STOCHASTIC OPTIMISATION MODEL OF OIL REFINERY INDUSTRY AND UNCERTAINTY QUANTIFICATION IN SCENARIO TREE OF PRICING AND DEMAND

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DEDICATION

This thesis is dedicated to my father. Even though he has passed away, his spirit and enthusiasm remain with me toward completing my doctoral degree. It is also dedicated to my mother, who has sacrificed a lot and has the outmost patience with me, and most of all, to my husband for being very supportive and tolerant. To my children who are always understanding and pray for my success, this is for you all.

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Finally, infinite thanks to my family for their endless support for me to not give up on my study. Without their encouragement, this thesis will not be completed.

ABSTRACT

Uncertainties in oil prices and product demands affect oil refinery industry profits. The fluctuations in oil prices and unstable product demands result in disruptions at procurement, production, and inventory stages. This issue has increased awareness among managers and decision-makers to include uncertainty characteristics in refinery planning. Stochastic programming is an approach to optimising the profit of oil refineries under uncertainty. A crucial assumption for this approach is the use of scenario trees to characterise the probability distribution of the underlying stochastic process. However, there are limited studies on accurate forecast methods to generate scenario trees with low error. The existing stochastic programming approaches do not include uncertainty quantification of stochastic parameters with an accurate forecast model. Thus, this study has developed a framework to formulate uncertainty quantification of stochastic parameters in a stochastic programming model. In modelling oil price dynamics, information on whether the structural break exists is crucial due to the long memory property that might be camouflaged by the existence of the structural break. In this study, oil prices are modelled and forecasted based on the hurst value, and stochastic differential equations are explored to analyse the uncertainty of the time series. Meanwhile, the Holt-Winter method is adopted to describe the uncertainties of petroleum product demand with seasonal variation. The long memory analysis for the before-break and after-break series did not present similar results, which confirmed that the returns of oil prices did not possess true long memory during this period. The results indicate that Geometric Brownian Motion (GBM) and mean-reverting Ornstein-Uhlenbeck (OU) are accurate forecast models to represent future oil prices. It is found that the Holt-Winter seasonal method is an accurate model to represent future petroleum products demand as its mean absolute percentage error (MAPE) value is less than 10. The study obtained 64 scenarios for oil price uncertainty and 32 scenarios for product demand uncertainty as an effective scenario tree for the input of stochastic programming. This newly developed stochastic programming with uncertainty quantification gained 9% more profit than the stochastic programming based on expert judgment, amounting to approximately USD 269,000 per day (~USD 98 million per year). Thus by incorporating uncertainty quantification of stochastic parameters in stochastic programming, more profit could be gained compared to that using stochastic programming based on an expert judgement approach. This new method would also be able to capture more information in managing the supply and demand of petroleum products. The optimal process flow rate in the oil refinery and the amount of shortfall and surplus petroleum finish products in every possible scenario could be determined so the management could plan for future events. Future work for this study could apply more general techniques and reasonable estimates for the distribution of stochastic parameters. Matching the first four statistical moments such as mean, variance, skewness, and kurtosis that are sufficient to explain the characteristics of the uncertain parameters could also be considered.

ABSTRAK

Ketidaktentuan harga minyak dan permintaan produk mengakibatkan keuntungan industri penapisan minyak terjejas. Turun naik harga minyak dan permintaan produk yang tidak stabil mengakibatkan gangguan pada peringkat perolehan, pengeluaran dan inventori. Isu ini telah meningkatkan kesedaran dalam kalangan pengurus dan pembuat keputusan untuk memasukkan ciri ketidaktentuan dalam perancangan penapisan. Pengaturcaraan stokastik adalah satu pendekatan untuk mengoptimumkan keuntungan kilang penapisan minyak di bawah ketidaktentuan. Satu andaian penting pendekatan ini adalah pokok senario bercirikan taburan kebarangkalian proses stokastik. Walau bagaimanapun, kajian mengenai kaedah ramalan yang tepat untuk menjana pokok senario dengan ralat yang rendah agak terhad. Pendekatan pengaturcaraan stokastik sedia ada tidak termasuk kuantifikasi ketidaktentuan parameter stokastik dengan model ramalan yang tepat. Oleh itu, kajian ini telah membangunkan sebuah kerangka untuk memformulasi kuantifikasi ketidaktentuan parameter stokastik dalam model pengaturcaraan stokastik. Dalam pemodelan dinamika harga minyak, maklumat tentang kewujudan pemisahan struktur adalah penting kerana sifat memori panjang yang mungkin dikaburi kerana kewujudan pemisah struktur. Siri masa telah dimodelkan dan diramalkan berdasarkan nilai Hurst, dan persamaan pembeza stokastik telah diterokai untuk menganalisis ketidaktentuan harga minyak. Sementara itu, kaedah Holt-Winter telah digunakan untuk menerangkan ketidaktentuan permintaan produk petroleum dengan variasi bermusim. Analisis memori panjang untuk siri sebelum dan selepas pemisah struktur tidak menunjukkan keputusan yang sama, yang mengesahkan bahawa pulangan harga minyak tidak mempunyai memori panjang yang sebenar dalam tempoh ini. Hasil menunjukkan bahawa Gerakan Geometrik Brown (GBM) dan min-berbalik Ornstein-Uhlenbeck (OU) adalah model ramalan yang tepat untuk mewakili harga minyak masa hadapan. Kaedah bermusim Holt-Winter didapati adalah model yang tepat untuk mewakili permintaan produk petroleum masa hadapan kerana min nilai ralat peratusan mutlak (MAPE) kurang daripada 10. Kajian ini memperoleh 64 senario untuk ketidaktentuan harga minyak dan 32 senario untuk ketidaktentuan permintaan produk sebagai pokok senario yang berkesan dalam input pengaturcaraan stokastik. Kaedah pengaturcaraan stokastik yang baru ini memperoleh 9% lebih keuntungan daripada pengaturcaraan stokastik berdasarkan pertimbangan pakar, berjumlah kira-kira USD 269,000 sehari (~ USD 98 juta setahun). Justeru dengan menggabungkan kuantifikasi ketidaktentuan parameter stokastik dalam pengaturcaraan stokastik, lebih banyak keuntungan boleh diperolehi berbanding cara pengaturcaraan stokastik berdasarkan penilaian pakar. Kaedah baru ini juga dapat memberi lebih banyak maklumat dalam menguruskan bekalan dan permintaan produk petroleum. Kadar aliran proses penapisan minyak yang optimum dan jumlah kekurangan dan lebihan produk petroleum dalam setiap senario masa hadapan dapat dikenalpasti supaya pihak pengurusan boleh merancang untuk masa hadapan. Kajian akan datang boleh mempertimbangkan pengggunaan teknik yang lebih umum dan anggaran yang lebih munasabah untuk taburan parameter stokastik. Pemadanan empat pengiraan statistik momen seperti min, varians, kepencongan dan kurtosis yang mencukupi untuk menerangkan ciri-ciri parameter ketidaktentuan juga boleh dipertimbangkan.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

ACF	-	Autocorrelation function
ARFIMA	-	Autoregressive fractionally integrated moving average
BM	-	Brownian motion
CRR	-	Cox, Ross and Rubeinstein
CUSUM	-	Cumulative sum
DFA	-	Detrended fluctuation analysis
EEV	-	Expectation of expected value
EV	-	Expected value
GBM	-	Geometric Brownian motion
GPH	-	Geweke Porter-Hudak test
HN	-	Here and now
JR	-	Jarrow Rudd
LMSV	-	Long memory stochastic volatility
LPG	-	Liquid petroleum gas
MAPE	-	Rescaled range method
MLE	-	Maximum likelihood estimation
NYMEX	-	New York Mercantile Exchange
OU	-	Ornstein-Uhlenbeck
PDU	-	Primary distillation unit
R/S	-	Maximum likelihood estimation
RMSE	-	Root mean square error
RP	-	Recourse problem
SDE	-	Stochastic differential equations
SP	-	Stochastic programing
WS	-	Wait and see
WTI	-	West Texas Intermidiate

LIST OF SYMBOLS

d	-	Fractional differencing parameter
H	-	Hurst parameter
J	-	Set of processes j
S	-	Set of scenarios s
$b_{i,j}$	-	Stoichiometric coefficient for material i in process j
$C_{j,t}$	-	Operating cost of process j in period t
$d_{i,t,s}, d^L_{i,t,s}, d^U_{i,t,s}$	-	Demand for product i in period t per realization of scenario s with its corresponding constant lower and upper bounds
$I^{f\min}_{i,t}, I^{f\max}_{i,t}$,	-	Minimum and maximum required amount of inventory for material i at the end of period t
$h_{i,t}$	-	Unit cost of outsourcing the production of product type i in period t
p^L_t, p^U_t,	-	Lower and upper bounds of the availability of crude oil during period t
r_t, o_t	-	Labour cost for per man-hour of regular and overtime in period t
$\alpha_{j,t}$	-	Cost coefficient for the investment cost of capacity expansion of process j in period t
$\beta_{j,t}$	-	Fixed cost charge for capacity expansion investment cost of process j in period t
$\gamma_{i,t}$	-	Unit sales price of product type i in period t
$\tilde{\gamma}_{i,t}$	-	Value of the final inventory of material i in period t
$\lambda_{i,t}$	-	Unit purchase price of crude oil type i in period t
$\tilde{\lambda}_{i,t}$	-	Value of the starting inventory of material i in period t
p_s	-	Probability of scenario s
$\lambda_{t,s}$	-	unit purchase price of crude oil in period t per realization of scenario s

$\gamma_{i,s,t}$	-	Unit sales price of product type i in period t per realization of scenario s
$d_{i,s,t}$	-	Demand for product i in period t per realization of scenario s
c_i^+	-	Fixed penalty cost per unit demand $d_{i,s}$ of underproduction product i per realization of scenario s
c_i^-	-	Fixed penalty cost per unit demand $d_{i,s}$ of underproduction product i per realization of scenario s
P_t	-	Amount of crude oil purchase in period t
$x_{\mathrm{j},t}$	-	Production capacity of process j during period t
$S_{\mathrm{i},t}$	-	Amount of product i sold in period t
$L_{\mathrm{i},t}$	-	Amount of lost demand for product i in period t
$H_{\mathrm{i},t}$	-	Amount of product i to be outsourced in period t
$z_{i,s}^+$	-	Amount of underproduction of product type i per realization of scenario s

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Uncertainty in Oil and Gas Industry

The oil and gas industry is a major player in the energy market that transforms oil and gas into various petroleum products. It plays a vital role in the global and domestic economy. Annually, the oil and gas industry in the U.S. invested an average of USD 227 billion on infrastructures from 2012 to 2016, accounting for 16.0% of the total capital expenditures in all U.S. industries (*American Petroleum Institute (API),* 2018). Every year, the increasing consumption of petroleum products increases the demand for crude oil. In 2018, the total world consumption of petroleum was about 100 million barrels per day (b/d); the United States (U.S.) was the largest petroleum consuming country (20.5 million b/d), whereby its transportation sector consumed the highest (66.0%) (*Use of oil*, 2021). In 2020, the total petroleum consumption in the U.S. decreased by 13% from 2019 due to the coronavirus disease (COVID-19) pandemic that causes declining demand for transportation fuels, as planes are grounded and cars parked. Overall, petroleum consumption increased from 1985 to 2020 (Sonnichsen, 2021d). In line with the increasing consumption of petroleum products, the oil and gas industry has to compete for global energy resources and maintains a healthy earning capability to allow reinvestment in the country's facilities, infrastructures, and new technologies, while generating returns that meet the shareholders' expectations (*American Petroleum Institute (API)*, 2016).

The oil and gas industry is divided into three major sectors: upstream, midstream, and downstream (Koroteev & Tekic, 2021) as shown in Figure 1.1. Each sector consists of complex activities that link with one another. The upstream sector, commonly known as exploration, involves identifying deposits, drilling wells, and recovering raw materials from the ground, including field development. Depending on the standards, some crude oils are exported to the international market, and some are processed in the local refineries. The midstream sector is an intermediate sector, which involves transportation to move crude oils to refineries. At times, the operation in the midstream sector is classified as part of the downstream sector. The downstream sector focuses on the refining, processing, marketing, and distribution of refined petroleum products. Because crude oil itself has minimal consumer value, downstream activities play an important role in process the crude oil into the range of petroleum products. There are more than 400 oil refineries worldwide, and most refineries operate in North America (*IHS Markit*, 2019). For example, 18 refineries with the capacity to refine 2 million b/d are located in Canada, contributing to gross domestic product (GDP) of 2.5 billion and the employment of 17,500 Canadian workers (Philip Cross, Pierre Desrochers, & Hiroko Shimizu, 2013). Meanwhile, there are 53 refineries in South East Asia, and seven of them operate in Malaysia, with a capacity of 880,000 b/d (U.S. Energy Information Administration (EIA), 2021).

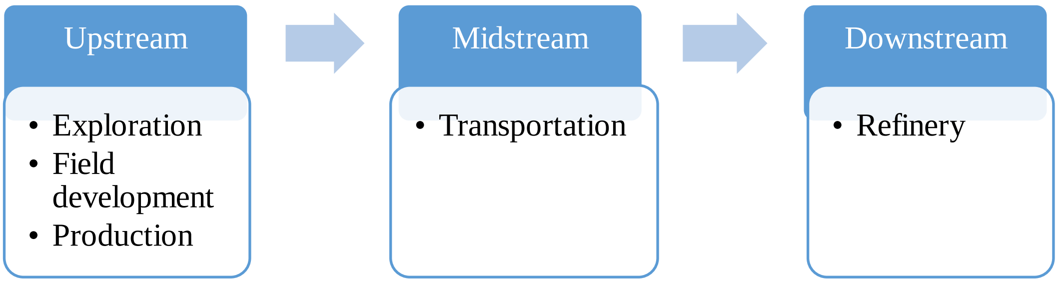

Figure 1.1 Sectors in the oil and gas industry

The oil industry is highly dependent on changes in oil prices because oil is an essential input for many goods and services in the economy (Hoque, Low and Zaidi, 2020). Lower oil prices reduce oil companies' businesses input costs and operating expenses and increase corporate profits and cash flow. The opposite is true when oil prices go up. In general, profitability in refining can be measured by their financial performance (Andrews, Pirog and Sherlock, 2010). The comparative financial performance for world refining companies, Exxon Mobil, Chevron, BP and Shell for the period 2011 to 2020 is shown in Figure 1.2. In general, it shows the profit downtrend from 2011 to 2019. The combination of high crude oil price and weak demand are factors that contribute to the decline in profit from 2011 to 2014. Crude oil is the cost that determines profits in refineries. When the crude oil price is high, the product demand evolves with the increasing income, and the sensitivity of demand to the increase of price is low. Refineries then pass on the high crude oil price to consumers by raising the product price. If the demand is stagnant or low, the transition of high crude oil price to the final product price is unlikely. The high petroleum products inventories pushed down product prices compared to the cost of crude oil, which reducing refining profit margins (Andrews, Pirog, & Sherlock, 2012). The total petroleum consumption in the U.S. decreased due to the COVID-19 pandemic has affected the prices of crude oils to various petroleum products which causes the lowest profit recorded in 2020.

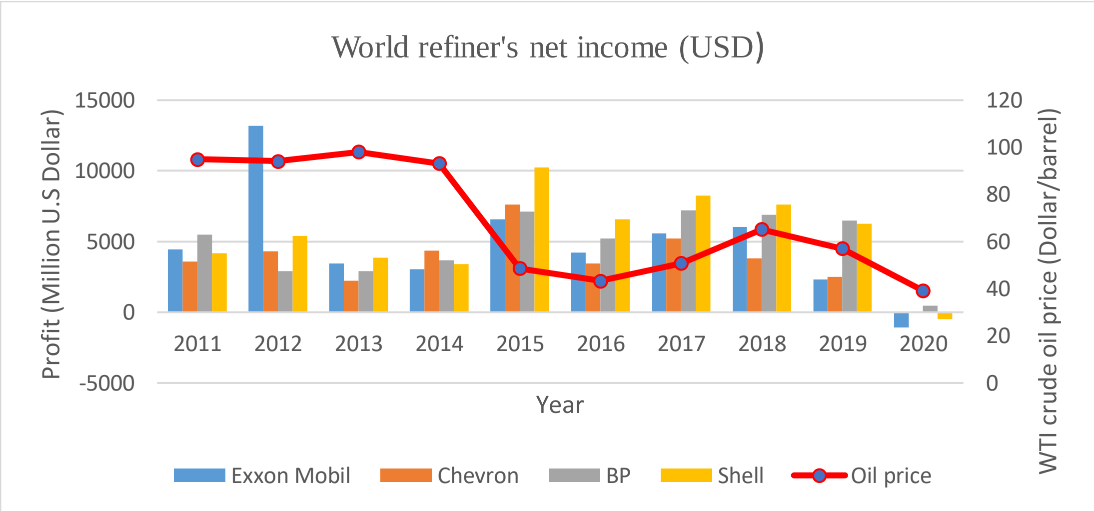

Figure 1.2 World refiner’s net income from 2011 to 2020

Source: (N. Sonnichsen, 2021)(Chevron, 2020)(BP, 2020)(Shell, 2020)

According to Energy Information Administration (EIA) (U.S. Energy Information Administration (EIA), 2021), Malaysia’s national oil and gas natural company, Petroliam Nasional Berhad (PETRONAS) owns a share in the majority of Malaysia's oil and gas blocks, and its financial contributions to government income in the form of taxes, dividends, and cash payments accounted for around 35% of total government revenue in 2019. Petronas' primary activity is the production, refining, and distribution of oil and gas, as well as the manufacture of refined goods such as gasoline, lubricants, and petrochemicals. In the upstream segment, the higher the price of crude oil and gas, the higher the profit, and vice versa. Meanwhile, the profit in downstream segment is determined by the difference between the cost of raw materials and the selling price of petroleum finished products. This implies that the price of crude oil and natural gas, as well as the selling price of its refined products, have a significant influence on the company's profitability (Aziz, 2020).

PETRONAS refinery’s comparative financial performance with crude oil price for the past ten years, from 2011 to 2020, is presented in Figure 1.3. The decline in profit from 2011 to 2014 is attributable to several factors, including the combination of high crude oil prices and lower petroleum product sales volumes (PETRONAS, 2010)(PETRONAS, 2011)(PETRONAS, 2012)(PETRONAS, 2013)(PETRONAS, 2014). The increased profit from 2015 to 2018 is due to a higher refining margin benefitting from lower crude oil prices as well as higher petrochemical products sales volume (PETRONAS, 2015)(PETRONAS, 2016)(PETRONAS, 2017)(PETRONAS, 2018). The lower petrochemical product spreads and refining margins were the fundamental causes of the profit drop in 2019 (PETRONAS, 2019). Lower petroleum product sales volume due to the impact of the COVID-19 outbreak causes profit loss in 2020 (PETRONAS, 2020). Because crude oil and petroleum product prices are the two most important factors that affect oil refining industry profit, changes in oil prices have a significant impact on profitability (Energy Information Administration (EIA), 2016). Meanwhile, sales volume is an important figure in business, as it provides information about the market demand. These indicate that uncertainties in oil prices and product demands affect the worldwide oil refining industry profit and Malaysian oil refining industry profit.

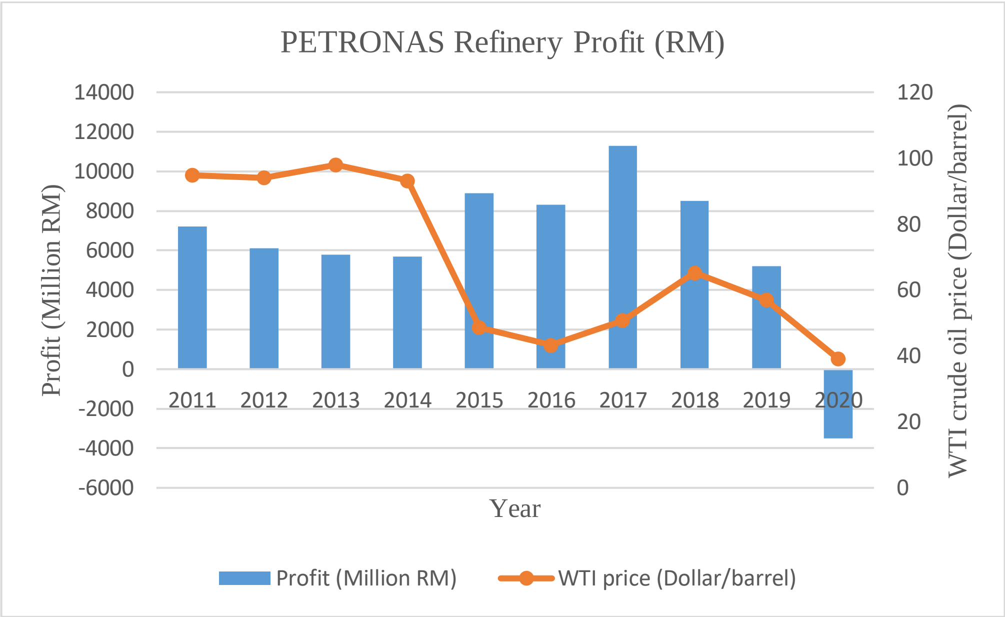

Figure 1.3 PETRONAS's refinery profit from 2011 to 2020

1.2 Challenges in Optimising Oil Refinery Profit

Fluctuating crude oil prices and unstable demand for finished products result in inefficiency that is transferred down to the final product cost. This also disrupts the procurement, production, and inventory stages, which eventually affect the profitability of the oil refining industry. Hence, decision making becomes more complex, and accurate uncertainty quantification is crucial to ensure the decision process reflects the behaviour of the uncertainties.

1.2.1 Uncertainty in Oil Prices

Crude oil is the primary raw material and input for the oil refinery process. There are several oil types in this world, and they are classified and priced according to the density and sulphur content. West Texas Intermediate (WTI) is one of the well-known world's crude oils. WTI crude oil is the longstanding benchmark for pricing crude oil futures contracts traded on the New York Mercantile Exchange (NYMEX).

In this study, WTI crude oil price is chosen because WTI is a widely used benchmark price and forms the basis of many crude oil price formulas. Refineries convert crude oil into various valuable products through several different processes: separation process, conversion process, treatment process, and blending process. The resulting petroleum products are classified as light, medium, or heavy products. Light products consist of liquid petroleum gas (LPG), gasoline, and naphtha. Medium products consist of middle distillates, diesel fuel, kerosene, and related jet aircraft fuel. Heavy products consist of fuel oils, lubricating oils, paraffin wax, asphalt, tar, and petroleum coke.

The majority of the world's crude oil reserves are located in areas prone to political instability or where oil production has been disrupted due to political events. There were three major events that dramatically disrupted the flow of oils from global producers, resulting in the price movement during the late 1970s (J. D. Hamilton, 2009): the Iranian revolution in 1978, Iraq's invasion of Iran in September 1980, and Iraq's invasion of Kuwait in August 1990. Geopolitical events that interrupt crude oil and petroleum product supply to the market might impact crude oil and petroleum product prices. Figure 1.4 represents WTI crude oil prices from 1985 to January 2020. Crude oil prices were more stable until 2000. After 2000, there was one event where the oil price reached its maximum price in history (USD 145 per barrel) in July 2008 before the price dramatically collapsed to USD 30 per barrel in December 2008. Supply and demand and the role of speculations were the main causes of the oil shock from 2007 to 2008 (J. D. Hamilton, 2009). It has been a failure of production to increase between 2005 and 2007, rather than a dramatic reduction in supply. Saudis followed a deliberate strategy of adjusting production to stabilize prices. Saudi production for 2007 was about 850,000 barrels a day lower than it had been in 2005. The decline was one important factor contributing to the stagnation in world oil production from 2005 to 2007.

Although the global supply was stagnant, the global demand continued to increase back then—for instance, the oil consumption in China rose 7% compound annual rate since 1990. In 2007, Chinese consumption was 870,000 barrels per day higher than in 2005. Apart from that, speculation also played an important factor in the oil shock from 2007 to 2008, where investors purchased oil not as a commodity but as a financial asset. Such financialization of commodities introduces a speculative bubble in the oil price. This scenario is different from what caused oil shock in the past decade, primarily referring to the disruption of oil production due to geopolitical events.

It took a year to recover from 30 dollars per barrel in December 2008 to a price range between 80 dollars per barrel and 100 dollars per barrel. In the second half of 2014, the crude oil price dropped to 40 dollars per barrel. It was even worse in 2015 when it dropped to only 30 dollars per barrel. U.S. shale oil producers dominated the market, causing a shift in the global crude oil supply and demand balance (Lu *et al.*, 2021). Then, the price started to increase, and recently, it increased up to 60 dollars per barrel in January 2020. Traditionally, the oil industry has been less focused on procurement management with volatile prices due to relatively stable crude oil prices (Chen *et al.*, 2015). However, since the new millennium, crude oil prices have been highly volatile, forcing management to incorporate price volatility into policy-making decisions. The industries and governments continuously question the behaviour of oil prices in the future due to the uncertainty in oil prices.

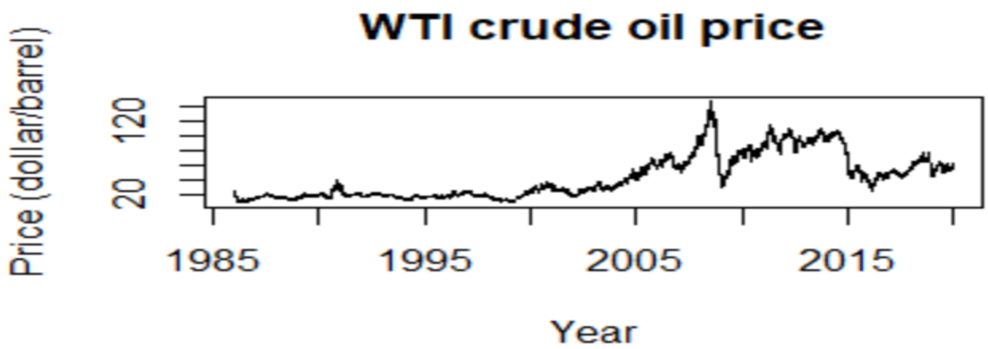

Figure 1.4 WTI crude oil prices from 1985 to January 2020

Source: EIA, WTI spot price

1.2.2 Uncertainty in Demand for Finished Products

The demand for crude oil is derived from the need for petroleum products (Brouwer, 2011). For example, if consumers demand more gasoline, refiners will purchase more crude oils to produce more gasoline. According to the International Energy Agency (IEA), the global economic slowdown since 2010 has significantly reduced the growth rate of global crude oil demand; its growth rate declined from 3.2% in 2010 to 0.9% in 2012. In Europe, the European debt crisis in 2009 has significantly impacted the economic growth and reduced demand for crude oils and refined products. Meanwhile, in the U.S., economic recession and lower demand for motor fuel have reduced oil consumption. As the world's second-largest consumer of crude oil, China's slower economic growth in 2012 has also significantly impacted the demand for crude oils and refined products. All these scenarios represent the uncertainty in demand, which has affected the planning and decision making of refineries in procurement, production, and inventory management.

1.2.3 Optimisation Problem

The decision-making process is typically treated as an optimisation problem. It is always required in many fields, primarily in computer science, economics, engineering design, operation research, environmental control, agriculture, and biological sciences (Sahinidis, 2004). A generic optimisation problem is represented as follows:

$$\begin{aligned} &\min_{x,y} f\left(x, y;\theta\right) \\ &s.t\ g\left(x, y;\theta\right) \le 0 \\ &h\left(x, y;\theta\right) = 0 \\ &x \in \mathbb{R}^{n^x}, y \in \left\{0,1\right\}^{n^x} \end{aligned} \tag{1.1}$$

where some continuous variables, x, represent the decisions being made, such as sizing decision of reactor; $0-1$ variables y represent the discrete choices, such as to select a given reactor or not; an objective function f serves to minimise or maximise, such as to minimise total costs and constraints g and h that the variables have to satisfy, such as the mass balance; variable x is a continuous variable with a dimension n^x that can take a real value; variable y is a binary variable with a dimension n^y that can only take value 0 or 1, which is usually used to represent logic relations or choices; vector θ represents the parameters involved in the optimisation problem, such as price, product demand, and processing cost.

Optimisation problems are divided into deterministic optimisation problem and stochastic optimisation problem. Depending on the forms of f, g, h, x, y, the deterministic optimisation problem can be classified into several categories (Li and Grossmann, 2021):

1) Problem Equation (1.1) is a mixed-integer non-linear programming (MINLP) if some of f, g, h are non-linear functions.

2) Problem Equation (1.1) is a mixed-integer linear programming (MILP) if f, g, h are all linear functions.

3) Problem Equation (1.1) is a non-linear programming (NLP) if some of f, g, h are non-linear functions and there is no y variable, such as $n^y = 0$.

4) Problem Equation (1.1) is a linear programming (LP) if f, g, h are linear functions and there is no y variable, such as $n^y = 0$.

The selection of LP, NLP, MILP, and MINLP depends on the nature of the problem. For examples, non-linear equations describe the kinetic behaviour in chemical engineering problems; integer variables describe the process synthesis problem; binary variable describes the need for capacity expansion in oil supply chain investment planning problem. However, the parameters θ in the deterministic optimisation problem are assumed to be known, which does not reflect the actual situations. In the industrial design and operation of the chemical processes, the decision-making process often involves parameters with uncertainty, such as chemical costs, product demand, and the availability of raw materials. The failure to account for uncertainty in the decision-making process may result in inferior or infeasible solutions. Hence, it is necessary to include uncertainty in the optimisation problem.

1.3 Refinery Planning under Uncertainties

Planning can be described as a developed strategy to allocate equipment, utility, or labour resources to carry out a specific task to develop a single product or multiple products (Leiras *et al.,* 2011). In general, the planning level is characterised into strategic planning (long-term), tactical planning (medium-term), and operational planning (short-term). Strategic or long-term planning covers the longest time horizon, ranging from one year to several years, and the decisions cover the whole organisation, focusing on major investments, such as facility location problems and platform investment planning. Meanwhile, tactical or medium-term planning covers the mid-term horizon, ranging from a few months to a year, and the decisions cover production, inventory, and distribution. Operational or short-term planning covers a short time horizon, ranging from one week to three months, and the decisions cover actual operation and resource allocation. Refinery planning activities determine the types of crude oils for the production of specific products to be sold in the market.

Stochastic dynamic programming, stochastic programming, robust programming, and fuzzy programming are the main techniques for dealing with uncertainty in the refinery planning optimisation problem (Leiras *et al.*, 2011). Stochastic dynamic programming requires too large a state space that leads to the computational burden, even with modern computing capabilities (Begen, 2011). Meanwhile, in fuzzy programming, the problems are not well defined either in terms of the objective function or constraints due to the way uncertainty is modelled as fuzzy numbers, and constraints are as fuzzy sets (Sahinidis, 2004). The accuracy of this approach is jeopardised since they rely on incorrect data and inputs. Robust programming assumes limited information about the distributions of the underlying uncertainties (Leiras, Hamacher and Elkamel, 2010). The stochastic programming approach deals with optimisation problems using parameters with a discrete or continuous probability distribution , separated into recourse models and probabilistic models (Leiras *et al.*, 2011). The risk notation in the robust stochastic programming with recourse's objective function adds another variable to resolve and the risk not being reduced by the lower error of the stochastic parameter. Corrective action for recourse models is avoided due to second stage constraints that can be violated by incorporating a risk measure in probabilistic stochastic programming. Thus, in this study, we choose two-stage stochastic programming with recourse because the first stage decision variables have to be made before the realization of uncertainty which is the optimal operation mode of units and stream flows and the second-stage decision variable can be adjusted after the realization of uncertainty which is the amount of shortfall and surplus petroleum finished products. Stochastic programming is the prominent approach in the refinery planning optimisation under uncertainty (Leiras *et al.*, 2011)(Lima, Relvas and Barbosa-Póvoa, 2018)(Li and Grossmann, 2021), and the crucial assumption is that a scenario tree is given to characterize the probability distribution of the underlying stochastic process. However, there is no better forecast method to generate a scenario tree that has a low error which the existing stochastic programming approaches do not include uncertainty quantification of stochastic parameters with an accurate forecast model. Thus, the problem in the oil refinery business is that the oil refinery business profit decreases from 2011 to 2019 due to there being no uncertainty quantification of stochastic parameters in developing a stochastic programming model. There is also no probabilistic scenario tree with a low error as an input parameter to the stochastic programming model, as shown in Figure 1.5.

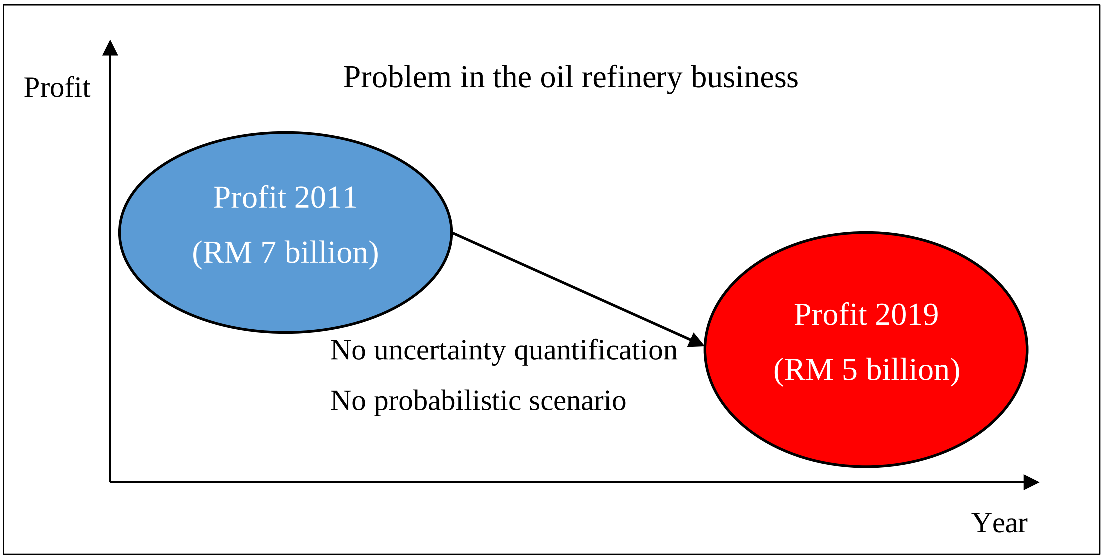

Figure 1.5 Oil refinery business problem infographic

Oil refineries face larger risks than what they encountered 20 years ago due to the fluctuation of crude oil prices. The instability of oil prices has attracted researchers to determine the best model to describe the fluctuations of oil prices. Time series models, econometric models, qualitative methods and artificial intelligence techniques are the four main forecast method categories used in modelling and forecasting oil prices (Lu *et al.*, 2021). The time series models are the simplest model (Suganthi and Samuel, 2012) and essentially continuous probability distributions of random variables. In earlier studies, Brennan and Schwartz (1985) and Paddock, Siegel, and Smith (1988) modelled the commodity price as geometric Brownian motion (GBM) in the application of option's evaluation. GBM is one of the continuous stochastic processes, and the choice of the stochastic process significantly affects the decision to invest in the oil and gas industry (Postali & Picchetti, 2006). Kaffel and Abid (2009), Mostafei, Sani, and Askari (2013), and Nwafor and Oyedele (2017) suggested that GBM works effectively as a proxy for the modelling of crude oil price. With an unexpected price change, the tractability, operational simplicity, and ability to assess all predictions at the same ratio are the advantages of this approach. On the other hand, (E. S. Schwartz, 1997) argued that the mean-reverting process (or also known as OU process) can accurately model the oil price. A mean-reverting process reflects the tendency to reach long-term mean over time. Besides, Lima, Relvas, and Barbosa-Póvoa (2018) proposed ARIMA model to represent the oil price series. ARIMA models require stationary process that may take more than one time lags to transform the data into stationary process. This will complicate the tractability of the continuous probability distribution of the time series.

In modelling energy prices, Barros, Caporale, and Gil-Alana (2012) showed the importance to consider structural breaks, as the results suggested long memory properties if the breaks are not allowed. For the testing of long memory in the crude oil price, Aloui and Mabrouk (2010) and Cunado, Gil-Alana, and Gracia (2010) found no evidence of long memory in the crude oil price return, but they found strong evidence on the long memory in the volatility. Mostafei, Sani, and Askari (2013) run the Perron 1997 unit root test with structural break and concluded that Iranian light and heavy crude oils have one break date. Jibrin *et al.* (2015) identified long memory characteristics and discovered three structural breaks in both time series. It is important to check the subseries of the time series because Yusof, Kane, and Yusop (2013) had shown that although the time series exhibited long memory property, the display of long memory property in the subseries (after detecting structural breaks).

Meanwhile, (Chen *et al.*, 2017) detected a long memory process on the financial time series of the FTSE Bursa Malaysia KLCI index prices. However, the question is whether it is a true long memory or short memory with structural breaks? The confusion on the behaviour of long memory and structural change requires an understanding of the long memory property, but little attention has been given to this aspect in the analysis of stochastic parameters in optimisation problem. Disregard and misspecification of structural breaks potentially lead to poor forecasting performance and policy making. To date, there has been no study on the modelling of oil price uncertainty considering the long memory process in the refinery operation. Thus, the current study examined whether oil prices exhibit the property of long memory (with the existence of structural breaks) in order to choose the appropriate stochastic process for the modelling of oil price uncertainty.

There are many methods to detect the existence of long memory and estimate the fractional differencing parameter, d, which can be summarised into three methods: heuristic, maximum likelihood, and semi-parametric methods (Boutahar, Marimoutou and Nouira, 2007). Heuristic method, such as rescale range (R/S), is useful to determine the first estimate of d. However, this method is generally inaccurate and sensitive to short range serial correlation. Meanwhile, the Whittle approximate maximum likelihood method gives a more accurate estimate of d, but generally requires knowledge of the true model that is often unknown (Wang *et al.*, 2007). Semi-parametric method like the GPH method proposed by Geweke and Porter-Hudak (1983) is based on the behaviour of the spectral density when frequencies approach zero without specifying a finite parameter model for the $d-th$ difference of the time series. Thus, the current study used the GPH method to estimate the fractional differencing parameter, as this model only requires information on the behaviour of spectral density near to origin, not necessary for the specific model.

Demand uncertainty disrupts the procurement of raw materials, production flow, and inventory stages, which have attracted the management to identify the best model to describe demand uncertainty for oil refinery planning. Time series, regression, econometric, ARIMA, as well as soft computing techniques are the modelling and forecasting models of oil demand (Suganthi and Samuel, 2012). Carneiro, Ribas, and Hamacher (2010) modelled the product demand according to different economic growths whereas Ejikeme-Ugwu, Liu, and Wang (2011) sampled product demand according to a normal distribution. Fabrício Oliveira and Hamacher (2012) followed the first-order autoregressive model, and Fernandes, Relvas, and Barbosa-Póvoa (2015) considered to model the product demand with market demand evolution.

As for the time series model, Lima, Relvas, and Barbosa-Póvoa (2018) handled demand uncertainty through time series analysis according to the Box-Jenkins methodology in order to fit the seasonal autoregressive integrated moving average (SARIMA) model to the oil demand data. SARIMA models require stationary process that may take more than one-time lags to transform the data into stationary process which will complicate the tractability of the continuous probability distribution of the time series. The Holt-winter method is another suit of technique that uses historical data to model demand data that have trend and seasonal components. This method is a time series analysis that is appropriate to predict product demands (Dewi and Listiowarni, 2020). This method represents demand uncertainty in stochastic programming to optimise oil refinery profit.

Solving stochastic programming with continuous distribution directly is generally computationally intractable due to the integration over the continuous distribution (Li and Grossmann, 2021). In stochastic programming, randomness is taken into account in the scenario tree, which requires the probability distribution function (PDF) of the stochastic parameter to approximate the discrete distribution of a limited number of outcomes. If the number of scenarios is too large, the model scale and calculation time will be increased. This modelling of the stochastic parameter using a scenario tree as its approximation is known as scenario generation. The binomial tree is a discrete approximation to the underlying stochastic process that can be used to obtain a solution that is computationally efficient for stochastic programming. Using a two-stage stochastic programming method explicitly combines all scenarios and optimises expectations in an objective function.

1.4 Problem Statement

Every day, oil refinery production planning needs to make crucial decisions to improve or sustain the company's production profitability, such as determining the right amount of crude oil to purchase and products to produce and optimise the production with the best use of the existing resources. It is difficult to reach a consensus on where profitability is headed in the next few years with the current oil prices and products demands uncertainty. Discovering the behaviour of oil prices and petroleum products demands is not a simple task in optimising oil refinery production planning. Managements are wondering what is the oil price tomorrow, how much it will differ from today's price and how much demand of petroleum products in the future. The fluctuation of oil prices makes it difficult to forecast the raw material procurement prices. Meanwhile, demand uncertainty causes difficulty to determine the correct quantity of raw material to order and the number of finished products to produce. An inaccurate forecast leads to inefficient decision making in optimising the company's profit margin. One of our primary concerns in this study is to formulate stochastic input parameters into an optimisation problem by identifying the characteristics of data series before forecasting future oil prices uncertainty and seasonal variation in forecasting future product demands uncertainty.

Generating scenario tree that has a low error requires better forecast method. One of the perplexing issues with regards on how an accurate forecast model of the stochastic parameters generate a scenario tree that has a low error. Naturally, time series models are continuous probability distributions of random variables. It is complicated and computational intractable to solve two-stage stochastic programming directly with continuous distribution due to its integration over the continuous distribution. It is important to discretise continuous probability distribution with a limited number of outcomes. Therefore, the construction of a probabilistic binomial scenario tree based on the forecast model as an accurate input parameter to stochastic programming becomes second task in our study.

Numerous prior studies on downstream oil supply chain management under uncertainties adopted stochastic programming as the mathematical model to determine the optimal solution to maximise the profit or minimise the cost (Tong, You and Rong, 2014)(Lima, Relvas, & Barbosa-Póvoa, 2018)(Wang *et al.*, 2019)(Zhang *et al.*, 2019)(Zang *et al.*, 2020). Recently, the improvement of mathematical programming software results in increasing interest to use stochastic programming for process system engineering (PSE) applications including oil refinery (Li and Grossmann, 2021). However, those studies mainly focused on designing the algorithm for the stochastic programming and paid less attention on generating scenario tree that has low error although it is an essential component to develop stochastic programming that is robust in facing uncertainties. The question is how to quantify stochastic parameters in developing two-stage stochastic programming for optimising oil refinery profit? What are the effects of uncertainty quantification of stochastic parameters in two-stage stochastic programming with recourse? Therefore, to manage uncertainties in optimisation model, frameworks are developed in this research to formulate uncertainty quantification in stochastic programming model. This study tends to propose the formulation of stochastic input parameters into the two-stage stochastic programming to optimise oil refinery profit. Applying mathematical programming models to solve issues of the oil refinery optimisation model with uncertainties is relatively new, where the development of stochastic modelling and technique is still required.

1.5 Research Questions

The research questions of this study are as follows:

(a) How to mathematically formulate oil refinery profit optimisation problem with uncertainty?

   i) Does the data series exhibit the property of true long memory or short memory with structural breaks? What is the accurate forecast technique to represent future oil prices that possesses with long memory property for objective function coefficients?

   ii) How to forecast stochastic product demand with seasonal variation for optimisation constraints?

(b) How to establish a binomial scenario tree for discretisation of the continuous probability distribution?

   i) How to incorporate the stochasticity into the input parameters?

(c) How to develop a two-stage stochastic programming in optimising oil refinery profit?

   i) What are the effects of uncertainty quantification of stochastic parameters in two-stage stochastic programming with recourse?

1.6 Research Objectives

The objectives of this study are as follows:

(a) To formulate stochastic input parameter for oil refinery profit optimisation problem with uncertainty quantification

i) To forecast prices uncertainty with consideration of long memory process for objective function coefficients

ii) To forecast stochastic product demand with seasonal variation for optimisation constraints

(b) To establish a binomial scenario tree by incorporating stochasticity of input parameters for the two-stage stochastic programming

(c) To develop a two-stage stochastic programming for optimising oil refinery midterm production planning profit

1.7 Scope of Study

The scope of this study is as follows:

(a) This study established a general framework to analyse the stochastic parameters, the prices of crude oils and finished products (Table 1.1), and the demand for petroleum finished products (Table 1.2) at oil refinery production as input to the optimisation model.

Table 1.1 Prices of crude oils and finished products

No.	Price Data	Date
1	WTI crude oil	1986-2020
2	Gasoline	1993-2020
3	Naphtha	2007-2020
4	Jet fuel	1990-2020

5	Heating oil	1990-2020
6	Fuel oil	1983-2020

Table 1.2 Demand for petroleum finished products

No.	Demand Data	Date
1	Gasoline	2000-2020
2	Naphtha	2000-2020
3	Jet fuel	2000-2020
4	Heating oil	2000-2020
5	Fuel oil	2000-2020

(b) This study presented the structural break test for the stochastic parameters. Following that, the long memory parameters before and after the break periods were estimated using the semi-parametric method.

(c) The drift and diffusion coefficient parameters for data after the break period were estimated through maximum likelihood estimation. The stochastic parameters were modelled and forecasted based on the stochastic differential equations (SDEs).

(d) The demand uncertainties were modelled based on the trend and seasonal components in the data series.

(e) The binomial model for each stochastic parameter was constructed and combined to develop a scenario tree that represents all possible scenarios as input parameters for the stochastic programming.

(f) This study considered the deterministic oil refinery production planning proposed by Allen (1971) and Khor *et al.* (2008) as the base case of a numerical example. Following that, the base case model was reformulated to include uncertainties, and two-stage stochastic programming with fixed recourse was used to maximise the oil refinery profit margin.

1.8 Significance of Study

The contribution of this study is highlighted through methodology, formulation and theoretical perspectives. From a methodology perspective, uncertainty quantification of stochastic input parameters for oil refinery profit optimisation had been done. Involving uncertainty quantification of stochastic programming parameters, the study determined an accurate forecast model to represent the future value of oil prices and petroleum product demands in the optimisation model. Therefore, this study established a probabilistic scenario tree that has low error for oil prices and product demands uncertainty. Developing two-stage stochastic programming for optimising oil refinery profit with accurate forecast leads to reduced stochastic programming risk by the lower error of scenario tree, resulting in efficient decision-making and improved petroleum refinery profits.

A framework to formulate uncertainty quantification in stochastic programming had been established. The stochastic model framework in this study is divided into three modules: module 1 refers to time series analysis, module 2 refers to the discretisation of the continuous probability distribution, and module 3 refers to the stochastic optimisation model. Following the three modules, the obtained results of the time series analysis were translated into a scenario tree for the study to implement in stochastic programming. This study determined the advanced knowledge in improving forecast accuracy of stochastic parameters to represent the uncertainties in the optimisation model based on the characteristics of the data series.

The advancement of knowledge in the fields of applied stochastic modelling and optimisation methods had been made. The proposed model in this study integrated the uncertainty quantification into the stochastic programming that contributed to the growing body of knowledge on the interface of stochastic and operation research management. Thus, the current study provides the practical tool to optimise refinery margin and inculcate a data-driven decision-making environment.

1.9 Thesis Organisation

Overall, the thesis is structured as follows: Chapter 1 introduces the background of the study, problem statement, objectives of the study, as well as the scope and significance of the study; Chapter 2 reviews literature on stochastic optimisation for oil refinery; Chapter 3 presents the methodology; Chapter 4 focuses on the result of the analysis of stochastic parameters, scenario tree construction and optimisation model; Chapter 5 presents the conclusion and recommendations for future research.

Chapter 2 reviews literature on oil refinery production planning under uncertainties, especially in the two-stage stochastic programming model. In order to incorporate uncertainties into the oil refinery problem, the methodology for dealing with uncertainties is the key component of developing a two-stage stochastic programming model that is robust against uncertainties. Thus, the literature review on modelling and forecasting uncertainties are discussed in this chapter. After selecting the appropriate model to describe the behaviour of uncertainties, the study proceeded to construct all possible scenarios in the future. Thus, the literature review on scenario construction for uncertainties is also presented in this chapter.

Chapter 3 presents the fundamental methodology to deal with uncertainties, discretises the probability distribution to produce scenarios assigned with probabilities, and constructs a scenario tree as input for the optimisation problem. When it comes to price uncertainty, the observation of a true long memory process in this study was defined in terms of detecting long memory and structural break. This chapter also describes the construction of Brownian motion, the geometric Brownian motion (GBM), and mean-reverting process or also known as Ornstein-Uhlenbeck (OU) process. In this study, uncertainties were modelled and forecasted, corresponding to each of Hurst parameter. The Holt-Winters seasonal method was adopted in this study to describe the uncertainties of product demand considering the trend and seasonal components. Then, this chapter explains the scenario generation for the stochastic parameters. The scenario-based approach was used to represent uncertainties in this study. Moment matching method in the scenario generation model was used to discretise continuous distribution, with a limited number of outcomes for price uncertainty. Meanwhile, the prediction interval in this study represented the future realisation of demand uncertainty. A scenario construction for price and demand uncertainties is thoroughly discussed in this chapter. Lastly, Chapter 3 demonstrates problem formulation for the uncertainties in the application of oil refinery production planning. The chapter begins with the structure of the deterministic petroleum refinery planning model based on the production planning proposed by Allen (1971). The study reformulated the deterministic model with the addition of stochastic parameters to address uncertainties in the commodity price and demand for finished products based on Khor *et al.* (2008). The details of the framework to maximise oil refinery profit margin with consideration of uncertainties are thoroughly discussed in this chapter.

Meanwhile, Chapter 4 discusses the major findings of the current study with respect to the objectives of study and corresponding research questions. This chapter explains the mathematical model of two-stage stochastic programming with recourse in applying the refinery production planning problem. In this study, the test of the proposed stochastic model was performed using the Generic Algebraic Modelling System (GAMS) to calculate the profit and determine the optimality. The comparison with the shortcut discretisation method, involving an expert judgment, is discussed in this chapter.

The final chapter, Chapter 5 concludes the overall findings according to the outline of the objectives of the study. This chapter also includes recommendations for future research, specifically on further development of the proposed model.

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Appendix D List of Publications

Journal:

1) Bahar, A., Noh, M. N., Zainuddin, Z. M., (2017, November). Forecasting model for crude oil price with structural break. In Malaysian Journal of Fundamental and Applied Sciences (MJFAS), Special Issue (2017), 421-424.

2) Noh, M. N., Bahar, A., Zainuddin, Z. M., (2018, December). Scenario Based Two-Stage Stochastic Programming Approach for the Midterm Production Planning of Oil Refinery. In MATEMATIKA, Special Issue (2018), 45-55.

Conference:

1) Noh, M. N., Chen, K. C., Bahar, A., Zainuddin, Z. M., (2016, June). Analysis of oil price fluctuations. In AIP CONFERENCE PROCEEDINGS of the 23rd National Symposium on Mathematical Sciences (SKSM23) 2015 (Vol.1750, No. 060011, pp.1-5). AIP Publishing.

2) Zainuddin, Z. M., Bahar, A., Noh, M. N., (2020, February). Two-stage stochastic programming approach for oil refinery production planning. In Proceeding ISI World Statistics Congress 2019, Special Topic Session volume 1, 208-215.

3) Noh, M. N., Bahar, A., Zainuddin, Z. M., (2021, August). Formulating a deterministic equivalent of stochastic programming in describing behaviour of prices and demand uncertainty. In AIP CONFERENCE PROCEEDINGS of the 5th ISM International Statistical Conference 2021 (ISM-V 2021)