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Influence of static and dynamic economic indicators on the feasibility study of chemical plants: the styrene monomer case-study

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*The most common misunderstanding about science is that scientists seek and find truth. They don’t. They make and test models… Making sense of anything means making models that can predict outcomes and accommodate observations. Truth is a model***.**

Neil Gershenfeld

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List of Acronyms

BTZ	“Basso Tenore di Zolfo”- Low Sulfur Content
CAPEX	Capital Expenses
CAPM	Capital Asset Pricing Model
CD	Conceptual Design
CF	Cash Flow
CO	Crude Oil
CPU	Central Processing Unit
DCD	Dynamic Conceptual Design
DCF	Discounted Cash Flow
DEP	Dynamic Economic Potential
DOF	Degrees of Freedom
DNPV	Dynamic Net Present Value
EA	Activation Energy
EB	Ethylbenzene
EE	Electric Energy
EP	Economic Potential
FCI	Fixed Capital Investment
LP	Low Pressure
LPS	Low Pressure Steam
MRP	Market Risk Premium
M&S	Marshall and Swift index
NIAT	Net Income After Taxes
NIBT	Net Income Before Taxes
NPV	Net Present Value
OPEX	Operative Expenses
PNPV	Predictive Net Present Value
PSE	Process Systems Engineering
SSE	Sum of Square Errors

TCI	Total Capital Investment
TPC	Total Product Cost
USD	United States Dollar
WACC	Weighted Average Cost of Capital

Abstract (English)

Aim of this manuscript is to perform a feasibility study of a styrene production plant. This analysis is carried out through the identification of the optimal configuration among 39889 different ones, which are obtained by varying four degrees of freedom of the process/plant: reactor inlet temperature, LP vapor flow rate, splitting factor, and reactor volume The identification of the optimal configuration and possible revenues from the styrene plant operation are evaluated through several economic indicators. First the analysis focuses on two static indicators, *i.e.* Conceptual Design and Net Present Value, and foremost, the manuscript concerns the dynamic indicators, such as Dynamic Conceptual Design and Dynamic Net Present Value. This second class of indicators is far more appropriate to carry out a feasibility study of a chemical plant, since it takes into account prices variability and market fluctuations along the plant life. The comparison between these indicators is achieved with historical price series over a time period from 2004 to 2014, where DNPV results to be the most reliable and exhaustive indicator. However, the evaluation of possible future revenues should be based on suitable predictive models for future market quotations of plant commodities and utilities. In particular, econometric models are used and the indicator obtained is a predictive and dynamic version of the Net Present Value. The PNPV is evaluated by generating 3000 economic scenarios through which the percentage of configurations that returns positive revenues and the most recurring optimal configurations is evaluated. This analysis allowed assessing the goodness of an investment for the construction and operation of a styrene plant.

Abstract (Italian)

Il principale obiettivo di questo lavoro di tesi è quello di realizzare uno studio di fattibilità di un impianto di produzione di stirene. Tale analisi viene effettuata attraverso l'identificazione della configurazione ottimale tra le 39889 possibili, ottenute tramite la variazione di quattro gradi di libertà all'interno del processo: temperatura in ingresso al reattore, portata del vapore LP, Splitting Factor e volume del reattore. L'identificazione della configurazione ottimale e i possibili ricavi provenienti dalla messa in opera dell'impianto vengono valutati attraverso l'utilizzo di indicatori economici. La prima analisi si concentra su indicatori di tipo statico, quali il Conceptual Design e il Net Present Value, in secondo luogo la trattazione riguarda gli indicatori di tipo dinamico, quali il Dynamic Conceptual Design e il Dynamic Net Present Value. Questa seconda classe di indicatori risulta di gran lunga più adeguata al tipo di studio che si vuole effettuare, in quanto prende in considerazione la variabilità dei prezzi durante la vita dell'impianto. Il confronto tra questi indicatori viene realizzato utilizzando serie storiche delle quotazioni di mercato in un arco temporale tra il 2004 e il 2014, grazie a cui è possibile identificare lo NPV dinamico come l'indicatore più affidabile e completo. Alla luce di tale conclusione, la valutazione della configurazione ottimale e dei possibili ricavi provenienti dalla messa in opera dell'impianto vengono valutati utilizzando solo l'NPV dinamico. La valutazione dei possibili ricavi, però, viene fatta utilizzando modelli predittivi per le future quotazioni di mercato di tutte le correnti e dei fluidi di servizio presenti nell'impianto, si parla quindi di NPV dinamico e predittivo. La valutazione del PNPV viene fatta attraverso la generazione di 3000 scenari rispetto ai quali viene valutata la percentuale di configurazioni che restituisce ricavi positivi e le configurazioni ottimali più ricorrenti. Grazie a queste analisi è possibile valutare se sia redditizio o meno investire nella costruzione e nella messa in opera di un impianto di stirene.

Motivation and structure of the work

Purpose of this manuscript is to perform a feasibility study of a styrene plant, identifying the optimal configuration among the 39889 obtained by changing the process degrees of freedom. In order to perform this analysis, two economic indicators, such as Conceptual Design and Net Present Value, was considered. These are static indicators, as they do not take into account price variations and market fluctuations over time. Aim of this manuscript is to compare static indicators with their dynamic version and analyze the main differences. Among the dynamic indicators, Dynamic Conceptual Design and Dynamic Net Present Value were considered to identify the differences in terms of styrene plant future revenues and optimal configurations. Thus, the analysis on the dynamic indicators concerns an investigation on the level of detail needed to perform a reliable feasibility study. It wants to understand if it is sufficient to use static indicators and if the indicators that consider only CAPEX and OPEX are reliable or not.

In order to carry on this analysis, the manuscript was divided into five chapters with a progressive depth of investigation. **Chapter 1** is an explanation of what is a feasibility study and its importance. It presents the tools available and the differences between static and dynamic methods, analyzing Conceptual Design, Net Present Value and their dynamic version. It also introduces the main elements of the aforementioned indicators. **Chapter 2** presents an overview of the styrene monomer and plant. It also provides an explanation of the four degrees of freedom (reactor inlet temperature, LP steam flowrate, reactor volume, and Splitting Factor) adopted in order to produce the different plant configurations and identify the optimal one. **Chapter 3** explains the methodology used to evaluate the economic indicators with an approach that produces results increasingly more accurate by upturning the investigation detail. In addition, this chapter covers the numerical input data selected for the styrene production plant, used in the MATLAB code. **Chapter 4** concerns the analysis of the results given by the different indicators. It starts from the evaluation of the static indicators and goes to the definition of the Dynamic Conceptual Design and the Dynamic Net Present Value. Eventually, the chapter presents a comparison between the dynamic indicators and a specific analysis on the DNPV. discusses the difference between the economic and the econometric models and provides a description of the econometric models used to foresee the commodity and utility quotations. The second part of the chapter is about the forecast of the PNPV scenarios and the analysis of the obtained results.

Chapter 1

Feasibility study of a chemical plant

The first chapter concerns the explanation of what is a feasibility study and why is so important to perform it. It presents the tools available and the differences between the static and the dynamic methods. It also explains how to evaluate the different indicators used to run a feasibility study such as the Conceptual Design, the Dynamic Conceptual Design, the Net Present Value, and the Dynamic Net Present Value.

1.1 Introduction

Running a project as big as the construction of a chemical plant is something that requires a huge effort: big investment, long time, and a number of resources are needed. A preliminary evaluation of the effectiveness of an investment is something that must not be neglected. For this purpose, several methods are applicable. Among these methods there are two big classes according to the usage of the time factor. The ones, which consider time in their calculations, are dynamic methods, as Dynamic Conceptual Design (DCD). The ones, which do not consider time, are static methods, as Conceptual Design (CD). The latter class presents the advantage of the simplicity and thus the usability by a large number of professionals. Despite the easiness of the static methods, it is preferable to use the dynamic indicators as the absence of the time factor may end up to a misleading interpretation of an investment. As a matter of fact, the market is governed by large a number of fluctuations due to the variation of the prices. An effective approach to the search of the maximum possible earning is considering the problem from a dynamic point of view.

1.2 Conceptual Design

Conceptual design is a hierarchical process used to evaluate the best configuration of a chemical plant from a large number of alternatives. The possible process configurations to obtain a product are countless, but only a very little number of ideas, usually minus than 1%, are operable and profitable on the industrial scale. To define an optimal layout, it is necessary to follow some economic guidelines related to process constraints, environmental safety, and sustainability. This approach progressively goes in-depth and produces results that are more accurate by increasing the investigation detail. Five levels of decision have to be considered. From the second to the fifth level it is possible to summarize all the decisions taken in the "*Economic Potential"* (EP), evaluated as the difference between the gains arising from the plant and the plant capital expenditure (CAPEX) and operative expenditure (OPEX). The CD assessment ensues the following sequence:

- The first level decision is about the process definition, the choice between a continuous operation and a batch one.

- In the second level, the input-output structure of the process flowsheet is analyzed. Is possible to evaluate the EP2 with the following formula:

$$EP2 = \sum_{j=1}^{Nproduct} C_{P,j} * \dot{n}_j - \sum_{i=1}^{Nreactant} C_{R,i} * \dot{n}_i \tag{1}$$

Where:

- $C_{P,j}$ is the molar cost per product j,
- n_j is the molar flow per product j,
- $C_{R,i}$ is the molar cost per reactant i,
- n_i is the molar flow per reactant i.

EP2 is measured in USD/y.

- In the third level the focus is on the identification of the recycle and the evaluation of the reactor and compressor costs. Is possible to evaluate the EP3 with the following formula:

$$EP3 = EP2 - (\frac{CAPEX_{Reactors+Compressors}}{YearsOfOperation} - OPEX_{Reactors+Compressors}) \tag{2}$$

Also the EP3 is measured in USD/y.

- In the fourth level, the separation section design and costs are taken into account. Is possible to evaluate the EP3 with the following formula:

$$EP4 = EP3 - (\frac{CAPEX_{Separation}}{YearsOfOperation} - OPEX_{separation}) \tag{3}$$

The EP4 is measured in USD/y.

- In the fifth level the heat exchange network is considered in order to evaluate the energetic efficiency of the plant. And even though is frequently not considered, due to the complexity of its evaluation, is calculated as follows:

$$EP5 = EP4 \pm (HeatExchangeNetwork) \tag{4}$$

The value of the EP must be significantly greater than zero to ensure an economic convenience. In particular, in order to have a profitable plant the EP4 must be greater than zero. Conceptual Design approach is largely used in the industry because of its immediacy: a little number of calculations allows the designers to draw conclusions on the most relevant plant choices. However, the main disadvantage of the CD is that costs are assumed fixed and constant, whereas the market prices can change significantly. An effective approach to the search of the maximum possible earning is considering the problem from a dynamic point of view. This means that product and reactant costs vary in time, according to the market quotations.

1.3 Dynamic Conceptual Design

Among the dynamic methods for the assessment of the economic feasibility of industrial processes, the Dynamic Conceptual Design (DCD) methodology plays a key role. The strongest aspect of this method is the easiness of the calculations, as it uses only the CAPEX and OPEX terms, where CAPEX includes the equipment cost and OPEX accounts for the cost of raw materials and utilities. DCD adopts the same hierarchical approach reported in paragraph 1.2 and the only difference with respect to the CD is the prices variation. Considering that the life of a chemical plant can be rather long, the most widespread method to evaluate the feasibility of a chemical plant is the evaluation of cumulated DEP4. This indicator considers the variation of prices every month and is calculated as follows:

$$DEP4 = \sum_{j=1}^{nMonth} Revenues_i * nHoursPerMonth - \sum_{i=1}^{nEquipment} EquipmentCost_i \qquad (5)$$

Where the revenues are the difference between the incomes coming from the sold or internally used (by)products, which allow saving expenditures for further utilities, and the costs of raw materials and utilities. It must be pointed out that, even though this method considers the variability of the market, it neglects several other elements, which raise significantly the costs of a chemical plant.

1.4 Net Present Value

Among the static methods is possible to count another indicator, the Net Present Value (NPV). This indicator has the advantage of considering many other expenses of a plant, not only the raw materials and the equipment costs. NPV is calculated as the algebraic sum of all discounted cash flows generated by the considered project, less the value of the cash flow at time zero. It represents the incremental wealth generated by a project, as if it were immediately available:

$$NPV = \sum_{t=1}^{Ny} \frac{f_t}{(1+i)^t} - C_0 \tag{6}$$

Where:

- f_t is the cash flow at year t,
- i is the Weighted Average Cost of Capital (WACC),
- C_0 is the fixed-capital investment.

If the NPV is negative there are no reasons to undergo an investment that instead of generating value would create a loss in terms of money, resources, and time. A positive NPV means that the project can lead to sufficient earnings and repay the initial investment. On the other hand, a negative NPV is the proof of economic losses, which would be generated by running the project.

1.4.1 FCI

The evaluation of the NPV starts from the calculation of the Fixed Capital Investment. For this purpose, several methods are applicable, according to the preliminary information level of detail. For the sake of simplicity, in this manuscript the "percentage of delivered-equipment" method has been chosen. This method requires the evaluation of the delivered-equipment cost and all the other items are than estimated as its percentage. The cost of the delivered-equipment can be easily calculated according to the Guthrie's Formula. The Guthrie's Formula uses the Marshall and Swift (M&S) index, the cost of the same piece of equipment already assessed at some time of the past, and the characteristic dimensions of the equipment. Using these simple tools, allows evaluating the equipment cost of the plant. Once the costs of the delivered equipment are calculated, it is possible to estimate all the other components. **Error! Reference source not found.** shows a description of the number of items that contribute to the Fixed Capital Investment.

Table 1 – Total direct and indirect plant costs.

Total direct plant cost	Total indirect plant cost
Purchased Equipment	Engineering
Purchased equipment installation	Supervision
Instrumentation and controls (installed)	Legal expenses
Piping (installed)	Contractor's fee
Electrical system (installed)	Contingencies
Buildings	
Yard improvement	
Service facilities	
Land	

1.4.2 Cash Flow

Once the FCI has been calculated it is possible to move to the Total Product Cost (TPC), which represents the operative costs of the plant. It is possible to calculate the TPC as a percentage of the raw material and utilities cost as follows:

$$TPC = n * (\sum_{i=1}^{Nrawmaterial} Raw\ Material_i + \sum_{j=1}^{Nutilitiy} Utility_i) \tag{7}$$

Where n represents the value of the percentage selected, according to the guidelines proposed.

Several items are included in the formation of the TPC and are shown in Figure 1.

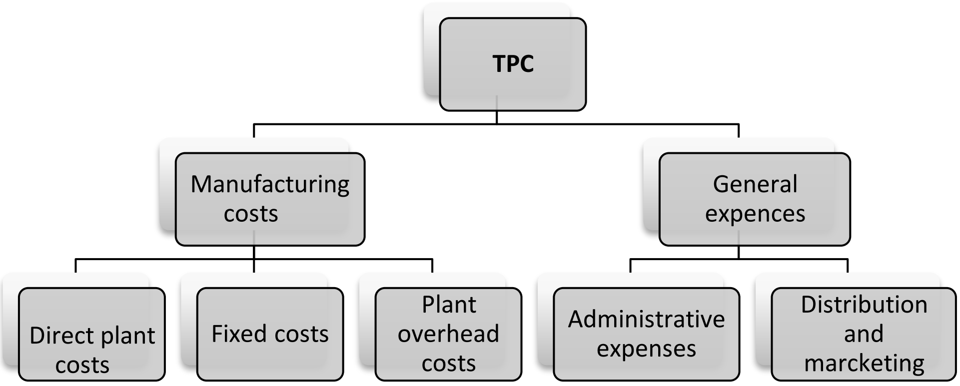


Figure 1 – Total Product Cost division.

When the value of the total product cost is obtained, it is possible to proceed with the calculation of the cash flow:

- Earnings, calculated as the sum of the products earning:

$$Earnings = \sum_{i=1}^{Nproduct} ProductsSold_i \qquad (8)$$

- Profits, calculated as the difference between the earning and the total product cost:

$$Profits = Earnings - TPC \qquad (9)$$

- Net Incomes Before Taxes, calculated as the difference of the profit and the annual depreciation:

$$NIBT = Profits - Depreciation \qquad (10)$$

The depreciation is the decrease in value that occurs to equipment, buildings, and other assets. The depreciation rate is usually higher at the beginning and then decreases in the last years of the depreciation period. However, the sum of every single annual depreciation percentage must be equal to 100%. For the sake of simplicity, the straight-line depreciation model has been chosen, *i.e.* throughout the plant life the rate of discount is equal every single year.

- Net Income After Taxes, calculated as the difference between the NIBT and the taxed amount:

$$NIAT = NIBT * (1 - TaxRate) \tag{11}$$

The tax rate is something difficult to be calculated, it varies in the different Countries and it includes different items according to the business, which is being ran.

- Cash Flow, the cash flow is the sum of the NIAT and the depreciation value:

$$CF = NIAT + Depreciation \tag{12}$$

As shown by the previous formulas, the cash flow evaluation is the most important step within the feasibility study.

1.4.3 Discounted Cash Flow

As aforementioned, the NPV uses the discounted cash flow. The discounted cash flow or actualized cash flow (DCF) is an investment evaluation method used to estimate an investment attractiveness. DCF uses future cash flow and discounting them allows reaching a present value estimation. The aim of this indicator is to estimate the money an investor would gained adjusted for the time value of money. It is worth observing that, in its estimation, the risk factor is taken into account.

Let CFi be the generic expected cash flow for the period i and be WACC the correct rate for the activity risk to be evaluated. Let n be the number of periods in which this activity provides cash flows. The value of this activity is given according to the discounted cash flow formula:

$$DCF = \sum_{i=1}^{n} \frac{CF_i}{(1 + WACC)^i} \tag{13}$$

This is the current value of all future cash flows.

1.4.3.1 WACC

In order to better understand the meaning of the discounted cash flow, a focus on the WACC is in order. The WACC can be defined as the weighted average rate of return required by those who supply capital, both debt and equity. Its value should be related to the relevant risk of the investment: an increase in the WACC underlines a decrease in valuation and an increase in risk. WACC can be estimated as follows:

$$WACC = k_s \frac{Equity}{Equity + Debt} + k_d (1 - tax) \frac{Debt}{Equity + Debt} \tag{14}$$

Where:

- k_d is the debt cost of the firm,
- k_s is the equity cost,
- tax is the corporate tax rate,
- Debt and Equity are the market values of the debt and the equity of the firm, respectively.

As shown, WACC can be split into two components, the cost of equity and the cost of debt, each weighted with suitable "weights." Each term of the formula must be analyzed in order to deeply understand the meaning of this factor.

The cost of equity is the most complex component to be calculated. The difficulties in estimating the cost of the owned resources lies in the fact that this is not a certain value. The cost of equity can be determined by reference to different economic models, where CAPM (Capital Asset Pricing Model) is the most widespread one. With CAPM, the cost of equity is determined as the sum of the risk-free return and a risk premium that depends on the systemic risk of the company being assessed, measured by a "beta" coefficient. The CAPM formula is as follows:

$$Ke = Kf + \beta * MRP \tag{15}$$

Where:

- K_e is own equity cost,
- K_f is yield of zero risk securities,
- ß is systemic risk factor,
- MRP is the market risk premium.

The companies with a high value of “beta” are very risky: they are typically start-ups with high financial risk and with extremely volatile cash profits and cash flows. On the other hand, companies with small “beta” are considered moderately risky:

- $ß > 1$: The title moves in the same direction of the market and with higher fluctuations of the market itself.

- $0 < ß < 1$: The title moves in the same direction of the market, but with lower oscillations of the market itself.

- $-1 < ß < 0$: The title moves in the opposite direction of the market and with lower fluctuations of the market itself.

- $ß < -1$: The title moves in the opposite direction of the market and with greater fluctuations of the market itself.

The cost of debt can be defined as the rate that the company would pay in current market conditions to obtain a new medium-long term loan. In the formula, the cost of debt is decreased by deductibility of interest expenses, according to the tax rate. Despite the wide use in business practice, this approach is rather risky as it tends to underestimate the cost of debt.

The weight of equity and debt plays an important role as well. The determination of the weight of equity and indebtedness must be related to the entire projection time span. Generally speaking, equity and debt should be determined on the basis of their market prices, but often business practice prefers accounting based.

According to this method, the companies calculate the values of the WACC. Usually the WACCs are calculated with a quarter frequency. However, not all the companies share this information publicly.

1.5 Dynamic Net Present Value

As a matter of fact, prices are not constant and their variation is governed by the volatility of prices, market fluctuations, demand modification, financial fluctuations, offer and demand oscillation, periodic variation, calamities, and several others. The presence of the aforementioned elements creates a large number of variations on the prices of the markets goods. If these variations are neglected the evaluation of the profitability of a chemical plant are biased. In order to use an indicator, which considers both the market fluctuation and the expenses related to the lifecycle of a chemical plant, it is advisable to evaluate a modified version of the NPV. DNPV is calculated as described in the previous paragraph but the prices are not kept constant, as well as in the DCD, and at the same time the WACC is considered variable. The aim of this manuscript is first to evaluate if the DNPV is worth or the computational complexity and burden, given by the evaluation of the prices variation, can be neglected; and foremost the relation between the DCD and DNPV: if there is a proportion between these indicators and if all the elements neglected in the calculation of cumulated DEP4 have an important influence on the plant costs.

Chapter 2

Styrene monomer and production

This chapter presents an overview of the styrene monomer and its toxicity, the important role played in the worldwide market, and the plant layout. The final part of the chapter provides an explanation of the four degrees of freedom adopted in order to produce the different plant configurations and identify the optimal one.

2.1 Styrene

Phenyl ethylene, *i.e.* the IUPAC name of styrene (C_6H_5-CH=CH_2), is an aromatic, colorless, flammable compound with a strong odor. Also known as ethenylbenzene, vinyl benzene ad phenylethene, at room temperature is an oily liquid. It has a melting point of -31°C and a boiling temperature of 145°C, it is soluble in acetone, benzene, ether, n-heptane, and ethanol. In **Error! Reference source not found.** is shown the styrene monomer molecule.

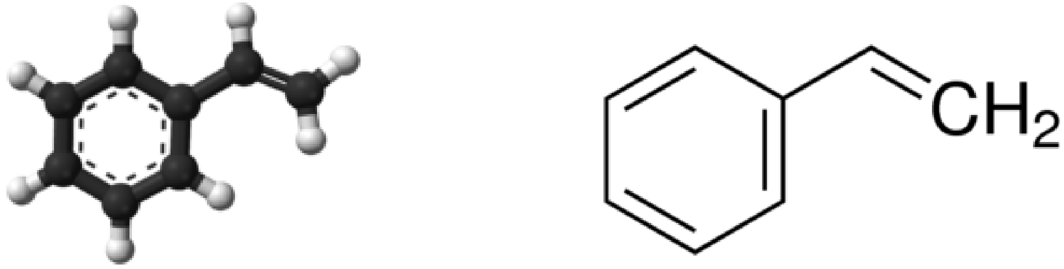


Figure 2 – Styrene monomer representation.

Styrene is mainly used in the production of polystyrene plastics and resins. It is also used as an intermediate in the synthesis of materials used for ion exchange resins and to produce copolymers. After ethylene and vinyl chloride, it is the most important monomer in the production of plastics. It is used as an intermediate in the production of several plastomers and elastomers (polystyrene, SBR, ABS and SAN resins). Figure 3 shows the most widespread usages of styrene.

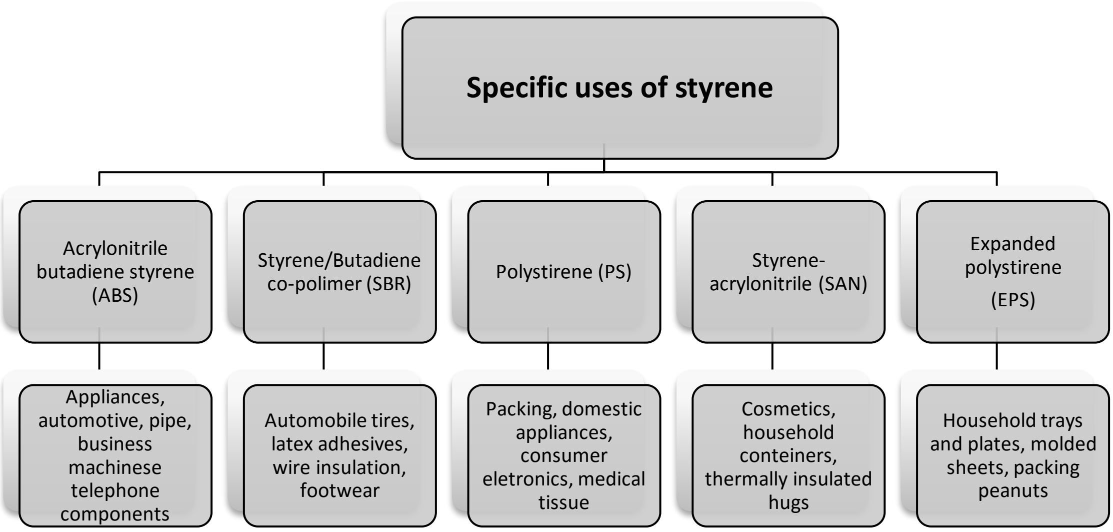


Figure 3 – Styrene specific usages.

Styrene world production is about 26.5 million of tons per year, thus, is one of the most important products of the organic chemical industry. The production of styrene is spread all over the world, particularly in North America, Europe, Japan, and Korea. The worldwide production of styrene, divided by geographic area, is shown below in Figure 4.

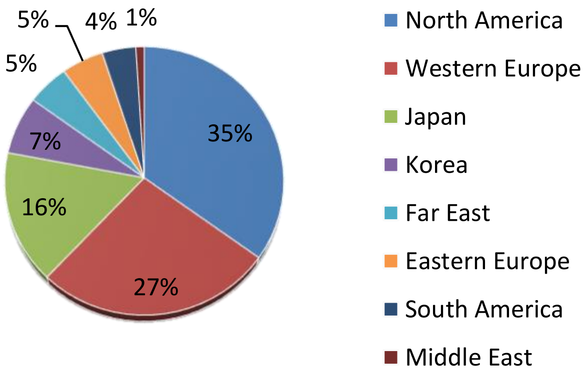


Figure 4 – Styrene production by geographic areas.

2.2.1 Styrene toxicity

Styrene is regarded as a "hazardous chemical", is harmful if inhaled, it causes skin and serious eyes irritation, may irritate the respiratory tract, it causes damage to central nervous system, liver, respiratory system and auditory organs in case of prolonged and repeated exposure, it may be lethal if ingested and if it penetrates into the respiratory tract . Styrene oxide is considered toxic, mutagenic, and possibly carcinogenic. The U.S. EPA does not have a cancer classification for styrene, but it has been the subject of their Integrated Risk Information System (IRIS) program.

2.2.2 Styrene Production

The industrial production of styrene is mainly run via catalytic dehydrogenation of ethylbenzene. The first process was finalized in Germany (IG Farben, Ludwigshafen, 1931), using a ZnO, Al2O3 + CaO based dehydrogenation catalyst. As aforementioned, styrene is produced by ethyl benzene-based technology. There is another technology, which co-products styrene with propylene oxide by the PO/SM process. Although, more than the 90% of EB is first made by the catalytic alkylation of benzene with ethylene, using either aluminum chloride or, more recently, zeolite catalysts. The reaction can be carried out in either vapor or liquid phases. The EB is dehydrogenated to styrene in the presence of steam. The main reaction is:

$$C_6H_5\text{-}CH_2CH_3 \rightarrow C_6H_5\text{-}CH{=}CH_2 + H_2 \qquad \Delta H = +29\ kcal/mol \tag{16}$$

This is a catalytic endothermic reaction, with unfavorable equilibrium constant with $\Delta G° = 0$ is reached at about 700 °C. In order to increase the yield of the reaction it is possible to operate at low pressure, due to the absence of equimolarity. It is also possible to add steam in the inlet flow in order to decrease the partial pressures and supply the heat of reaction. Thus, the operating condition of the process are 550-620 °C for the temperature and 1-3 bar for the pressure. Fe2O3, the active phase; Cr2O3, the support, and K2CO3, the promoter, make the catalyst. The conversion of ethylbenzene is about 40% and selectivity towards styrene is more than 90%. Three main byproducts are produced within the process: toluene, benzene and tars. They are formed by the following parasite reaction:

$$C_6H_5CH = CH_2 + 2H_2 \rightarrow C_6H_5CH_3 + CH_4 \qquad (17)$$

$$C_6H_5CH_2CH_3 \rightarrow C_6H_6 + C_2H_4 \qquad (18)$$

$$C_6H_5CH_2CH_3 \rightarrow 8C + 5H_2 \qquad (19)$$

In order to mitigate the coke formation, the steam added to the inlet flowrate is really helpful. The reaction to eliminate tar is the following one:

$$C + 2\ H_2O \rightarrow CO_2 + 2\ H_2 \qquad (20)$$

One of the biggest problems of this styrene production process is the final separation of styrene from the byproducts and the ethylbenzene. Considering the different boiling temperature of toluene, benzene, ethyl benzene and styrene a sequence of distillation columns are used for the separation. **Error! Reference source not found.** shows the boiling temperature of the styrene production components.

Table 2 – Products, byproducts and reactants boiling temperature.

Component	Boiling temperature (°C)
Styrene	145
Ethyl benzene	136
Toluene	110

Considering the different boiling temperature of the components, the separation of benzene and toluene occurs in the first column and the byproducts are either sent to a toluene dehydrogenation plant or further separated into benzene. Ethylbenzene is then separated and recycled to the reactors, and considering the small difference of the boiling temperature of toluene and ethylbenzene, a high level of reflux is needed. Finally, styrene is distilled from tars and polymers under vacuum in order to keep the temperature as low as possible. It is important to keep in mind that the residence time and the temperature of the distillation section must be kept as low as possible in order to avoid the polymerization of the styrene. There is one other possible scheme for the separation section, the so-called Monsanto approach, which carries out first the most difficult separation, followed by separation of the benzene – toluene mixture. Here below the standard and Monsanto scheme of the separation are shown in Figure 5.

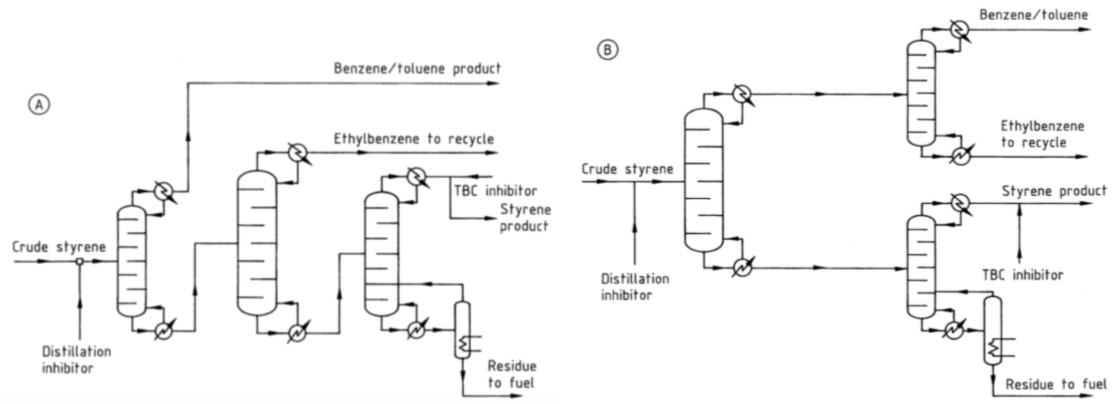


Figure 5 – Standard (A) and Monsanto (B) separation section schemes.

2.2.2.1 Styrene plant

The styrene production is achieved in the plant described in Figure 6. The ethylbenzene is mixed with a stream of low-pressure steam and fed to the plant at a constant rate of 132.8 kmol/h. This value allows meeting a styrene production of around 100,000 ton/y and is reported in by Luyben (2011), Vasudevan et al. (2009), Barzaghi and Conte (2015), and Buscemi e Pagnoncelli (2016). The vapor pressure is about 3 bars and the temperature is about 200 °C. The feeding stream is heated with a fraction of the steam in E-1, a heat exchanger, with the stream coming from the second reactor. In order to reach the inlet temperature of the first reactor, the remaining steam is heated in a furnace E-2. In as a consequence of the temperature threshold for the catalyst deactivation that is 600 °C. In this thesis work the inlet temperature to the reactor is one of the degrees of freedom and belongs to the 535-565 °C interval. This choice is a consequence of the kinetic “Power Law”, better discussed in Barzaghi and Conte (2015). The inlet stream passes through a catalytic reactor. The adiabatic operation of the reactor makes the temperature dropping, thus the outlet stream is heated by means of the E-3 furnace before entering the second reactor.

Exiting the second reactor, the stream is sent to a separation section, composed of a decanter and three distillation columns. The decanter removes the light gases from the feed, the first column C-1 is used to separate Benzene, the second column C-2 for the toluene separation and the third column C-3 for the ethylbenzene. According to this plant scheme, the aim of this thesis work is to evaluate which is the optimal configuration among thousands of possible alternatives. In order to investigate different plant configurations four degrees of freedom are taken into account: inlet temperature, splitting factor, LP steam pressure and reactor volume. The only way to better understand which is the most profitable solution is to run a feasibility study and calculate the revenues coming from each plant configuration.

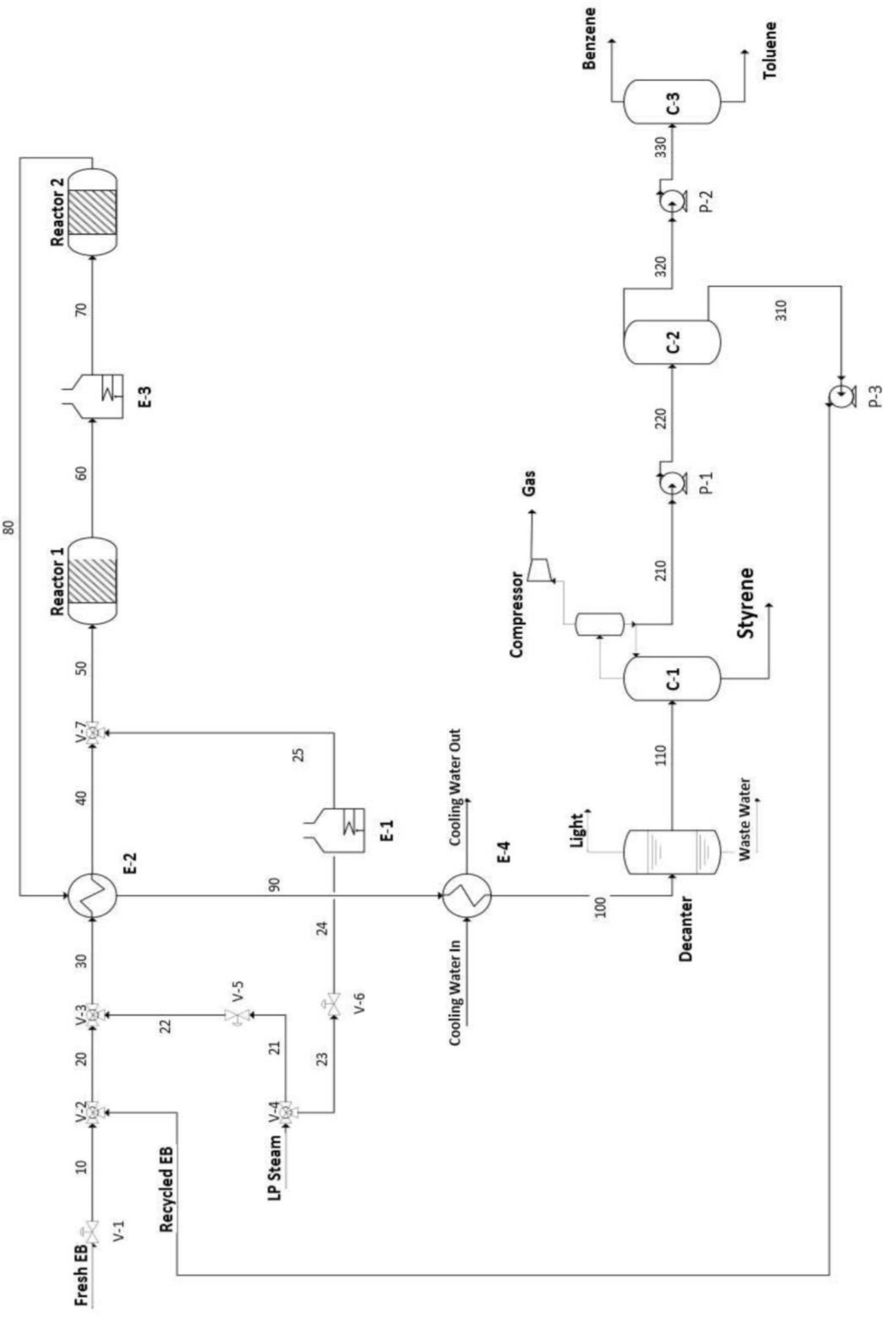


Figure 6 – Styrene production plant.

2.2 Degrees of freedom

Two different external aspects must be considered in order to identify the optimal plant configuration: price variability and the WACC instability. In order to analyze the different configurations some degrees of freedom must be chosen and varied to produce the different configurations. It is worth understanding what elements can be considered constant during the conceptual design of the plant and which should be varied due to their influence on the plant profitability. Four degrees of freedom have been chosen to deploy the different plant configurations to be economically assessed. The four degrees of freedom chosen for this plant are:

- Low pressure (LP) steam inlet flow

- Inlet temperature to the reactors (the same for each reactor)

- Reactor volume (the same for each reactor)

- Splitting factor of the “LP Steam” flowrate

The first three degrees of freedom are the same adopted in Luyben (2011), whilst the “LP Steam” splitting factor was first proposed in Buscemi and Pagnoncelli (2015). It is worth observing that the reactor volume is something that is assigned at the design stage of the equipment. The other three degrees of freedom can be modified while the plant is running and are degrees of freedom at the design stage in terms of nominal operating conditions. The possibility of modifying the design variables on-line allows a possible further increase of the plant profitability. The influence and the upper and lower limits of these decision variables must be further analyzed.

2.2.1 Influence and bounds of the LP steam flowrate

As discussed in Paragraph 1.2.2, steam has a leading role in the partial pressures decrease, supplies the heat of reaction and reduces the formation of coke. Considering that “LP steam” flow controls all these aspects, the importance of this design variable is very high. The lower and upper bounds are set at 2000 and 5000 kmol/h respectively as proposed by

Luyben (2011) and further discussed in Barzaghi and Conte (2015). This flow rate has been selected to fall in the range of an EB/LP Steam ratio of 12-17, proposed in Sheel and Crowe (1969), and in Vasudevan et al. (2009). The discretization step selected for the grid-search algorithm is 100 kmol/h, as reported in Buscemi and Pagnoncelli (2016). By fixing the other three degrees of freedom and varying the “LP steam” flowrate, it is possible to evaluate the influence on the other plant variables.

2.2.2 Influence and bounds of the reactor inlet temperature

As a simplification, proposed by Luyben (2011), the conditions of the two adiabatic reactors are exactly the same, which allows reducing the number of degrees of freedom from five to four, and avoiding the introduction of the second reactor inlet temperature as a degree of freedom. The inlet reactor temperature influences the conversion and selectivity of the styrene production reaction. The temperature must also be controlled due to the upper thermal limit of all the materials of the piping system and the equipment. All these aspects lead to the need of an optimization and a tight control on the inlet temperature in the first reactor. An increase in selectivity is something positive for the styrene production but the decrease of the conversion leads to a higher recycle ratio and thus higher costs. A tradeoff between the selectivity and the conversion is therefore highly recommended. Considering that the reaction of styrene production is endothermic, the reaction should be run at the highest possible temperature. As aforementioned, the upper thermal limit of the material does not allow the possibility of running the reaction at the highest possible temperature. A tradeoff between these aspects should be attained. The inlet temperature window covers the 535-565 °C interval with a discretization step of 3°C, as proposed by Barzaghi and Conte (2015).

2.2.3 Influence and bounds of the reactor volume

The reactor volume, which is the same for both the adiabatic reactors, is the degree of freedom that must be set in advance and cannot be modified during the plant operation. The upper and lower limits are 21.38 and 72.70 m^3, as proposed by Barzaghi and Conte (2015). The volume is calculated by setting the reactor diameter at 3.3 m, as proposed in Luyben (2011), and varying the length from 2.5 to 8.5 m with a discretization step of 0.5 m.

The size of the reactor is strictly related to the CAPEX and affects both the selectivity and conversion. A longer reactor would lead to a higher level of conversion but also to an unaffordable cost of the reactor itself. Also the yield is strongly related to the reactor volume.

2.2.4 Influence and bounds of the splitting factor for the “LP Steam”

The reason of the Splitting Factor optimization was discussed in Buscemi and Pagnoncelli (2016). The influence is on both CAPEX and OPEX terms, in particular related to the E1, E2, and E4 furnaces. The optimal ratio of LP Steam inlet flow (the splitting factor) has to be between 21 and 23. Varying the splitting factor values different aspects change along the plant: E4 increases in area but the CAPEX and OPEX for the E1 and E2 decreases. As proposed in Vasudevan et al. (2009), the splitting factor is set between 0 and 1. In this thesis work the splitting factor goes from 0.1 to 0.9 with a discretization step of 0.1. It is worth underlining that the ratio between LP steam and fresh EB is already well controlled by the LP steam flow rate. Increasing the latter increases the ratio between LP steam and fresh EB, and decreasing it lowers the ratio. Thus, it makes no sense to try to change the flowrate of fresh EB because it is already enough to twist the steam stream, considering that, it is important to evaluate the ratio 22/20 but it can be done by changing either LP steam or the Splitting Factor.

Chapter 3

Fixed and operative expenses estimation

This third chapter concerns the methodology utilized to evaluate the different items of the economic indicators. It starts from the evaluation of the plant CAPEX and OPEX for the CD and DCD and it progressively goes in-depth till the evaluation of the fixed and operative expenses for the NPV. This approach produces results that are increasingly more accurate by upturning the investigation detail. In this chapter are also explained all the numerical input selected for the styrene production plant.

Regardless of the type of economic indicator, whether static or dynamic, a feasibility study starts from the evaluation of the plant CAPEX and OPEX. The differentiation between such indicators is due to the level of detail with which capital and operative expenses are calculated. As aforementioned the simplest one is the Conceptual Design and the most complicated, from a computational point of view, is the Dynamic Net Present Value. Whether the analysis is deeply developed or not, the evaluation of the fixed expenses is based on the computation of the equipment purchase and installation costs, and the assessment of the operative expenses is based on the computation of the raw material costs.

3.1 Fixed costs evaluation

The first step to be completed is the plant CAPEX estimation. The starting point for the evaluation of the fixed cost is the calculation of the equipment prices and their installation costs. The equipment considered in the styrene production plant are two furnaces, two reactors, three columns, one decanter, two heat exchangers, one condenser and one reboiler. For all these equipment cost evaluation, it is advisable to use the Guthrie's formulae. These formulae use geometric, pressure, design, and other parameters in order to find the cost of a piece of equipment at the present time, by comparing it with a corresponding past cost of the same piece of equipment. This comparison is made through the M&S, an index value for a given moment representing the cost at that moment relative to a certain base time. The equivalent cost at the present can be estimated by multiplying the cost at the time in the past to the ratio between the present index value and the one at the moment when the original cost was obtained. There are many different cost index, it has been chosen to use the M&S which gives a fairly accurate estimation if the time period considered is less than ten years. It is worth underlining that the price obtained through all the cost index is just an estimation, several factors, such as the technological advancement and the local conditions, are not taken into account. The plant equipment cost is evaluated as follows:

- The furnaces cost is estimated using the following formulae:

$$C_{Fournace} = \left(\frac{M\&S}{280}\right) * (5.52 * 10^3) * Q^{0.85} * (1.27 + F_d + F_m + F_p) \qquad (21)$$

  Where:

  - Q is the adsorbed duty [MBtu/h] and is estimated between 20 and 300 MBtu/h,
  - F_d is the designed variation,
  - F_m is the material variation,
  - F_p s the pressure variation,
  - M&S is the Marshall and Swift index updated to 2010, which was the last index available.

  The cost of the furnaces is evaluated in USD.

- The heat exchangers, the reboiler, and the condenser costs are estimated using the following formulae:

$$C_{HeatExchanger} = \left(\frac{M\&S}{280}\right) * 101.3 * A^{0.65} * \left[2.29 + (F_d + F_p) * F_m\right] \quad (22)$$

Where F_d, F_m, F_p, and M&S represents the same parameters used for the evaluation of the furnaces costs, A is the heat exchanger area [ft^2] and is estimated between 200 and 5000 ft^2. In order to measure the heat exchange area, the following formula has been used:

$$\mathrm{A} = \frac{Q}{\mathrm{U} * \Delta T_{ml}} \quad (23)$$

Where:

- U is the overall exchange coefficient [W/m^2/K],
- Q is the heat exchanged which directly given from UniSim,
- ΔT_{ml} is the average logarithmic temperature difference and it is calculated in different ways for the reboilers, the condensers and the heat exchangers:

$$\Delta T_{ml} = \frac{(T_{hot1} - T_{hot2}) - \ (T_{cold1} - T_{cold1})}{log\,\frac{T_{hot1} - T_{hot2}}{T_{cold1} - T_{cold2}}} \quad (24)$$

Equation (24) is used for the condensers and the heat exchangers while equation (25) is used for the reboilers.

$$\Delta T_{ml} = T_{steam} - T_{reboiler} \quad (25)$$

The values used for the evaluation of the different heat exchangers area are summarized in Table 3.

Table 3 – Heat Transfer Phenomena Coefficients.

Factors	Value	UoM
U Heat Exchanger 2	0.3	[kW/m^2/K]
U Heat Exchanger 4	0.7	[kW /m^2/K]
U Reboiler	1	[kW /m^2/K]
U Condenser	0.7	[kW /m^2/K]
H2O Temperature IN	20	[°C]
H2O Temperature Out	40	[°C]
Reboiler Vapor Temperature	200	[°C]

It is worth observing that the cost of the heat exchangers is evaluated in USD.

- The decanter, the columns, and the reactor costs are estimated as follows:

$$C_{Vessel} = \left(\frac{M\&S}{280}\right) * 101.9 * D_{Vessel}{}^{1.066} * L_{Vessel}^{0.802} * (2.18 + F_m * F_p) \qquad (26)$$

Where F_d, F_m, F_p, and M&S represent the same parameters used for the evaluation of the previous piece of equipment, D is the diameter of the vessels, and L represents the height in the case of the columns and the length in the case of the decanter and the reactors. Both D and L are measured in ft. The cost of the vessels is evaluated in USD.

It is worth observing that the cost of the columns is not only related to the costs of the vessels but is also related to the costs of the trays for the second column, which is a tray column, and the cost of the filling for the first and the third column, which are filling columns.

$$C_{Column\ 1,3} = C_{Filling} + C_{VesselColumn} \qquad (27)$$

$$C_{Column\ 2} = C_{Trays} + C_{VesselColumn} \tag{28}$$

The cost of the trays is evaluated using the following relation:

$$C_{Trays} = \left(\frac{M\&S}{280}\right) * 4.7 * {D_{tray}}^{1.55} * H * (F_s + F_t + F_m) \tag{29}$$

Where F_m and M&S represents the same parameters used for the evaluation of the previous equipment, D is the diameter [ft], H is the tray stack height [ft], F_t is the mechanical refrigeration factor is set at 1.8 when a bubble cup column is used, and F_s is the tray spacing factor set at 1 due to the space in 24 in.

In order to evaluate the costs of the columns some additional parameters are needed and reported in Table 4.

Table 4 – Column costs estimation constants.

Factors	Value	UoM
Packed cost	1000	[\$/m^3]
Tray height	2	[ft]
Real trays number	52	[kW/m^2/K]

- The heat exchangers, the reboiler, and the condenser costs are estimated using the following formulae:

$$C_{Compressor} = \left(\frac{M\&S}{280}\right) * 517.5 * D^{0.82} * (2.11 + F_d) \tag{30}$$

Where F_d and M&S represents the same parameters used for the evaluation of the furnaces costs and D is the duty evaluated in bph. The costs of the compressor is in USD.

As aforementioned, the costs of the different equipment depend on three different parameters F_m, F_p, and F_d.

The first parameter is the material factor (F_m), which is set at 1 when the equipment is made of carbon steel; all the columns items are made of carbon steel only the furnaces are made of stainless steel, in case of stainless steel the material factor is set at 0.75. The choice of the materials depends on the resistance needed for the equipment, in the case of the furnaces, due to the high temperatures is better to use a more resistant material.

The second parameter is the pressure factor (F_p), which is set at 1 when the equipment pressure is up to 50 psig while it is set at 0 when the pressure is up to 150 psig. All the vessels have a pressure lower than 50 psig; the furnaces, heat exchangers, reboiler, and condenser have a higher pressure, between 50 and 150 psig.

The third parameter is the design factor (F_d), it depends on the equipment configuration. The values of the design factor for the different equipment are reported in Table 5.

Table 5 – Guthrie's Formula design factor (F_d).

Unit	Value	Features
Compressor	1.0	Centrifugal motor
Furnace	1.0	Process heater
Heater	0.8	Fixed tube sheet
Reboiler	1.35	Kettle reboiler
Condenser	0.8	Fixed tube sheet

3.1.1 NPV fixed capital investment

Capital investment is the total amount of money necessary to supply the plant and manufacturing facilities plus the amount of money required as working capital for operation of the facilities. As aforementioned the evaluation of the equipment purchase and installation cost would be enough to evaluate the fixed costs if just the Conceptual Design and the Dynamic Conceptual Design were taken into account. Nevertheless, this manuscript considers also other indicators as the Net Present Value and its dynamic version, thus the evaluation of the fixed expenses is more complicated. As reported in paragraph 1.3.1, the FCI is made of different items divided in direct and indirect costs.

The direct costs are those directly related to plant erection and are composed of several contributions:

- Purchase and Installation of the Equipment, the basis of several predesign methods such as CD, they represent respectively 15-40% and 6-14% of the fixed capital investment;

- Instrumentation and Controls, represent 2-6% of the fixed capital investment;

- Piping, which covers labor, valves, fittings, pipe, supports, and other items involved in the complete erection of all piping used in the plant, the percentage of the installed pipe line is 3-20% of the fixed capital investment;

- Electrical Installations, which consists primarily of installation labor and materials for power and lighting, with building-service lighting usually included, in ordinary chemical plants, electricals and their installations cost is 2-10% of the fixed capital investment;

- Buildings, including services consists of expenses for labor, materials, and supplies involved in the erection of all buildings connected with the plant, also the cost of heating, lighting, ventilation, and similar building services are included, the percentage is 3-18% of the fixed capital investment;

- Yard Improvements, includes the cost for fencing, grading, roads, sidewalks, railroad sidings, landscaping, and similar items, cost for chemical plants is approximately 2-5% of the fixed capital investment.

- Service Facilities, consists in the utilities for supplying steam, water, power, compressed air, fuel, waste disposal, fire protection, and miscellaneous service items, such as shop, first aid, and cafeteria equipment and facilities, it represents 8-20% of the fixed capital investment;

- Land, includes also the accompanying surveys and fees depends on the location of the property, as a rough average, land costs for industrial plants is 1-2% of the total capital investment.

The remaining part of the fixed capital investment is constituted by the indirect costs composed of:

- Engineering and Supervision, for construction design and engineering, drafting, purchasing, accounting, construction and cost engineering, travel, reproductions, communications, and home office expense including overhead constituting the capital investment for engineering and supervision, 4-21% of the fixed capital investment;

- Construction Expense, includes construction or field expense temporary construction and operation, construction tools and rentals, home office personnel located at the construction site, construction payroll, travel and living, taxes and insurance, and other construction overhead, it is 4-16% of the fixed capital investment;

- Contractor’s Fee, varies for different situations, but it can be estimated to be about 2-6% of the fixed capital investment;

- Contingencies, is usually included in an estimate of capital investment to compensate for unpredictable events, such as storms, floods, strikes, price changes, small design changes, errors in estimation, and other unforeseen expenses, is 5-15% of the fixed capital investment.

In order to proceed with the evaluation of the fixed capital investment it is advisable to choose an intermediate value between the upper and the lower limit of the percentage shown before, by considering that the styrene plant has a medium productivity, and the location of the plant is set to be in the north of Italy.

According to the amount of detailed information available and the accuracy desired, several methods can be employed to evaluate the capital investment. The method chosen in this manuscript calls for the evaluation of the delivered-equipment cost. The other items included in the total direct plant cost are then estimated as percentages of the delivered-equipment cost. The additional components of the capital investment are based on average percentages of the total capital investment. The value of the FCI is estimated through the following equation:

$$FCI = \sum_{i=1}^{Nequipment} (CostE_i) * (1 + DirectCosts + IndirectCosts) * (1 + Others) \tag{31}$$

Where the direct costs are constituted by instrumentation, piping, electrical, buildings, yard improvement, service facilities, and land; the indirect cost are constituted by engineering, supervising, and construction; and others are constituted by contractor’s fee and contingency. All the factors used to evaluate the FCI are summarized in Table 6.

Table 6 – Selected Fixed Cost Factors.

Factors	Value
Instrumentation	0.28
Piping	0.31
Electrical	0.1
Buildings	0.22
Yard Improvements	0.10
Service Facilities	0.55
Land	0.6
Engineering and Supervision	0.32
Construction Expenses	0.34
Contractors Fee	0.05
Contingency	0.1

In the evaluation on the NPV and its dynamic version the FCI is not the ultimate step for the evaluation of the fixed expenses, the working capital has to be taken into account. The working capital is the amount of money needed for the operation of the plant. The sum of the fixed-capital investment and the working capital is termed as the total capital investment.

$$TCI = \frac{FCI}{1 - 0.15} \tag{3. 1}$$

3.2 Operative cost evaluation

Evaluation of the necessary capital investment is only a piece of a complete cost estimation. Another equally important part is the calculation of costs for operating the plant and selling the products. As aforementioned, in order to estimate the operative costs, the starting point is the calculation of the raw material costs. This procedure has an additional difficulty compared to the previous calculations, since some of the indicators used in this manuscript include variation of prices over time. Whilst the costs of the equipment can be considered fixed throughout the plant life, the cost of the raw material is characterized by strong variations even in a small period of time, due to the market fluctuations. Therefore, to calculate the cost of raw materials, it is not possible to determine a unique value, but a number of values obtained according to the established temporal characteristics, such as the plant life and the time span. In this manuscript, the plant life has been set at 10 years and the prices of raw materials are evaluated once every month.

In a styrene plant, several raw material and utilities are used. In order to run a feasibility study of a styrene plant, the price of benzene, toluene, ethylbenzene, styrene, steam and electricity are taken into account.

Crude Oil

It is worth underlining that the price of many of these components is strongly related to price of crude oil, which vary according to the market trend shown in Figure 7. The price of the Crude Oil has been taken from the Italian website *Il Sole 24 Ore – Finanza e Mercati.*

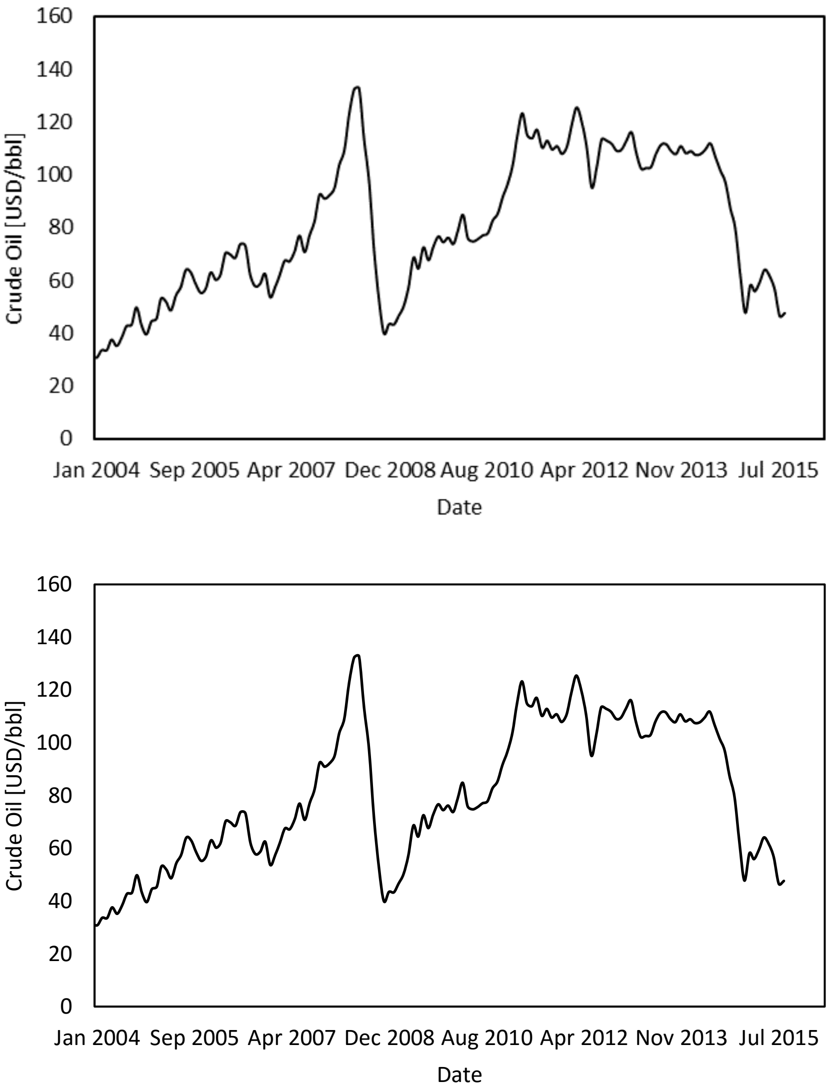


Figure 7 – Crude Oil prices [USD/kmol] over a time period from January 2004 to July 2015.

Benzene, Toluene, and Styrene

Considering a time period going from 2004 to 2015, the price of all products, by-products, reactants, and utilities has been studied in order to point out the importance of the price variability. The price of benzene, toluene and styrene has been taken from the major databases (HIS, ICIS, Orbichem…) and are shown respectively in Figure 8, Figure 9, and Figure 10.

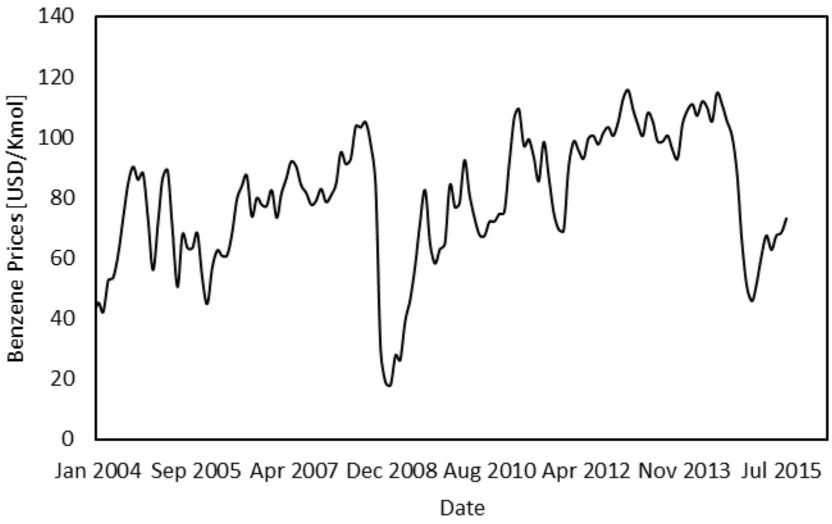


Figure 8 – Benzene market prices [USD/kmol] over a time period from January 2004 to July 2015.

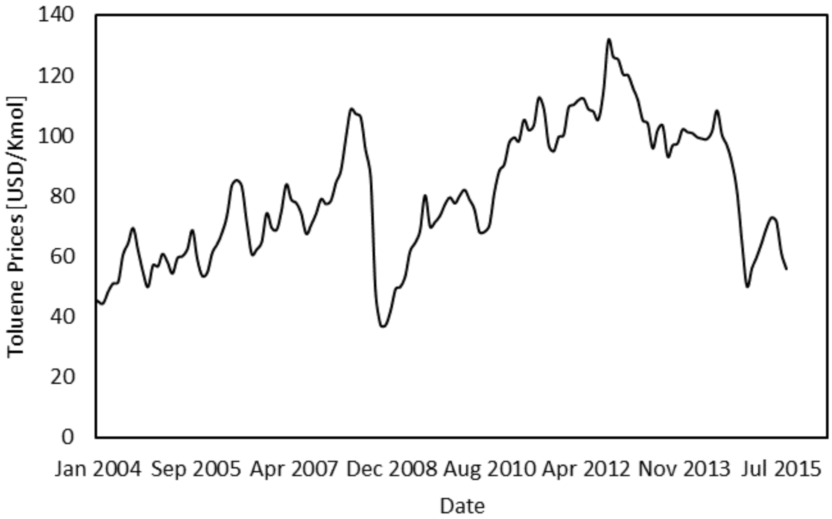


Figure 9 – Toluene prices [USD/kmol] over a time period from January 2004 to July 2015.

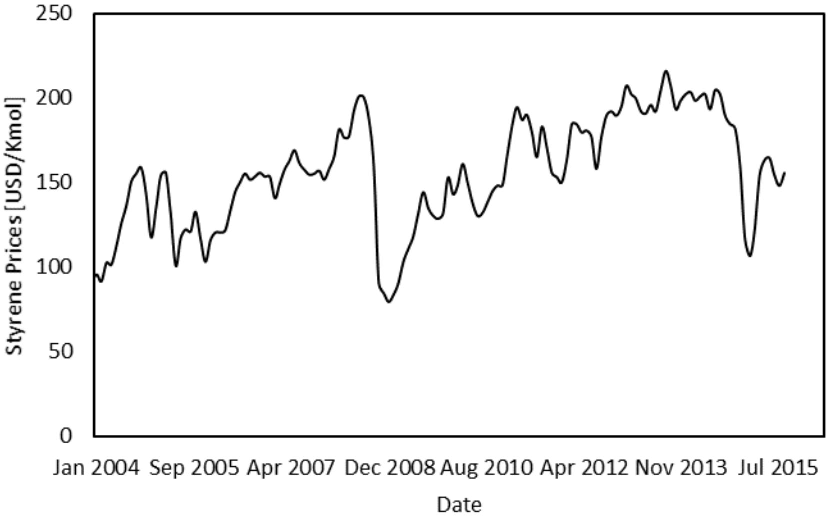


Figure 10 – Styrene prices [USD/kmol] over a time period from January 2004 to July 2015.

Ethylbenzene

Unfortunately, it was not possible to find all the prices required for any time period, and, as in the case of ethylbenzene quotation, the prices must be estimated through some correlations. The correlation used for ethylbenzene links the price of the latter to the price of ethylene and benzene, the main products used for its production.

$$Et - B\ Price = Benzene\ Price + Ethylene\ Price + \ 8{,}6697 \qquad (32)$$

Since the production of styrene itself provides low profitability, it is reasonable to assume that the production of benzene and ethylene is carried out by the same company, considering that one of the highest expenses of a chemical plant is given by raw materials. This allows getting the latter at a lower price with respect to the market one. In particular, as done for the ethylbenzene, is useful to analyze the production cost of the two chemicals. This value varies considering different factors such as raw materials involved in their production, location of the plant, reactor type and reactions involved.

As far as ethylene is concerned, it can be produced mostly from steam cracking using naphtha or ethane as raw material. The first one is generally used in Europe since ethane is in short supply, while the second is generally used is in the USA. Considering that both naphtha and ethane come from crude oil, ethylene production cost can be related to the price of crude oil. Figure 11 illustrates the production cost of ethylene generated for a model of a medium sized naphtha cracker against the ethylene market price by switching the crude oil price.

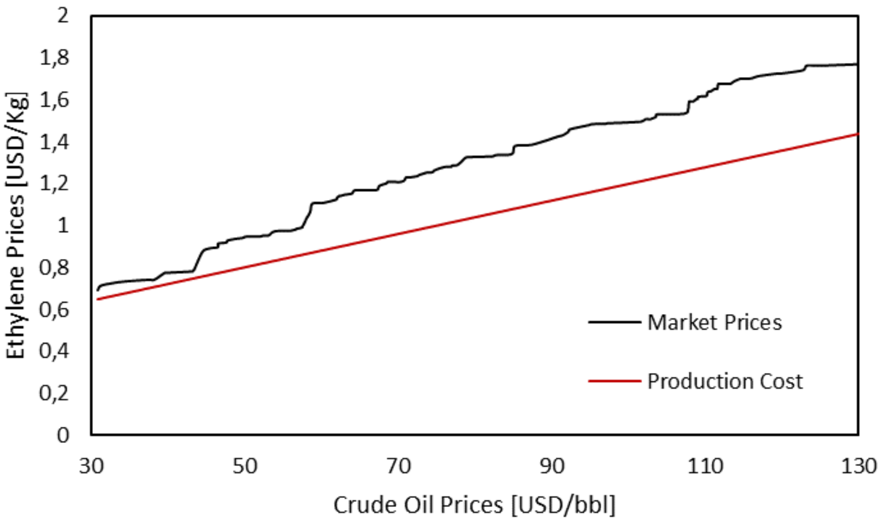


Figure 11 – Production cost of ethylene against the ethylene market price.

Clearly this is an idealized representation, since the slope of the line depend on several variables, but a single line will serve the purposes needed. The production cost varies linearly with the crude oil price. By comparing these costs to the market ones, is possible to assume that the raw materials cost is 10% to 30 % less than the market value. For sake of simplicity in this manuscript an average percentage of 20% has been chosen.

Benzene can be produced through different processes such as catalytic reforming, hydrodealchilation of toluene, pyrolysis of by-products formed in the production of olefins by steam cracking of liquid feeds such as naphtha, and steam cracking of naphtha. As aforementioned the market prices of benzene depend on different factors such as the crude oil quality, the extraction site, the easiness of the latter operation, the production process, the local taxation rate, and thus it is not easy to estimate the difference between the production costs and the market prices. Nevertheless, a literature research has shown that the biggest part of the difference ranges is between 15% and 30%. For sake of simplicity in this manuscript an average percentage of 20% has been chosen. By fixing the price of styrene and other commodities, and lowering the price of ethylbenzene, the gains become visibly higher because the revenues are still the same but the expenses are lower, due to the lower price of ethylbenzene (gains are calculated as the difference between revenues and expenses). Since the aim is to maximize the earnings, it was decided to perform an ethylbenzene cost analysis, in order to obtain a lower price and, consequently, higher earnings. Thus, it was decided to produce benzene and ethylene internally in company instead of purchasing them form third parts, in order to lower the quotations of the two raw materials from the market price to the production cost. Consequently, the price of ethylbenzene obtained by using ethylene and benzene as precursors is reduced. It is worth observing that market prices are always raised with the respect to the production cost. Thus, as a result of bibliographic research, it was decided to reduce the value of both benzene and ethylene prices in equation (32) by 20%, in order to obtain a lower price of ethylbenzene and maximize the earnings.

The prices of ethylene and ethylbenzene are respectively shown in Figure 12 and Figure 13.

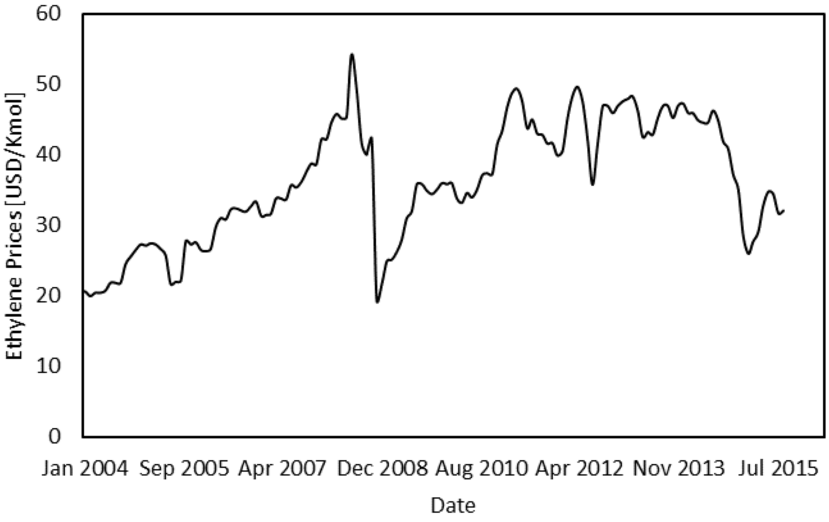


Figure 12 – Ethylene market prices [USD/kmol] over a time period from January 2004 to July 2015.

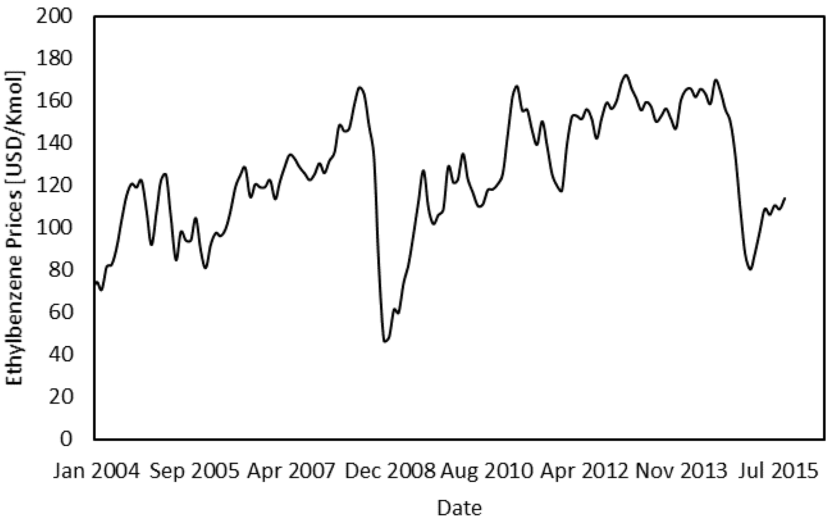


Figure 13 – Ethylbenzene prices [USD/kmol] over a time period from January 2004 to July 2015.

BTZ Oil

For the fuel oil utility, in order to produce steam a low Sulphur content fuel oil has been chosen. This is known as BTZ ("Basso Tenore di Zolfo" in Italian) and it has a lower heat of combustion of 9600 kcal/kg (ENI S.p.A. (2015)). The price of the utilities as BTZ Fuel oil has been taken from the Italian website *Ministero dello sviluppo e dell'economia,* and the the source for the euros/dollars ratio is Italian website *Il Sole 24 Ore – Finanza e Mercati*. The price of BTZ Oil is shown in Figure 14.

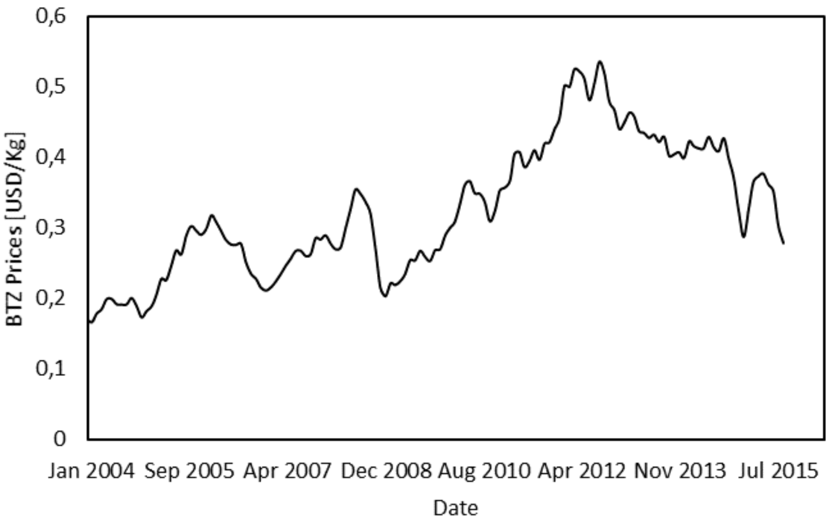


Figure 14 – BTZ Oil prices [USD/kmol] over a time period from 2004 to 2015.

Water

Water price estimation is crucial because is used has a cooler for the heat exchanger and for all the condensers. Water quotations are not easy to be estimated, considering that the price of water changes from country to country and often from region to region. It is advisable to set water price has at 0.048 USD/m3 as proposed by Ulrich and Vasudevan (2006).

Electric Energy

The last utilities considered for the styrene production plant is the electric energy, which has been considered due to the compressor consumption. Electric energy price has been estimated by the model proposed in Manca (2016) based on Italian prices of electric energy. It is worth underlining that the electric energy prices are governed by frequent changes. The prices of electricity have a particular daily and seasonal trend: there are differences between working days and holidays and also among seasons. There are also some stochastic oscillations which cannot be prevented due to their random variations. The price of electric energy has a strong dependence on the price of the crude oil quotations with a three months delay. The model proposed is the following one.

$$EE\ Price = a_j + b_j * P_{CO,i-t} + c_j * \sin(\frac{2\pi i}{T} + \varphi_j) \tag{33}$$

Where i is the i-th week, j is the time band (there are four bands in a day: morning, afternoon, evening, night), a is a reference value of EE price, b is a coefficient for the dependency of EE price from CO, td is time delay, c is parameter of the periodic component, T is period of the sinewave function (the period can be compared to a season), φ is the phase of the sinewave function. In order to be consistent with the other commodities prices, the weekly quotation has to be turned in monthly quotation assuming constant prices during the weeks of the same month. The resulting trend is shown in Figure 15.

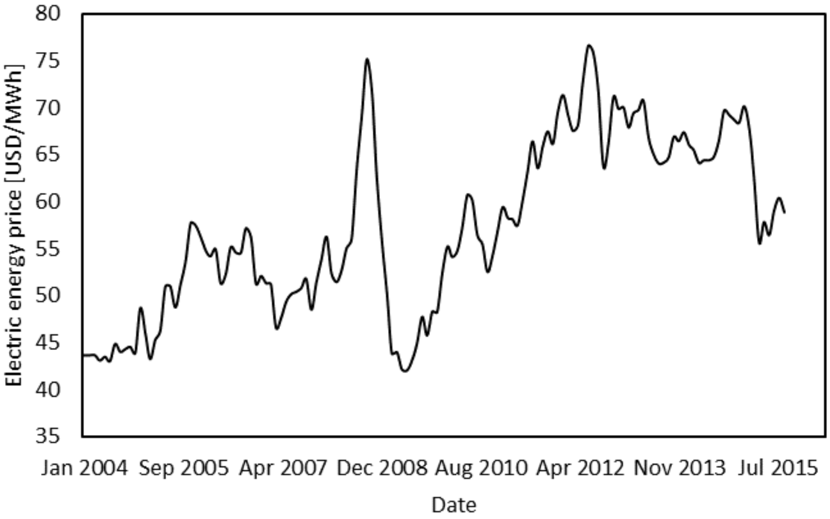


Figure 15 – Electric energy prices [USD/MWh] over a time period from 2004 to 2015.

Once the prices of products, by-products, reagents and utilities have been defined, the evaluation of the operative costs for CD and DCD is simply performed as the difference between the gains generated by the sale or the internal use of products and by-products, and the resulting costs from the purchase of reagents and utilities. The only difference between the two indicators is that the CD uses fixed prices, which are kept constant throughout the plant life, while the DCD changes its prices according to the market variations presented above.

3.2.1 NPV total product cost

As aforementioned the evaluation of the raw materials cost would be enough to evaluate the operative cost if just the Conceptual Design and the Dynamic Conceptual Design were taken into account. However, other indicators such as the Net Present Value and its dynamic version call for a more in-depth investigation, which includes the biggest part of the expenses characterizing the plant life. The costs for operating the plant and selling the products can be gathered under the name of total product cost. This is divided in two different categories: the first one is under the heading of manufacturing costs and the second one under the name of general expenses.

3.2.1.1 Manufacturing Cost

The manufacturing costs represent all the expenses connected with the manufacturing operation of a process. They are divided into direct production costs, fixed charges, and plant-overhead cost.

Direct production costs include expenses directly associated with the manufacturing activities and can be divided into different categories, as shown in Table 7.

Table 7 – Direct production costs range and description.

Item	Range	Inclusions
Raw Materials	30-60 % TPC	Freight and Transportation
Operating Labor	15% TPC	Skilled and Unskilled Labor
Supervisory and Clerical Labor	15% Operating Labor	
Maintenance and Repairs	6% FCI	
Operating Supplies	15% Maintenance and Repairs	
Power and Utilities	10-20% TPC	Steam, Electricity, Water, Air, Natural Gas, and Fuel Oil.
Patents and Royalties	0-6% TPC	
Catalysts and Solvents	-	

It is worth underlining that not all the processes need patents and that the definition of a range for the catalyst and solvent is unlikely predictable. The styrene production process does not use any kind of catalyst.

The second item of the TPC is represented by the fixed charges, which are expenses that remain practically constant throughout the plant life and do not vary with the production rate. They include:

- Depreciation is a measure of the reduction in value of all the plant physical assets, due to several reasons such as deterioration, technological advances, change in demand for the property employment, market variation, and other factors. The total value of the depreciation is calculated as the difference between the initial and the final value of the properties, divided by the service life that is the amount of time for which an equipment is theoretically designed without breaking. It is worth noticing that the final appraisal and the depreciation duration it is unlikely known, even though these costs are distributed along the plant assets life. Consequently, these values are to be estimated at the time the plant is ready for the initial use. In this manuscript, for the sake of simplicity, the period of depreciation for each asset will coincide with the life of the plant itself and the final value, also known as savage value, is considered to be zero. There are several methods for the depreciation accounting, among these there are two big classes according to the consideration to interest costs. In this manuscript, the straight-line strategy has been used, it does not take into account the interest cost and the value of the property decreases linearly with time. Under this model, equal amounts of money are charged for depreciation every year throughout the entire service life of the properties. The annual depreciation cost may be expressed in equation form as follows:

$$D = \frac{V - SV}{n} \tag{34}$$

Where V represents the original value of the property at start of the service-life period, completely installed and ready for use in USD; SV is the salvage value of property at end of service life; and N is the service life of the equipment.

Since is assumed that the equipment will be dismissed after the service life, depreciation value is calculated without considering the salvage value as follows:

$$D = \frac{V}{n} \tag{35}$$

A typical example of a straight-line depreciation is shown in Figure 16.

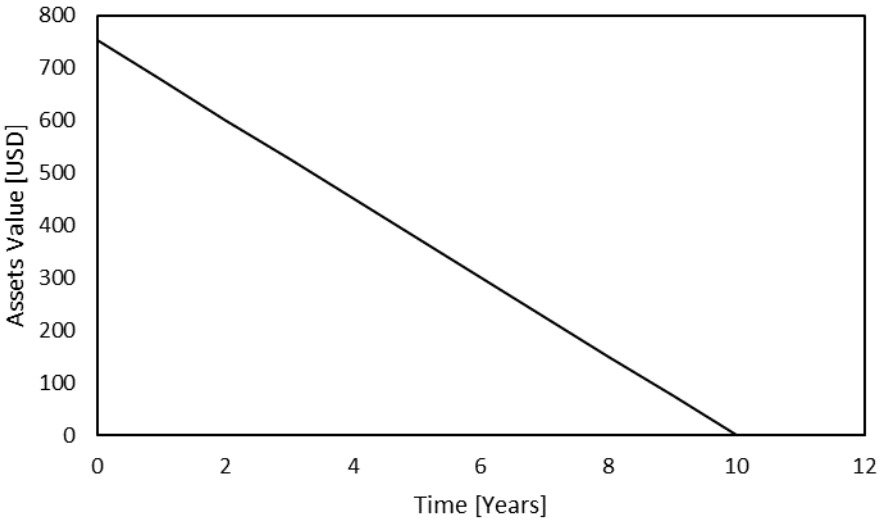


Figure 16 – Example of a straight-line depreciation on a plant life of 10 years.

- Local taxes, this item wildly varies with the location of the plant. Usually, it is 1-2% of the fixed capital investment. The taxation of companies in Italy is differentiated according to the legal nature of the companies: individual companies and companies of persons firstly, capital companies secondly. The first are subjected to Irpef while the latter are subjected to Ires. Whatever the legal nature of the business, taxes are applied to the total income, which is the net income earned during the tax period. The basic steps for Ires evaluation are two: the determination of the tax base and the application of the rate. For the sake of simplicity, the taxation rate has been fixed at 30%.

- Insurance strongly depends on the process type, but as a rough approximation, the annual value of the insurance can be estimated as 1% of the fixed capital investment.

Plant overhead cost does not vary along time and includes basically all the other items especially related to the employee's insurance, medical expenses, vacation, recreation facilities, benefits packaging, laboratory control, property protection, storage, and many others.

3.2.1.2 General Expenses

In addition to the manufacturing costs, there are also the general expenses classified as administrative expenses, distribution and marketing expenses, research and development expenses, financing expenses, and gross-earnings expenses (a direct function of the gross earnings).

In this manuscript, it has been decided to asses TPC by dividing the cost of raw materials for 0.6. This means that the raw materials represent the 60% of the TPC value, which is evaluated as follows:

$$TPC = \frac{Raw\ Materials}{0.6} \tag{36}$$

It is worth underlining that if the cost of the reactants is very high, raw materials represent a very large part of the operative costs of a chemical plant. Since Ethylbenzene is a very expensive reactant, considering that it is obtained from benzene and ethylene, a factor equal to 0.6, which is the highest eligible value, has been chosen, in order to take into account the high cost of ethylbenzene in the assessment of the TPC.

3.3 Discounted Cash Flow evaluation

Once the TPC, the taxation rate, and the depreciation have been evaluated, it is possible to proceed with definition of the Cash Flow as shown in paragraph 1.2.3. Nevertheless, the NPV and its dynamic version use the discounted cash flow which is defined as follows:

$$DCF = \sum_{i=1}^{n} \frac{CF_i}{(1 + WACC)^i} \tag{37}$$

As aforementioned, the companies calculate the values of the WACC as shown in paragraph 1.4.3.1, with a quarter frequency. However, not all the companies share this bit of information publicly. In order to go ahead with the evaluation of the DCF, WACC has to be set. Since this manuscript is about a feasibility study of a chemical plant, it is advisable to select the major chemical industry and use the WACC shared by these companies. Figure 17 shows WACC values for both BASF and Total.

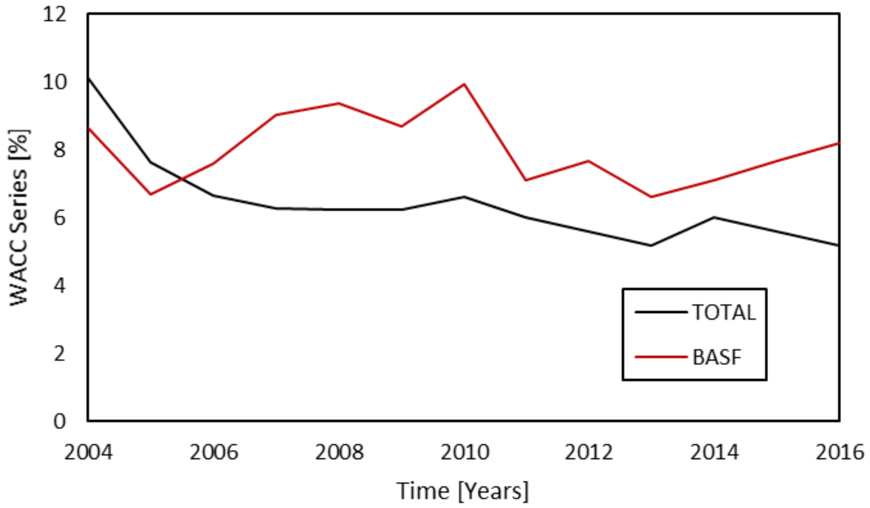


Figure 17 – BASF and Total WACC value from 2004 to 2016.

It is possible to observe that all the WACC values fall between 5% and 10%. In addition, throughout the years the variations are minimal. Several other companies have the same WACC trend, it is worth underlining that these values have been published by the companies on the Italian website *GuruFocus (https://www.gurufocus.com).* Considering that most of the companies has similar values of WACC and the range of existence of these values is small for all these companies, for this manuscript, the selection of a company's data rather than another is arbitrary. This will be confirmed by further investigations on the sensitivity analysis. Once the selected WACC is chosen, it is possible to proceed with the calculation of the discounted cash flow, as reported above. Figure 18 shows the cash flow for two different plant configurations, the first one is the one giving the maximum earnings, the second one is the one gives the minimum earning at the end of the plant life, corresponding to the degrees of freedom shown in Table 8.

Table 8 – Values of the different degree of freedom for the configurations with the maximum and minimum earning.

Degree of freedom	Maximum Earning	Minimum Earning
LP flowrate [kmol/h]	2000	2000
Reactor Temperature [k]	535	565
Reactor Length [m]	2.5	8.5
Splitting Factor [-]	0.3	0.7

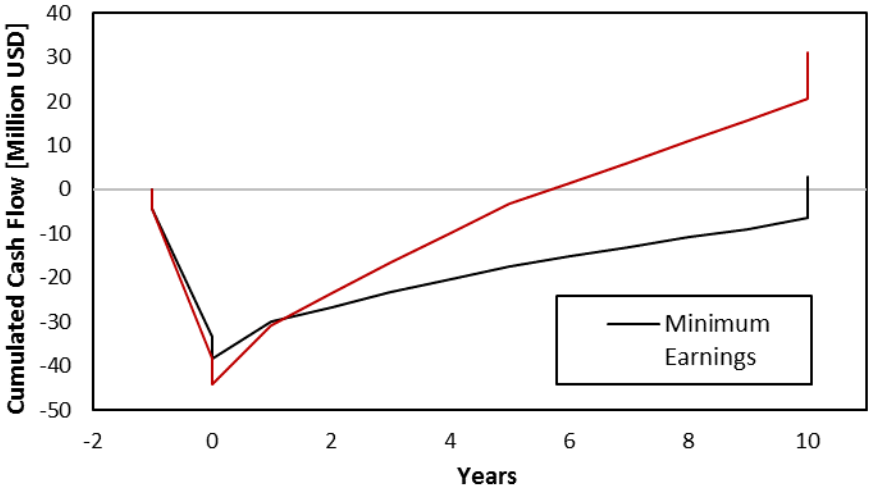


Figure 18 – Discounted cash flow [million USD] for the maximum and minimum earnings configuration.

To obtain this graph a cash flow analysis was carried on. This plot starts at the year -1 since the year 0 is the startup of the plant activity. Here an amount of money called working capital must be subtracted in order to ensure the initial operations consisting in the first batch of raw materials and several other activities. At the end of the plant service life, supposing to sell the land, is possible to add to the revenues the amount of money subtracted at the year -1 to buy the land. It is also possible to add the working capital and the scrap value of the remaining pieces of equipment.

Chapter 4

Results analysis and discussion

This chapter analyzes and discusses the results produced by the different economic indicators. It starts from the evaluation of the dynamic conceptual design and it proceeds with the assessment of the dynamic NPV. A comparison between these indicators follows and investigates both qualitative and quantitative similarities and differences. The end of the chapter covers the conclusions on which is the most reliable indicator and reports a sensitivity analysis of the dynamic NPV.

As aforementioned, aim of this manuscript is first to evaluate the results given by the different indicators and calculate the economic revenues obtainable throughout the plant life. The second goal of this work is to understand if the Dynamic NPV is worth the higher computational complexity. Eventually, we identify if there is any a relationship between the DCD and DNPV not only from a qualitative point of view, but also from a quantitative one. The data used for this work are obtained connecting at the software level UNISIM DESIGN and MATLAB. This connection is well explained in Buscemi Pagnoncelli (2016). UNISIM DESIGN simulates the styrene plant and allows retrieving plant details such as equipment sizes and flowrates. MATLAB is used to elaborate the economic indicators that will be shown in the following. A number of 39889 plant configurations has been supplied to UNISIM of which only 32144 converged. Since processing all this information takes a quite long CPU time, the single simulations are performed by adopting the so-called “snake grid” algorithm, which allows reducing the computation time needed by the software as shown in Buscemi Pagnoncelli (2016).

4.1 Static indicators: CD and NPV

It has been determined that the results provided by the Conceptual Design are inadequate for a complete and reliable feasibility study. Indeed, CD considers fixed prices of commodities and neglects the significant market price fluctuations as discussed in Paragraph 3.2. In addition, CD does not even consider a number of factors that NPV accounts for. Due to these two shortcomings, the results produced by CD estimation are inadequate for a rigorous economic assessment of an industrial project. It is worth underlining that also the NPV, even though it considers more factors than CD in the plant expenses, faces the same problem of fixed prices. Thus, the results discussed in this chapter are not focused on the static indicators, but on the dynamic ones, which consider the fluctuations of the market prices. To better explain the problem of fixed prices, Table 9 shows the prices of raw materials and utilities in November 2008 and September 2013.

Table 9 – Raw materials and utilities prices of November 2008 and September 2013.

Raw Material and Utilities	Nov 2008 [USD/kmol]	Sep 2013 [USD/kmol]
Crude Oil	52.45 [USD/barrel]	111.6 [USD/barrel]
Benzene	29.83	100.60
Toluene	37.32	93.06
Styrene	90.26	215.84
Ethylbenzene	80.73	147.56
Ethylene	42.23	46.96
BTZ Oil	0.27	0.43
Electricity	71.7509 [USD/MWh]	64.1497 [USD/MWh]

It is worth considering November 2008 and September 2013, since the first one provides the lowest revenues, according to the difference between product price and raw material/utility costs, and the second one has the highest revenues of the all life plant period, January 2004 to December 2013 (120 months). This choice is made because it is important to emphasize the huge difference in the quotations according to the selected period. The results based on the November 2008 and September 2013 prices are shown in Table 10 and Table 11.

Table 10 – Configurations results based on November 2008 quotations.

	EP4 cumulated	NPV
Number of positive configurations	32144	0
Number of negative configurations	0	32144
Maximum value [million USD]	8.745e7	-1.621e7
Minimum value [million USD]	1.821e7	-5.094e7

Table 11 – Configurations results based on September 2013 quotations.

	EP4 cumulated	NPV
Number of positive configurations	32144	32144
Number of negative configurations	0	0
Maximum value [million USD]	4.0255e8	7.8073e7
Minimum value [million USD]	2.4408e8	1.6539e7

As shown by the results above it is not advisable to use a static indicator due to the strong dependence on the market prices. By changing the reference month, the variability is too high to consider reliable such an analysis.

4.2 Dynamic indicators estimation and comparison

4.2.1 Dynamic Conceptual Design and DEP4 evaluation

As shown in equation (5), using DCD calls for the evaluation of cumulated DEP4, which is computed as the economical earnings equal to the difference between revenues and expenses. Where revenues are the income coming from the selling product and by product, and the expenses are represented by the purchasing of raw materials and equipment. It is worth advising that the operative cost, such as the incomes coming from the product and byproduct and the expenses for the raw materials, are spread over the plant life, whilst the equipment purchasing are limited to the construction stage. The evaluation of the commodities cost considers monthly quotations which are a good compromise between accuracy of calculation and complexity of computation. Aim of the DCD assessment applied the past months, is to show which were the plant optimal design variables, which maximize the incomes in the 10-year period (120 months), from January 2004 to December 2013.

Figure 19 shows the first analysis performed and represents the fluctuation of the cumulated DEP4 produced by each configuration. Since the computation follows the snake grid of degrees of freedom, which produces a confused up and down representation, it was decided to expose the same results also in ascending order to better highlight in which range of values the DEP4 lays.

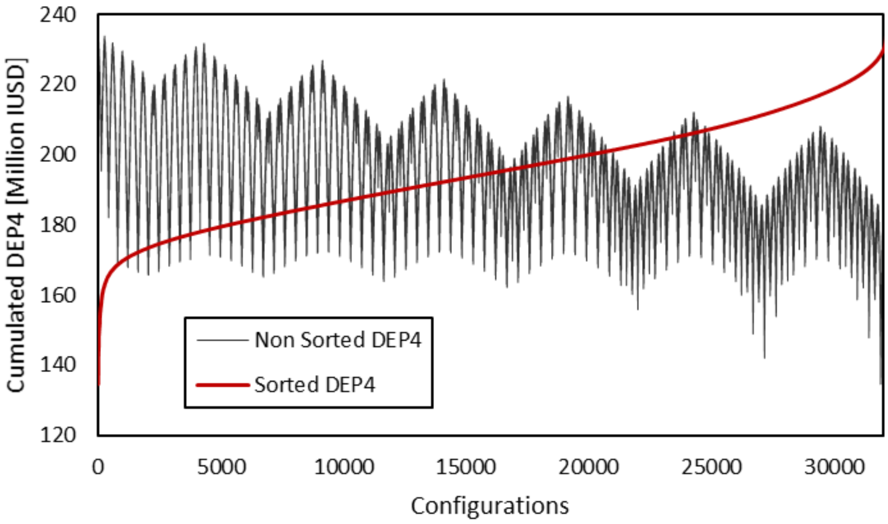


Figure 19 – Sorted and not sorted DEP4 trend for each scenario.

From the evaluation of the DCD it is possible to observe that all the configurations give positive incomes, where the lowest one is about 138 million USD and the highest one is about 238 million USD.

The second analysis represents the DEP4 as a function of a pair of DoFs, whereas the other two are kept constant. This is important in order to understand which kind of relation exists between the economic indicator and the DoFs. In each 3-D plot, the degrees of freedom considered are written on the axes, while the remaining two are kept constant. The fixed value for the DoFs are 0.3 for the Splitting Factor, 2000 kmol/h for the steam flowrate, 535 °C for the reactor inlet temperature, and 2.5 m for the reactor length. The results are shown in Figure 20, Figure 21, Figure 22, and Figure 23.

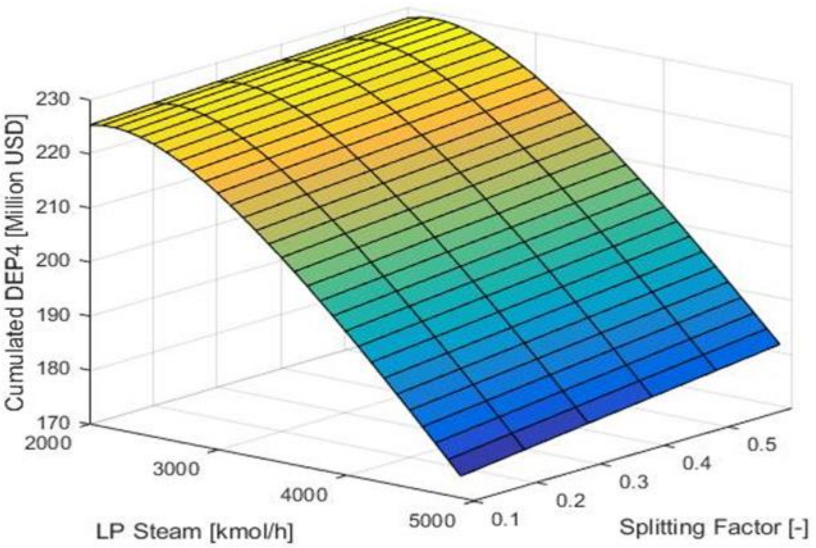


Figure 20 – Cumulated DEP4 value as a function of two degrees of freedom: LP steam flowrate and Splitting Factor.

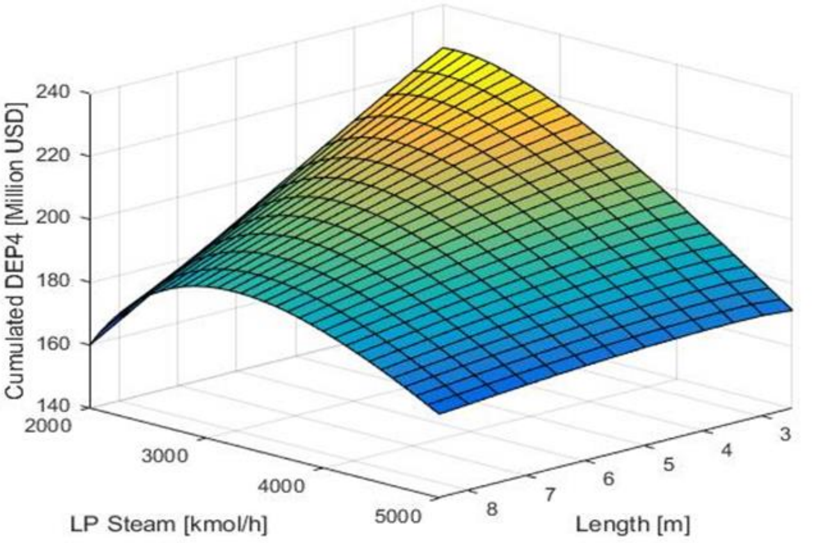


Figure 21 – Cumulated DEP4 value as a function of two degrees of freedom: LP steam flowrate and reactor length.

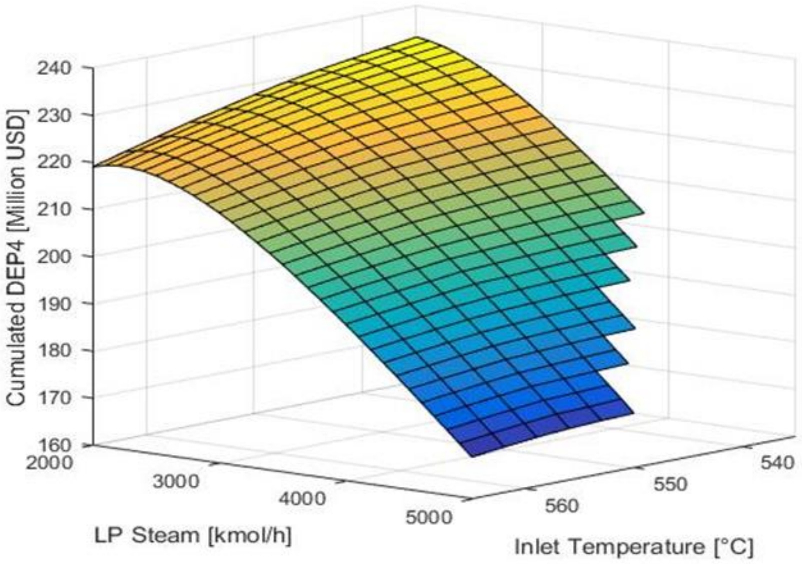


Figure 22 – Cumulated DEP4 value as a function of two degrees of freedom: LP steam flowrate and inlet temperature.

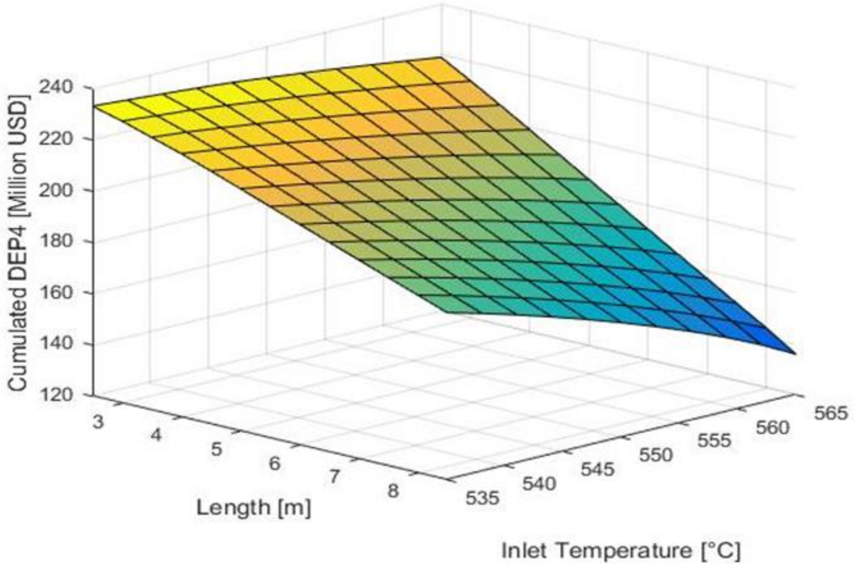


Figure 23 – Cumulated DEP4 value as a function of two degrees of freedom: reactor length and inlet temperature.

These plots show that there is a linear relation between the different variables except when the steam flowrate is considered as an independent variable, in particular for the lowest values where a maximum point is shown, highlighting the strong importance of this variable for the optimum calculation.

4.2.2 Dynamic Net Present Value

In order to perform a consistent comparison between DCD and DNPV, the same analysis shown in the previous paragraph is repeated for the Dynamic Net Present Value. Aim of this analysis is to show which are the plant optimal design variables, which maximize the incomes in the 10-year period (120 months), from January 2004 to December 2013.

Figure 24 shows the first evaluation performed and represents the variation of DNPV for each scenario, sorted in ascending order and as a function of the snake grid of degrees of freedom.

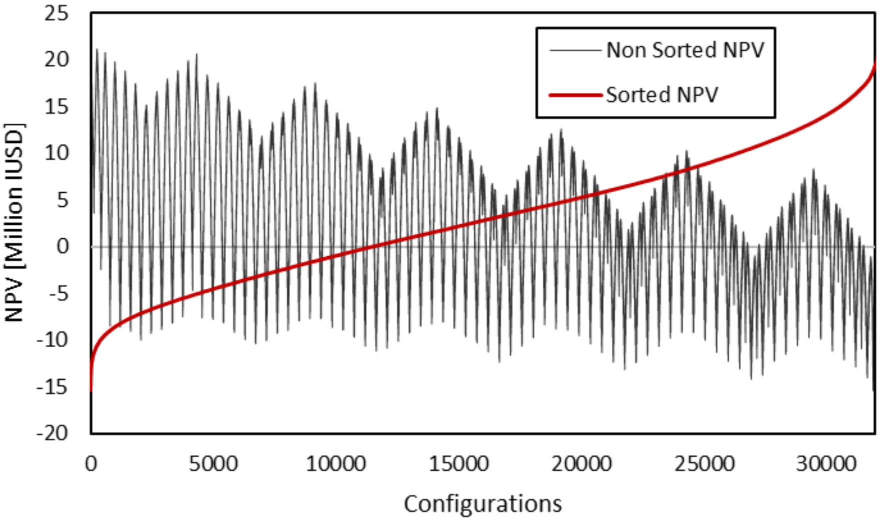


Figure 24 – Sorted and not sorted DNPV trend for each scenario.

It is possible to observe that not all the configurations give positive incomes, and a not negligible number of negative values is recorded. This underlines the great difference between the two indicators. In particular, the lowest value of the NPV is -15 million USD and the highest one is about 25 million USD.

In addition, Figure 25, Figure 26, Figure 27 and Figure 28show the 3-D plots, that represent the dynamic NPV as a function of two DoFs, while the remaining two are kept constant. The same values of the assigned DoFs used for the cumulated DEP4 are used for the dynamic NPV.

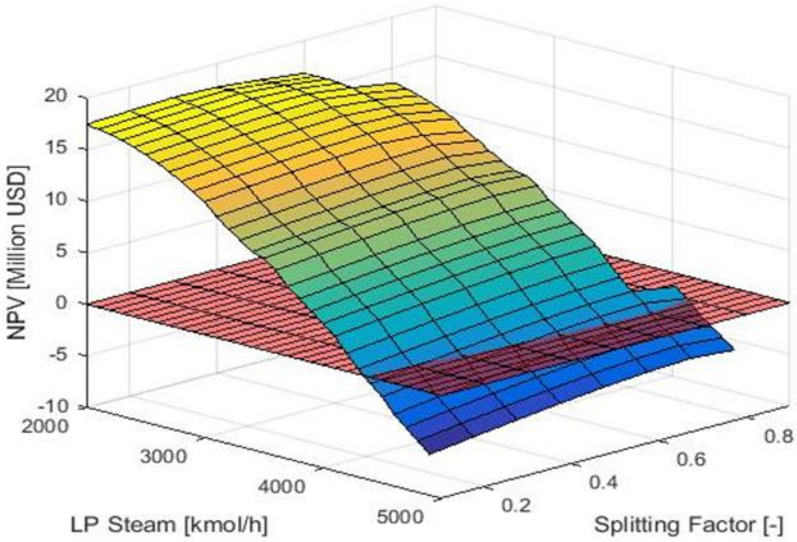


Figure 25 – Dynamic value as a function of two degrees of freedom: LP steam flowrate and Splitting Factor.

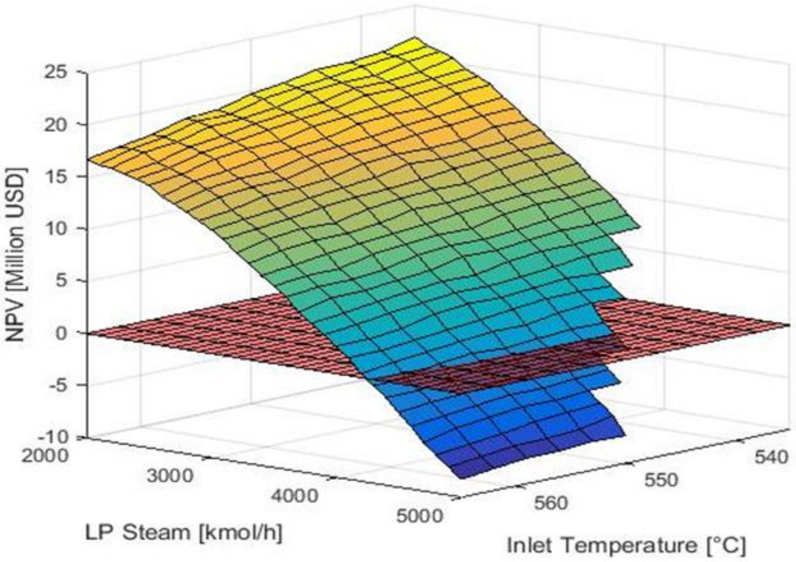


Figure 26 – Dynamic value as a function of two degrees of freedom: LP steam flowrate and inlet temperature.

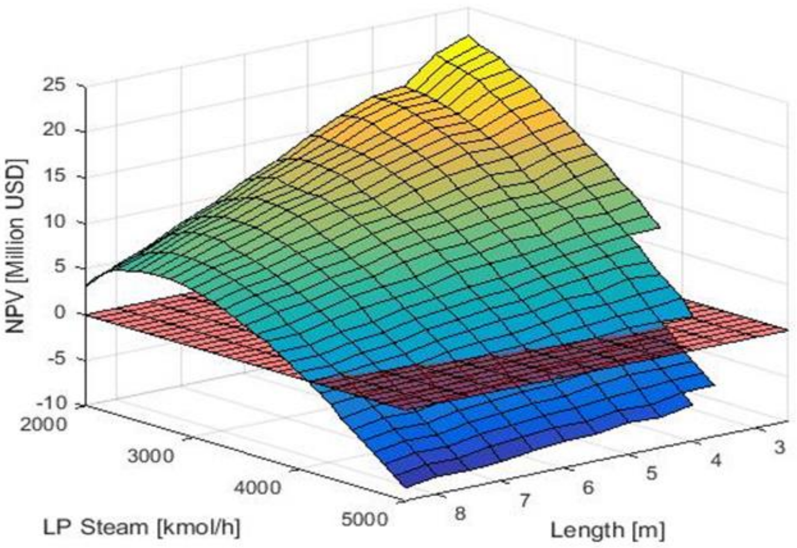


Figure 27 – Dynamic value as a function of two degrees of freedom: LP steam flowrate and reactor length.

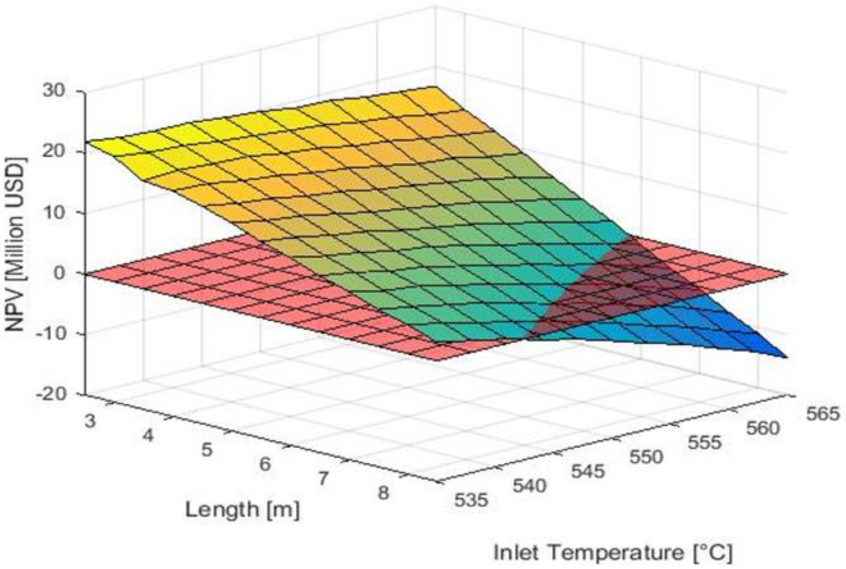


Figure 28 – Dynamic value as a function of two degrees of freedom: reactor length and inlet temperature.

It is worth underlining that the red plane is used to highlight the intersection of the curve with the zero values of the NPV. The 3D plots comparison between the cumulated DEP4 and the DNPV allows concluding that the same conclusions about the maximum point are also valid for the dynamic NPV. Only the shape of the curves is not completely coincident, since the NPV is not smooth as the other. This is due to the total capital investment, which has a higher impact on the indicator with respect to CAPEX.

4.2.3 A comparison between the DCD and the DNPV

As shown in paragraphs 4.3.1 and 4.3.2, there are substantial differences between DCD and DNPV. The first major difference is a quantitative one, as the numerical evaluation of the two indicators gives very different results. On one hand DCD always returns positive incomes (in the order of 100 million USD), on the other hand dynamic NPV does not always return positive incomes. Furthermore, all the results are in the order of tens million USD, an order of magnitude less than DCD. All the results discussed above are reported in Table 12.

Table 12 – Configurations results for cumulated DEP4 and DNPV.

Configuration	cumulated DEP4	DNPV
Number of positive configurations	32144	20600
Number of negative configurations	0	11544
Maximum value [million USD]	2.35E+08	2.18645e7
Minimum value [million USD]	1.35E+08	-1.5370e7

A statistical analysis was performed. Figure 29 and Table 13 show the distributions of the incomes for the DCD and the DNPV configurations.

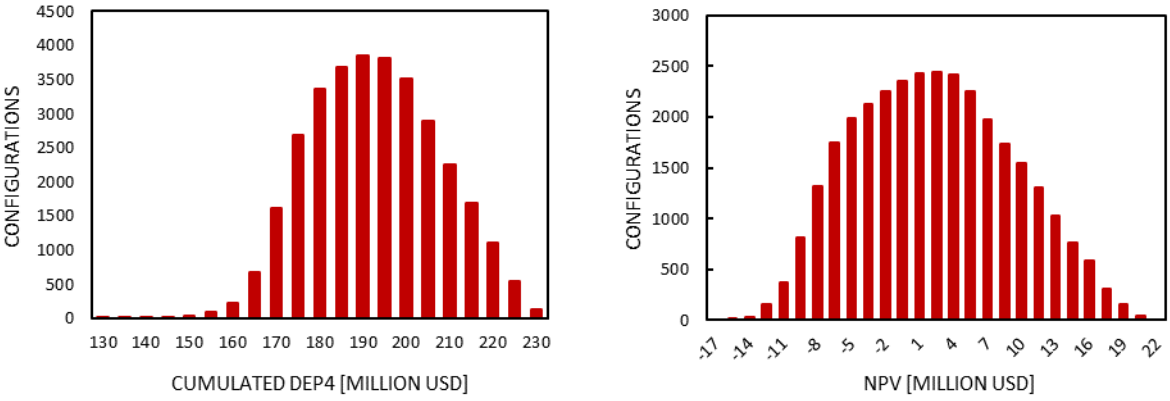


Figure 29 – Configurations income distribution for DCD and DNPV.

Table 13 – Distributions characteristics [USD] for cumulated DEP4 and DNPV.

	cumulated DEP4	DNPV
Average	1.95E+08	3.04E+06
Median	1.947E+08	2.82E+06
Skewness	0.054490071	0.160267
Standard Deviation	7.84	6.34

As for the previous analysis, this study highlights the big difference between the two indicators from a quantitative point of view.

As aforementioned, the goal of this manuscript is to carry out not only a quantitative analysis but also a qualitative one. In particular, the search for the optimum is one of the main tasks f an engineering investigation and, in this manuscript, it does not depend on the numerical differences between DEP4 and NPV, but on how they are computed.Table 14 shows the combination of degrees of freedom that maximize and minimize the incomes depending on the specific indicator.

Table 14 – Maximum and minimum configurations for cumulated DEP4 and DNPV.

	Configuration	SF	LPS Flowrate [kmol/h]	L Reactor [m]	Inlet T [K]
Max DNPV	3	0.3	2000	2.5	535
Min DNPV	39625	0.7	2000	8.5	565
Max DEP4	6	0.6	2000	2.5	535
Min DEP4	39619	0.1	2000	8.5	565

The results in the table emphasize the great diversity of the two indicators, since the optimal set of degrees of freedom is different. This testifies a quite important difference between DCD and dynamic NPV, which cannot be considered interchangeable. The fact that indicators cannot be exchanged with each other is also evidenced by the proportionality analysis shown in Figure 30, calculated as the ratio between DNPV and DEP4 for each configuration.

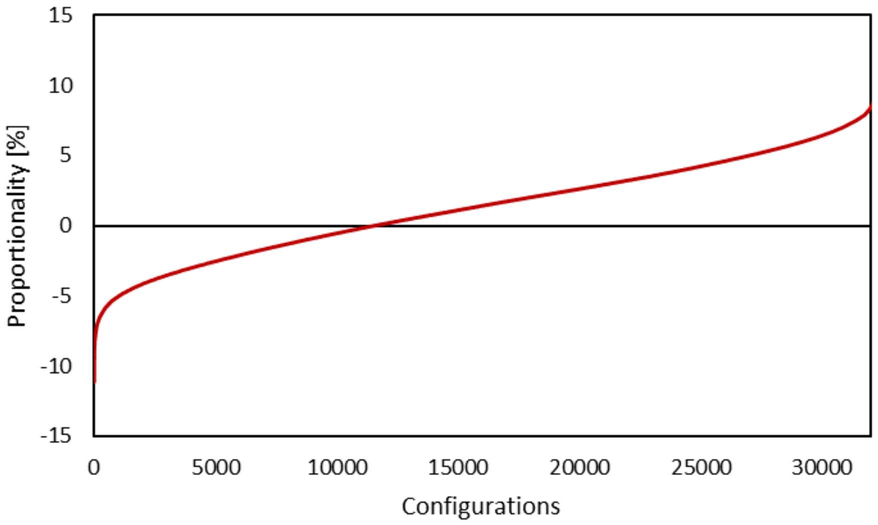


Figure 30 – Proportionality between DNPV and Cumulated DEP4.

The plot shows that the ratio between DEP4 and DNPV does not produce a constant value, with which would easily allow passing from one indicator to the other by a simple numerical operation.

In the face of this analysis, it is possible to state that Dynamic Conceptual Design is a less sophisticated indicator, since it returns too high incomes and a different optimal configuration with the respect to dynamic NPV, a far more complete indicator. It is worth observing that, despite the greater abundance of dynamic NPV details, computational difficulties are almost negligible compared to the goodness of the returned results. As a matter of fact, the computation of DNPV with respect to DCD is rather simple, as the data required for the evaluation of both of them are the same.

From now on, we have therefore decided to concentrate future analysis only on DNPV.

4.3 Dynamic Net Present Value sensitivity analysis

Purpose of this paragraph is to determine which are the most relevant factors that affect the dynamic NPV assessment and how the latter varies by changing one of them. In particular, four different elements have been selected: WACC, TCI, benzene price, and ethylene price. Figure 31 shows the Dynamic Net Present Value sensitivity analysis with respect to the aforementioned factors.

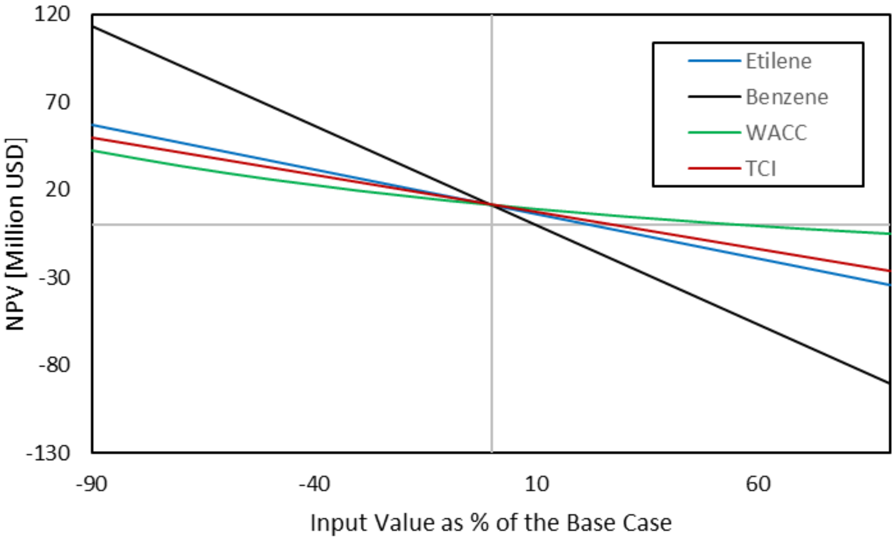


Figure 31 – Sensitivity analysis of WACC, TCI, benzene price, and ethylene price.

The analysis highlights that the most influent factor on the DNPV is first the price of benzene and then the price of ethylene. These results corroborate what was observed in the previous paragraphs about the importance of price fluctuations. If the commodities prices changes, the variation of DNPV is consequently large. Total Product Cost also plays an important role in the assessment of dynamic NPV, and this is due to the fact that fixed costs are a large fraction of the costs needed to build and operate a chemical plant. However, even if this item must be taken into consideration, its influence is not as big as the price of benzene and ethylene. WACC is the only factor that can be neglected, as its variation causes a reduced change in DNPV.

Chapter 5

Predictive Net Present Value

This chapter is an introduction to the difference between the economic and the econometric models. Follows a description of the econometric models used in order to foresee the commodities and utilities quotations. The second part of the chapter is about the forecast of the DNPV scenario and the analysis of the results obtained.

In order to obtain the results discussed in chapter four, price series of the past have been used. Consequently, the prices of utilities and commodities were the real market prices corresponding to the months considered, except for the price of ethylbenzene which was estimated by a correlation between benzene and ethylene quotations. The choice of using price series of the past was essential to achieve a real assessment of DCD and dynamic NPV. However, the purpose of these indicators is not to analyze the past, but rather to investigate the potential gains of a future investment, such as the construction of a chemical plant. In order to do so, it is necessary to rely on data concerning the future rather than the past.

We decided to keep constant all fixed costs and consider variable both commodities and utilities prices. Also, we assumed that all fixed costs are sustained in a short time span from the analysis and thus can be assumed equal to those of present time. Conversely, utility and commodity prices vary widely throughout the plant life.

5.1 Economic and econometric models

Two different classes of models: economic and econometric can be adopted to forecast the prices of both commodities and utilities.

Economic models consider actual prices variations as they follow the supply and demand law trend. They are based on economic, physical, and financial features and thus on real

economic variables. However, the main limit of these models is that they need a constant update and they do not show a significant validity for long-term forecasts.
On the other hand, econometric models are based on statistical analysis of historical price series. They do not take into account the causes of price fluctuations, but consider only their trend. These models are more appropriate for long-term forecasts, such as the price variations occurring over a chemical plant life. Thus, it is advisable to use this kind of models to estimate the future prices of commodities and utilities rather than the economic one.

5.1.1 Commodities and utilities quotations modeling

In order to foresee future quotations of commodities and utilities, it is necessary to consider the quotations of the component that is taken as a reference. As mentioned in Chapter 3, the reference component is the Crude Oil. It is the precursor of many chemical processes and thus the price fluctuation of commodities and utilities, such as benzene, ethylene, and all the others, are strictly connected with its future quotations. As discussed in Buscemi and Pagnoncelli (2016), the econometric model for the quotation of crude oil is based only on the crude oil price at a different time in the past, whilst the price quotations of the other components are based on the price of crude oil and on the price of the commodity itself at a different time in the past. The models used in this manuscript are the following.

$$P_{CO}(t) = A + B * P_{CO}(t-1) + C * P_{CO}(t-2) \tag{38}$$

$$P_{BTZ}(t) = A + B * P_{BTZ}(t-1) + C * P_{CO}(t) \tag{39}$$

$$P_{Toluene}(t) = A + B * P_{CO}(t) + C * P_{CO}(t-1) + D * P_{Toluene}(t-1) \tag{40}$$

$$P_{Benzene}(t) = A + B * P_{Toluene}(t) + C * P_{Toluene}(t-1) + D * P_{Benzene}(t-1) \tag{41}$$

$$P_{Ethylene}(t) = A + B * P_{Toluene}(t) + C * P_{Toluene}(t-1) + D * P_{Benzene}(t-1) \tag{42}$$

$$P_{Ethylbenzene}(t) = P_{Ethylene}(t) + P_{Benzene}(t) + P_{Production}(t) \tag{43}$$

$$P_{Styrene}(t) = A + B * P_{Styrene}(t-1) + C * P_{Benzene}(t) \tag{44}$$

Where t is the time and parameters A, B, C, and D are summarized in Table 15.

Table 15 – Commodities and utilities modeling parameters

	A	**B**	**C**	**D**	**# Equation**
Crude Oil	2.596	1.846	-0.880	-	(38)
BTZ	0	0.939	2.763e-4	-	(39)
Toluene	4.26	0.85	-0.77	0.87	(40)
Benzene	-1.63	0.95	-0.89	0.96	(41)
Ethylene	3.43	0.678	0.103	-	(42)
Ethylbenzene	-	-	-	-	(43)
Styrene	11.474	0.538	0.735	-	(44)

All these models are obtained by using a correlogram, a plot that shows the dependence of a component with itself in the past or with the reference component. It helps in identifying the time dependence and any possible delay between the quotation of the reference component and the ones of the depending commodities. Correlation index varies from -1 to +1. If it is equal to -1, the trend of the two variables is perfectly opposite. If it is equal to +1, the correlation is perfectly positive: the two variables follow the same trend and the relationship is linear. In general, the higher the correlation, the greater the influence of that price product on the quotation of the commodity of interest. Every parameter is thus calculated by using a regression that minimize the sum of squared errors (SSE) between modeled prices of the i-th commodity and its past real prices.

The evaluation of the modeled prices for the electric energy is not as simple as the other commodities and utilities, since they are affected not only by daily fluctuations, but also by seasonal trends. The model is as follows:

$$P_{EE,i,j}(t) = a_j + b_j * P_{CO,i-t_d} + c_j * \sin(\frac{2\pi * i}{T_j} + \varphi_j) \quad (45)$$

Where:

- i is the i-th week;
- j is the time band (there are four bands in a day: morning, afternoon, evening, night);
- a is a reference value of EE price [USD/MWh];
- b is coefficient for the dependency of EE price from CO [bbl/ MWh];
- td is time delay [week] (i.e. number of weeks of delay between the EE and CO prices);
- c is parameter of the periodic component [USD/MWh];
- T is period of the sinewave function (the period is expected to be comparable to a season) [week];
- φ_j is the phase of the sinewave function [-].

The values of the previous parameters are summarized in Table 16.

Table 16 – Electric energy modeling parameters.

	a	b	c	phi	T [month]
Morning	58.68456	0.231302084	3.018953	2.9559	9.9151
Afternoon	44.96224	0.295241441	3.716831	1.8282	19.94852
Evening	41.48949	0.385253342	4.829762	2.5654	19.50937
Night	19.96115	0.264435858	1.930759	1.286	13.72645

Figure 32, Figure 34 shows the results of the selected models and propose a comparison between the historical price series and the modeled quotations of crude oil and electric energy. The price of the latter one is strongly influenced by the fluctuations of the first.

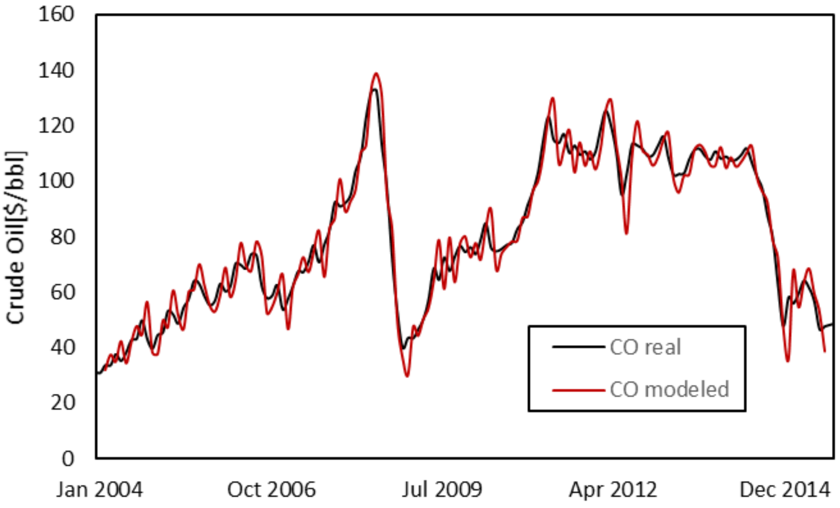


Figure 32 – Crude Oil modeled quotations and historical price series.

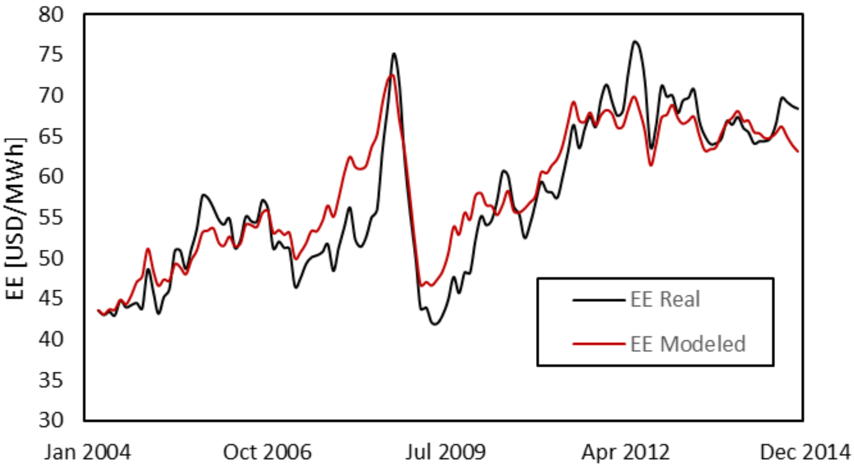
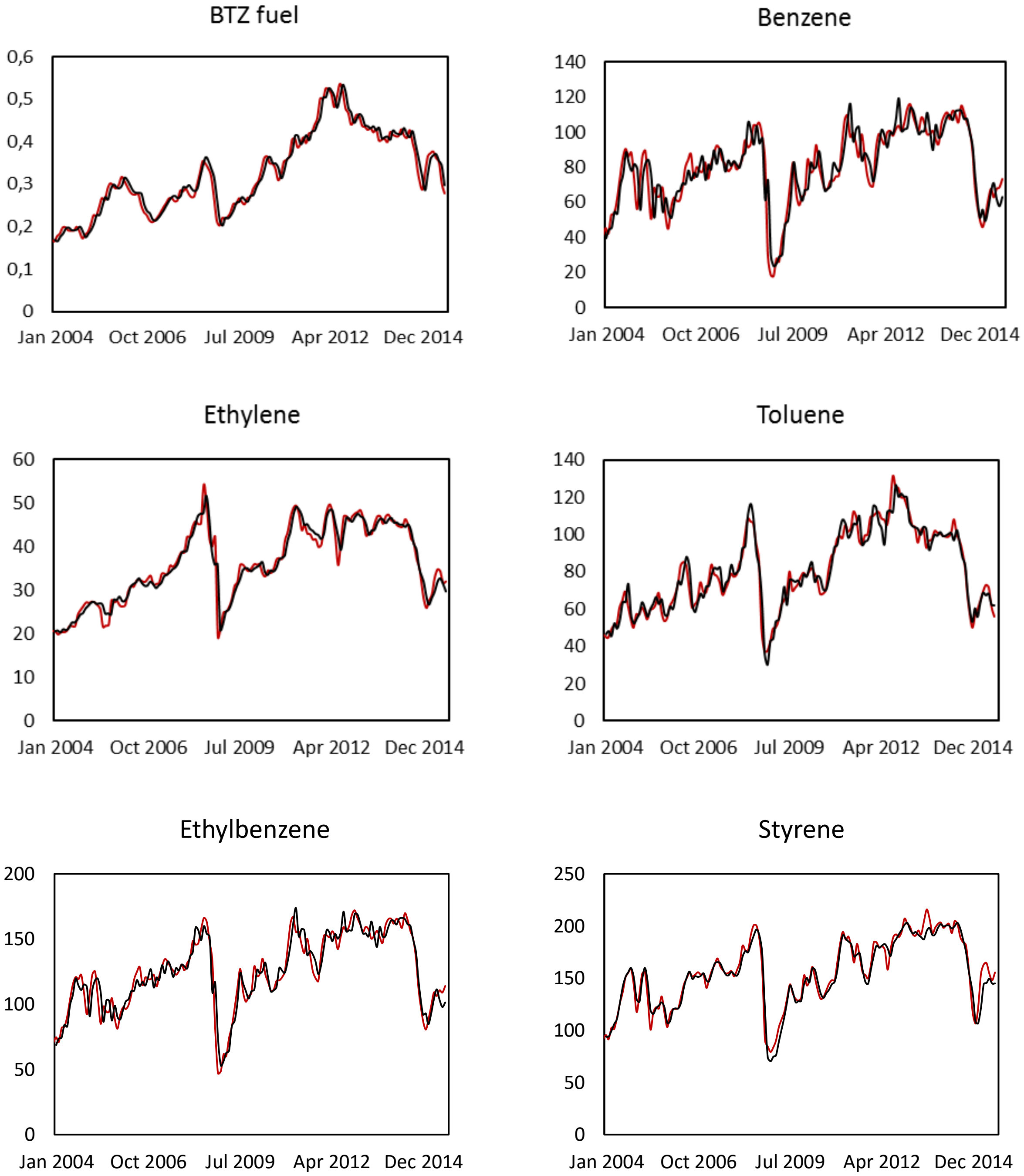


Figure 33 – Crude Oil modeled quotations and historical price series.


BTZ fuel

Benzene

Ethylene

Toluene

Ethylbenzene

Styrene

Figure 34 – Comparison between historical price series (black line) and modeled quotations (red line) [USD/kmol]

The previous analysis shows that the modeled quotations are pretty similar to those of the historical series and thus the econometric models can be considered valid also to forecast future trends (*i.e.* for predictive purposes supported by a distribution of future economic scenarios).

5.2 Scenarios production and analysis

Relying on a single value of a commodity at a certain time may end up to a misleading interpretation of the results, due to the future unpredictability. This uncertainty generates the need to create a large number of scenarios for future quotations, in order to have a reliable set of data. In this manuscript, we decided to create 3000 economic scenarios over a 10-year time span. The following equations are used to generate the scenarios.

$$P_{CO}(t) = P_{CO,Econometric}(t) * (1 + \sigma_{P_{CO}} * rand(-1;1) + \mu_{P_{CO}}) * (1 + g(t)) \qquad (46)$$

$$P_{CO,Econometric}(t) = \ [A + B * P_{CO}(t-1) + C * P_{CO}(t-2)] \qquad (47)$$

Where:

- σPCO is the standard deviation of errors between the model and CO real price in moving average. Its value is 0.031081405 [USD/bbl],
- µPCO is the average value of errors between the model and CO real price in moving average. Its value is -0.000172734 [USD/bbl],
- rand(−1; 1) is a random number between -1 and +1,
- g(t) is a function that adds a background noise, making the whole scenario more realistic with the addition of peaks typical of CO price.

For the other commodities, the formula is as follows:

$$P_i(t) = P_{i,Econometric}(t) * (1 + \sigma_i * rand(-1;1) + \mu_i) \qquad (48)$$

Where:

- i, is the i-th commodity,
- $P_{i,Econometric}$ is the price of the commodity evaluated as the econometric model,
- σ_i, is the standard deviation of the error for that specific commodity or utility between the model and moving average value,
- μ_i, is the average value of the error for that specific commodity or utility between the model and moving average value.

Table 17 shows the values of σ_i and μ_i.

Table 17 – Commodities and utilities modeling parameters

	σ_i	μ_i
Toluene	0.028867024	-0.046716
Benzene	0.070056575	0.004779251
Styrene	0.036794306	-0.010971858
Ethylene	0.036412378	0.001505031
BTZ	0.034249484	0.004279642

5.2.1 Dynamic Net Present Value scenarios

The equations and parameters reported in Paragraph 5.2 allow producing a stochastic distribution of different scenarios for crude oil and the corresponding commodities involved in the styrene process. For the sake of clarity, the following illustrations show only 50 out of 3000 economic scenarios. In Figure 35, Figure 36, and Figure 37 are shown the future quotations scenario of crude oil, benzene and ethylene.

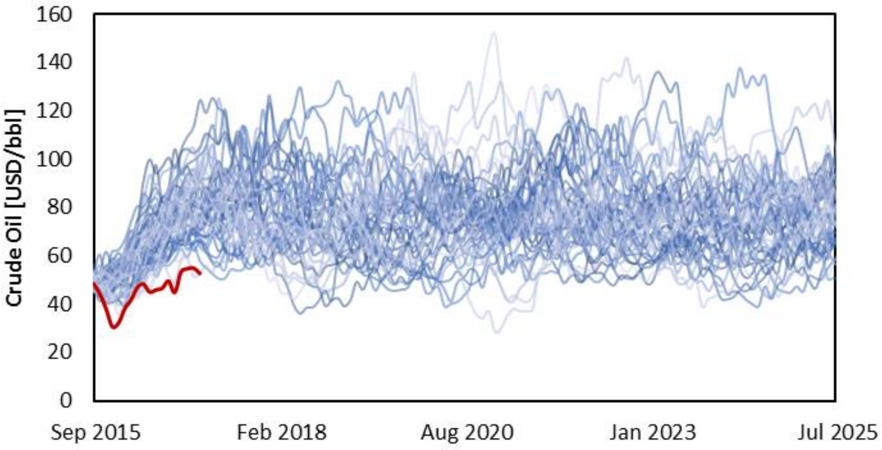


Figure 35 – Crude Oil quotation scenarios and historical price series.

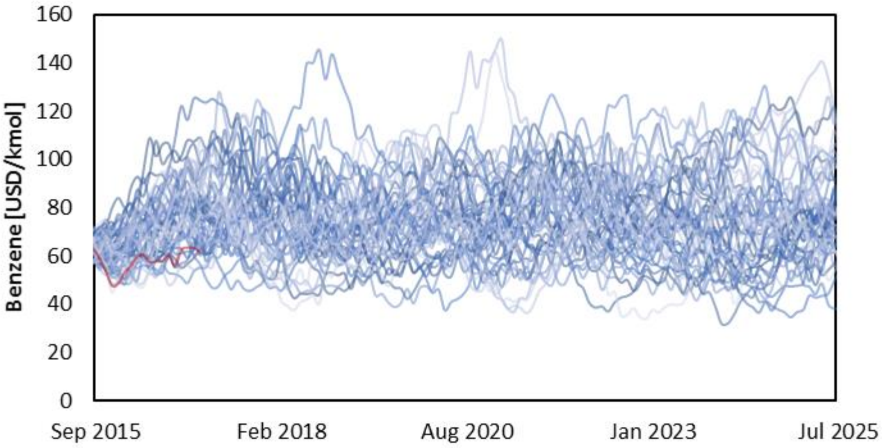


Figure 36 – Benzene quotation scenarios and historical price series.

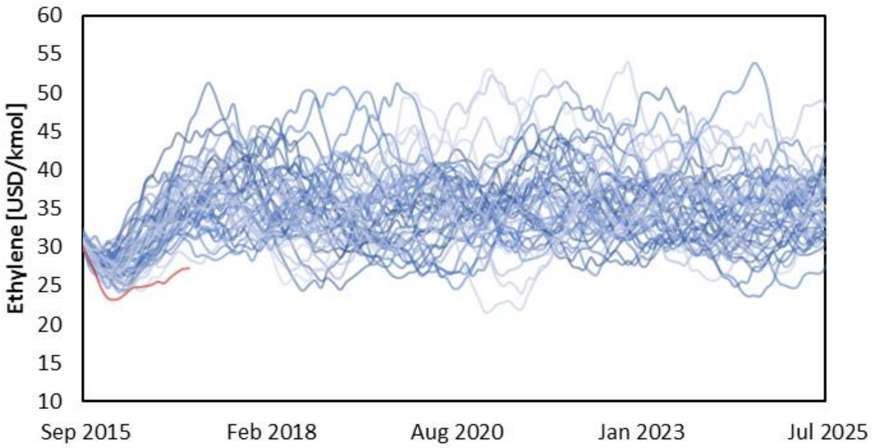


Figure 37 – Ethylene quotation scenarios and historical price series.

Commodities and crude oil future price scenarios show that the generated ranges contain only some of the real market quotation, marked with the red line. This is due to the fact that only 50 scenarios have been taken into account. In case of 3000 scenarios, the stochastic distribution embraces the real market quotations from Sep-2015 to Aug-2017.

It is possible to generate a very high number of PNPV scenarios, 3000 times 32144 configurations. Each scenario has two degrees of freedom combinations, which return respectively the maximum and the minimum PNPV. For the sake of representation simplicity, only the configurations linked to the utter maximum and minimum are represented in Figure 38; while Figure 39 represents the average of the 32144 configurations for each scenario.

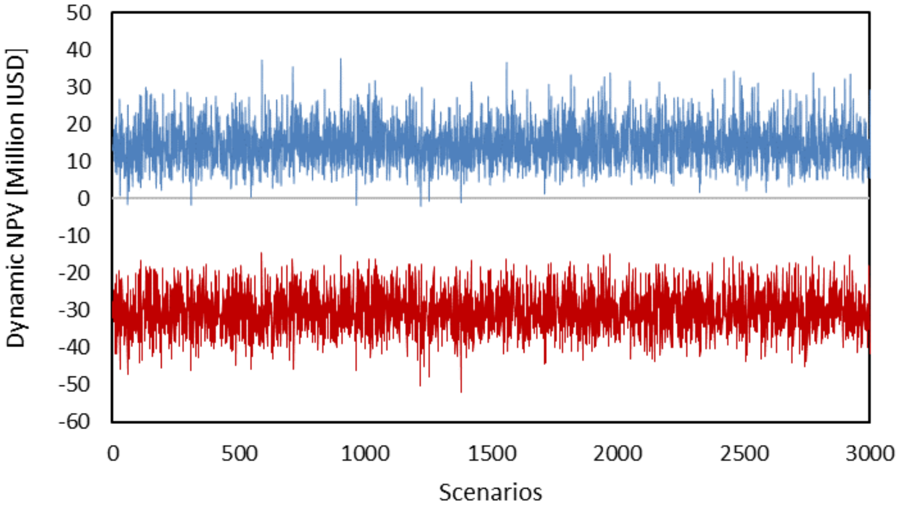


Figure 38 – Maximum and minimum DNPV for 3000 scenarios.

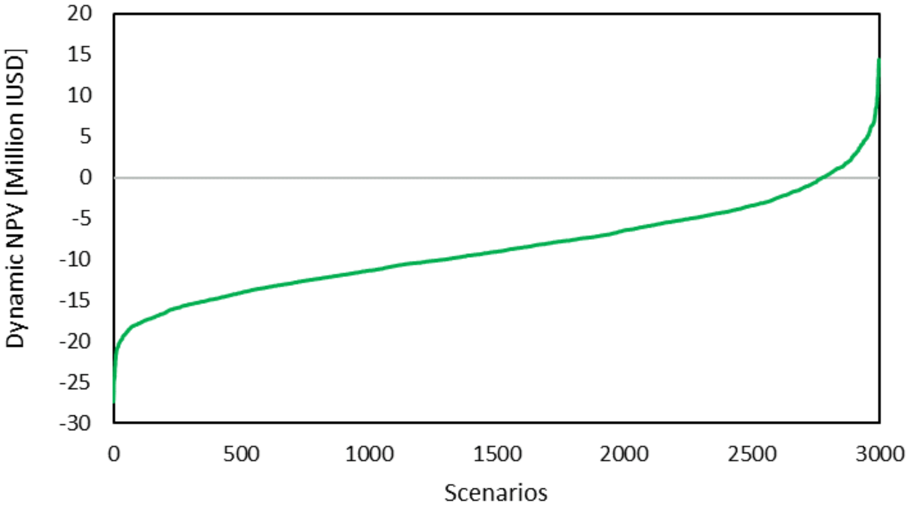


Figure 39 – Medium DNPV for 3000 scenarios.

It is important to point out that in the case of the maximum DNPVs, all the scenarios give the same result in terms of combination of degrees of freedom. Whilst In the case of the minimum DNPVs, not all the scenarios return the same configuration but there is a prevailing one. Table 18 and Table 19 show the degrees of freedom combinations that return respectively the maximum and minimum PNPV, with a focus on the percentage of scenarios In particular in case of maximum PNPV, 100% of scenarios are have the same combination of the degrees of freedom, while in the case of minimum NPV there is no equity between the scenarios.

Table 18 – Degrees of freedom combinations for the Maximum PNPVs for each scenario.

	Configuration	**SF [-]**	**LP steam [kmol/h]**	**Inlet T [K]**	**Reactor L [m]**	**Number of scenarios [%]**
Maximum	3	0.3	2000	535	2.5	100

Table 19 – Degrees of freedom combinations for the Minimum PNPVs for each scenario.

	Configuration	**SF [-]**	**LP steam [kmol/h]**	**Inlet T [K]**	**Reactor L [m]**	**Number of scenarios [%]**
Minimum	39625	0.7	2000	565	8.5	5.37
Minimum	39889	0.1	5000	565	8.5	94.63

The fact that only 5.37% of the scenarios return the same result DNPV calculated with the historical price series, is a further evidence of the fact that using the scenarios is extremely important to have a more detailed evaluation of an investment. Thus, it is not advisable to rely on a single dynamic trend (*e.g.*, the past one) of quotations.

As a further investigation, it was decided to perform a series of statistical analysis of the configurations that returns the maximum DNPV. The results are shown in Figure 40 and in Table *20*.

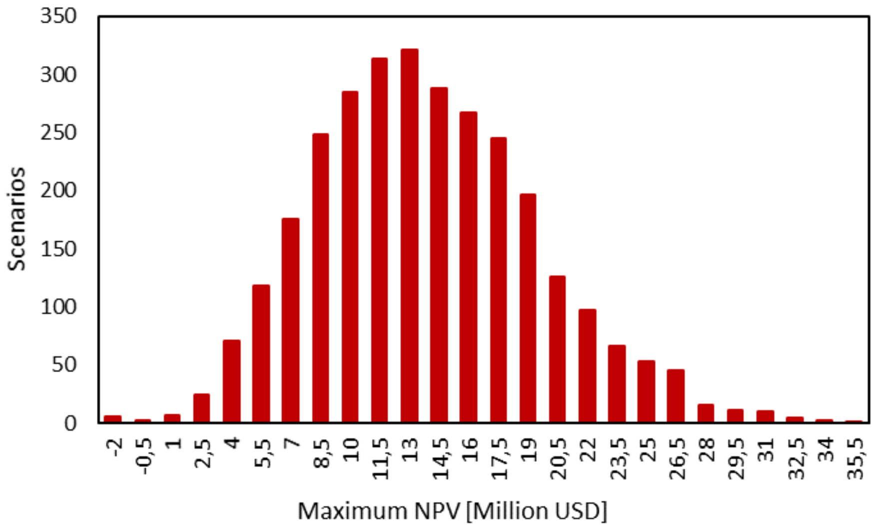


Figure 40 – Distribution of the maximum dynamic NPV.

Table 20 – Statistical parameter the maximum dynamic NPV.

	Value
Average	14.61
Median	14.148202
Skewness	0.43425
Standard Deviation	5.6645
Maximum	37.332867
Minimum	-1.794388

The analysis performed show that the numerical values are different than those obtained using historical series but still of the same order of magnitude.

Conclusions and future developments

Aim of this thesis was to compare not only quantitatively, but also qualitatively, the economic indicators, which differ one from the other for the level of detail used for their assessment. First, it was shown that static indicators produce results that may end up in a misleading interpretation that depends on the period when the investment is assessed. Furthermore, the difference between Dynamic Conceptual Design and Dynamic Net Present Value was analyzed. It turned out that the second indicator returns results of an order of magnitude lower than the first one. It is worth underlining that it is still a rough estimation, since it uses only an estimation of the TCI. However, DNPV is much closer to a realistic analysis than DCD is, even though the complexity of calculation is negligible. From this analysis, it was also found that the two indicators are not in a proportional relation, and thus it is not possible to determine one from the evaluation of the other.

Despite the scenarios created by econometric models are not 100% reliable, as they provide future quotations, the drafting of a large number of them may prove a winning economic strategy as they are not only able to define the probability that leads to positive results, but also allow understanding which combination of degrees of freedom most often brings to the optimal solution

As far as NPV is concerned, the sensitivity analysis showed that the NPV dependency from WACC is significantly less strong than the dependency from both fixed and operative costs. Therefore, it is legitimate for a rough estimation to use an approximated parameter rather than obtaining equity and debt values that would lead to a heavy work, in terms of data collection and analysis. Finally, unlike DEP4, NPV depends heavily on the area where it is set to invest because it depends on local taxes and import prices.

The major problem of this methodology is the computation time needed to obtain all the configurations from UNISIM-MATLAB. An improvement can be reached by creating a database of possible plant configurations to accelerate a future real-time optimization of the considered plant, once the reactor volume is assigned. Furthermore, the CPU time needed from MATLAB to process the PNPV for all the configurations and for each scenario is very high, especially if one decides to increase either the number of the configurations or the number of the scenarios. Reducing the computational time would be a great improvement.

Future applications could be to couple a downstream polystyrene plant to further increase revenues. Beyond this, it seems viable to consider the idea of combining the search for the optimal economy with the search for the optimal environmental impact, looking for the combination of DoF that maximizes both. Finally, the use of economic models to create future models of commodities prices may prove more detailed for future price estimates.

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