ON THE APPLICATION OF MODERN PORTFOLIO THEORY TO PROCESS PLANT INVESTMENTS

A Thesis

by

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ABSTRACT

Decision-making among process plant investments has been, and still is, commonly based on typical profitability measures like the Net Present Value (NPV) and the Return on Investment (ROI). This evaluation is done based on single plant-to-plant performance. However, the portfolio nature of processes, such as a company that produces several products from various technologies, is not evaluated. The study of portfolio optimization, that guides investment decision-making, has been implemented in several fields outside the chemical engineering domain. For instance, the Modern Portfolio Theory (MPT) is used to determine the risk return relationship of various portfolios. Then, this study will evaluate its applicability and potential on process plant portfolio investments to aid at the decision-making stage.

The MPT-based methodology was developed for process plant portfolios. Then, this methodology was applied on a case study of six process plants. Various MPT curves were developed that differ by variability rate (Annual and Monthly). Another MPT analysis studies the effect of including economies of scale. Several MPT portfolios will be contrasted with alternatively produced portfolios constructed from the commonly used economic metrics (e.g. NPV/ROI). Results show that NPV/ROI indicators miss more than 50% of attractive portfolio investments when considering annual variability. For monthly variability, MPT portfolios constantly outperformed the alternatively produced portfolios. The same is observed when economies of scale were accounted for. Then, MPT under uncertainty may guide investors to select better process plant portfolios.

DEDICATION

To my lovely family

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NOMENCLATURE

w_n	Percent investment allocated
$\overline{\mu_n}$	Expected return on an asset
$\overline{\mu_{port}}$	Average expected return of an asset portfolio
$\overline{\mu_M}$	Average expected return on a market
R_F	Return on the risk-free asset
β_i	Asset variability
β_{Port}	Asset portfolio variability
σ^2	Variance
σ	Standard deviation (Risk)
ρ	Correlation factor
$F_{p,r}^{net}$	Net flow of a plant
$C_{p,r*}$	Plant capacity
$a_{p,r}$	Amount of resource per ton of product produced
GVA_p	Gross value added
c_r	Cost per unit resource
$TCC_{p,r*}$	Total capital cost
$D_{p,r*}$	Depreciation cost
$FCost_{p,r*}$	Fixed operating cost
$GP_{p,r*}$	Gross profit
$ROI_{p,r*,t}$	Return on investment
$\overline{ROI_{p,r*}}$	Average return on investment of a plant
T	Time
$Return_{PF}$	Portfolio return
Var_{PF}	Portfolio variance
$Risk_{PF}$	Portfolio risk

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1. INTRODUCTION

The basis of chemical engineering lies in the successful economic, environmental, and safety performance of process plants. These plants give rise to chemicals that are either used locally or exported to meet global market demands. To have attractive plant investments, individual processes are evaluated based on several metrics, but the greatest emphasis is usually put on their economic performance. As chemical plants require a great allocation of capital, decision-making between several chemical plant projects is crucial and such an evaluation is done with extreme care.

As the norm suggests, chemical plants are evaluated through typical economic measures such as the Net Present Value (NPV) and the Return on Investment (ROI). Furthermore, plants that do not appear attractive (i.e. having a high NPV and/or ROI value) are eradicated before proceeding further into the investment decision. As a result, there might be an oversupply in the market of specific chemicals, and other products might remain at a disadvantage (unless a more attractive technology is put forth). However, as investment decision-making comes with uncertainty, such a black-and-white approach may not be the best. Consequently, other decision-making tactics that provide an array of various investments, should be considered.

In general, several companies invest in a multitude of process technologies that produce a spectrum of products. Even if these companies own such process portfolios, a blind eye is turned towards the evaluation of portfolio investment performance and instead only individual plant performance is studied. Then, evaluating process plant investments in a collective matter would be of interest for investors, as they can have the complete picture when assessing such investments.

Then, the goal of this thesis is to evaluate the potential of applying a novel based MPT model on process portfolios for guidance on decision-making. The objectives of this study are summarized as follows:

- To evaluate the economic performance of portfolios developed using MPT with respect to alternative portfolios determined by typical economic measures (NPV and/or ROI).
- To evaluate several MPT curves that differ in terms of variability duration (Annual and Monthly) and whether economies of scale were accounted for.

These objectives will serve to tackle the gap presented in literature regarding the lack of evaluation methods for process portfolios especially those that consider multi-criterions (i.e. risk and return).

2. RESEARCH QUESTIONS

This section highlights what are the research inquires intended to be studied. This study is meant to answer whether (1) Can Modern Portfolio Theory (MPT) provide insight to process plant portfolio development? (2) How to develop MPT methodology in such a way to become applicable on process plant selections? (3) Can MPT outperform the status quo of applying profitability metrics (e.g. NPV and ROI)? The remaining of this thesis is comprised of the literature review, methodology development, case study, results and discussions, conclusion, and future work.

3. LITERATURE REVIEW

The following section highlights the literature found to support this research study. First, the literature surrounding typical economic metrics will be highlighted. Next, the background information and some applications of the Modern Portfolio Theory (MPT) will be discussed.

3.1. Typical economic measures

As mentioned, the most typically used economic indicator for chemical process plant projects is the Net Present Value (NPV) (Towler and Sinnott 2013a). NPV has always been used to evaluate the profitability performance of a single plant. In general, NPV is used to distinguish between various plant investment candidates in terms of their relative plant profitability performance. However, this metric does not determine the required allocation of investment across process plants to yield an attractive portfolio. Then, NPV does not set guidelines for the most crucial steps an investor has to take when considering process portfolio investment. Namely, (1) to determine which plants to invest in and (2) how to divide the capital among them has to be done guideless, and the investor can just hope that he/she is holding an attractive portfolio.

Furthermore, NPV is calculated through fixed chemical prices at a specific point in time, and so its labeled as a static model that does not consider real options (Berkovitch and Israel 2004). By definition, real options appear to managers throughout the company’s lifetime due to a variation in investment uncertainty and/or attractiveness. As managers would be able to assess the current risk situation a company is in, it might choose to abandon, expand, or even to switch investments (Mun 2002). NPV does not consider investment risk, and so when it comes to process plants, their profitability fluctuates over time due to the constant variation in chemical prices on both ends (i.e. inputs and outputs), which NPV consequently fails to capture its effect. As raw materials, products, and energy prices fluctuate on the market, they in turn alter the profitability performance of a plant which imposes a risk on the investment. Furthermore, investing in several processes simultaneously may also impose an overall profit variability (i.e. risk). This again has to be accounted for. Nevertheless, price fluctuations are difficult to correctly predict as social, economic, and environmental externals are continuously subjected to change. Another pitfall of using the traditional NPV metric lies in its great sensitivity to the chosen discount rate, which can lead to different investment outcomes (Gallant 2019).

As a result, the NPV metric was further expanded to account for such variations. Several modifications include altering the discount rate, evaluating the discounted cashflows through probability distribution functions, and carrying out a sensitivity analysis (Gaspars-Wieloch 2019). In some cases, the raw NPV model was transformed to give rise to more advanced indicators, such as the stochastic NPV (SNPV) metric (Creemers 2018). This model considers cashflows to be variable and in turn allows the NPV to become changeable. Recently, this metric (SNPV) has been used to aid in power portfolio section where again the risk return relationship was studied (Mari 2020). Furthermore, several statistical equations that define the mean and standard deviation of various sensitivity variables have also been suggested (Humphreys 2005). These variables may even include interest rate variation and/or plant lifetime alteration. Modern simulations have also been developed to study the economic performance of process plants when subjected to such sensitivities, such as the Monte-Carlo simulator (Towler and Sinnott 2013a). More sophisticated methods and/or criteria have been developed to consider the risk reward relationship of investments and are summarized in a latest publication (Vetrova et al. 2019).

Even if the previously mentioned methods shed light on the relationship between plant profitability and price fluctuations and/or rate assumptions, they do not consider such an effect on multiple process portfolios. In turn, they cannot deliver which process plants to invest in and how the capital division should be in such a way to achieve maximum portfolio benefit at minimum risk.

3.2. Modern Portfolio Theory

A method that studies the risk-return relationship of portfolios based on historic price fluctuations and can in turn guide decision-makers for attractive investment, has already been developed in the field of economics and finance. This method is called the Markowitz theory and is interchangeable with the commonly known Modern Portfolio Theory (MPT) (Harry Markowitz 1952). AMPT was first developed to evaluate which asset mix should an investor hold to have an attractive portfolio in terms of risk-return tradeoff (Lhabitant 2017). Then, MPT defines the risk as the standard deviation of an asset's expected return, and the mean return average to be the return on an asset. MPT also requires the prior determination of a correlation matrix which highlights how do the assets' returns move with respect to each other among the considered investments (Elton et al. 2014). This is used to understand the effect of holding several assets on portfolio variability. MPT is a multivariate model as it presents several investment opportunities (i.e. multiple random variables) to invest in while assuming normal distribution (i.e. linear relationship between asset risk and return) (Rachev et al. 2011). In such models, the correlation matrix is the most crucial parameter to study.

The MPT model searches for the optimum capital distribution that can satisfy the risk-return tradeoff defined by the user. These pareto-optimal solutions are presented in what is called 'the efficient frontier' curve. The efficient frontier contains the non-dominated portfolios, which are portfolios that have the highest return at a specific risk value and the lowest risk at a specific return value (Markowitz 1991). Then, it is not possible for portfolios to exist above and/or beyond these points. Furthermore, MPT determines the appropriate division of capital among the assets in such a way to obtain the efficient portfolios. In a nutshell, MPT generates several efficient portfolios that balance the risk-return tradeoff by specifying the optimum capital division among portfolio constituents. Then, the efficient frontier contains the pareto-optimal solutions of a multi-objective problem, which in this case is maximizing return whilst minimizing risk. This multi-objective is subjected to a constraint which limits the development of portfolios to ones that do not surpass the total available capital. This model defines the risk (i.e. variability) as the standard deviation.

As the efficient frontier contains a range of pareto optimal solutions, an investor can choose projects depending on their comfort level with risk. The pareto-optimal curve can be determined by either scalarization or vectorization methods (Chircop and Zammit-Mangion 2013). The former involves transforming a multi-objective problem into a single-objective problem while enforcing the other as a constraint (Ghane-Kanafi and Khorram 2014). If such an approach was used, it is possible to obtain non-global pareto solutions. In turn, such models require the use of a pareto-filter to remove such solutions (Mattson, Mullur, and Messac 2004). The latter includes evolutionary algorithm models which follow the Darwinian approach (i.e. survival-of-the-fittest) by generating, reproducing, and mutating individuals to meet the presented goals (i.e. fitness function) (Qu et al. 2017). For instance, genetic algorithm (GA) has been used as a multi-objective solver in fields of engineering (Chipperfield, Fleming, and Fonseca 1994), biology (Pond et al. 2006), and finance (Sinha, Chandwani, and Sinha 2015). Furthermore, GA can be coupled with other solvers (i.e. a hybrid model) to allow another model to further locate possible solutions (i.e. refine results) that have been missed by GA (Wan and Birch 2013). Due to its ease of application and robustness a GA-hybrid solver will be utilized in this study.

Since MPT has been introduced, it has been used to guide portfolio selection in various fields. In finance, MPT is used to determine the optimum division of capital among a pool of financial investments to hold an efficient portfolio (Elton et al. 2014). MPT gave rise to the well-known Capital Asset Pricing Model (CAPM) which allows a user to determine the expected return on a financial stock (Wang and Xia 2002). There has been a recent study that utilizes the CAPM on financial stocks whilst considering their momentum and inertia for portfolio optimization (Lim, Kim, and Ahn 2020). In the policy-making sector, MPT was used to aid in policy-making by determining the risk-return relationship for a diverse set of energy technologies (Stempien and Chan 2017). MPT was used to determine suitable policy-decisions by evaluating portfolio risk and return of minerals on the Mongolian market (Puntsag 2020). In the energy sector, MPT was used to establish the optimum power generation mix in China (Zhang, Zhao, and Xie 2018). Similarly, the model was used to study the possible electricity generation options in the poverty-stricken country Kenya (Malala and Adachi 2020). This theory has also been applied on the food-energy-water nexus to establish ideal crop selections while considering the risk present in national food security (Raboy, Linke, and Najdawi 2010). A more recent study utilized MPT to determine the optimum soybean varieties whilst considering different weather conditions (Marko et al. 2017). The impact of portfolio diversification on the risk-return relationship for oil and gas portfolios has been studied (Costa Lima et al. 2008) along with determining the optimum capital allocation among oil and gas investments to hold attractive portfolios (Xue et al. 2014). In waste management, the theory was utilized to assess the efficient distribution of groundwater resources whilst incorporating the impact of urbanization and climate change (Hua et al. 2015). In a recent study, MPT was used under uncertainty to evaluate future performance of several environmental investments (Ando et al. 2018). In sustainable development, MPT was used to study different energy portfolios, while considering inexpensive and clean power options, to meet the environmental goals set by the United Nations Sustainable Development (Brandi and Silvio 2020).

This study adjusts and applies MPT to explore ideal portfolios for process plant investments. Even if there are numerous applications of the MPT-based strategy in different fields, such an approach on the process portfolio optimization problem has, to our knowledge, not been previously attempted in the chemical engineering domain. In particular, the suggested novel-MPT approach can evaluate ideal portfolios in terms of (i) which processing plants to include, and (ii) their respective capital distribution to hold an efficient portfolio (i.e. at optimum risk-return conditions). These pareto-optimal portfolios constitute the efficient frontier as they balance the opposing risk-return objectives, from which a decision-maker can pick from a list of possible portfolios depending on attitude towards risk.

4. METHODOLOGY

The following section shows the method used to obtain the results. First, the general MPT application is demonstrated through financial investment applications. Then, the method is transformed to work on process portfolio investments.

4.1. Financial asset portfolios

First, the general concepts and/or equations that are embedded in an MPT application on financial investments is demonstrated. Then, additional model equations, specific to the analysis of processing plant portfolios, are established to produce the complete MPT-based approach.

Let a portfolio hold a set of financial assets A = {a_1, a_2, …., a_n}, n ∈ ℕ, and the fraction (weight) of asset a_i in the portfolio be w_i ∈ [0,1]. The weights of all assets in the portfolio sum up to one (Lhabitant 2017):

$$\sum_{n=1}^{N} w_n = 1 \qquad (1)$$

This constraint ensures that all portfolios developed should divide the total capital available. A portfolio can contain asset n, which translates to $w_n > 0$. If a portfolio doesn't contain asset n, $w_n = 0$ holds. In a portfolio, $w_n < 0$ applies if the user is selling the asset short which is an unattractive investment. As a portfolio studies the risk return relationship, determining these two variables comes next. Then, the risk and return of each portfolio is calculated as follows. Let PORT = {$port_1$, $port_2$, ..., $port_N$}, n ∈ ℕ be a set of portfolios constituted of assets a_i combinations. The expected return of a portfolio is determined as shown in (2) (Elton et al. 2014).

$$\overline{\mu_{port}} = \sum_{n=1}^{N} w_n \times \overline{\mu_n} \qquad \forall\ (\text{port} \in \text{PORT}) \qquad (2)$$

where $\overline{\mu_{port}}$ is the average expected return on a portfolio and $\overline{\mu_n}$ is the expected return on a single asset. The variable $\overline{\mu_n}$ is most commonly obtained on a monthly basis. The variance of a portfolio is computed as (Elton et al. 2014),

$$\sigma_{port}^2 = \sum_{n=1}^{N} w_n^2 \sigma_n^2 + 2\sum_{n=1}^{N} \sum_{m \neq n}^{N} w_n w_m \rho_{n,m} \sigma_n \sigma_m \quad \forall \text{ (port} \in \text{PORT)} \tag{3}$$

where σ_{port}^2 is the portfolio variance and σ_n^2 is the variance of a single asset. The variable σ_n^2 is also obtained on a monthly basis. The first term on the right hand side of (3) is the unsystematic risk (i.e. variance) whereas the following term is the systematic risk (i.e. covariance). As the number of assets held in a portfolio increases (N→∞), the covariance term surpasses the variance term resulting with $\sum_{n=1}^{N} w_n^2 \sigma_n^2 \rightarrow 0$. This observation happens through portfolio diversification. Consequently, in portfolio theory, the covariance is of more importance than the individual variance. The covariance explains the direction a couple of assets move with respect to each other. Further, the term $\rho_{n,m}$ represents the correlation between two assets, which explains the strength of this relationship. Then, the Pearson correlation coefficient ($\rho_{n,m}$) shows in what direction do asset returns move and their relative strength with respect to each other. It has a value between -1 and +1 (Elton et al. 2014). As $\rho_{n,m} \rightarrow 1$ translates to both assets having expected returns that move in the same direction and have a strong alike relationship. As $\rho_{n,m} \rightarrow -1$ translates to both assets moving opposite to one another and have a strong opposing relationship. As $\rho_{n,m} \rightarrow 0$ means the two assets have a weak/to no apparent relationship with one-another. For financial investments, if such correlations cannot be determined, it is most commonly assumed to be 0.5 (Elton et al. 2014). The terms σ_n and σ_m represent the standard deviation of assets n and m respectively. The portfolio standard deviation (risk) is determined as:

$$\sigma_{port} = \sqrt{\sigma_{port}^2} \quad \forall \text{ (port} \in \text{PORT)} \tag{4}$$

Then, the return on a single asset can be found using the Sharpe-Lintner Capital Asset Pricing Model (CAPM) (Elton et al. 2014):

$$\overline{\mu_n} = R_F + (\overline{\mu_M} - R_F) \times \beta_i \qquad \forall \ (a \in a_n) \tag{5}$$

Where R_F represent the return on the risk-free asset. It is most commonly assumed to be a 10-year note treasury bill. The variable $\overline{\mu_M}$ represents the expected average return on the market, which is about 10% (if the S&P 500 was taken as the reference market). Then, the variable β_i is a measurement of the asset's return variability (i.e. risk) with respect to the market return and is calculated using (Elton et al. 2014):

$$\beta_i = \frac{\sigma_{n,M}}{\sigma_M^2} \qquad \forall \ (a \in a_n) \tag{6}$$

Where the numerator represents the covariance between the return on the asset and the return on the market. The denominator is defined to be the variance of the market return. As (5) is a linear model, it is expected that as β_i increases (i.e. asset risk increases), the higher the expected return. Then, the portfolio beta can be found using (7), and market beta is always one (Elton et al. 2014).

$$\beta_{Port} = \sum_{n=1}^{N} w_n \beta_i \qquad \forall \text{ (port} \in \text{PORT)} \tag{7}$$

The expected mean return, and standard deviation of each portfolio are plotted to yield the risk-return relationship. To evaluate which portfolios are pareto-optimal the efficient frontier has to be determined. The efficient frontier is the curve that connects the non-inferior portfolios from the highest return portfolio (A) to the lowest risk portfolio (B) as illustrated in Figure 1, where efficient portfolios fall in-between the two. The highest return portfolio is most commonly a single asset.

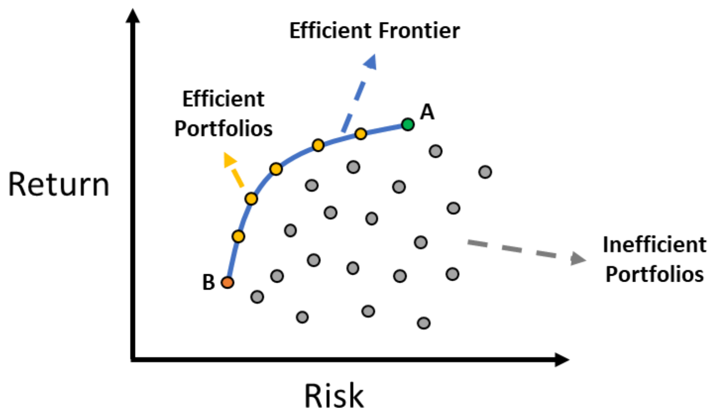

Figure 1: Typical efficient frontier

Any other portfolios that do not fall on the efficient frontier are taken as inefficient (i.e. unattractive). This is because they do not yield maximum return for a specified risk value, and/or they obtain a higher risk for a specified return value. No portfolios fall above the efficient frontier. The following section will demonstrate how to obtain the efficient frontier for process plant portfolios.

4.2. Process plant portfolios

To apply MPT on process portfolios, the profitability performance of a plant has to be determined prior to analysis. The profit of a plant is a function of operating costs for raw materials and energy inputs, which continuously undergo significant price fluctuations and can result in substantial variability in plant profit. In this study, it has been assumed that the processing plant portfolio investments are built at the same point in time and their respective capital costs are assumed to be calculated. Then, the capital cost charges are fixed in contrast to the variable material and energy inputs and valuable product outputs. Figure 2 illustrates the variability in profit for a plant of known capital investment.

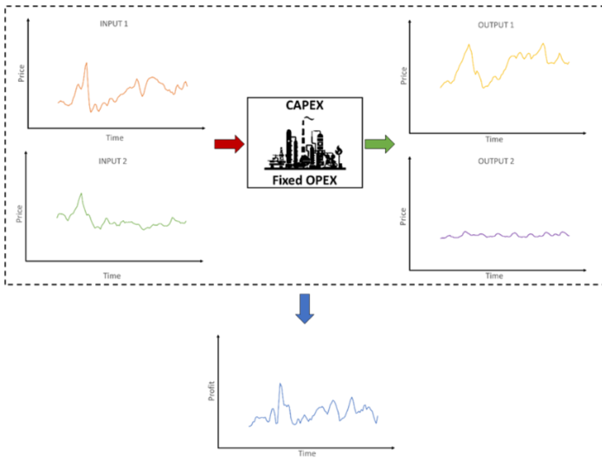

Figure 2: Plant profit instability due to fluctuating input and output prices

Let a portfolio hold a set of plants P = {p_n}, n ∈ ℕ, and let the fraction (weight) of capital invested into a plant (p_i) in a portfolio be w_i ∈ [0,1]. The capital allocation should meet the requirement of (1) i.e. the capital is entirely invested in each portfolio developed. Moreover, let there be a set of material and energy resources R = {r_n}, n ∈ ℕ, which contains the resource inputs and outputs associated with the plants in P. Then, a user is required to know the overall mass balance, utility requirements and/or surpluses, capital costs, and other fixed operating costs of each process plant. Let the material and energy inputs and outputs of a processing plant be defined through parameter ($a_{p,r}$), which represents the specific net amount of material and energy resource r ∈ R (raw materials, utility, and power requirements) per ton of product produced in plant p

(Ahmed et al. 2020). The main output produced in plant p is set as reference product r* for which the parameter has a value of one ($a_{p,r*} = 1$). The mass balance for a plant p is:

$$C_{p,r*}\left(a_{p,r}^{in} - a_{p,r}^{out}\right) = F_{p,r}^{net} \qquad \forall\ (\mathrm{r} \in \mathrm{R}) \tag{8}$$

Where $C_{p,r*}$ is the capacity of a processing plant p that produces a reference resource r* and $F_{p,r}^{net}$ represents the net flow of resource r from and/or to the plant. The parameter $a_{p,r}^{in}$ shows the amount of raw material, utility requirement, and power input per ton of product whereas $a_{p,r}^{out}$ represents the amount of product, by-products, waste, and/or power output per ton of reference product. The variable $C_{p,r*}$ falls in-between upper and lower bounds, where the lower bound was defined for reasonable and/or realistic small plant capacities, and the upper bound is based on the total capital investment available for allocation. This is shown in (9).

$$C_{p,r*}^{Lower\ Limit} \leq C_{p,r*} \leq C_{p,r*}^{Upper\ Limit} \qquad \forall\ (\mathrm{r} \in \mathrm{R}) \tag{9}$$

By convention, net inputs flows are negative, whereas product or other net output flows are positive. The parameter $a_{p,r}^{in}$ represents the amount of raw material, utility requirement, and power input per ton of product whereas $a_{p,r}^{out}$ represents the amount of product, by-products, waste, and/or power output per ton of reference product. Then, the gross value added by a plant p is the subtraction the of total cost inputs from the plant sale outputs:

$$GVA_p = \sum_r \left(F_{p,r}^{net} \times c_r\right) \qquad \forall\ (\mathrm{p} \in \mathrm{P}) \tag{10}$$

Where c_r is the specific cost (price) per unit of resource. To find the net profit of a process, additional costs should be removed from the revenue obtained in (10). These costs include fixed operating costs and annualized capital or depreciation. The total capital cost of a process $TCC_{p,r*}$ of a capacity $C_{p,r*}$ can be estimated using the typical capacity ratio:

$$TCC_{p,r*} = TCC_{p,r*}^{Ref} \times \left(\frac{C_{p,r*}}{C_{p,r*}^{Ref}}\right)^{b} \qquad \forall\ (\mathrm{p} \in \mathrm{P}) \tag{11}$$

Where $TCC_{p,r*}^{Ref}$ is the capital cost of a reference plant at a certain capacity $C_{p,r*}^{Ref}$. The depreciation $D_{p,r*}$ of the capital cost can be determined through the straight-line, double declining, or MACRS methods. Fixed operating costs can then be calculated (12), and its respective breakdown is shown in Table 1. It was assumed each plant has 4 shift positions with a 4.8 operator/shift position and an operator salary of USD 30,000/shift position each year (Towler and Sinnott 2013b).

$$FCost_{p,r*} = Labor_{p,r*} + Maintenance_{p,r*} + Overhead_{p,r*} \qquad \forall\ (\mathrm{p} \in \mathrm{P}) \tag{12}$$

Table 1: Fixed OPEX breakdown

Labor	Shift Positions	
	Supervisions	25% of Shift positions
	Direct Overhead	45% of Shift positions and Supervisions
Maintenance		3% of Total Fixed Capital Cost
Overhead Expense	Plant Overhead	65% Labor and Maintenance
	Tax and Insurance	1.5% of Total Fixed Capital Cost

The labor, maintenance and overhead costs were estimated from Towler's book (Towler and Sinnott 2013b). The gross profit of plant p is evaluated through:

$$GP_{p,r*} = GVA_{p,r*} - FCost_{p,r*} - D_{p,r*} \quad \forall\ (\mathrm{p} \in \mathrm{P}) \tag{13}$$

To promote clarity, it has been assumed that MPT calculations do not consider taxes on plant profits as this would necessitate assumptions on geographical locations as well as the overall tax situation of the company studying the plant portfolio assessment. Due to the fluctuations of input and output prices, the gross profit ($GP_{p,r*,t}$) and in-turn the return on investment (ROI) varies over time. The $ROI_{p,r*,t}$ in a given time interval t and the average ROI $\left(\overline{ROI_{p,r*}}\right)$ over multiple time intervals T of plant p can be calculated as:

$$ROI_{p,r*,t} = \frac{GP_{p,r*,t}}{TCC_{p,r*}} \times 100 \qquad \forall\ (\mathrm{p} \in \mathrm{P}) \tag{14}$$

$$\overline{ROI_{p,r*}} = \frac{\sum_{t=1}^{T}(ROI_{p,r*,t})}{T} \qquad \forall\ (\mathrm{p} \in \mathrm{P}) \tag{15}$$

Over the time period T, the variance of plant ROI, due to input and output price fluctuations, and its respective standard deviation is determined through:

$$\sigma_{ROI_{p,r*}}^{2} = \frac{\sum_{t=1}^{T}(ROI_{p,r*,nt} - \overline{ROI_{p,r*}})^2}{T-1} \qquad \forall\ (\mathrm{p} \in \mathrm{P}) \tag{16}$$

$$\sigma_{ROI_{p,r*}} = \sqrt{\sigma_{ROI_{p,r*}}^{2}} \qquad \forall\ (\mathrm{p} \in \mathrm{P}) \tag{17}$$

Then, the return on a portfolio PF holding processes p ∈ PF can be determined through:

$$Return_{PF} = \frac{\sum_{p\epsilon PF} GP_{p,r*}}{\sum_{p\epsilon PF} TCC_{p,r*}} \times 100 \qquad \forall\ (\mathrm{pf} \in \mathrm{PF}) \tag{18}$$

The portfolio variance is a measure of the change in ROI over the time period T of study. Similarly to (3) above, the risk includes both the individual risk of holding a plant and the risk present between the individual plants held and can be quantified according to:

$$Var_{PF} = \sum_{p=1}^{P} \sigma_{ROI_{p,r*}}^{2} + 2\sum_{p=1}^{P} \rho_{ROI_p,ROI_{p+1}} \sigma_{ROI_{p,r*}} \sigma_{ROI_{p+1,r*}}\ \forall\ (\mathrm{pr} \in \mathrm{PR}) \tag{19}$$

The correlation factor ($\rho_{ROI_p,ROI_{p+1}}$) shows the strength of the relationship present between each pair of plants studied, and can be calculated using:

$$\rho_{ROI_p,ROI_{p+1}} = \frac{\sum_{n=1}^{N}(ROI_{p,r*} - \overline{ROI_{p,r*}}) \times (ROI_{p+1,r*} - \overline{ROI_{p+1,r*}})}{\sqrt{\sum_{n=1}^{N}\left(ROI_{p,r*} - \overline{ROI_{p,r*}}\right)^2}\sqrt{\sum_{n=1}^{N}\left(ROI_{p+1,r*} - \overline{ROI_{p+1,r*}}\right)^2} \tag{20}$$

Where the numerator represents the covariance between the plants' ROIs and the denominator represents the product of each plant's ROI variability (i.e. standard deviation). Similar to the financial asset case, as $\rho_{ROI_p,ROI_{p+1}} \rightarrow +1$ it translates to the fact that pair of the plants' ROI move together in the same direction and have a strong alike relationship. As $\rho_{ROI_p,ROI_{p+1}} \rightarrow -1$ translates as the pair of the plants' ROI move opposite to one another and have a strong opposing relationship. Lastly, as $\rho_{ROI_p,ROI_{p+1}} \rightarrow 0$ signifies there is a weak and/or no relationship present between the plants' ROI. The correlation factor between a plant and itself is always one. As the number of plants held increases, it means the further diversified the portfolio is (i.e. more products produced). As shown in (19), the covariance term will surpass the variance term. As a result, to reduce portfolio risk, it is preferred to include plant combinations that have low correlation factors (e.g. negative to zero correlation). Then, the risk (standard deviation) of a process portfolio investment is determined as:

$$Risk_{PF} = \sqrt{Var_{PF}} \quad \forall\ (\mathrm{pf} \in \mathrm{PF}) \tag{21}$$

Similar to the financial investment case, the risk of a portfolio is defined to be the standard deviation. To obtain the efficient frontier, a multi-objective optimization problem that maximizes portfolio return and minimizes portfolio risk is formulated (22). The constraint ensures that all the process portfolios generated will divide all the available capital among its constituents.

$$\begin{gathered} \text{Maximize Return}_{\mathrm{PF}} \qquad \text{Minimize Risk}_{\mathrm{PF}} \\ \text{Subject to:} \qquad \textstyle\sum_{\mathrm{p}=1}^{\mathrm{P}} \mathrm{w_p} = 1 \end{gathered} \tag{22}$$

The multi-objective optimization (22) was evaluated through MATLAB by using a hybrid solver comprised of a multi-objective genetic algorithm (gamultiobj) and a goal attainment algorithm (fgoalattain) (MATLAB 2020) as shown in Figure 3.

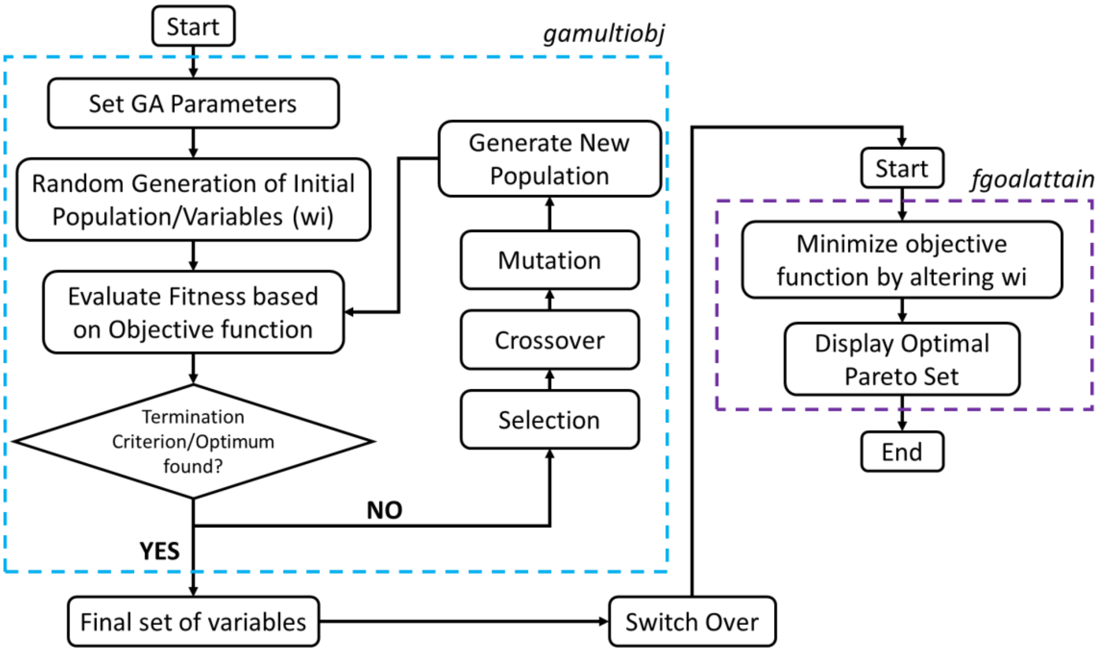

Figure 3: Evaluation using the GA-Hybrid solver

Some of the GA parameters had to be set prior to running the MPT analysis. The population size was defined to be 400. The cross over function was set to be ‘cross over heuristic’. The mutation function was defined as ‘mutation adapt feasible’. Such parameters gave good estimation of the true pareto-optimal frontier. The multi-objective optimization was solved initially to render an initial set of results. This result was fed again in the Hybrid-model as an initial population. This process was repeated until there was no change in the initial and final population obtained.

5. RESULTS AND DISCUSSION

The following section highlights the results obtained in this study with a thorough discussion. The MPT analysis was applied on a set of single plants. Several efficient frontier curves were obtained. The base case was constructed using annual variability of historic profitability performance while assuming fixed specific plant CAPEXs. Another case alters the base case by using a monthly variability basis instead. The final case alters the base case by considering the economies of scale.

5.1. Development of MPT portfolios

The case study assumes the available capital for the portfolio investment to be USD 250 million and considers six chemical production process plants for inclusion into process investment portfolios: Methanol, Acetic acid, Formalin, Nitric acid, Ammonia, and Urea. In order to assess the performance of selected portfolios in a known future, the portfolios are designed using the presented MPT based approach using historic monthly pricing data for the years 2007 through 2014. Investments are assumed to be made with plant operation beginning in 2015 to allow future data to be known for a 5-year horizon from 2015 to 2019. This is done to be able to evaluate future profitability performances of some selected portfolios. Table 2 shows the a_{pr} parameters for each process, and the references used to determine these parameters are shown in Table 3. Maximum capacity limits for each process have been set to ensure processes do not produce more that 2% of the global market demand for each product produced (Table 4).

Table 2: a_{pr} parameters for each process

Resource	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
Methane	-0.526	-	-	-	-0.505	-
Oxygen	-0.402	-	-	-	-	-

Table 2: Continued

Resource	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
Methanol	+1.000	-0.542	-0.424	-	-	-
Carbon Monoxide	-	-0.473	-	-	-	-
Carbon Dioxide	-	-	-	-	-	-0.733
Air	-	-0.074	-1.167	-4.410	-1.146	-
Acetic Acid	-	+1.000	-	-	-	-
Formalin	-	-	+1.000	-	-	-
Ammonia	-	-	-	-0.279	+1.000	-0.567
Nitric Acid	-	-	-	+1.000	-	-
Urea	-	-	-	-	-	+1.000
Methanol Waste	+0.663	-	-	-	-	-
Acetic Acid Waste	-	+0.089	-	-	-	-
Formalin Waste	-	-	+0.841	-	-	-
Nitric Acid Waste	-	-	-	+3.989	+0.891	-
Ammonia Waste	-	-	-	-	-	-
Pure CO_2	+0.264	-	-	-	+1.275	-
Urea Waste	-	-	-	-	-	+0.300
Condensate	-	-	-	-	-	+1.084
Steam to Power	-	-	+199.193	+201.945	+22.80	-
HP Steam	-	-0.230	-	-	-4.373	-
MP Steam	-1.000	-	-	-	-1.515	-
LP Steam	-	-	-	-0.10	-	-1.20
Process Water	-	-	-0.250	-0.3	-	-
Cooling Water	-140	-2.631	-42	-130	-157	-70
Makeup Water	-	-	-	-	-1.515	-
Fuel NG	-	-	-	-	-0.217	-
Power	-89	-40.03	-49	-9	-50	-125

Table 3: References for each a_{pr} parameter

a_{pr} Type	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
Mass Balance	(Hinderink et al. 1996)	(Garrett 1989)	(Bolch 2006)	(Laue, Thiemann, and Scheibler 2006)	(Flórez-Orrego and De Oliveira 2015),(Prevention 2007)	(Stamicarbon 2020)

Table 3: Continued

a_{pr} Type	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
Utility needs	(Collodi et al. 2017),(Dybkjær and Hansen 1997)	ASPEN simulation	(Bolch 2006)	(Laue et al. 2006)	(Flórez-Orrego and De Oliveira 2015)	(Hignett 1985b)
Route	Combined Reforming of NG (Mega-Methanol) by Lurgi	Celanese	Formox	Dual-Pressure	Steam-Methane Reforming ICI	Stamicarbon

Table 4: Global Market size of each chemical

Plant	Market Size (USD) × 10^9	Reference
Methanol	31.81	(Grand View Research 2019)
Acetic Acid	8.92	(Grand View Research 2020a)
Formalin	4.00	(Ahuja and Amit 2019)
Nitric Acid	24.00	(Grand View Research 2020b)
Ammonia	48.65	(Grand View Research 2017)
Urea	38.00	(Adroit Market Research 2019)

Product and raw material prices are obtained from Intratec (Intratec 2020). For materials not tracked by Intratec, prices have been determined through other methods as explained in the Appendix. Figure 4 and Figure 5 display various historic chemical prices and several historic utility prices used in this case study. Additional case study data are available in the Appendix. Straight-line depreciation over a 20-year plant life is assumed with a salvage value that is equal to zero. It has been assumed there is no profit from excess steam, additional power, or waste gases (such as CO_2). Then, the multi-objective optimization (22) is solved through MATLAB using a hybrid solver of a multi-objective genetic algorithm (gamultiobj) and a goal attainment algorithm (fgoalattain).

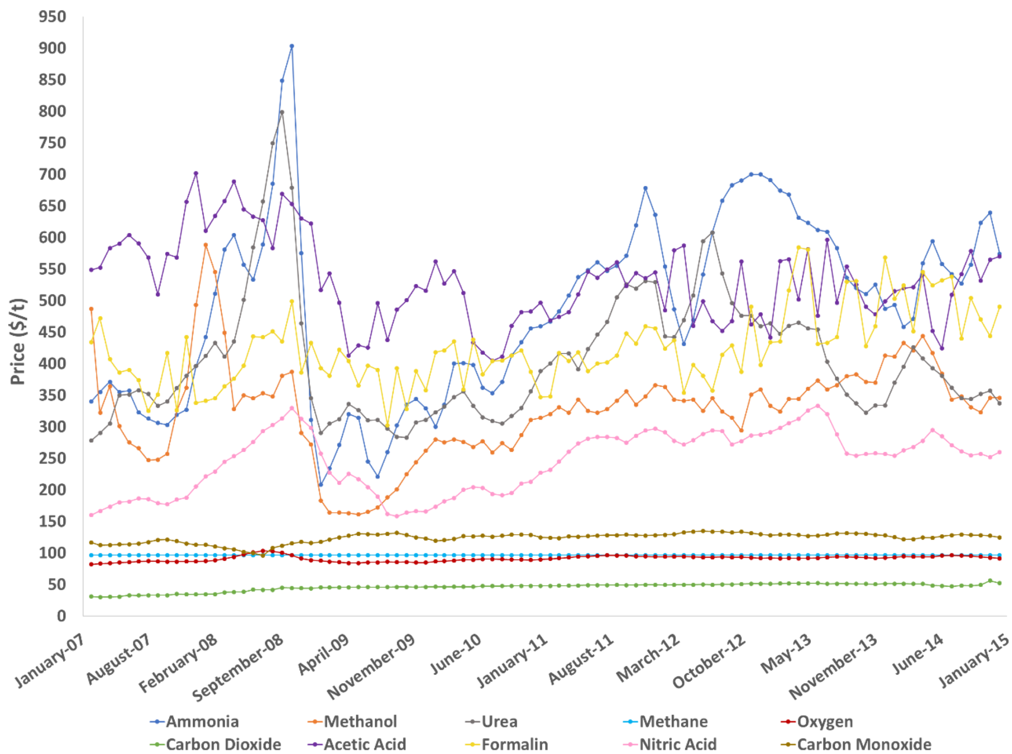

Figure 4: Historic chemical pricing data

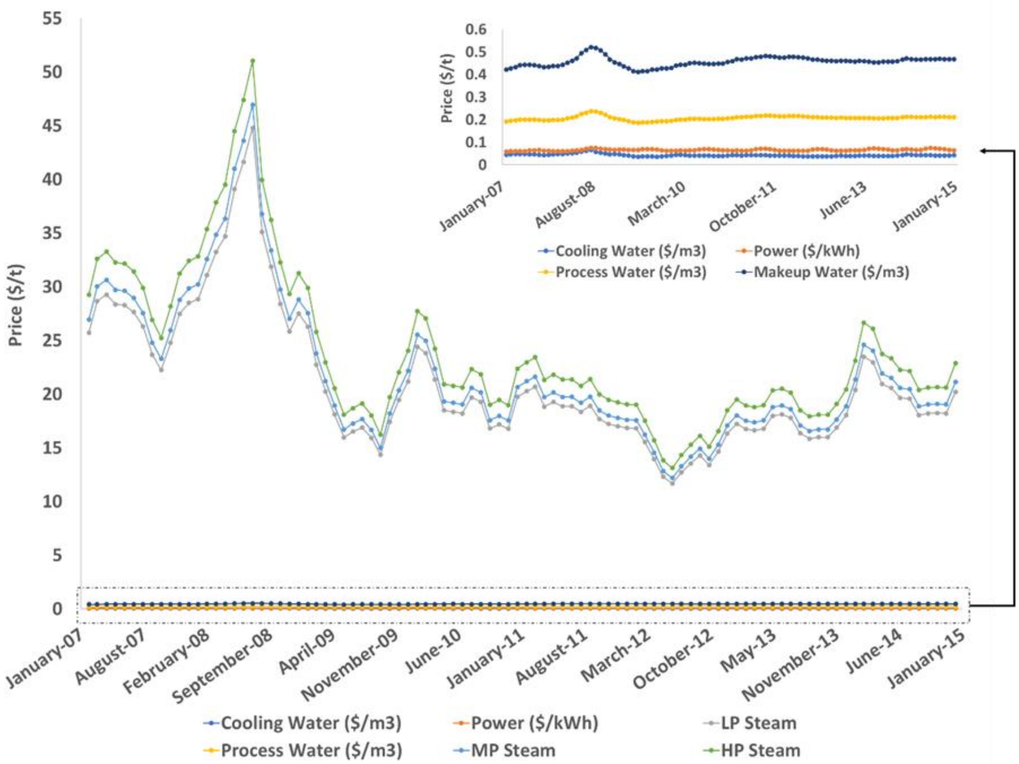

Figure 5: Historic utility pricing data (USD/t unless mentioned)

To be able to compare MPT portfolios, which are developed by considering profit variability, against conventional portfolios, which are based on a stable profitability criterion, a reference must be chosen. In this study, alternative portfolios were constructed using NPV and ROI metrics. As NPV and ROI do not have the ability of distributing capital among a set of process portfolios, such an approach is guideless. Then, these reference portfolios are constructed by selecting processes in order of decreasing profitability, while assuming equal investment across the selected processes. In total, there are six reference portfolios for each profitability criterion containing a different number of processes (NPV-1 to NPV-6; ROI-1 to ROI-6). For instance, NPV 6 /ROI 6 contains six plants. Then, the study aims to determine if there are efficient MPT portfolios that can outperform the NPV and ROI based portfolios. This comparison happens by obtaining the net profit of each portfolio when projected into the future (i.e. year 2015 to 2019). The comparison between each pair of portfolios (e.g. MPT 2 and NPV 2) based on their net profits is then computed. Besides illustrating the approach and comparing efficient portfolios against reference portfolios, the study investigates the effect of profit variability duration (i.e. annual versus monthly) and the effect of economies of scale on portfolio selection.

5.1.1. Annual variability frontier

A base case is developed assuming linear plant capital cost models in the calculation of profits and returns. Consequently, the specific CAPEX and the specific fixed OPEX were calculated for each plant operating at mid-capacity (between the upper and lower capacity limits). These parameters do not alter and are shown in Table 5. The total capital cost and fixed operating costs of the plants are then calculated according to equations (23) and (24) respectively.

Table 5: Specific capital cost and fixed operating cost

Plant	Capital Cost (USD/t)	Fixed Capital Cost (USD/t)
Methanol	23.20	34.57
Acetic Acid	36.54	57.83
Formalin	41.64	77.88
Nitric Acid	22.11	33.02
Ammonia	44.51	65.81
Urea	11.11	16.81

$$TCC_{p,r*} = \text{Specific CAPEX}\left(\frac{\text{USD}}{\text{t}}\right) \times C_{p,r*}\left(\frac{\text{t}}{\text{y}}\right) \times \text{Lifetime (y)} \qquad \forall\ (\text{p} \in \text{P}) \qquad (23)$$

$$FCost_{p,r*} = \text{Specific Fixed OPEX}\left(\frac{\text{USD}}{\text{t}}\right) \times C_{p,r*}\left(\frac{\text{t}}{\text{y}}\right) \quad \forall\ (\text{p} \in \text{P}) \qquad (24)$$

As economies of scale were not considered at the base case, the individual plant risk is independent of plant size and the portfolio investment risk is a linear function of individual plant investment risk. Then, the individual variance is defined as shown in equation (25). Then, the risk model will have the form shown in (26).

$$\sigma^2_{ROI_{p,r*}} = w^2_{p,r*} {\sigma^2}^{Fixed}_{ROI_{p,r*}} \tag{25}$$

$$Var_{PF} = \sum_{p=1}^{P} w^2_{p,r*} {\sigma^2}^{Fixed}_{ROI_{p,r*}} + 2\sum_{p=1}^{P} w_{p,r*} w_{p+1,r*} \rho_{ROI_p,ROI_{p+1}} \sigma_{ROI}{}^{Fixed}_{p,r*} \sigma_{ROI}{}^{Fixed}_{p+1,r*} \tag{26}$$

Where the terms ${\sigma^2}^{Fixed}_{ROI_{p,r*}}$ and $\sigma_{ROI}{}^{Fixed}_{p,r*}$ represent the fixed plant variance and fixed standard deviation at any given capital investment. Plant capital and capacity limits are given in Table 6. The individual risk and return for each plant are summarized in Table 7. The correlation factors used in equation (26) are given in Table 8.

Table 6: Capacity limits for a 250 million USD investment

Plant	Minimum weight Investment	Maximum Capacity (t/y)	Maximum weight Investment
Methanol	0	538,888	1
Acetic Acid	0	244,141	0.714
Formalin	0	96,054	0.320
Nitric Acid	0	565,412	1
Ammonia	0	280,833	1
Urea	0	1,124,760	1

Table 7: Annual plant return and risk at maximum investment

Plant	Average Annual ROI (%)	Annual σ^2 (%)	Annual σ (%)
Methanol	31.47	1.71	13.06
Acetic Acid	26.55	0.40	6.33
Formalin	19.37	0.19	4.34
Nitric Acid	10.42	0.11	3.35
Ammonia	21.51	2.26	15.04

Table 7: Continued

Plant	Average Annual ROI (%)	Annual σ^2 (%)	Annual σ (%)
Urea	14.24	4.42	21.01

Table 8: Correlation matrix for annual return and risk

	Correlation factors (ρ)					
	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
Methanol	1.000	-0.126	0.100	0.162	0.758	-0.250
Acetic Acid	-0.126	1.000	-0.625	-0.370	-0.507	0.634
Formalin	0.100	-0.625	1.000	0.508	0.254	-0.928
Nitric Acid	0.162	-0.370	0.508	1.000	0.634	-0.220
Ammonia	0.758	-0.507	0.254	0.634	1.000	-0.217
Urea	-0.250	0.634	-0.928	-0.220	-0.217	1.000

The multi-objective optimization problem in equation (22) is solved to determine the efficient frontier (Figure 6). The frontier was color-coded to visualize changes in portfolio constituents (plants) along the efficient frontier. Tables 9 and 10 provide further details on which plants were included in each segment and what is their respective capital weight range.

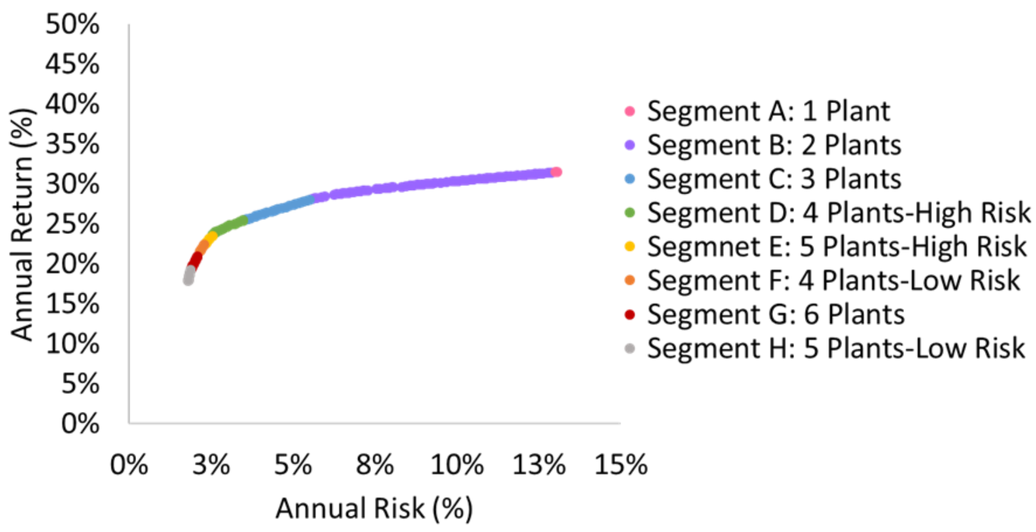

Figure 6: Segmented efficient frontier for annual return and risk

Table 9: Plant constituents for each frontier segment

Segment	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
A	✓					
B	✓	✓				
C	✓	✓	✓			
D	✓	✓	✓		✓	
E	✓	✓	✓	✓	✓	
F		✓	✓	✓	✓	
G	✓	✓	✓	✓	✓	✓
H	✓	✓	✓	✓		✓

Table 10: Weight allocation range of frontier plants for annual return and risk

	Weight Range (%)					
Segment	**Methanol**	**Acetic Acid**	**Formalin**	**Nitric Acid**	**Ammonia**	**Urea**
A	100	0	0	0	0	0
B	32-99	1-68	0	0	0	0
C	16-32	54-70	1-27	0	0	0
D	1-18	53-57	24-32	0	1-12	0
E	1-3	49-53	32	3-8	9-10	0
F	0	44-49	32	8-14	1-7	2-3
G	1-5	30-41	31-32	18-29	0	3-4
H	3-5	23-29	32	30-37	0	3-4

Tracking the efficient frontier from the highest return-risk segment (top right) to the lowest risk-return segment (bottom left), the highest return portfolio (Segment A) is a single plant portfolio containing only the Methanol plant. This is expected as the methanol plant has the highest individual return (Table 7). As the risk is lowered, the next portfolio (Segment B) holds the Methanol together with the Acetic acid plant. The Acetic acid plant is chosen due to its overall dampening effect on the portfolio risk while still offering high return. The overall risk considers the individual plant risk as well as the risk present between two plants (Equation (26)) and the Methanol plant has a low correlation value with the Acetic acid plant (-0.126). Note the Methanol plant has the lowest correlation with the Urea plant (-0.250), but the plant is not chosen due to its low return. Moving further along the frontier, the next portfolio contains the Formalin plant in addition to the Methanol and Acetic Acid plants (Segment C). The Formalin plant was added as it further decreases portfolio risk of both the Acetic Acid and Methanol plants. As the number of plants included in the frontier increases (i.e. diversification) the covariance risk term becomes more crucial to follow. Then, as the Formalin plant had a negative and a weak correlation factor with the Acetic Acid plant (-0.625) and the Methanol plant (0.100), its inclusion would be attractive. Further reductions in risk is achieved when the Ammonia plant was added (Segment D) to the existing plants from Segment C. The Ammonia plant was attractive as it had a high return (21.51%) and has one of the lowest correlation factors with the Acetic Acid plant (-0.507), which had the highest investment allocation (Table 10). Then, the Nitric Acid plant was added (Segment E) as it again further dampens portfolio risk due to its negative correlation with the Acetic Acid plant (-0.370), which still held the highest investment allocation (Table 10). As the portfolio risk decreases, the Methanol plant became deactivated (Segment F). The Acetic acid and Formalin plants remain in the portfolio due to their low standard deviations (6.33% and 4.34% respectively), with the remaining Ammonia plant reducing the risk of the Acetic Acid-Formalin plant combinations more than the deactivated high-risk Methanol plant. Moreover, the Methanol plant has the highest individual return (31.47%), and so it is not possible to be included at low risk-return portfolios. This however may happen, but that plant might have a minor capital allocation. Moreover, the Nitric Acid plant remained due to its diminishing effect on the Acetic acid plant risk and its low individual risk (3.35%) compared to the Urea plant alternative (21.01%). Moving to even lower risk (Segment G), all the plants remained active and the Urea plant along with the Methanol plant are added. Methanol has a weak negative to no relationship with all the plants (-

0.250 to 0.162) except Ammonia (0.758). However as the Ammonia plant is included at minor investments (Table 10) the reactivation of the Methanol plant became possible. As mentioned, because the Methanol plant has a high individual return (31.47%), it was present at a minor investment (maximum of 5%). As Segment G contains a high capital allocation to the Acetic acid, Formalin, and Nitric acid plants, the Urea plant was added as it dampens the portfolio risk (-0.928 and -0.220 for the Formalin and the Nitric acid plant respectively). Reaching the final Segment (H), all previous plants remain except Ammonia. As shown in Table 10, the Nitric acid plant had the highest weight allocation in Segment H. This is expected as the Nitric acid plant has the lowest individual risk (3.35%). As the Ammonia plant had the highest correlation with the Nitric acid plant (0.667), it had to be removed to maintain the low-risk environment.

The efficient frontier contains up to six-plant portfolio combinations. Further, the frontier has four-plant and five-plant portfolio combinations at different risk levels (i.e. High and Low). The portfolios offer returns between 31.49 % (highest risk) to 17.82 % (lowest risk). Then, several portfolios were chosen from the frontier (Table 11). These portfolios will then have their net profit computed from years 2015 to 2019 and be contrasted with the alternatively developed portfolios (section 5.1.4). The next section explains the monthly efficient frontier.

Table 11: MPT portfolio combinations for annual return and risk (*High risk)

Plant	**Weights (%)**							
Methanol	100	68.67	31.31	18.36	3.38	0	1.21	4.89
Acetic Acid	0	31.04	67.14	52.83	52.91	49.17	40.61	29.22
Formalin	0	0	1.04	27.58	31.79	31.75	31.91	31.97
Ammonia	0	0	0	1.27	8.72	10.41	6.60	0
Nitric Acid	0	0	0	0	3.10	8.22	18.05	29.75
Urea	0	0	0	0	0	0	1.64	3.68
Label	MPT 1	MPT 2	MPT 3	MPT 4*	MPT 5*	MPT 4	MPT 6	MPT 5

5.1.2. Monthly variability frontier

The efficient frontier in Figure 6 considers annual variability of returns for the 2007 to 2014 period. The study has been repeated considering monthly variability (Figure 7) to investigate the effect of such changes on MPT portfolio construction and performance (section 5.1.5). The results show that considering monthly variability brings about changes to portfolio construction.

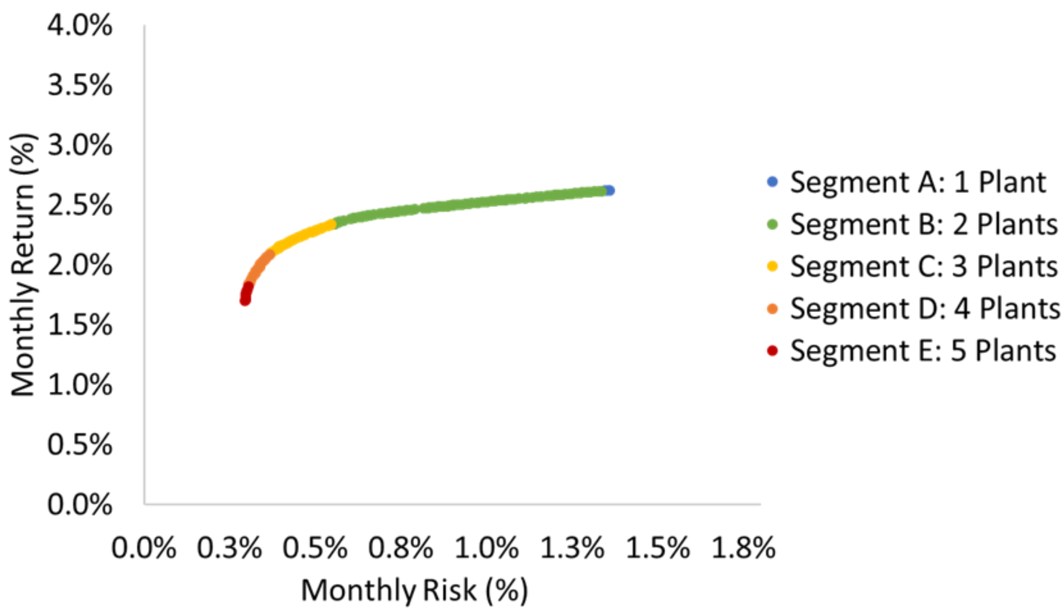

Figure 7: Segmented efficient frontier for monthly return and risk

The same specific CAPEX and fixed operating cost (Table 5) were used in this analysis. The bounds on capital investment remain as mentioned in Table 6. In turn, no plant can produce more than 2% of the global market demand for each product. Then, the return and risk for each plant are summarized in Table 12 and the correlation factors used in equation (26) are given in Table 13.

Table 12: Monthly plant return and risk at maximum investment

Plant	Average Annual ROI (%)	Annual σ^2 (%)	Annual σ (%)
Methanol	2.62	0.0185	1.36
Acetic Acid	2.21	0.0055	0.74
Formalin	1.61	0.0034	0.58
Nitric Acid	0.87	0.0027	0.52
Ammonia	1.79	0.0195	1.40
Urea	1.19	0.0623	2.50

Table 13: Correlation matrix for monthly return and risk

	Correlation factors (ρ)					
	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
Methanol	1.000	-0.299	-0.227	-0.092	0.478	-0.177
Acetic Acid	-0.299	1.000	-0.121	-0.050	-0.268	0.314
Formalin	-0.227	-0.121	1.000	0.256	0.200	-0.296
Nitric Acid	-0.092	-0.050	0.256	1.000	0.017	0.206
Ammonia	0.478	-0.268	0.200	0.017	1.000	-0.184
Urea	-0.177	0.314	-0.296	0.206	-0.184	1.000

Evidently from Table 12, the ROIs and standard deviations are lower than the annual variability base case. As shown, the correlation factors differ between the cases. Such differences can result with changes in portfolio constituents of the efficient frontier, as the covariance term becomes important when portfolios diversify. Tables 14 and 15 provide further details about which plants were included at the various segments and their respective capital allocations. As shown in Table 14, Ammonia was never active along the frontier. Similar to the base case, several MPT portfolios based on monthly variability were chosen and are shown in Table 16. The portfolios offer returns between 2.62 % (highest risk) to 1.70 % (lowest risk).

Table 14: Selected plants in frontier for monthly return and risk

Segment	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
A	✓					

Table 14: Continued

Segment	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
B	✓	✓				
C	✓	✓	✓			
D	✓	✓	✓	✓		
E	✓	✓	✓	✓		✓

Table 15: Weight allocation range of frontier plants for monthly return and risk

	Weight Range (%)					
Segment	**Methanol**	**Acetic Acid**	**Formalin**	**Nitric Acid**	**Ammonia**	**Urea**
A	100	0	0	0	0	0
B	32-99	1-68	0	0	0	0
C	22-36	43-63	4-32	0	0	0
D	17-22	33-46	29-32	2-19	0	0
E	13-16	26-33	31-32	19-27	0	1

Table 16: MPT portfolio combinations for monthly return and risk (*High risk)

Plant	**Rank**	**Weights (%)**				
Methanol	1	100	71.22	35.92	20.92	15.57
Acetic Acid	2	0	28.75	60.02	46.12	32.82
Formalin	3	0	0	4.06	30.99	31.64
Nitric Acid	4	0	0	0	1.58	18.87
Urea	5	0	0	0	0	1.03
Ammonia	6	0	0	0	0	0
Label		MPT 1	MPT 2	MPT 3	MPT 4	MPT 5

Both frontiers included the Methanol plant as the most attractive and the Nitric Acid plant as the least attractive (due to its low individual return). The risk and return ranges for the monthly variability frontier had smaller values than the annual variability frontier. The frontier developed with annual variability contains up to six plant-portfolios, whereas the monthly variability frontier contains up to five-plant portfolios. The annual variability frontier contains portfolios at different risk levels whereas the monthly variability frontier did not. Both frontiers have the same constituents in segments A, B, and C. The annual variability frontier contained the Ammonia plant whereas the monthly variability frontier did not. Segment D in the monthly variability frontier, did not include the Ammonia plant as it has a high individual risk (1.40%), where instead the plant with the lowest individual risk at 0.52% (Nitric acid plant) was added. As the risk lowered (Segment E), the Formalin plant had the highest investment due to its low individual risk (0.58%) and return (1.61%). In turn, as the Formalin plant had the lowest correlation with the Urea plant (-0.296), it was included in the portfolios. However, the Urea plant had a high individual risk (2.50%), and so was present at minor investments (1%). Both frontiers contained the same constituents in the lowest risk segment (all plants except Ammonia).

5.1.3. Alternatively produced portfolios for the linear capital cost model

As described above, a total of 12 reference portfolios are developed based on common profitability criteria NPV and ROI (NPV-1 to NPV-6; ROI-1 to ROI-6). The NPV and ROI of each plant at their respective maximum investment was determined using the monthly material and energy prices for year 2015 (Table 17).

Table 17: NPV and ROI of each plant based on 2015 prices

	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
NPV (MMUSD/y)	83	34	14	31	63	-51
ROI (%)	33	19	17	13	25	-20
CAPEX (MMUSD)	250	178.4	80	250	250	250

The plants are ranked based on a descending order of their NPV and ROI values. To develop NPV and ROI portfolios it has been assumed each portfolio, depending on the number of plants held, has an equal capital allocation among its constituents. This division still has to meet each plant's capacity limits (Table 6). The resulting reference portfolios are summarized in Tables 18 and 19.

Table 18: NPV combinations in 2015

Plant	Rank	Weights (%)					
Methanol	1	100	50	33.33	25	20	16.67
Ammonia	2	0	50	33.33	25	20	16.67
Acetic Acid	3	0	0	33.33	25	20	16.67
Nitric Acid	4	0	0	0	25	20	16.67
Formalin	5	0	0	0	0	20	16.67
Urea	6	0	0	0	0	0	16.67
Label		NPV 1	NPV 2	NPV 3	NPV 4	NPV 5	NPV 6

Table 19: ROI combinations in 2015

Plant	Rank	Weights (%)					
Methanol	1	100	50	33.33	25	20	16.67
Ammonia	2	0	50	33.33	25	20	16.67
Acetic Acid	3	0	0	33.33	25	20	16.67
Formalin	4	0	0	0	25	20	16.67
Nitric Acid	5	0	0	0	0	20	16.67
Urea	6	0	0	0	0	0	16.67
Label		ROI 1	ROI 2	ROI 3	ROI 4	ROI 5	ROI 6

The performance of the efficient portfolios (for both annual and monthly variability cases) and the reference portfolios have been assessed for the 5-year (future) period from 2015 to 2019. The net profit earned by each portfolio during this future period is summarized in Tables 20 and 21 for the annual and monthly variability cases respectively.

Table 20: Net profit of each portfolio with annual variability (*High risk)

	MPT	NPV	ROI
Portfolio Type	**Profit (MMUSD)**		
1-plant	391.42	391.42	391.42

Table 20: Continued

	MPT	NPV	ROI
Portfolio Type	**Profit (MMUSD)**		
2-plant	333.52	259.24	259.24
3-plant	265.03	242.34	242.34
4-plant	249.16*	219.38	241.13
	203.54		
5-plant	214.84*	223.00	223.00
	196.40		
6-plant	198.82	166.08	166.08

Table 21: Net profit of each portfolio with monthly variability (*High risk)

	MPT	NPV	ROI
Portfolio Type	**Profit (MMUSD)**		
1-plant	391.42	391.42	391.42
2-plant	338.71	259.24	259.24
3-plant	275.39	242.34	242.34
4-plant	254.01	219.38	241.13
5-plant	231.70	223.00	223.00

5.1.4. Portfolio comparison for annual MPT variability

This section compares the net profit of each portfolio pairs developed from the annual variability frontier. The difference of each pair of portfolios' net profit is shown in Table 22.

Table 22: Difference between each portfolio pair for annual return and risk

Combination	Difference (MMUSD)	Combination	Difference (MMUSD)
MPT 1 - NPV 1	391.42 - 391.42 = 0	**MPT 1 - ROI 1**	391.42 - 391.42 = 0
MPT 2 - NPV 2	333.52 - 259.24 = 74.28	**MPT 2 - ROI 2**	333.52 - 259.24 = 74.28
MPT 3 - NPV 3	265.03 - 242.34 = 22.69	**MPT 3 - ROI 3**	265.03 - 242.34 = 22.69
MPT 4* - NPV 4	249.16 - 219.38 = 29.78	**MPT 4* - ROI 4**	249.16 - 241.13 = 8.03
MPT 4 - NPV 4	203.54 - 219.38 = -15.84	**MPT 4 - ROI 4**	203.54 - 241.13 = -37.59
MPT 5* - NPV 5	214.84 - 223.00 = -8.16	**MPT 5* - ROI 5**	214.84 - 223.00 = -8.16
MPT 5 - NPV 5	196.40 – 223.00 = -26.60	**MPT 5 - NPV 5**	196.40 - 223.00 = -26.60
MPT 6 - NPV 6	198.82 – 166.08 = 32.74	**MPT 6 - ROI 6**	198.82 – 166.08 = 32.74

Both MPT and NPV/ROI chose the Methanol plant as the most attractive, and so the same consensus was reached with single-plant portfolios. As a result, there was no difference for those portfolio pairs. However, as additional plants were added to the portfolios, their performance differed. For the two-plant portfolios, MPT outperformed both NPV and ROI by generating additional profits of 74.28 MMUSD (for both cases). This was mainly due to the additional 19% capital investment that was allocated to the Methanol plant in the MPT-portfolio. This Methanol plant generated an extra 73 MMUSD solely. The minor 1 MMUSD was obtained from the Acetic acid plant. Then, NPV and ROI portfolios fell short as they lack guidance on capital distribution in process portfolios.

For the three-plant portfolio, MPT outperformed both NPV and ROI by generating additional profits valued at 22.69 MMUSD (for both cases). These profits were obtained from the additional 34% capital allocation to the Acetic acid plant. The Acetic acid plant generated 70 MMUSD, and surpassed NPV/ROI's collective profits from the Methanol and the Ammonia plants (48 MMUSD). The four-plant portfolios were assessed next.

NPV 4 and ROI 4 had different annual profits due to their mismatched plant rankings. There were two types of four-plant portfolios developed by MPT which differed in their risk level. The high-risk MPT 4 portfolio outdid both NPV 4 and ROI 4 portfolios by obtaining an additional profit of 29.78 MMUSD and 8.03 MMUSD respectively. For the NPV 4 case, the additional profits made by MPT were mainly due to the 28% extra investment allocated to the Acetic acid plant. The Acetic acid plant gave 58 MMUSD. An additional profit of 28 MMUSD was provided by the Formalin plant held by the MPT portfolio. The NPV portfolio made profits through the Methanol plant (26 MMUSD) and the Ammonia plant (30 MMUSD). In turn, the NPV portfolio fell short when compared to the MPT portfolio. Then, MPT 4 - high risk and ROI 4 held the same plants but differed in terms of capital division. For the MPT portfolio, the Acetic acid and the Formalin plants generated most of the profit (58 MMUSD and 6 MMUSD respectively). In contrast, ROI 4 generated greater profits from the Methanol and Ammonia plants (26 MMUSD and 30 MMUSD). Then, due to the capital division set by MPT, the Acetic acid and Formalin plants achieved higher overall profits. If ROI was equipped with the ability of capital distribution, this portfolio wouldn't be overlooked, and additional profits would've been obtained.

The low-risk MPT 4 portfolio was outdone by both NPV 4 and ROI 4 where extra profits of 15.84 MMUSD and 37.59 MMUSD were acquired respectively. MPT 4 - low risk and NPV 4 portfolios differed in terms of plant choice. The additional profits generated in NPV 4 were roughly equally obtained from the Methanol (22 MMUSD), Nitric acid (25 MMUSD), and Ammonia (18 MMUSD) plants. The additional capital allocation to the Nitric acid plant (17%) and the Ammonia plant (15%) allowed the NPV portfolio to outperform the MPT portfolio. Note that the profits generated by the MPT portfolio were solely from the Acetic acid plant (50 MMUSD). Nevertheless, NPV 4 surpassed MPT 4-low risk by luck due to the guideless capital division. This scenario might not be repeated in other plant portfolio applications. Then, the MPT 4-low risk and ROI 4 portfolios varied in plant choice (Nitric acid plant in place of the Methanol plant). Due to this, most of the additional profit was obtained from the Methanol plant (85 MMUSD), and the remaining was from the Ammonia plant (18 MMUSD). This rendered the ROI 4 portfolio to overcome the MPT portfolio, which had a net additional profit of 66 MMUSD from the Acetic acid and Formalin plants.

NPV and ROI had the same five-plant portfolios, and so their difference with MPT 5 portfolios will be alike. Like MPT 4, MPT 5 had two portfolio types that differ in their risk level. The MPT 5-high risk portfolio held the same plants as the NPV and ROI portfolios. Then, the

MPT 5-high risk portfolio was surpassed by both NPV 5 and ROI 5 which gave additional profits valued at 8.16 MMUSD. The extra profits originated mainly from the Methanol plant (65 MMUSD) due to the extra 17% capital allocation. Extra profits were obtained from the Nitric acid plant (25 MMUSD) and the Ammonia plant (14 MMUSD) due to their additional 17% and 11% capital allocation. Then, because of the guideless capital division, the alternatively produced portfolios outperformed by chance. The profits generated by the MPT portfolio originated from the Acetic acid plant (68 MMUSD) and the Formalin plant (28 MMUSD). Moreover, the MPT 5-low risk portfolio had its net profit surpassed by both NPV 5 and ROI 5 portfolios by a surplus of 26.60 MMUSD. A portion of this profit (59 MMUSD) was achieved by the additional 15% capital investment that was allocated to the Methanol plant. Similarly, this outcome as a cause of the guideless investment assumption. The remaining profit was obtained from the Ammonia plant (30 MMUSD), where instead the MPT held the Urea plant. MPT chose the Urea plant to dampen portfolio risk, and in turn it rendered lower profits. The MPT portfolio generated profits from the Acetic acid (19 MMUSD), Nitric acid (14 MMUSD), and Formalin (28 MMUSD) plants.

Lastly, NPV 6 and ROI 6 behaved in an identical manner as they both held the same plants and had the same capital division among them. MPT 6 outperformed both NPV 6 and ROI 6 by generating an additional profit of 32.74 MMUSD. Part of these profits was obtained from the extra 24% capital allocation to the Acetic acid plant (50 MMUSD). Further profits resulted from the additional 15% capital investment allocated to the Formalin plant (36 MMUSD), and the lower 15% capital investment given to the Urea plant (17 MMUSD). In this case, NPV/ROI gained its extra profits through the Methanol (60 MMUSD) and the Ammonia (13 MMUSD) plants. Likewise, NPV and ROI portfolios cannot identify such attractive process portfolio investments as they lack the ability to do so.

5.1.5. Portfolio comparison for monthly MPT variability

This section compares the net profit of each portfolio pairs developed from the monthly variability frontier. A comparison of the portfolios' total profits is shown in Table 23.

Table 23: Difference between each portfolio pair for monthly return and risk

Combination	Difference (MMUSD)	Combination	Difference (MMUSD)
MPT 1 - NPV 1	391.42 - 391.42 = 0	**MPT 1 - ROI 1**	391.42 - 391.42 = 0
MPT 2 - NPV 2	338.71 - 259.24 = 79.47	**MPT 2 - ROI 2**	338.71 - 259.24 = 79.47
MPT 3 - NPV 3	275.39 - 242.34 = 33.05	**MPT 3 - ROI 3**	275.39 - 242.34 = 33.05
MPT 4 - NPV 4	254.01 - 219.38 = 34.63	**MPT 4 - ROI 4**	254.01 - 241.13 = 12.88
MPT 5 - NPV 5	231.70 - 223.00 = 8.70	**MPT 5 - ROI 5**	231.70 - 223.00 = 8.70

Similar to the annual variability case, the metrics chose the Methanol plant as the most attractive, and so no difference was present for the single-plant portfolios. Both NPV and ROI had the same two-plant portfolio, which MPT 2 outperformed both by generating supplementary profits valued at 79.47 MMUSD. These profits were obtained from the additional 21% capital allocation to the Methanol plant in the MPT portfolio (83 MMUSD). Whereas the NPV and ROI portfolios had minor additional profits from the Ammonia plant (3 MMUSD) when compared to the Acetic acid plant held by the MPT. As mentioned, MPT's ability to allocate capital was able to determine this more attractive portfolio.

For the three-plant portfolios, NPV and ROI generated a similar profit as they held the same portfolio constituents. The profit generated by the MPT 3 portfolio surpassed both NPV 3 and ROI 3 by 33.05 MMUSD. The additional profits gained by the MPT portfolio mainly originated from the extra 27% capital allocation to the Acetic acid plant (55 MMUSD). Some additional profits were obtained from the Methanol plant (10 MMUSD). The NPV and ROI portfolio again obtained high profits from the Ammonia plant (33 MMUSD) when compared to the Formalin plant held by MPT. As MPT can determine which plants to invest in and the respective capital allocation, it rendered a more attractive option than the alternatives.

The MPT 4 portfolio outperformed both NPV 4 and ROI 4 portfolios by obtaining a surplus of 34.63 MMUSD and 12.88 MMUSD. Both NPV and ROI held different portfolio constituents. For the NPV case, the MPT portfolio had an additional 21% capital allocation to the Acetic Acid plant, which allowed it to gain profits valued at 44 MMUSD. Another main source of income was from the Formalin plant (42 MMUSD) when compared to the Ammonia plant held by the NPV portfolio. The NPV portfolio generated higher profits from the Nitric acid plant (35 MMUSD) and the Methanol plant (16 MMUSD). However, this overall was still lower than the net profit MPT provided. For the ROI case, the MPT plant again generated additional profits from the Acetic acid plant (44 MMUSD) and the Formalin plant (14 MMUSD). The profits gained by the ROI portfolio were from the Methanol plant (16 MMUSD) and the Ammonia plant (29 MMMUSD). The ROI portfolio had a lower difference when compared to the NPV portfolio.

NPV and ROI held the same five-plant portfolio. The MPT 5 portfolio outperformed both NPV 5 and ROI 5 by generating an additional profit valued at 8.70 MMUSD. A portion of the supplementary profit, gained by MPT 5, originated from the extra 13% capital allocated to the Acetic acid plant (26 MMUSD). Another portion was obtained from the additional 12% capital allocation to the Formalin plant (27 MMUSD). Whereas for the NPV and ROI portfolios, the additional profits were obtained from the Methanol plant (17 MMUSD), the Ammonia plant (26 MMUSD), and the Nitric acid plant (1 MMUSD). The MPT portfolio held the Urea plant to decrease portfolio risk. As Urea is not as profitable when compared to the Ammonia plant, it allowed the NPV and ROI portfolios to obtain higher profits from that plant. Overall, MPT again was successfully able to determine a more attractive investment and its profitability performance overcame both NPV and ROI portfolios.

5.1.6. Summary for annual and monthly frontiers

In this case study, the metrics reached the same consensus for single-plant portfolios. Yet, their differences became apparent when process plant portfolios were introduced. Overall, MPT portfolio performance vary depending on variability level (annual or monthly). For the annual variability case, when NPV and/or ROI is utilized as a decision-making metric, it misses more profitable projects more than 50% of the time when compared with MPT portfolios developed. MPT outperformed in two-plant, four-plant, and six-plant portfolio combinations when compared to NPV and/or ROI portfolios. Nevertheless, there were cases at which NPV and/or ROI outperformed MPT. In most of these cases, due to the guideless capital distribution assumption for the alternatively produced portfolios, the NPV and/or ROI portfolio outperformed that of MPT. This was fortunate to occur but may not happen again in future process portfolio studies. In one case (MPT 4 Low Risk - ROI 4), due to a variation in plant choice, MPT's net profit fell short. For the annual variability case, MPT performed better over a wider variety of process plant portfolios (two plant, four plant, and six plant) whereas NPV and/or ROI had a better performance at a limited number of process portfolios (four plant and mainly five plant). Furthermore, the MPT portfolios developed using monthly variability performed better than the portfolios generated by annual variability. MPT-generated portfolios (based on monthly variability) outdid all the alternatively produced portfolios (NPV and ROI). Nevertheless, MPT's process portfolio construction presents potential, and its ability to choose and distribute capital among portfolio constituents will remain a benefit that typical NPV and/or ROI indicators cannot provide. Moreover, utilizing monthly variation might be more effective for process plant portfolio development.

5.2. Development of MPT portfolios when considering economies of scale

As economies of scale are now being considered, the total capital investment and fixed operating cost are calculated as shown in equations (11) and (12). To develop the efficient frontier, the plant investment and risk relationship should be determined. The same applies for the plant investment and return relationship. Then, using equations (15) to (18) the average net profit and the respective ROI variability (risk) can be computed for each plant at various capital investments. This allows the user to estimate the return and/or risk for each process depending on the capital investment allocated. As economies of scale were considered, these relationships will be non-linear. Then, at different investments, plant risk and return will alter according to their determined non-linear relationships. Then, portfolio variance was determined through equation (19) and consequently portfolio risk (standard deviation) was calculated through equation (21).

It has been assumed the frontier is unbounded and so investment limits presented in Table 6 were applied. The returns and risks for each plant at its maximum investment is shown in Table 24. The correlation factors were determined to be the same as the linear case (Table 8). The efficient frontier was then obtained and is shown in Figure 8.

Table 24: Plant return and risk at maximum investment (considering economies of scale)

Plant	Average Annual ROI (%)	Annual σ^2 (%)	Annual σ (%)
Methanol	44.22	2.81	16.76
Acetic Acid	35.59	0.59	7.70
Formalin	29.43	0.31	5.54
Nitric Acid	17.86	0.19	4.39
Ammonia	32.61	3.94	19.85
Urea	20.75	6.65	25.79

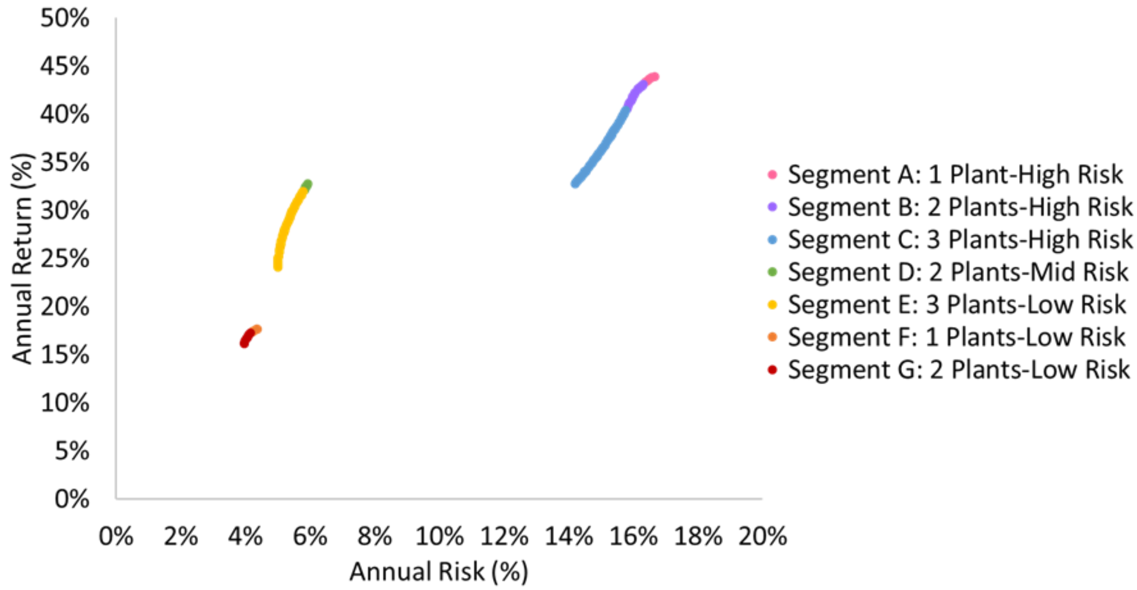

Figure 8: Efficient frontier when considering economies of scale

Segment A contains the Methanol plant only as it has the highest return (44.22%). Segment B added the Urea plant as it has the lowest correlation with the Methanol plant (-0.250). However, as the Urea plant has one of the lowest returns (20.75%), it was included at minor investments (maximum 3%). Then, segment C contained the Formalin plant in addition to the Methanol and Urea plants. As the Formalin plant had the lowest correlation with both the Methanol plant (-0.250) and the Urea plant (-0.928), its attractive inclusion dampens portfolio risk. As the Formalin plant return falls at mid-range (29.43%), its weight allocation increases from right to left (segment C). Further, segment D contained lower risk portfolios, and so the Methanol and Urea plants were removed as their individual standard deviations were relatively high (16.76% and 25.79% respectively). The Formalin plant remained as it has a relatively low standard deviation (5.54%). To further decrease portfolio risk, the Acetic acid plant was added due to its negative correlation (-0.625) with the Formalin plant. Further, the Acetic acid plant has a low individual risk (7.70%)

and a return of 35.59% (i.e. mid-high return) making it attractive to include at this segment. As the risk decreases, Segment E contained the Ammonia plant along with the Formalin and Acetic acid plants. The Urea plant was not added as it had the highest correlation with the Acetic Acid plant (0.634). The Nitric acid plant was not added as it has a high correlation with the Formalin plant (0.508). Then, the Methanol and Ammonia plants remain as candidates. The latter was chosen due to its greater dampening effect on risk (correlations of -0.507 and 0.254) when compared to the former (correlations of -0.126 and 0.100). Moreover, the Ammonia plant (32.61%) had a lower return than the Methanol plant (44.22%), allowing it to be active at lower return portfolios. As the risk is further reduced, all the previously included plants were removed, and the Nitric Acid plant was solely active (Segment F). This is expected as the Nitric Acid plant has the lowest risk (4.39%) and return (17.86%). To further reduce risk, Segment G had the Nitric acid plant included with the Acetic acid plant as it had the lowest correlation factor (-0.370) with it. As noticed from Figure 8, there exists disconnected areas throughout the frontier. Table 25 provides further information on the plant constituents and capital distribution before and after each disconnected region.

Table 25: Portfolio constituents at ends of disconnected frontier regions

Plant	**Weight**			
Methanol	0	0	0	0.846
Acetic Acid	0	0.544	0.680	0
Formalin	0	0.320	0.320	0.118
Nitric Acid	1	0	0	0
Ammonia	0	0.125	0	0
Urea	0	0.009	0	0.038
Risk (%)	4.38	5.00	5.93	14.20
Return (%)	17.65	24.09	32.79	32.79

As shown in Table 25, there are great differences between the plants and their respective capital distribution at the disconnected ends. For the first disconnected region (between 4.38% and 5% risk), the Nitric acid capital allocation decreases. It is expected that overall portfolio return will decrease initially until it reaches a low return point. As the Acetic acid and the Formalin plants have an increase in capital weight, it is expected that portfolio returns will start increasing again. As the investments to these plants increases, the portfolio return will increase until an efficient portfolio has been determined. There was a change in both return and risk as no plant has a standard deviation as low as the Nitric acid plant (4.38%). Consequently, the lowest possible portfolio risk is 5% provided by the Acetic acid, Formalin, and Ammonia plants. For the second disconnected region, there was no change in portfolio return but a great change in portfolio risk (5.93% to 14.20%). The Acetic acid plant weight decreases fully, whereas the Formalin plant weight decreases slightly. Then, portfolio return will drop eventually reaching a low return point. However, as the Methanol plant has a great increase in capital allocation (from 0 to 0.846), it is expected at some point the portfolios will start to gain higher returns. This continues to happen until the same initial portfolio return has been achieved, but by another portfolio combination. Then, as the changes in capital weights are known, the disconnected frontier regions may be estimated and are shown in Figure 9.

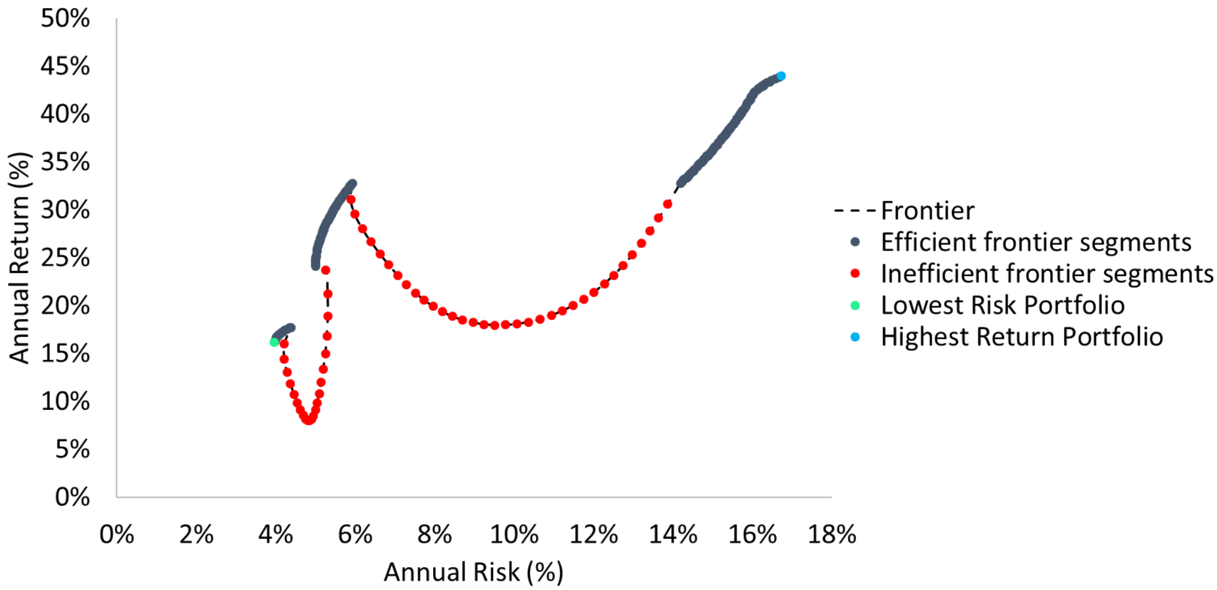

Figure 9: Frontier with inefficient portfolios

As shown, the frontier contains both efficient and non-efficient portfolios (i.e. the disconnected regions). These non-efficient portfolios were estimated as the pareto-optimal solutions would not consider these results. These portfolios were considered inefficient as there exists other portfolios (i.e. efficient ones) that have lower risk at their specific return value. For instance, there exists two portfolios that have a return of 30% where one has a risk value of 6% (efficient) and the other 14% (inefficient). Also, other portfolios were considered inefficient as there exists higher portfolios returns for a specific value of risk. For example, there exists two portfolios that have a risk of 5% where one has a return value of 24% (efficient) and the other 9% (inefficient). These non-efficient portfolios resulted due to the consideration of economies of scale. In this case, the effect of investment alteration results with a greater impact on both portfolio return and risk because of the nonlinearity of the objectives. As shown in Figure 9, the determined inefficient portfolios have lower returns (than the previously calculated pareto-optimal solution) as the risk increases. This is expected based on the previous discussion. Then, due to the non-linearity present from considering the economies of scale, only a unique plant-capital distribution can surpass the previous pareto-optimal performance (i.e. at the other end of the disconnected region). As the model searches for that point, the frontier may develop gaps. As soon as the newly found portfolio surpasses the previous pareto-optimal trade-off, another segment then begins to develop. Then, the user may expect vast changes in portfolio capital allocation between the efficient segments (Table 25). This phenomenon was not observed in the linear case.

The annual variability frontier was continuous whereas the non-linear frontier was disconnected. The portfolio return range was higher for the non-linear frontier as economies of scale were considered. In terms of plant choice, both frontiers had portfolios that contained the Methanol plant at higher returns and the Nitric Acid plant at lower returns. Both frontiers contained the Formalin, Acetic Acid, and Ammonia plants throughout the mid-risk return profile. The non-linear frontier contained less plant portfolio combinations than the annual variability frontier. Another difference between the annual variability frontier and non-linear frontier is that the former contained the Acetic Acid plant at higher returns whereas the latter contained the Urea plant instead. As the annual variability frontier had a smoother transition in the Acetic Acid-Methanol segment. More specifically, for minor changes in portfolio return, there was a minor change in portfolio risk. Whereas the non-linear frontier had abrupt transitions, and so both risk and return decrease at a steeper rate. Due to this, each frontier presented pareto-optimal solutions depending on the type of objective studied (linear vs non-linear). Several MPT portfolios where then chosen from the frontier and are presented in Table 26. Note that segments F and G were not included in the analysis.

Table 26: MPT portfolio combinations when considering economies of scale (*High Risk)

Plant	Rank	Weights (%)				
Methanol	1	100	97.66	90.58	0	0
Urea	2	0	2.26	3.39	0	0
Formalin	3	0	0	6.10	32.00	31.99
Acetic acid	4	0	0	0	68.00	61.22
Ammonia	5	0	0	0	0	6.27
Nitric Acid	6	0	0	0	0	0
Label		MPT 1	MPT 2*	MPT 3*	MPT 2	MPT 3

5.2.1. Alternatively produced portfolios considering economies of scale

Considering economies of scale, the NPV and ROI of each plant at their respective maximum investment were determined using material and energy prices for year 2015 (Table 27). The NPV and ROI portfolios were again developed and are shown in Tables 28 and 29. The Formalin plant had a maximum investment of 32%, and so the division was slightly altered for the ROI 3-plant portfolio.

Table 27: NPV and ROI of each plant using 2015 prices (considering economies of scale)

	Methanol	Acetic Acid	Formalin	Nitric Acid	Ammonia	Urea
NPV (MMUSD/y)	116	47	22	52	94	-54
ROI (%)	46	26	27	21	38	-22
CAPEX (MMUSD)	250	178.4	80	250	250	250

Table 28: NPV portfolio combinations in 2015 (considering economies of scale)

Plant	Rank	Weights (%)					
Methanol	1	100	50	33.33	25	20	16.67
Ammonia	2	0	50	33.33	25	20	16.67
Nitric Acid	3	0	0	33.33	25	20	16.67
Acetic Acid	4	0	0	0	25	20	16.67
Formalin	5	0	0	0	0	20	16.67
Urea	6	0	0	0	0	0	16.67
Label		NPV 1	NPV 2	NPV 3	NPV 4	NPV 5	NPV 6

Table 29: ROI portfolio combinations in 2015 (considering economies of scale)

Plant	Rank	Weights (%)					
Methanol	1	100	50	34	25	20	16.67
Ammonia	2	0	50	34	25	20	16.67
Formalin	3	0	0	32	25	20	16.67
Acetic Acid	4	0	0	0	25	20	16.67
Nitric Acid	5	0	0	0	0	20	16.67
Urea	6	0	0	0	0	0	16.67
Label		ROI 1	ROI 2	ROI 3	ROI 4	ROI 5	ROI 6

5.2.2. Portfolio comparison considering economies of scale

This section will highlight the profitability difference between the portfolio pairs developed. The total profit made by each portfolio was computed and is shown in Table 30. The difference between each portfolio's profit was calculated and is shown in Table 31.

Table 30: Net profit of each portfolio considering economies of scale (*High risk)

	MPT	**NPV**	**ROI**
Portfolio Type	**Profit (MMUSD)**		
1-plant	550.24	550.24	550.24
2-plant	514.83*	161.40	161.40
	309.06		
3-plant	434.97*	52.74	166.17
	260.30		

Table 31: Difference of each portfolio pair when considering economies of scale

Combination	Difference (MMUSD)	Combination	Difference (MMUSD)
MPT 1 - NPV 1	550.24 - 550.24 = 0	**MPT 1 - ROI 1**	550.24 - 550.24 = 0
MPT 2* - NPV 2	514.83 - 161.40 = 353.43	**MPT 2* - ROI 2**	514.83 - 161.40 = 353.43
MPT 2 - NPV 2	309.06 - 161.40 = 147.66	**MPT 2 - ROI 2**	309.06 - 161.40 = 147.66
MPT 3* - NPV 3	434.97 - 52.74 = 382.23	**MPT 3* - ROI 3**	434.97 - 166.17 = 268.80
MPT 3 - NPV 3	260.30 - 52.74 = 207.56	**MPT 3 - ROI 3**	260.30 - 166.17 = 94.13

Similar to the previous cases, MPT, NPV, and ROI chose the Methanol plant as a single-process portfolio, and so there was no difference present for those pairs. The MPT had portfolios that differed in risk level (i.e. High and Low) with both two-plant and three-plant combinations. The profit obtained by the MPT 2 – high risk portfolio surpassed both NPV 2 and ROI 2 by 353.43 MMUSD. This originated from the additional profits made by the extra 48% capital investment in the Methanol plant (385 MMUSD). Whereas the NPV and ROI portfolios made minor profits (32 MMUSD) from the Ammonia plant. Then, the MPT 2 – Low risk outperformed both NPV 2 and ROI 2 by obtaining a surplus in profits valued at 147.66 MMUSD. The MPT portfolio obtained its additional profits from the Acetic acid plant (172 MMUSD). In contrast, the NPV and ROI portfolio obtained minor profits from the Methanol plant (25 MMUSD). Further, the MPT 3 – high risk portfolio outdid both NPV 3 and ROI 3 by obtaining 382.23 MMUSD and 268.80 MMUSD respectively. For the NPV case, the MPT portfolio had an additional 57% capital allocation to the Methanol plant which gave a surplus profit of 400 MMUSD. Whereas, the NPV portfolio made the additional profits from the Nitric acid plant (19 MMUSD) when compared to the Urea plant held by MPT. For the ROI case, the additional profits made by MPT again originated from the Methanol plant (398 MMUSD). However, the ROI portfolio generated most of its additional profits from the Formalin plant (125 MMUSD). Further, minor profits were from the Ammonia plant (4 MMUSD) which was replaced by the Urea plant in the MPT portfolio. This replacement again was due to a reduction in portfolio risk. The MPT 3 – low risk portfolio outperformed both NPV 3 and ROI 3 by an additional 207.56 MMUSD and 94.13 MMUSD. The MPT portfolio generated more profits from the Formalin (59 MMUSD) and Acetic acid (154 MMUSD) plants when compared to the Methanol and Nitric acid plants held by NPV 3 respectively. For NPV, the only additional profits were from the Ammonia plant (6 MMUSD) due to the supplementary 27%

capital allocation. For the ROI 3 case, MPT differed by holding the Acetic Acid plant instead of the Methanol plant which generated supplementary profits for the MPT portfolio (101 MMUSD). Similar to the NPV portfolio, the ROI portfolio made extra profits from the Ammonia plant (7 MMUSD) due to the added 28% capital allocation.

Like the previous cases, the NPV, ROI, and MPT metrics reached the same conclusion for single-plant portfolios but differed when additional processes were included. Unlike the previous cases, when economies of scale where considered, there was a significant difference between the portfolios developed by MPT and the alternatively produced portfolios (NPV and/or ROI). This is crucial as in reality, economies of scale are most commonly accounted for. Then, this result further stresses the importance of MPT's ability to evaluate plant choice and determine their respective capital allocation to render a set of efficient process portfolio investments.

6. CONCLUSION

The goal of this thesis was to study the potential of using the Modern Portfolio Theory (MPT) as a decision-making tool with process plant investments. MPT can evaluate which plants to include in a portfolio and what should their respective capital division be by studying the risk return trade-off. The typical decision-making approach, throughout the chemical engineering domain, is done through process evaluation of economic indicators, such as NPV and ROI. However, these standard metrics do not consider the risk imposed by price fluctuations in raw materials, utilities, and power needs. MPT requires the input of historic pricing data of such resources to assess a plant's profit variability (risk) over a certain time period. Then a case study that includes Methanol, Ammonia, Urea, Nitric acid, Acetic acid, and Formalin plants as potential investment candidates was presented. The MPT curves for the case study were developed using pricing data from 2007 to 2014. Moreover, several MPT curves were determined which differed depending on annual and/or monthly variability, and whether economies of scale were accounted for. Then, to obtain the pareto-optimal solutions, a multi-objective optimization that maximizes return whilst minimizing risk needed to be solved subjected to a total investment constraint. The optimization was evaluated through a hybrid solver using both genetic algorithm (gamultiobj) and a goal attainment algorithm (fgoalattain) on MATLAB. Simultaneously, alternative portfolios were developed based on the typical NPV and ROI metrics. It has been assumed these plants were bought and were ready to operate in year 2015. For comparison purposes, several MPT portfolios, along with ROI and NPV portfolios, had their net profit evaluated over years 2015 to 2019 (future). The portfolios differed in the number of plants invested in, which plants were invested in, and their respective capital division. The results rendered the following conclusions:

- For the annual variability case, NPV and ROI portfolios failed to present attractive investments more than 50% of the time.
- For the monthly variability case, MPT portfolios outperformed all of the NPV and ROI portfolios by profits that ranged from 8.70 MMUSD to 79.47 MMUSD.
- When economies of scale were considered, MPT portfolios outperformed all of the presented NPV and ROI portfolios by profits that ranged from 94.13 MMUSD to 382.23 MMUSD.

In general, MPT's performance improved upon increasing data frequency (annual versus monthly). This novel study is not suggesting proceeding with MPT decision-making over the commonly used metrics (NPV and/or ROI). Instead, the results obtained in this thesis suggest that utilizing MPT as a decision-making tool under uncertainty can be insightful and may guide investors to hold attractive process plant portfolios.

6.1. Future work

The results have been obtained and it was concluded that MPT under uncertainty may guide investors to select better process plant portfolios than those developed by the status quo of applying profitability metrics (e.g. NPV and ROI). In light of this, it would be interesting to further assess MPT's potential by evaluating the following:

- Studying MPT with various historic price durations on portfolio development.
- Utilizing other risk models (e.g. semi-variance and coefficient of variance).
- Applying MPT whilst considering a more diverse set of process plants.
- Evaluating the effect of process to process integration on portfolio risk through MPT.

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APPENDIX

This section provides additional information for the reader. The data used to calculate each plant CAPEX is shown in Table 32. The capital cost reference of each plant is shown in Table 33.

Table 32: CAPEX data for each plant in 2015

Plant	CAPEX Exponent	Reference CAPEX (MMUSD)	Reference Capacity (t/y)
Methanol	0.60	348.00	1,200,000
Acetic Acid	0.68	137.48	202,460
Formalin	0.55	25.19	15,000
Nitric Acid	0.59	174.35	402,340
Ammonia	0.53	202.89	250,000
Urea	0.70	56.52	165,000

Table 33: References for each plants' CAPEX

Plant	CAPEX Reference source	CAPEX exponent source
Methanol	(Garrett 1989)	(Peters, Max S. Timmerhaus and West 2003)
Acetic Acid	(El-Halwagi 2012)	(Humphreys 2005)
Formalin	(Kadambur and Kotecha 2016)	(Peters, Max S. Timmerhaus and West 2003)
Nitric Acid	(ICIS 2017)	(Garrett 1989)
Ammonia	(Hignett 1985a)	(Humphreys 2005)
Urea	(Hignett 1985b)	(Peters, Max S. Timmerhaus and West 2003)

The Methane price was assumed to be fixed at a value of 1.79 USD/MMBtu (Thomson Reuters 2020b) recorded in March 2020. Equation (27) was used to convert USD/MMBtu to USD/ton NG.

$$\mathrm{NG}\left(\frac{\mathrm{USD}}{\mathrm{ton}}\right) = 1.79\,\frac{\mathrm{USD}}{\mathrm{MMBtu}} \times \frac{1\ \mathrm{MMBtu}}{28.3\ \mathrm{m}^3} \times \frac{\mathrm{kg}}{0.656\ \mathrm{m}^3} \times \frac{1\ \mathrm{ton}}{10^3\ \mathrm{kg}} \tag{27}$$

The price of carbon monoxide (CO) was calculated through the operation of a partial oxidation syngas unit and a cryogenic separation unit. This process required NG and Oxygen as raw material. The H_2 price was calculated through the operation of an electrolysis unit. This process required waster as raw material. These chemical prices were calculated using the general equation (28), and their respective parameters are shown in Table 34. The parameters a, c, and e represent the amount of raw material, utility, and by-products used and/or produced per ton of reference chemical. The variables b, d, and f represent their prices, respectively. The prices of NG, water, oxygen, and power were obtained from (Intratec 2020).

$$\mathrm{X}\left(\frac{\mathrm{USD}}{\mathrm{ton}}\right) = \mathrm{a}_{\mathrm{RM/X}} \times \mathrm{b} + \mathrm{c}_{\mathrm{Utility/X}} \times \mathrm{d} - e_{\mathrm{byproduct/X}} \times \mathrm{f} \tag{28}$$

Table 34: Parameters for CO and H_2 price calculation

Chemical	**a**	**c**	**e**	**References**
CO	0.625, 0.625	1408	0.206	(Medrano-García, Ruiz-Femenia, and Caballero 2019) (Medrano-García, Ruiz-Femenia, and Caballero 2017)
H_2	9	54000	-	(Ayodele and Munda 2019)

Nitric acid and CO_2 prices were obtained by using the price producer index (PPI) as shown in equation (29). The references for the PPIs and the old chemical price are shown in Table 35.

$$\text{New Chemical Price}\left(\frac{\text{USD}}{\text{ton}}\right) = \text{Old Chemical Price}\left(\frac{\text{USD}}{\text{ton}}\right) \times \frac{\text{New Index}}{\text{Old Index}} \tag{29}$$

Table 35: References for CO_2 and Nitric acid price calculation

Chemical	Producer Price Index	Old Chemical Price	Source
Nitric acid	(U.S. Bureau of Labor Statistics 2020c) (U.S. Bureau of Labor Statistics 2020b)	51 USD/ton	(Pérez-Fortes et al. 2016)
CO_2	(U.S. Bureau of Labor Statistics 2020a)	263 USD/ton	(Kirschner 2008)

The price of Acetic acid was obtained using equation (30), with a reference value of 383 USD/ton (January 2016) found in (Thomson Reuters 2020a). The price variation was from (Intratec 2020).

$$\text{New Price}\left(\frac{\text{USD}}{\text{ton}}\right) = \text{Old Price}\left(\frac{\text{USD}}{\text{ton}}\right) + \left(\frac{\text{New price} - \text{Old Price}}{\text{Old Price}} \times \text{Old Price}\right) \tag{30}$$

Formalin and Nitric acid plants produced steam that was converted to power using a turbine, with an outlet steam at ambient conditions. Their respective power was obtained from ASPEN.