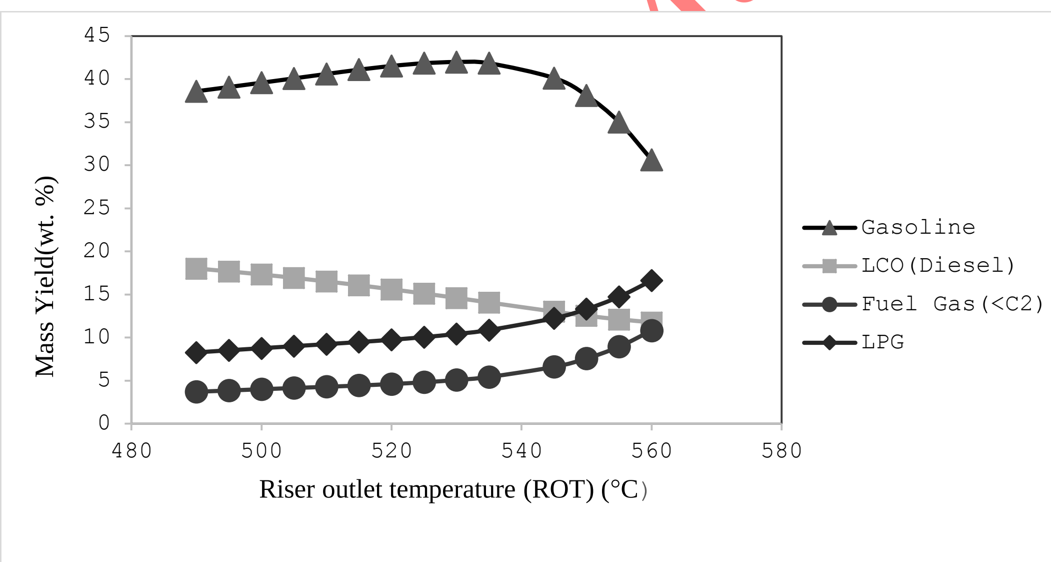

Fig. 2. Variation of product species with riser outlet temperature (ROT).

The changes in product mass yield from the catalytic cracking process with riser outlet temperature (ROT) are shown in Fig. 2. Figure 2 shows that the yield of gasoline (naphtha) increases with an increase in the riser outlet temperature (ROT) up to 530°C. After that, the gasoline yield decreases and the production of light gases increases sharply. Fig. 2's trend for the yield of gasoline is typical since an increase in ROT favors reactions that break the aromatic chain and increase the yield of C5+ components [1]. Diesel, another valuable product declines rapidly as ROT is increased. The reduction in LCO yield and increase in fuel gases(C1-C2) are caused by excessive thermal cracking and catalyst deactivation as the ROT increases. This is obviously an undesirable outcome. Operating at an ROT that simply takes the maximum gasoline into account is therefore not ideal; instead, an ROT that considers other premium products is optimum.

4.1.2 *Effect of Riser Outlet Temperature on Coke Yield*

Coke is an essential by-product deposited on the catalyst as cracking proceeds. The exothermic reaction from burning off this coke in the regenerator reaction provides the heat for the cracking reaction [1].

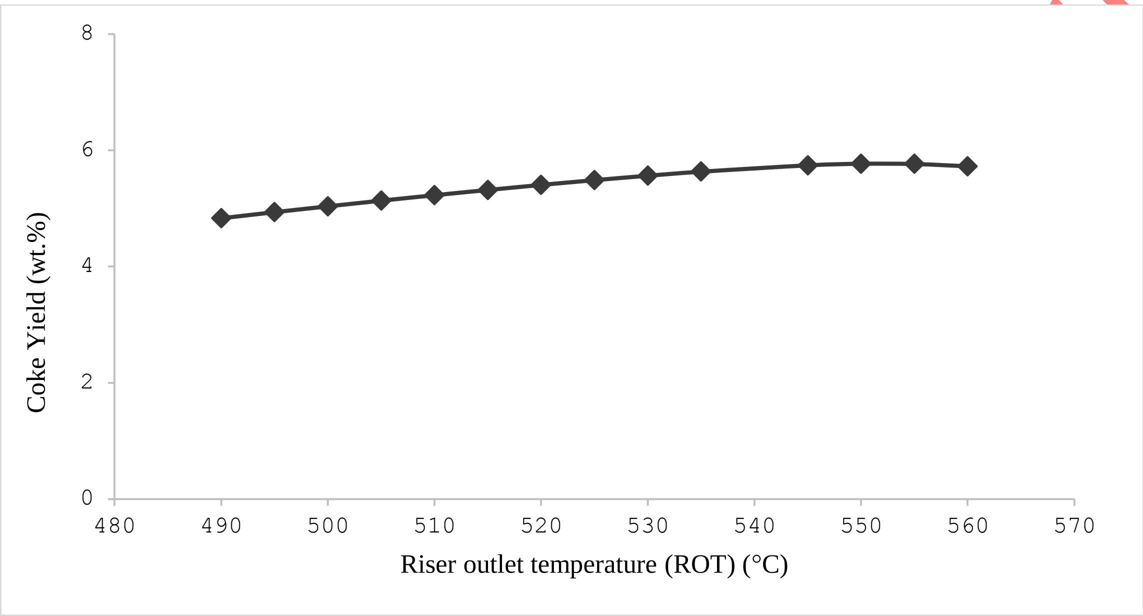

Fig. 3. Variation of coke with riser outlet temperature (ROT)

As a key function of ROT, Fig. 3 displays the amount of coke on the catalyst as it leaves the riser. Figure 3 illustrates the direct correlation between the coke yield and the riser output temperature. Increased coke deposits in the riser and the ensuing catalyst deactivation result in an increase in coke yield. Higher coke deposits in regenerating catalyst increase the amount of energy needed to regenerate the coke to the same activity. The permissible range of values for the riser reactor's ROT is constrained by these side effects.

4.1.3 *Effect of Riser Outlet Temperature on Combined Mass Yields*

Despite the refiner's intention to produce the most gasoline possible, as was previously indicated. The choice of a riser outlet temperature (ROT) is not solely based on this factor. To better comprehend this operational ROT of this refiner, two additional high-end products from the catalytic cracking reaction are considered alongside gasoline.

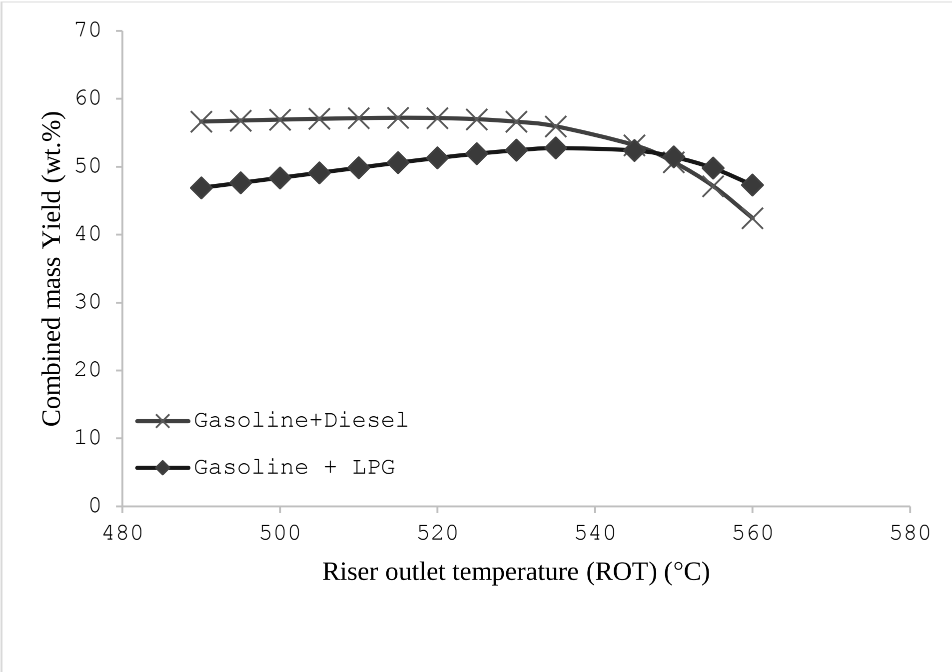

Fig. 4. Variation of combined mass yields with riser outlet temperature

Fig. 4 shows two hypothetical scenarios where the refiner may try to maximize the output of gasoline and diesel or gasoline and LPG as a function of the riser outlet temperature (ROT). As seen in Fig. 4, each of the many examples has its own ideal ROT values. The maximum temperature for the manufacture of gasoline and diesel is between 510 and 515°C, while the maximum temperature at which gasoline and LPG can be produced is between 524 and 535°C (this temperature range verifies the refiner's choice, which was obtained from the FCC of the case-study refinery).

4.1.4 *Effect of Change in Feed Flow Rate on Yields of Products*

Optimizing gasoline production can also be achieved by increasing the unit's throughput. Generally speaking, the refiner will rather process as much feedstock as possible than use less feed to achieve optimal conversion rates. According to Sadeghbeigi [1], it is a path that is not profitable. The most valued product (gasoline) should continue to have same bulk yield.

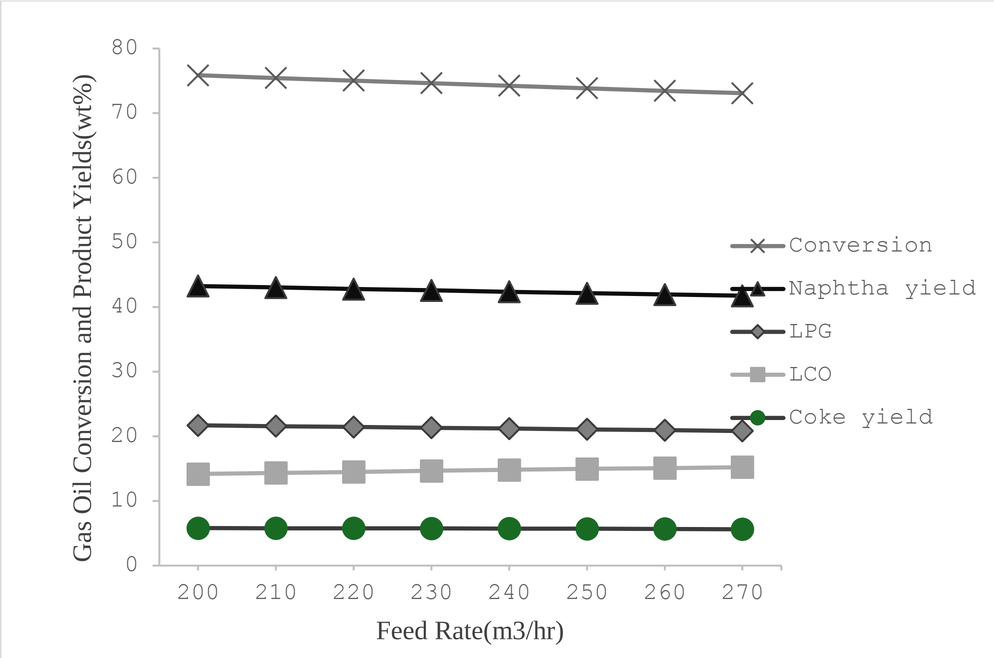

Fig. 5. Variation of gas oil conversion and product yields with feed flowrate

At a constant riser output temperature, Fig. 5 illustrates how changes in feed rate affect conversion and product yield. In Fig. 5, as the rate of feed oil increases to the unit, the conversion and the majority of product yields—aside from the LCO cut yield—show a negative trend. Because conversion fluctuates inversely with stream rates due to the limited reactor size available for cracking, the riser's shorter reaction time may be the cause of this overall reduction [19].

4.1.5 *Effect of Feed flow rate and ROT on Gasoline yield*

Reactions are categorized according to how the reactor's temperature changes during the reaction. Due to the nature of catalytic cracking reactions, the effect of reactor temperature is easily observed, therefore catalytic cracking of gasoil is not an exception. Catalytic cracking is an endothermic process, meaning that as the reaction proceeds, the reactor temperature decreases because the reaction mixture absorbs heat from the reactor. Feedstock conversion rises with reactor temperature, mostly due to an increase in the cat/oil ratio and a faster rate of reaction for the endothermic cracking reaction [19].

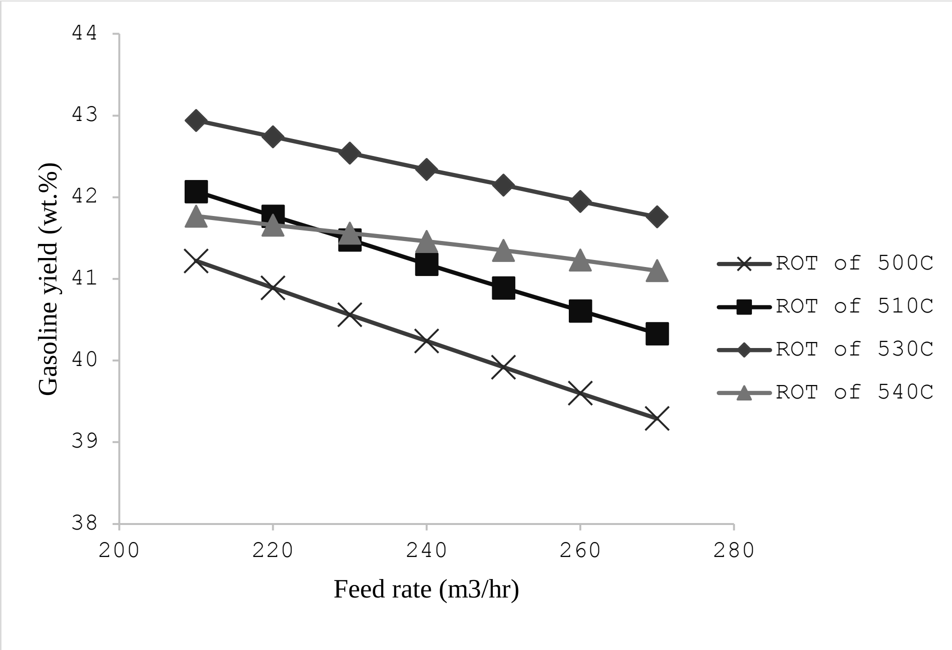

Fig. 6: Variation of gasoline yield with feed flowrate and riser outlet temperature (ROT)

Figure 6 displays the gasoline yield as a function of riser output temperature and gas-oil rate. Figure 6 shows that when both the feed flowrate and the reactor's ROT of are increased, the gasoline production rises. However, at an ROT between 530°C and 540°C, the gasoline output begins to decrease. This shows that the reactor temperature is currently higher than the fluid catalytic cracking unit's ideal conversion point, also known as the over cracking point. The picture also shows that a higher gasoline output with an increase in throughput is favored by an ROT of 530°C.

5. Conclusion

In order to provide the best gasoline possible, this effort uses a computer program that mimics how a fluid catalytic cracking unit would operate. For this simulation, the Aspen HYSYS Petroleum Refining model was used, which incorporates the 21 lump kinetic model schemes created by Aspen Tech to account for the chemical reactions occurring within the reactor section as well as additional sub-models for the regenerator, catalyst transfer, and riser reactor sections to depict the integrated nature of contemporary FCC units. Key process output variables, including product yields and characteristics, were adequately predicted by the steady state model's results, which were compared with data from an industrial plant.

This article addresses the previous limitation of using more complex kinetic models for the FCC unit simulation, which was caused by mathematical difficulties in the modeling processes and a lack of industrial or experimental data to validate the models. It suggests that sensitivity analysis be done to show that functional parameters like the feed flowrate and ROT have a big impact on the FCCU's performance. Additionally, the ROT's optimal control range with pertinent products as the primary output was attained. ROT should be between 524-535°C for gasoline and LPG and between 510-515°C for gasoline and diesel in order to maximize the overall production of these fuels. ROT must be adjusted to 530°C in order to simultaneously boost gasoline yield and output.

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