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Development of a New Method to Optimize Operations of an Existing Crude Unit

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Abstract

A nonlinear optimization method working with the Simplex Method was developed to find optimum operating conditions of a crude oil distillation unit subject to defined process constraints, product specifications and prevailing market conditions. Then the method was applied to a commercial crude unit. This crude unit was modeled using Aspen Hysys V12.1 process simulation software. Two sets of market scenarios designated as the maximum gasoline scenario and minimum gasoline scenario were applied to the simulation model. It was found that the model minimized naphtha production and maximized kerosene production for minimum gasoline scenarios where the price of kerosene and diesel products were higher than naphtha products. Similarly, the model maximized the naphtha product yield for the maximum gasoline scenario where the naphtha price exceeds the mid-distillate product price. The iterative procedure developed for the study monotonically converged to optimum operating conditions for both market scenarios. It was observed that the optimization scheme developed in this study could generate a significant profit increase in the conventional crude unit investigated in this study without and capital investment.

1. Introduction

The crude oil distillation unit is one of the most important refinery process units that influence the profitability of refineries. A significant amount of energy consumption occurs in crude distillation units. Consequently, it is essential that crude oil distillation units must be designed correctly and operated efficiently to produce oil products meeting the final product specifications, to operate downstream conversion units efficiently and to maximize the conversion of any given crude oil to valuable products.

The objective of this study is to develop a nonlinear method that systematically optimizes the operating conditions of a crude distillation unit and to apply the method to an existing conventional crude unit. The new method finds the optimum operating conditions of any crude distillation unit corresponding to any set of market conditions, product specifications and process constraints. It is found that optimization can generate a significant amount of savings in crude distillation unit operations, which, in turn, enhances the profitability of refinery operations under stringent economic conditions prevailing throughout the world.

In this study, a conventional crude oil distillation unit is modeled using the Aspen Hysys V12.1 process simulation program. Then the unit is optimized using a nonlinear optimization method working together with the Simplex Algorithm to determine the operating conditions.

The technical details related to design guidelines, operating conditions, and operation principles for crude oil distillation units have been given by Parkash [1], Meyers [2], Gary et al [3], Fahim et al [4], Steven et al [5], and Nelson [6] in great details. The details of the Simplex Algorithm have been explained in detail by Perry et al [7] and Peters et al [8]. Gürün et al. [9, 10] have applied the optimization method presented in this article to power stations composed of steam boilers,

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steam turbines, and gas turbines and supplying electrical power and steam at various pressures to refinery units. Similarly, Gürün et al. [11] have applied this optimization model to crude unit feed heaters. These references illustrate the application of the method to power stations and refinery process heaters. Kamışlı et al [14] have modeled a crude distillation unit in Hysys and investigated the effect of kerosene draw temperature, tower overhead vapor temperature, stripping steam flow rate and tower overhead pressure on kerosene yield. Yang et. al [15] have addressed a few references in literature discussing different methods of crude unit optimizations. Some of these references focus on heat exchanger network optimization using pinch technology. Others use surrogate methods to simulate crude units. Many applications concentrate on new unit optimization, revamp work, and heat integration improvement. The current work presented here differs from the previous work in that it optimizes the operating conditions of an existing unit without any capital investment subject to a set of process constraints, an objective function and current market data

2. Materials and Method

In this study, a commercial crude oil distillation unit with 100,000 bbl/day (662.4 m^3/h) crude processing capacity has been modeled by Aspen Hysys V12.1 process simulation software and optimized using the method summarized in Appendix B. A simplified process flow diagram for the unit is given in Figure A.1. Main equipment design data for the unit are given in Table A.1. Process description is given in Appendix A. Delawary [12] has published a test run data for this commercial unit for Kerkuk crude oil feed. The product flow rates and laboratory data were used to construct the crude oil feed to model the unit for test run and optimization calculations. The API of the crude feed used for this study is 34.1.

2.1. Fixed Process Parameters

The main process parameters assumed to be fixed in this study are listed in Table 1. Although some of these variables are controlled and can be included in the list of independent variables for optimisation purposes, these variables were assumed to be fixed here to simplify the example. The fixed variables were taken from the test run data presented by Delawary [12] to compare the optimisation results with the test run conditions.

2.2. Dependent Variable Definitions

Product specifications are given in Table 2. These are also the selected dependent variables used for the optimization. Other process variables in the units, such as temperatures in specific locations, heat duties of some heat transfer equipment, flow rates, and other product specifications can also be selected as dependent variables. However, only the product specifications listed in Table 2 have been selected as dependent variables for simplicity in this study.

2.3. Independent Variable Definitions

The process parameters that are independently controlled by a process control scheme are listed in Table 3. These are defined as independent variables in this study. There can be other process variables that are normally controlled by a process control system such as column pressures, overhead temperatures, flow distributions in in heat exchanger network systems of the units. However, 15 independent variables listed in Table 3 have been defined for each unit to illustrate the optimization method developed in this study for simplicity reasons.

Table 1. Major Process Parameters that are Assumed to be Fixed in Process Simulations

Process Variable	Units	Value
Atmospheric tower overhead temperature	^{0}C	92
Atmospheric tower overhead dram pressure	atm	1.4
Atmospheric tower bottoms pressure	atm	2
Light kero pumparound return temperature	^{0}C	67.8
Heavy kero pumparound return temperature	^{0}C	165.7
Diesel pumparound return temperature	^{0}C	268.2
Feed heater inlet temperature	^{0}C	279
Light kero pumparound rate	m^3/h	429.2
Heavy kero pumparound rate	m^3/h	240.9
Diesel pumparound rate	m^3/h	140.5
Atmospheric tower O/H cold drum temp	^{0}C	30
Atmospheric tower cold overhead drum pres	atm	1.11
Naphtha splitter feed temperature	^{0}C	143
Naphtha splitter overhead pressure	atm	5
Naphtha splitter overhead drum temperature	^{0}C	28
Stabilizer feed temperature	^{0}C	72
Stabilizer overhead pressure	atm	12
Stabilizer overhead drum temperature	^{0}C	39.5

2.4. Objective Function Definition

The objective function defines the parameter that is maximized or minimized in an optimization study. The optimization process tries to find the values of the independent variables so that the objective function is maximum or minimum while meeting predefined constraints imposed on dependent and independent variables. The objective function can be defined in different ways such as profit maximization, loss minimization, cost minimization, mid-distillate product maximization, and so on. Profit maximization has been selected as the objective function in this study.

A crude distillation unit receives crude oil as feed and produces LPG, naphtha, kerosene, diesel and fuel oil as products. Fuel and steam are consumed as energy sources to sustain the operations. Electrical power is also consumed in the process to run the process pumps. In this study, the total cost of electrical power is assumed to be constant and not to affect the optimization of the objective function. The profit is defined as the difference between the total revenues from the products and the total cost from crude oil, steam and fuel. Then the objective function can be written as given in Eqn 1.

Table 2. Product Specifications Used for the Optimizations

Product Specification	Units	Min	Max
LPG Sp. Gr.			0.56
Full Range Naphtha Sp. Gr.		0.71	0.74
LSRN Sp. Gr.		0.65	0.70
HSRN Sp.Gr			0.77
Light Kerosene Sp.Gr		0.78	0.81
Heavy Kerosene Sp.Gr		0.81	0.83
Diesel Sp. Gr.		0.84	0.87
Naphtha ASTM D 86 EP	^{0}C	150	195
LSRN ASTM D 86 %95 Point	^{0}C		120
HSRN ASTM D 86 %5 Point	^{0}C	95	120
Light Kero ASTM D 86 End Point	^{0}C		235
Heavy Kero ASTM D 86 End Point	^{0}C	255	290
Diesel ASTM D 86 End Point	^{0}C	355	400
Overhead naphtha product rate	m^3/h	80	200
Atmospheric tower bottoms temp.	^{0}C		370
LSRN product rate	m^3/h		50
HSRN product rate	m^3/h		150
LPG Product rate	m^3/h	4	20

$$\theta = \sum C_{prd}Q_{prd} - \sum C_{crd}Q_{crd} - \sum C_{stm}Q_{stm} - \sum C_{fuel}Q_{fuel} \quad (1)$$

2.5. Calculation Procedure

An iterative procedure has been used to find the optimum operating condition of the conventional crude unit. Constraints used in the calculations are given in Table 4. Test run data was used as the initial data to start iterations.

Table 3. Independent Variables

Process Variable	Units	Constraints used in simulation	
		Min	Max
Feed heater outlet temperature	^{0}C	340	380
Atm tower O/H reflux rate	m^3/h	80	150
Light kero stripper steam rate	kg/h	300	500
Light kero stripper steam rate	kg/h	200	400
Diesel stripper steam rate	kg/h	250	450
Main column stripping steam rate	kg/h	4000	6500
Light kero product rate	m^3/h	30	70
Heavy kero product rate	m^3/h	40	90
Diesel product rate	m^3/h	60	150
Light fuel oil product rate	m^3/h	200	400
Naphtha splitter overhead reflux rate	m^3/h	15	30
Naphtha splitter reboiler feed rate	m^3/h	100	250
Naphtha splitter reboiler temperature	^{0}C	200	240
Stabilizer overhead reflux rate	m^3/h	20	40
Stabilizer reboiler temperature	^{0}C	120	170

3. Results and Discussion

The initial and final values of the independent variables for the two market scenarios can be found in Table 4. The corresponding product characteristics and product flow rates are listed in Tables 5 and 6 for these scenarios. The results presented in this section apply only to the commercial crude facility considered in this study, to the market scenarios shown in Table-C.1, to the product specifications shown in Table-2, and to the independent process variables tabulated in Table-4 for illustrative purposes. The optimisation method is a general method that could be applied to any other crude distillation unit for any other set of valid market, design and product specification data. Consequently, the results of the optimisation may vary under different conditions.

The optimization calculations resulted in higher objective function values for both the minimum and maximum gasoline scenarios in relation to the test run conditions as shown in Table-6. The minimum gasoline and maximum gasoline scenarios provided a profit increase of \$19.2 million/year and \$11.7 million/year profit increase respectively. In general, the products of the crude distillation units are not final refinery products that meet the product specifications. As a result, crude unit product prices for crude oil products are normally lower than prices for the final products and crude oil products alone usually do not usually generate positive profit [13]. The value of objective function based on net profit turns out to be a negative number. Maximizing the objective function in this study actually means minimizing the negative value of the objective function.

Although the value of the objective function turns out to be negative, the difference between the optimal operating conditions and the test run conditions is positive for both market scenarios. The absolute values of the objective function for both scenarios do not mean that one scenario offers a higher profit than the other as the price basis for both scenarios is different.

Table 4. Initial and Final Values of Independent Variables Calculated for each Optimization Scenario

Process Variable	Units	Minimum Gasoline		Maximum Gasoline	
		Test Run	Optimum	Test Run	Optimum
Feed heater outlet temperature	^{0}C	374.0	367.2	374.0	368.6
Atm tower overhead reflux rate	m^3/h	122.9	112.4	122.9	125.6
Light kero stripper steam rate	kg/h	453.8	464.6	453.8	339.8
Heavy kero stripper steam rate	kg/h	359.5	279.6	359.5	259.9
Diesel stripper steam rate	kg/h	413.2	331.4	413.2	308.6
Main column st. stm rate	kg/h	5,977.0	5,697.5	5,977.0	4,761.0
Light kero product rate	m^3/h	45.7	54.3	45.7	47.1
Heavy kero product rate	m^3/h	62.6	66.9	62.6	58.0
Diesel product rate	m^3/h	122.2	122.5	122.2	124.8
Light fuel oil product rate	m^3/h	251.4	250.5	251.4	249.9
NS overhead reflux rate	m^3/h	24.4	27.0	24.4	23.9
NS reboiler feed rate	m^3/h	204.0	173.9	204.0	186.4
NS splitter reboiler temperature	^{0}C	224.0	223.0	224.0	226.6
Stabilizer overhead reflux rate	m^3/h	32.1	28.8	32.1	31.3
Stabilizer reboiler temperature	^{0}C	153.7	143.2	153.7	139.3
Objective Function (1000 $/h)		-35.7	-33.5	-12.3	-10.9
Annual Savings (Mil $/Year)		19.2		11.7	

The model adjusted the plant operating conditions for minimum gasoline operation such that the total flow rate of light kerosene and heavy kerosene increased from 108.3 m3/h for the test run conditions to 121.2 m3/h for the optimum conditions, while the sum of the flow rates of light naphtha and heavy naphtha decreased from 169.5 m3/h to 160.8 m3/h, as shown in Table-6. The switch from naphtha products to kerosene products resulted in a decrease in the specific gravity of naphtha products, the specific gravity of kerosene products and the specific gravity of naphtha across the range, as shown in Table 5. Similarly, the ASTM D-86 naphtha product endpoint decreased from 170.8 0C under the test run conditions to 164.9 0C under the optimum conditions, as shown in Table 5. The model also optimised the plant energy consumption compared to the test run conditions by reducing the feed heater outlet temperature, stripping steam rates, naphtha splitter reboiler output and stabiliser reboiler output as indicated in Table 3, provided the product specifications defined in Table 2 are still met. The model adjusted the process conditions of the plant in minimum gasoline mode to maximise the flow rates for light and heavy kerosene and minimise the flow rates for naphtha, as the naphtha price was set to a lower value than the diesel and kerosene price. This result in turn maximises the value of the objective function for the minimum gasoline scenario.

Table 5. Initial and Final Values of Product Properties for each Optimization Scenario

Process Variable	Units	Minimum Gasoline		Maximum Gasoline	
		Test Run	Optimum	Test Run	Optimum
LPG Sp. Gr.		0.5480	0.5400	0.5480	0.5360
Full Range Naphtha Sp. Gr.		0.7196	0.7164	0.7196	0.7202
LSRN Sp. Gr.		0.6691	0.6598	0.6691	0.6564
HSRN Sp.Gr		0.7385	0.7369	0.7385	0.7394
Light Kerosene Sp.Gr		0.7886	0.7827	0.7886	0.7905
Heavy Kerosene Sp.Gr		0.8162	0.8154	0.8162	0.8167
Diesel Sp. Gr.		0.8582	0.8586	0.8582	0.8589
Full Range Naphtha ASTM D 86 EP	^{0}C	170.8	164.9	170.8	171.6
LSRN ASTM D 86 %95 Point	^{0}C	97.7	96.9	97.7	98.7
HSRN ASTM D 86 %5 Point	^{0}C	111.7	111.4	111.7	112.9
Light Kero ASTM D 86 End Point	^{0}C	221.5	219.5	221.5	225.5
Heavy Kero ASTM D 86 End Point	^{0}C	281.5	283.1	281.5	281.2
Diesel ASTM D 86 End Point	^{0}C	394.0	400.0	394.0	400.0
Overhead naphtha product rate	m^3/h	180.7	168.3	180.7	182.7
Atmospheric tower bottoms tem.	^{0}C	354.4	350.2	354.4	353.7
LSRN product rate	m^3/h	20.2	26.1	20.2	27.5
HSRN product rate	m^3/h	149.2	134.6	149.2	149.0
LPG Product rate	m^3/h	11.1	6.5	11.1	4.4

Table 6. Initial and Final Product Flows for each Optimization Scenario

Product Flow Rate	Units	Minimum Gasoline		Maximum Gasoline	
		Test Run	Optimum	Test Run	Optimum
LPG	m^3/h	11.1	6.5	11.1	4.4
Light Naphtha	m^3/h	20.2	26.1	20.2	27.5
Heavy Naphtha	m^3/h	149.2	134.6	149.2	149.0
Light Kerosene	m^3/h	45.7	54.3	45.7	47.1
Heavy Kerosene	m^3/h	62.6	66.9	62.6	58.0
Diesel	m^3/h	122.2	122.5	122.2	124.8
Light Fuel Oil	m^3/h	251.4	250.5	251.4	249.9

The model shifted the plant operating conditions for the maximum gasoline mode so that the total flow of light naphtha and heavy naphtha increased from 169.5 m3/h for the test run conditions to 176.5 m3/h for the optimum conditions, while the sum of the flows of light kerosene and heavy kerosene decreased from 108.3 m3/h to 105.1 m3/h, as shown in Table-6. In addition, the total naphtha production increased from 160.8 m3/h in minimum gasoline mode to 176.5 m3/h in maximum gasoline mode, while the total kerosene production decreased from 121.2 m3/h to 105.1 m3/h under optimum conditions. As naphtha production increased from the minimum gasoline mode to the maximum gasoline mode, the specific gravities of light kerosene and heavy kerosene increased. The distillation endpoint according to ASTM D-86 for light kerosene also increased significantly.

Since the price of the kerosene products in Table 5 is slightly higher than that of the diesel products, the model produced more kerosene than diesel for both the minimum and maximum petrol modes. The model also adjusted the flow rates of diesel and light fuel oil for both market scenarios such that the end-point of the ASTM D-86 diesel product is shifted to the maximum limit of 400 0C defined in Table 5.

The convergence of the proposed calculation method is shown in Figure 1 and Figure 2 for both scenarios. These figures show that the values of the objective functions increase continuously up to a maximum value. These figures are given here to illustrate that optimising the operating conditions of a conventional crude oil distillation plant can lead to significant profit increases.

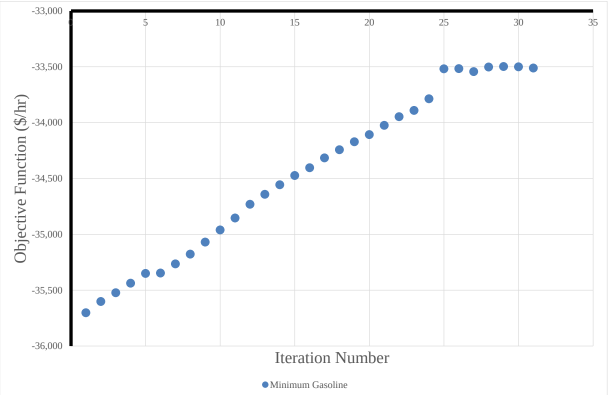

Figure 1. Convergence of the Calculation Procedure – Minimum Gasoline Scenario

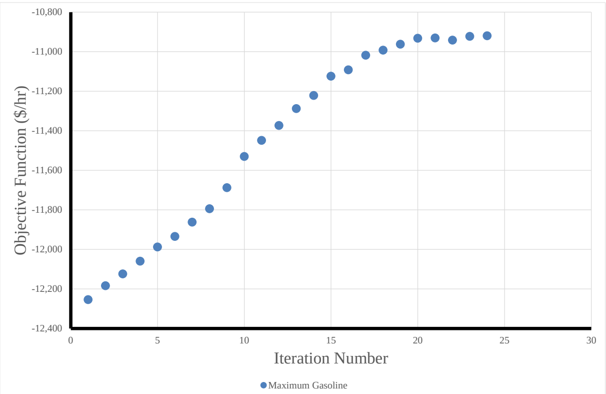

Figure 2. Convergence of the Calculation Procedure – Maximum Gasoline Scenario

4. Conclusions

A non-linear method was developed to optimise the operation of a crude oil plant depending on the prevailing market conditions, taking into account process constraints and product specifications. The method was applied to a conventional crude oil distillation plant for two different market scenarios. It was found that the iterative method converges monotonically to the optimal solution within a reasonable number of iterations.

The optimal operating conditions of the plants indicated that the profitability of the crude oil plant analysed in this study could be significantly increased for both scenarios. The optimisation calculations resulted in higher objective function values for both the minimum and maximum petrol scenarios in relation to the test run conditions. The minimum petrol and maximum petrol scenarios delivered a profit increase of $19.2 million/year and $11.7 million/year respectively.

Once a process unit, such as a crude distillation unit, has been designed and built, its mechanical configuration cannot be changed. However, due to changing market conditions, new product specifications and alternative strategic objectives, the unit may need to be operated within the permitted process limits under completely different operating conditions than the design conditions. This study proposes an optimisation method that can be applied to any existing process unit to determine alternative process conditions so that the unit can continue to operate under the strict economic conditions of a competitive market.

The commercial crude oil unit used in this study is just one example of a typical design. Many different configurations are possible. However, the optimisation method described in this study can be applied to any alternative configuration of the crude unit for any other optimisation criterion, such as minimum gasoline, maximum aviation gasoline and minimum middle distillate production.

Declaration of Ethical Standards

The author(s) of this article declare that the materials and methods used in this study do not require ethical committee permission and/or legal-special permission.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A: Process Description

Figure A.1 shows a simplified process flow diagram of the conventional crude oil distillation plant.

The crude oil feed first enters the atmospheric column after passing through a series of heat exchangers. While the products in the atmospheric column cool down, the crude oil heats up in these heat exchangers. The crude oil then passes through the feed heater before entering the atmospheric column at a controlled temperature. The atmospheric column considered for this study is equipped with three side strippers and three circulation streams. Light kerosene, heavy kerosene and diesel products are extracted from these side strippers. Stripping vapour is fed to these strippers to recover all the light hydrocarbons in these products. Stripping vapour is also fed to the bottom of the atmospheric column to recover any light hydrocarbons remaining in the light fuel oil product. The vapour leaving the top of the column is condensed by an overhead condenser and collected in a vessel. All non-condensed gaseous hydrocarbons leave the system as fuel gas from the overhead tank. Some of the condensing liquid in the overhead vessel is returned to the column as overhead reflux and the remaining liquid is withdrawn from the column as overhead product. The bottom product is withdrawn from the column as light fuel oil product.

The liquid overhead product withdrawn from the atmospheric column is basically a mixture of heavy naphtha, light naphtha and LPG products separated in naphtha splitter and debutaniser columns. The liquid overhead product from the atmospheric column is first fed into the naphtha splitter column where heavy naphtha is separated from the feed stream according to the product specification. The naphtha splitter is a distillation column where the overhead product is a mixture of LPG and light naphtha and the bottom product is heavy naphtha. The debutaniser is also a distillation column in which LPG and light naphtha products are separated. The debutaniser column is fed with the liquid overhead from the naphtha splitter column.

The most important design data for the equipment used in the plant can be found in Table A.1.

Table A.1. Main Equipment Design Data

Atmospheric Column	Number of Stages	35
	Feed Tray	30
	Lt Kero PA Return Stg	6
	Lt Kero PA Draw Stg.	8
	Hv Kero PA Return Stg	18
	Hv Kero PA Darw Stg	19
	Diesel PA Return Stg	26
	Diesel PA Darw Stg	29
	Condenser	Air, Partial
Light Kero Stripper	Number of Stages	4
	Vapor Return Stg	10
	Light Kero Draw Stg	12
Heavy Kero Stripper	Number of Stages	4
	Vapor Return Stg.	18
	Heavy Kero Draw Stg	19
Diesel Stripper	Number of Stages	4
	Vapor Return Stg.	24
	Heavy Kero Draw Stg	25
Naphtha Splitter	Number of Stages	20
	Feed Tray	10
	Condenser	Partial
	Reboiler	Heater, Partial
Debutanizer Column	Number of Stages	20
	Feed Tray	10
	Condenser	Partial
	Reboiler	S/T, Partial

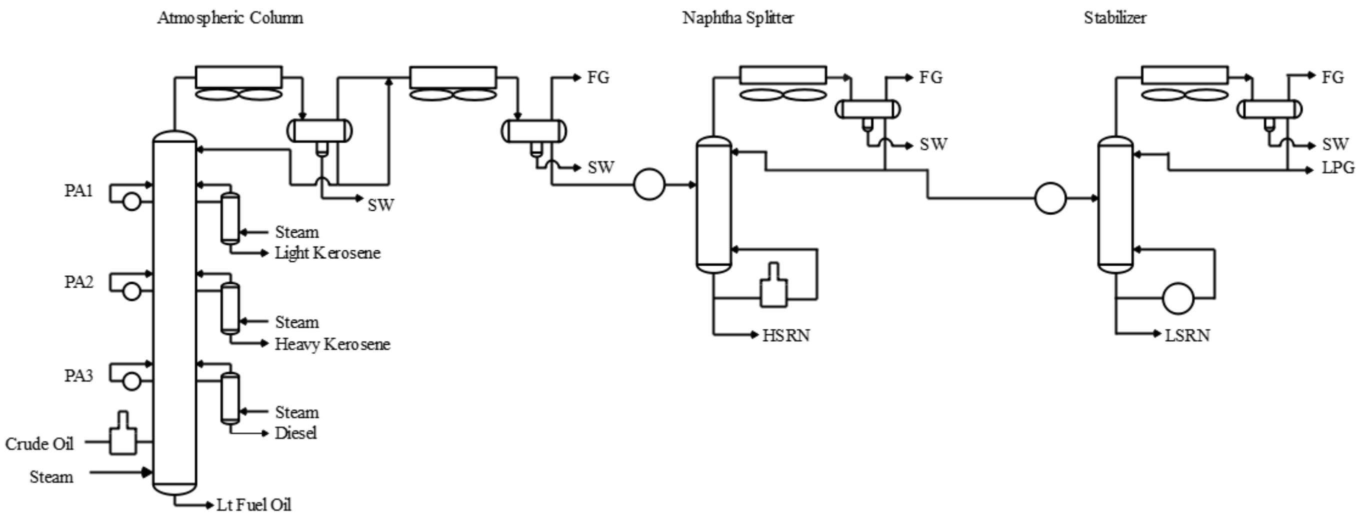

Fig A.1. Simplified Process Flow Diagram of a Conventional Crude Unit

Appendix B: Theoretical Background

When a crude oil plant operates in automatic mode with multiple process control loops under steady-state conditions, each of these process control variables can be changed independently. Each time a process control variable is changed, the process conditions in the entire plant change according to the change in the process control variable. These process control variables were defined as independent variables in this study. The outlet temperature of a heater, the pressure in a tower, the reflux rate in a column, the pumping rates in the column, the product withdrawal rates, the stripping vapour rates are just a few examples of these independent variables. When one of these variables is changed, there is a corresponding change in all process conditions and product characteristics in the plant. The variables that depend on the independent variables are defined as dependent variables in this study. The temperature at any point in a column, the specific gravity of a product, the distillation properties of a product can be given as examples of dependent variables, since any change in an independent variable causes a corresponding change in all dependent variables. The relationship between the independent and dependent variables is shown in Figure B.1.

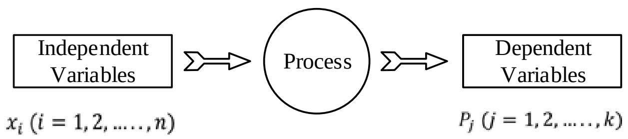

Figure B.1. Relations among Independent Variables, Process and Dependent Variables.

Let x_i be the value of any process variable that can be changed independently by the process control system operating the plant. There is n of these independent variables that are used for the operation of the plant or are included in the optimisation model of the plant. Therefore, i, the index of the independent variables, changes from 1 to n. Let P_j be any process variable that belongs to the plant. Any number of process variables can be defined for each raw plant or used as a dependent variable for the optimisation of the raw plant. Consequently, j, the index of the dependent variable, changes from 1 to k. All dependent variables change simultaneously when one of the independent variables in the plant changes. Therefore, each dependent variable is a function of all independent variables.

$$P_j = P_j(x_1, x_2, x_3, \ldots\ldots\ldots, x_n) \qquad j = 1, 2, 3, \ldots.., k \qquad \text{(B.1)}$$

Differentiation of this expression yields the following equation.

$$dP_j = \frac{\partial P_j}{\partial x_1}\, dx_1 + \frac{\partial P_j}{\partial x_2}\, dx_2 + \frac{\partial P_j}{\partial x_3}\, dx_3 + \cdots + \frac{\partial P_j}{\partial x_n}\, dx_n \qquad \text{(B.2)}$$

Each dependent variable shall be limited by a maximum and a minimum value. Therefore,

$$P_{j,min} \leq P_j \leq P_{j,max} \qquad \text{(B.3)}$$

Furthermore, each independent variable is also limited by a maximum and a minimum value.

$$x_{i,min} \leq x_i \leq x_{i,max} \qquad \text{(B.4)}$$

These equations can be expressed in dimensionless parameters defined as follows.

$$P_j^* = \frac{P_j - P_{j,min}}{P_{j,max} - P_{j,min}} \qquad \text{(B.5)}$$

$$x_i^* = \frac{x_i - x_{i,min}}{x_{i,max} - x_{i,min}} \qquad \text{(B.6)}$$

Then equations (3) and (4) can be written as follows.

$$0 \leq P_j^* \leq 1 \qquad \text{(B.7)}$$

$$0 \leq x_i^* \leq 1 \qquad \text{(B.8)}$$

The differential form of the dependent variable given in equation (2) can also be expressed in dimensionless form as follows.

$$dP_j^* = \frac{\partial P_j^*}{\partial x_1^*}\, dx_1^* + \frac{\partial P_j^*}{\partial x_2^*}\, dx_2^* + \frac{\partial P_j^*}{\partial x_3^*}\, dx_3^* + \cdots + \frac{\partial P_j^*}{\partial x_n^*}\, dx_n^* \qquad \text{(B.9)}$$

An objective function must be defined. In this study to optimise the operating parameters of a system. In this study, the objective function for optimisation is defined as the net profit. The net profit is defined as the difference between the revenue from the unit's products and the expenditure on crude oil, energy and steam to produce these products. Each time an independent variable is changed, the parameters in the objective function also change. Therefore, the objective function is also a function of all independent variables that can be changed by a process control system.

$$\theta = \theta(x_1, x_2, x_3, \ldots\ldots\ldots, x_n) \qquad \text{(B.10)}$$

Differentiation of the objective function yields the following expression.

$$d\theta = \frac{\partial \theta}{\partial x_1}\, dx_1 + \frac{\partial \theta}{\partial x_2}\, dx_2 + \frac{\partial \theta}{\partial x_3}\, dx_3 + \cdots + \frac{\partial \theta}{\partial x_n}\, dx_n \qquad \text{(B.11)}$$

Using the dimensionless definition of the independent variables given in equation (6), the differential form of the objective function can be written as follows.

$$d\theta = \frac{\partial \theta}{\partial x_1^*}\, dx_1^* + \frac{\partial \theta}{\partial x_2^*}\, dx_2^* + \frac{\partial \theta}{\partial x_3^*}\, dx_3^* + \cdots + \frac{\partial \theta}{\partial x_n^*}\, dx_n^* \qquad \text{(B.12)}$$

Optimising the operating conditions means finding a set of all independent variables that maximises the value of the objective function while satisfying the constraints imposed on the independent and dependent variables defined by equations (7) and (8) in dimensionless form. Since the operation of a crude oil distillation unit involves many complex processes, the mathematical model of the unit also requires a solution for highly nonlinear sets of equations. Therefore, an iterative procedure is developed in this study to find the set of independent variables that optimises the objective function. The iterative procedure attempts to find at each step the change in the independent variable (dx^*_i) that leads to an optimal change in the value of the objective function defined in equation (12), while maintaining the constraints on the independent and dependent variables defined in equations (7) and (8), until no change in the value of the objective function is observed.

Based on this approach, values of dependent and independent variables can be written as follows.

$$dx^*_{i,t} = x^*_{i,t+1} - x^*_{i,t} \tag{B.13}$$

$$dP^*_{j,t} = P^*_{j,t+1} - P^*_{j,t} \tag{B.14}$$

The subscript t in the above equations stands for the number of steps in the iteration procedure. Equations (7), (8), (13) and (14) can be combined to obtain the following constraint equations which define the limits for the change of the dependent and independent variables at each step of the iteration.

$$-x^*_{i,t} \le dx^*_{i,t} \le 1 - x^*_{i,t} \tag{B.15}$$

$$-P^*_{j,t} \le dP^*_{j,t} \le 1 - P^*_{j,t} \tag{B.16}$$

The partial derivatives in equation (9) define the contribution of a change in the value of each independent variable to the change in the value of the dependent variable. Equation (16) defines the limit of the total allowable change in the values of the dependent variable at each iteration step. By combining equations (9) and (16), the limits for the change of each independent variable for each iteration step can be defined as follows.

$$-\frac{P^*_{j,t}}{\frac{\partial P^*_{j,t}}{\partial x^*_{i,t}}} \le dx^*_{i,t} \le \frac{1-P^*_{j,t}}{\frac{\partial P^*_{j,t}}{\partial x^*_{i,t}}} \tag{B.17}$$

This expression can be calculated k times for each independent variable at each iteration step. The limits with the minimum absolute values specify the permissible maximum and minimum values for the change in the value of the independent variable. Equations (15) and (17) together define the limits for the change in the value of each independent variable at each iteration step. These equations can be written as follows.

$$\varepsilon_{i,min,t} \le dx^*_{i,t} \le \varepsilon_{i,max,t} \tag{B.18}$$

The aim of the solution is to find a set of dx*i,t that satisfies the constraints defined by equations (18) and (16) and maximises the change in the objective function specified in equation (12). The simplex algorithm can be used to find the desired solution. The following transformation can be implemented to apply the simplex algorithm.

$$du_{i,t} = \frac{dx^*_{i,t} - \varepsilon_{i,min,t}}{\varepsilon_{i,max,t} - \varepsilon_{i,min,t}} \tag{B.19}$$

Then the limits of $du_{i,t}$ are defined as follows.

$$0 \le du_{i,t} \le 1 \tag{B.20}$$

Equations (9), (16) and (19) can be combined to express the dependent variable differentials as follows.

$$-P^*_{j,t} - \sum_{i=1}^{n} \frac{\partial P^*_{j,t}}{\partial x^*_{i,t}} \varepsilon_{i,min,t} \le \sum_{i=1}^{n} \frac{\partial P^*_{j,t}}{\partial x^*_{i,t}} (\varepsilon_{i,max,t} - \varepsilon_{i,min,t}) du_{i,t} \le 1 - P^*_{j,t} - \sum_{i=1}^{n} \frac{\partial P^*_{j,t}}{\partial x^*_{i,t}} \varepsilon_{i,min,t} \tag{B.21}$$

Objective function differential given in equation (12) can be transformed into the following expression using equation (19).

$$d\theta - \sum_{i=1}^{n} \frac{\partial \theta}{\partial x^*_{i,t}} \varepsilon_{i,min,t} = \sum_{i=1}^{n} \frac{\partial \theta}{\partial x^*_{i,t}} \left(\varepsilon_{i,max,t} - \varepsilon_{i,min,t}\right) du_{i,t} \tag{B.22}$$

Simplex Algorithm is used to find a set of $du_{i,t}$ that maximizes the right hand side of equation (22) while meeting the constraints defined in equations (20) and (21) at each iteration step.

Appendix C. Market Data

Market data such as crude oil costs, product prices and energy costs are important factors that affect the profitability of a crude oil plant. These market data are constantly changing over time and lead to shifts in the optimal operating conditions of the plant. The data selected for this study are listed in Table C.1. As the market data changes over time, the optimisation calculations should be repeated to find a new optimal operating point that corresponds to the prevailing market conditions. In this study, the minimum petrol consumption scenario and the maximum petrol consumption scenario were considered. The market data shown in Table C.1 reflect the average conditions in the first quarter of 2022.

Table C.1. Market Data Used for Optimization Study as of the first quarter of 2022

Market Parameter	Units	Minimum Gasoline	Maximum Gasoline
Steam Cost	$/Ton	38,46	38,46
Natural Gas	$/MM kcal	49,11	49,11
Dated Brent	$/bbl	100	100
Kerkuk Crude Oil Spread	$/bbl	-1	-1
Naphtha Crack	$/bbl	-6	16
Kerosene Crack	$/bbl	14,5	14,5
Diesel Crack	$/bbl	14	14
Fuel Oil Crack	$/bbl	-22	-22
LPG	$/Ton	778	778

The minimum petrol demand scenario reflects the market case in which diesel and kerosene products are in greater demand than petrol. Therefore, the naphtha price is lower than the diesel and kerosene price. The scenario with maximum petrol demand reflects the case in which market demand for petrol is high, which is why the naphtha price is higher than in the case with minimum petrol demand. The only difference between the two scenarios is therefore the high naphtha price in the scenario with maximum petrol demand.

Appendix D. Nomenclature

C_{crd}	Purchase price of each crude oil feed stream ($\$/m^3$)
C_{fuel}	Fuel cost ($/kcal)
C_{prd}	Sale price of each product item ($\$/m^3$), for LPG product $/ton.
C_{stm}	Cost of steam stream ($/kg)
$du_{i,t}$	Transformed independent variable differential defined by equation (19)
P_j	Dependent variable j
P_j^*	Dimensionless form of dependent variable P_j as defined in equation (5)
$P_{j,max}$	Maximum value of dependent variable P_j
$P_{j,min}$	Minimum value of dependent variable P_j
$P^*_{j,t}$	Dimensionless independent variable j at iteration step t
$P^*_{j,t+1}$	Dimensionless independent variable j at iteration step t+1
Q_{crd}	Flow rate of each crude oil feed (m^3/h)
Q_{fuel}	Fuel consumption (kcal/h)
Q_{prd}	Flow rate of each product item (m3/h), for LPG product Ton/h.
Q_{stm}	Flow rate of steam (kg/h)
x_i	Independent variable i
x_i^*	Dimensionless form of independent variable x_i as defined in equation (6)
$x_{i,max}$	Maximum value of independent variable x_i
$x^*_{i,t}$	Dimensionless dependent variable i at iteration step t
$x_{i,min}$	Minimum value of independent variable x_i
$x^*_{i,t+1}$	Dimensionless dependent variable i at iteration step t+1
i	Independent variable index (i = 1, 2, 3, ……, n)
j	Dependent variable index (j = 1, 2, 3, ……., k)
t	Iteration step index
θ	Objective function
$\varepsilon_{i,max,t}$	Maximum limit for $dx^*_{i,t}$ at iteration step t
$\varepsilon_{i,min,t}$	Minimum limit for $dx^*_{i,t}$ at iteration step t