School of Industrial and Information Engineering

Department of Chemistry, Materials and Chemical Engineering
"Giulio Natta"

Master of Science in Chemical Engineering

CORO (Capex/Opex Robust Optimizer): An Automatic Simulation-based Process Optimization tool

Supervisor :
Prof. Flavio Manenti

Co-supervisor :
Ing. Kristiano Prifti

Co-supervisor :
Ing. Andrea Galeazzi

Candidate :
Lorenzo De Falco
926467

Academic Year 2020−2021

Contents

List of Figures

List of Tables

List of Symbols and Acronyms

ACEE	Association for the Advancement of Cost Engineering
APEA	Aspen Process Economic Analyzer
BFD	Block Flow Diagram
CAPEX	Capital Expenses
CEPCI	Chemical Engineering Plant Cost Index
CORO	Capex/Opex Robust Optimizer
CPSS	Chemical Process Simulation Software
DAE	Differential-Algebraic Equation
DLL	Dynamic Link Library
DOF	Degree Of Freedom
EOS	Equation Of State
FCI	Fixed Capital Investment
FOB	Free On Board
Ft	Correction Factor for heat exchange area
GUI	Graphic User Interface
ISBL	Inside Battery Limits
LMTD	Logarithmic Mean Temperature Difference
MOC	Material Of Construction
NPV	Net Present Value
OOP	Object Oriented Programming
OPEX	Operating Expenses
OSBL	Outside Battery Limits
PB	Payback
PFD	Process Flow Diagram

P&ID	Process & Instrumentation Diagram
ROI	Return On Investment
TAC	Total Annual Cost
TVM	Time Value of Money
U	Global Heat Transfer Coefficient
UML	Unified Modeling Language
VBA	Visual Basic for Applications
XML	eXtensible Markup Language

Abstract

In the framework of industrial feasibility analysis, the need for reliable information at the conceptual design stage raises interest in tools capable of producing such information quickly and accurately. At this stage, different alternatives have to be measured in terms of profitability in order to optimize the investment of time and resources.
Process simulation allows to gain knowledge of a plant before its construction, therefore it is an essential tool in the design phase. However, simulation software tools for cost estimation and process optimization turn out to be, respectively, lacking flexibility and inadequate in the resolution of non-convex problems characterized by multiple local minima.
The objective of this thesis project is to develop a system application capable of automatically performing cost estimation and robust optimization of industrial chemical processes, interfacing with a commercial process simulation software to retrieve the required data. The tool is designed in a two-layer architecture: a user interface consisting of an Excel file, containing macros written in VBA language, designed to enable data visualization and interaction; an algorithm for data-processing developed in C++ language, which implements the desired functionalities.
The developed software has proven to be particularly efficient when applied to demonstrative case studies. Particularly, the cost estimation of a complex ammonia separation plant has demonstrated more flexibility and accuracy than the cost estimation tool of a commercial chemical process simulation software. Furthermore, the optimization carried out on a specifically designed process has shown satisfactory efficiency and speed.
Therefore, the exploitation of the software developed in this project can generate added value in decision-making processes related to industrial plant design.

Keywords Process Optimization; Cost estimation; Process Simulation; Software Development

Estratto

Nell'ambito degli studi di fattibilità di processi industriali, la necessità di disporre di informazioni affidabili nella fase di progettazione concettuale genera interesse in strumenti che siano capaci di produrre tali informazioni velocemente e accuratamente. In questa fase, è necessario essere in grado di misurare la profittabilità di diverse opzioni in modo da ottimizzare l'investimento in termini di tempo e risorse.
La simulazione di processo permette di acquisire conoscenza di un impianto prima che lo stesso sia costruito, per questo motivo rappresenta uno strumento essenziale nella fase di progettazione. Tuttavia, nei programmi di simulazione, gli strumenti per la stima dei costi e l'ottimizzazione di processo risultano, rispettivamente, carenti dal punto di vista della flessibilità e inadeguati nella risoluzione di problemi non convessi caratterizzati da molteplici minimi locali.
L'obiettivo del presente progetto di tesi è lo sviluppo di un'applicazione di sistema capace di eseguire automaticamente la stima dei costi e l'ottimizzazione robusta di processi chimici industriali, interfacciandosi con un software commerciale di simulazione di processo per il reperimento dei dati necessari. Lo strumento è progettato in un'architettura a due livelli: un'interfaccia utente costituita da un file Excel, contenente blocchi di istruzioni scritte in linguaggio VBA, volta a dare la possibilità di visualizzare i dati e interagire con essi; un algoritmo per il trattamento dei dati sviluppato in linguaggio C++, il quale implementa le funzionalità desiderate.
Il software sviluppato ha dimostrato di essere particolarmente efficiente quando applicato a casi studio dimostrativi. In particolare, la stima dei costi di un complesso impianto di separazione dell'ammoniaca ha dimostrato flessibilità e precisione aggiuntiva rispetto al corrispondente strumento di un programma di simulazione di processo. Inoltre, l'ottimizzazione effettuata su un processo appositamente disegnato, ha evidenziato soddisfacente efficienza e velocità.
Pertanto, l'utilizzo del software sviluppato nell'ambito del presente progetto può generare valore aggiunto nei processi decisionali legati alla progettazione di impianti industriali.

Parole Chiave Ottimizzazione di processo; Stima dei costi; Simulazione di processo; Sviluppo software

Introduction

As pointed out by Martin *et al.*, 2017, during the conceptual design stage, the decisions made commit a large sum of money for the future phases of the project. This is the stage at which the majority of impactful decisions in terms of costs are taken. At the same time, it is the stage where changing the decisions is the cheapest. When a company has to bring modifications to the design while in the industrialisation stage, it is very costly because all the design process has to be done again. Therefore, there is a strong incentive to try to estimate project costs at as early a stage as possible, even if the design information is incomplete, so that the project can be optimized, evaluated or abandoned if it is not attractive. This concept is qualitatively pictured in Figure 0.1.

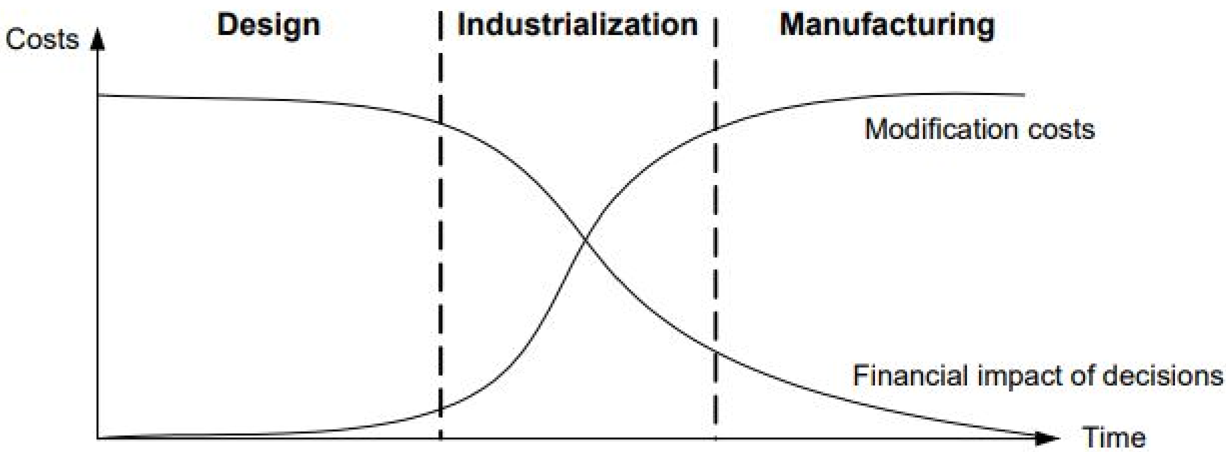

Figure 0.1: Decisions influence upon costs during a project (Martin *et al.*, 2017)

In recent years, process simulation has taken a key role in chemical process design. Through steady-state simulation, the engineer can model a process and determine its most important parameters with a high level of detail without requiring the huge amount of money and resources that the physical testing would imply. This type of simulation is usually carried out during the conceptual stage of a project to acquire a better understanding on how the process lay-out may be changed to maximize profit and to fine-tune the plant from an operational point of view. In this phase, multiple configurations can be considered. With the purpose of determining which of the options is the one to further investigate, profitability analyses are carried out.

In particular, for each of the alternatives, starting from the estimation of capital and operating expenses, several economic and financial parameters can be computed and used to determine its feasibility and its potential worth. The selection of the estimation procedure and of the indicator of interest depends on the available information, on the specific project requirements and on its progress.
Anyhow, a large part of estimation consists of the collection and storage of data obtained from records of actual plant costs. The data must be then correlated and updated and the required information rapidly retrieved for use in further cost estimations. It follows that this kind of procedure is time-consuming and rather repetitive; therefore, its automation is valuable in terms of time, costs and precision.
Analogously, optimization has found widespread use in chemical engineering applications, especially in the engineering of process systems. Problems in this sector frequently have several potential solutions with complicated economic and performance connections, making it difficult to determine the best answer by intuitive reasoning. Furthermore, system economics frequently show that discovering the best solution results in significant savings. Therefore, optimization has emerged as a significant method that assists the chemical sector in remaining competitive (Biegler, 2010).
The optimization of plants performances, by its nature, depends on a large set of variables. Its convergence can require a significant number of iterations, and for each iteration a slightly new problem has to be solved. Thus, the need to exploit computational power so as to solve problems that include hundreds of complex equations in a reasonable amount of time. As a result, process optimization strongly relies on process simulation software, on computational power as well as on the choice of appropriate numerical algorithms and optimization strategies. Automation ensures speed and eliminates human error if set up correctly.

Thesis Motivation

This project arises from the need for fast and reliable cost estimation and optimization in feasibility studies. Although cost estimation tools are a feature of many commercial process simulators, their use can be cumbersome. Sometimes, in order to obtain an estimate, very specific information on the equipment are required. The engineer might not be in possession of such details at the initial stages of the project. Also, the methodologies and the scope of the cost headings are not clearly defined for reasons related to proprietary information, this might result in miscalculations as some cost items could be double-counted or improperly neglected. Moreover, performances of optimizers implemented in process simulators are limited by high non-linearity of the problems, existence of multiple minima and presence of unfeasibility regions: a common solution to this problem is to interface the process simulator to external optimizer specifically designed to solve Non-Linear Problems (Biegler, 1985).
Concerning the approach to the process optimization, it has been observed that frequently only the operating expenses are minimized, or the profit is maximized without considering capital expenses. This is a conceptually wrong approach in a feasibility study, as all the

indexes of profitability depend strongly on both fixed investment expenses and manufacturing costs. Moreover, in most of the literature works in which capex and opex were optimized at the same time, an oversimplified approach was adopted and an incomplete definition of the terms was considered.
Although there have been endeavours whose purpose was the automation of economic estimation and process optimization, none of them provides a user-friendly interface and most importantly none of them has an approach that allows the software to be integrated with different process simulators.

Thesis Objectives

In the framework of the current state of the art, the aim of this thesis project is to provide an instrument that automates economic estimates and performs optimizations based on process simulation in the most flexible rigorous and robust way. This tool is conceived to be used in initial phases of the project (conceptual design). Once more precise information are available, factorial estimate may not be as accurate as required. However, simulation-based optimization can still provide important results in terms of decision making support, even if the absolute numbers are not highly precise.
To achieve these targets, the software has been structured in the following way:

- An Excel workbook functions as user interface. By using macros developed in VBA language, this workbook is able to connect with the commercial process simulator Aspen HYSYS, provided by AspenTech. In this workbook, the user can retrieve data from the simulation object of the analysis and then set the desired specifics for both cost estimation and process optimization.

- An XML (eXstensible Markup Language) file stores data, ready to be processed, in an organized way.

- A dynamic link library (DLL), developed in C++ language, processes the information to yield results. Firstly, the data are read from the input XML file. Then, such data are used for cost assessment performed by the implementation of factorial techniques. Finally, where required, the degrees of freedom and the objective functions are fed to the methods provided by the numerical library "BzzMath" (Buzzi-Ferraris and Manenti, 2013). The functions from this library are developed specifically for complex numerical problems and guarantee the robustness of the optimization.

It is worth to underline that the procedures of data extraction and data processing (i.e. cost estimation and optimization) have been intentionally decoupled in order to ensure the independence of the application core on the particular process simulator.
In order to guarantee a reliable, flexible and specific economic assessment, two different economic libraries are implemented: Turton *et al.*, 2012 and Peters and Timmerhaus, 2001. The presence of two economic libraries is fundamental to cross-check the results and to identify a reasonable span in which capital expenses and operating costs can range. Payback

time has been selected as objective function to minimize.
The resulting software is named CORO (Capex/Opex Robust Optimizer).

Thesis Outline

The present work is structured as follows:

Chapter 1 introduces the reader to the fields of process simulation and optimization. The chapter contains a brief review of these two topics and explicates their correlation. Initially, the discussion focuses on the fundamental features of commercial process simulation software and on the benefits that their application can produce. Successively, a definition of the optimization approach is provided; particular attention is placed on optimization strategies applied to typical problems of chemical engineering.

Chapter 2 discusses the subject of process economics. Initially, the cost estimation is contextualised in the framework of feasibility studies. In addition, capital and operating expenses are specified in all their sub-categories. Furthermore, methodologies proposed in literature for cost estimation are revised, with particular attention to the ones implemented in the software. In conclusion, a summary of profitability indicators is provided.

Chapter 3 is entirely dedicated to the description of the software development and of the solutions adopted to guarantee the correct functioning of cost estimation and economic optimization. In this section, the logic behind the software is clearly defined. The distinct layers of the program are presented, with a focus on their interaction. Samples from the source code are included in order to support the discussion.

Chapter 4 reports the results obtained from the application of the CORO to demonstrative case studies. The tool is tested in terms of efficiency and accuracy on complex flowsheets. The comparison with the corresponding tools of a commercial process simulation software validates the correct functioning of the produced program and highlights its advantages.

Conclusions summarize the goals achieved in this project and propose future developments found to be interesting and suitable for the implementation. Some of them could considerably widen the field of application of the software.

Chapter 1

Simulation-based Optimization in Process Industry

Effective optimization in process industry relies on fast and effective computation. As a matter of fact, the design and optimization of chemical process requires the solving of large amounts of equations. Before digital computers, the resolution was done manually and the errors would happen easily, leading to results far from the optimum. Consequently, the extensive application of the optimization methodology was unfeasible as the time and cost did not justify the obtained advantages. With the advancement of computer technology and the onset of the energy crisis in the 1970s, many chemical engineers and academics began to build softwares to solve chemical engineering problems exploiting numerical methods (Cai *et al.*, 2017). Those efforts eventually resulted in the development of multifunctional tools which allow to mathematically determine optimal operating conditions and process configurations rather than relying on heuristics or costly experimentation. As for today, the growth of machine learning and artificial intelligence has enabled the continuous analysis of big sets of data, whose exploitation can produce highly accurate grey box models for every particular case.

The availability of the virtual reproduction of entire processes through simulation enhances the field of application and the potential benefits of process optimization, reducing its cost at the same time.

This chapter has the goal to provide to the reader the fundamental knowledge on how a process simulator works and why its application leads to major benefits. Moreover, the mathematical approach to optimization and the formulation of strategies commonly applied to chemical engineering problems are covered. It should be noted that this discussion does not have the ambition of being comprehensive as the matter is quite complex and widely discussed in literature.

1.1 Process Simulation

An accurate definition of simulation is provided by Thomé, 1993: 'Simulation is a process of designing an operational model of a system and conducting experiments with this model for the purpose either of understanding the behavior of the system or of evaluating alternative strategies for the development or operation of the system. It has to be able to reproduce selected aspects of the behavior of the system modeled to an accepted degree of accuracy.' Chemical process models are often represented by a collection of individual unit models (the so-called unit operations) that usually correspond to major pieces of process equipment. Unit models are assembled within a process flowsheet that describes the interaction of equipment either for steady-state or dynamic behavior. As a result, models can be described by algebraic or differential equations. For example, steady-state process flowsheets are usually described by algebraic equations systems whilst dynamic process flowsheets are represented by lumped parameter models consisting of differential-algebraic equations (DAEs) (Biegler, 2010).

1.1.1 Chemical Process Simulation Softwares

The core structure of a process simulation is effectively summarized by Figure 1.1. In order

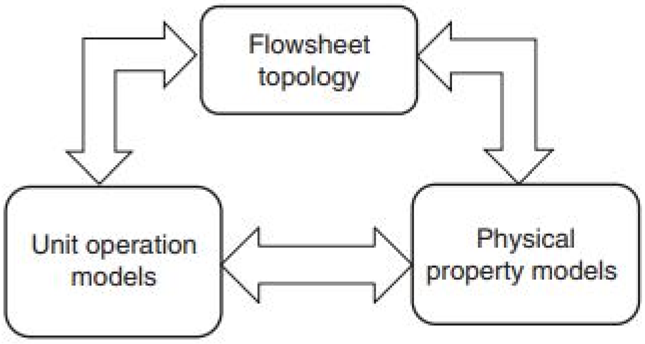

Figure 1.1: Structure of a process simulator (Haydary, 2019)

for the process model to be well defined, the user has to eliminate all the degrees of freedom by setting the required input data. Regardless of the Chemical Process Simulation Software (CPSS) used, the procedure to create a simulation consists in the same typical steps:

1. **Component Selection**: the user can select a list of chemical compounds to be used in the simulation. The software usually offer a large database from which hundreds of compounds can be retrieved along with their specific physical and chemical properties. The component list can consist of pure conventional compounds (having a well-known chemical formula) and also non-conventional components such as petroleum assays.

2. **Thermodynamic model definition**. Selection of the appropriate property method is a crucial step in process simulation. The accuracy and credibility of simulation results depend on the suitability of the chosen property method. Process simulators implement

tools for the calculation of physical properties of pure components and streams, as well as for the determination of phase equilibrium. The user has to select a property method or fluid package that provides a sufficiently accurate representation of the system. Selection of a suitable method requires good knowledge of the system thermodynamics and experience. Often, different models have to be checked against the measured data to select the most accurate model and, in some cases, it may be necessary to adjust some model parameters to achieve better description of the measured data (Haydary, 2019).
Among the most popular thermodynamic models in process engineering, there are the Soave-Redlich-Kwong (SRK) equation of state (EOS), particularly appropriate for hydrocarbons processing, and the Peng-Robinson (PR) EOS very accurate for the description of pure-component properties.

3. **Chemistry and Reactions**. In case the process involves a chemical reaction step, the user has to provide additional details about the reactive system, particularly, the set of the reactions to be considered, together with their stoichiometry and eventual other available information. For instance, if the dependence of the Conversion on the temperature is known, the simulator will take the equation as a constraint for the model. Moreover, equilibrium problems can be solved automatically when the value of the Equilibrium constant, or its dependence on the temperature, is known. Generally, the CPSS are able to solve heterogeneous catalytic reactions describable by the Langmuir−Hinshelwood kinetic model. It is worth pointing out that the process simulator can effectively solve both design and rating problems, depending on the type of information

4. **Flowsheet**. It is the phase where the actual building of the Process Flow Diagram (PFD) takes place. The user has to define all the material streams of interest and connect them to the unit operations. All the commercial CPSS offer a user-friendly environment that enables intuitive fruition of the application. Specifically, the Graphic User Interface (GUI) is responsible for the flowsheet designing and operation units connecting, parameters input and output, calculation control, and so on. It is the direct interaction between Process Simulator and the user: the convenience and functions of GUI are the most important factor of CPSS (Haydary, 2019).
Figure 1.2 shows the model palette available in Aspen HYSYS from which the user can select the model that represents the equipment. All the models describing conventional units are implemented. Moreover, the program provides some logical operators that are useful to correctly represent the plant such as recycle and adjuster operators. Many unconventional units are available as well. However, the results obtained from their simulation are not always accurate due to the intrinsic difficulty of modeling unconventional equipment. In any case, the function to import customized models is generally available: the user can supply his own model specifically developed for the operation of interest.

Figure 1.3 provides an outlook of a process simulation produced by using Aspen HYSYS.

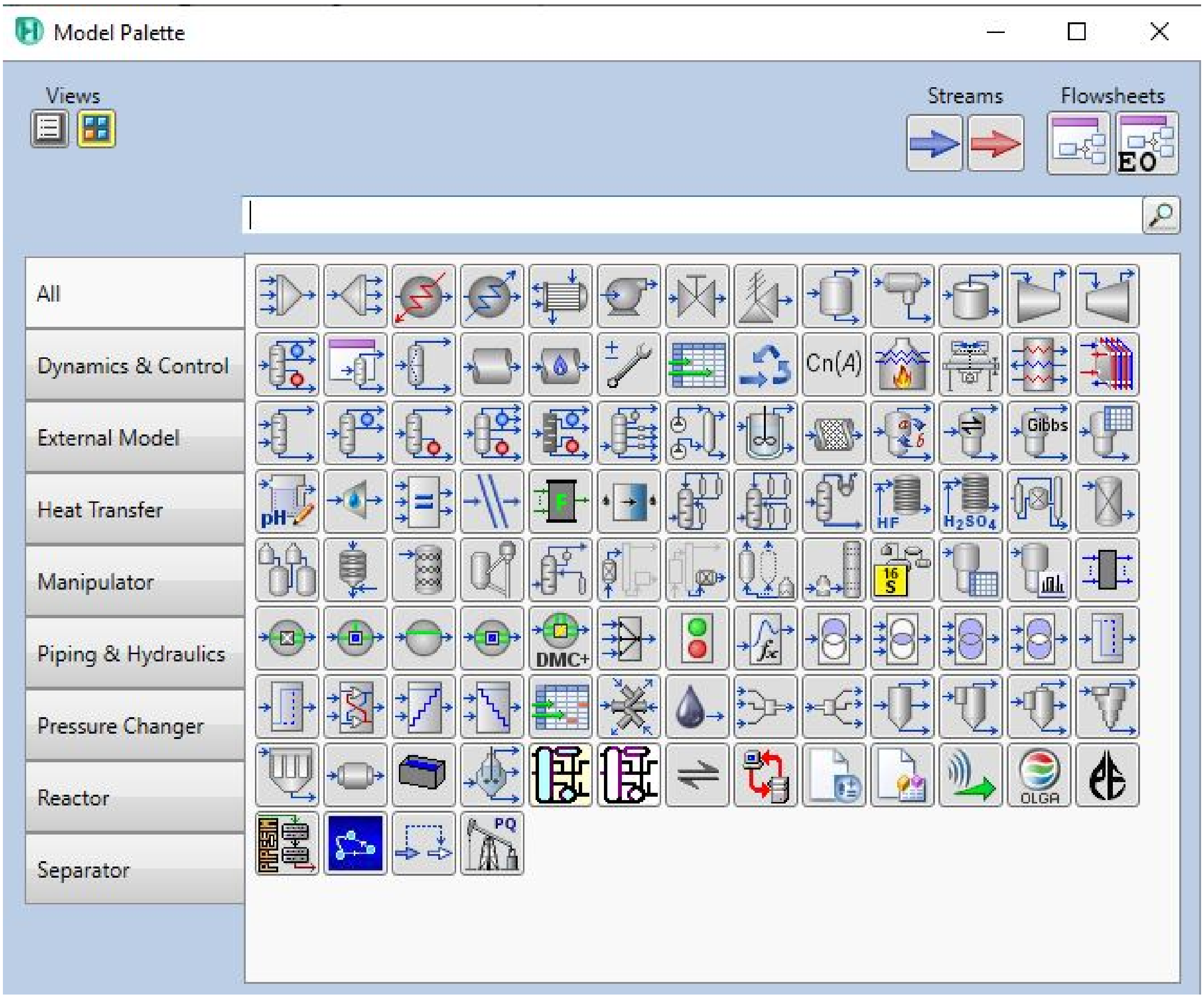

Figure 1.2: Available unit models in Aspen HYSYS

The plant performs the separation of ethanol from the fermentation broth, which is a mixture of water, ethanol and carbon dioxide. The flowsheet shows all the material streams (blue lines) involved in the process, the energy streams (red lines) required to perform the separation and most importantly the unit operations. In particular, five equipment can be distinguished:

- The flash separator carries out a first bulk separation, recovering on the bottom a stream 'Beer' more concentrated in ethanol than the feedstock; the top-stream is rich in CO_2 and it is sent to the 'CO2 Wash' Absorber.

- The 'CO2 Wash' absorber removes all the CO_2 from the light product of the flash, recovering small contents of ethanol that can be recycled to the fermentor.

- Absorber 'Conc' furtherly increases the concentration of ethanol thanks to the steam injection, which increases temperature from 30°C to 80°C.

- The refluxed absorber 'Lights' recovers part of the ethanol from the water and sends the bottom to a Rectification step.
- The Distillation column 'Rect' carries out the last part of the separation yielding the products respecting the specified purity.

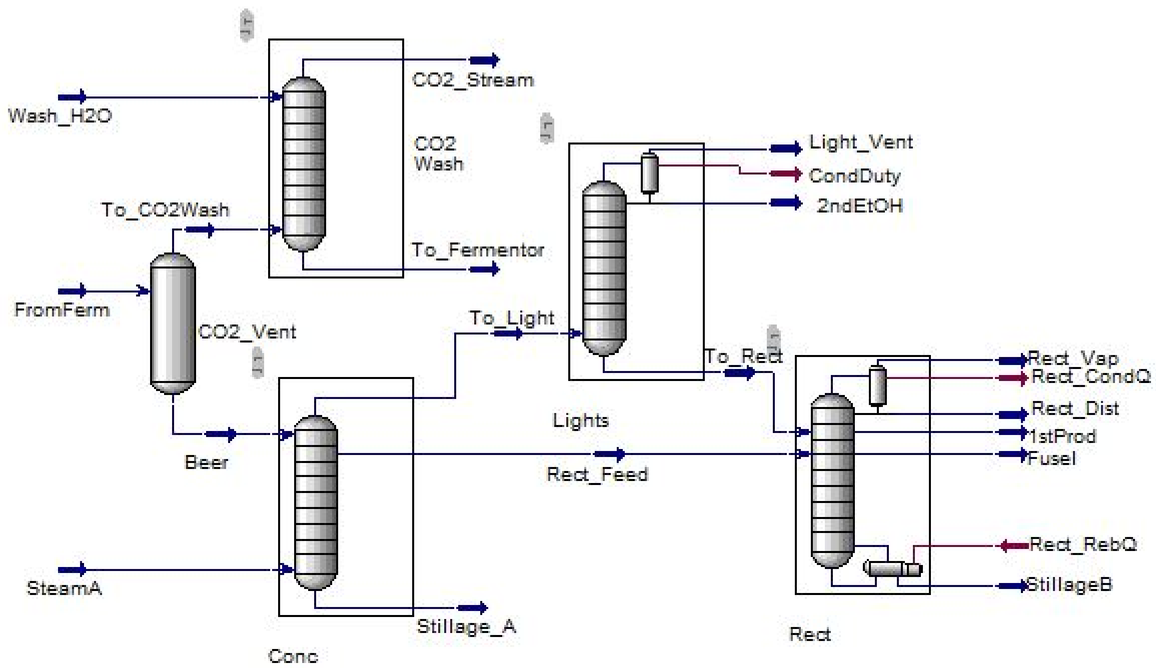

Figure 1.3: Aspen HYSYS Simulation case

It can be noted that the PFD is relatively simple and does not contain important information on utilities, instrumentations or control systems. On the other hand, process technological schemes available to the engineer are usually very detailed. The issue is that the more comprehensive flowsheets, such as the piping and instrumentation diagram (P&ID) are too complex to be used in simulation and optimization calculations. Only some information can be used for process simulation. Therefore, the process engineer has to carefully consider the simulation goals to extract the necessary information from the process technological schemes and documentation to create the simplified PFD. Subsequently, data from the plant operation have to be collected. Some plant data can be used as the input data to the simulator and some for the comparison of model and real plant data. After the preparation of a simplified PFD and the collection of all necessary information, process simulation with different scenarios can be realized. Based on the simulation results and their comparison with operational data and analysis of different scenarios, the process modification can be suggested.
Each software has its own functionalities and peculiarities, however, they are all developed

following a series of specifications defined by the CAPE-OPEN Interface Standard, which allows inter-operability between different environments.
Table 1.1 reports the most used CPSS. The process simulators upon which the CORO is

Table 1.1: List of main commercial Chemical Process Simulation software

Name	Source	Type
Aspen Plus	Aspen Technology Inc.	Stead-state
Aspen Dynamics	Aspen Technology Inc.	Dynamic
Aspen HYSYS	Aspen Technology Inc.	Steady-state and dynamic
PRO/II and dynamic	SimSci-Esscor	Steady-state and dynamic
UniSim desgin	Honeywell	Steady state and dynamic

based is Aspen HYSYS provided by AspenTech.
In addition to the essential features, all the CPSS provide supplemental functions to support the user in the analysis. Among others, spreadsheeting functionalities are provided to implement additional and customized calculations, cost estimation tools are present to allow evaluations on economics and utility management features can help in minimizing energy consumption.

1.1.2 Process Simulation Advantages

Chemical process engineers often work on two sorts of tasks: the design of a new process and the improvement of an existing plant. CPSS are an indispensable tool in both cases as the time to model and build the simulation is readily recovered in the analysis phase. Process simulation can help predict product outputs, illustrate the interdependencies of key unit operations and demonstrate consequences of process upsets. Moreover, process optimization routines can be easily applied to a simulation case (Haydary, 2019). As a result of stringent environmental regulations, increasing market competitivity and shortening of the margins it is mandatory to be able to implement intensification and optimization methodologies to processes, both in design and in operational phase. Increasing the unit operation efficiency, minimization of material and energy losses, and removal of different operational malfunctions are usual reasons for existing processes modeling.
Three main classes of improvement benefitting from process simulation can be identified: cost, time, and knowledge improvements. Cost improvements originate from the fact that conventional experiments are very costly. Conducting a simulation instead of a real experiment saves the expenses for experimental setting and operation. Time benefits can be expected from the fact that simulations can be run at any desired speed. While an experiment may take months, the simulation may be sped up almost arbitrarily by simply having simulation time pass faster than real time. On the other hand, simulation time may be slowed down arbitrarily. This is done when simulating biological processes, for example. It might be useful when too much data is accumulated within too little time and therefore cannot be analyzed properly. When the analysis is complete, the simulation can be continued with a

decision based on the thoroughly analyzed data. Knowledge improvements are a consequence of the possibility of observing the plant behaviours through simulation, independently on the actual plant operations. Furthermore, simulation of extreme or particular conditions can be used to predict performances and comportments when such conditions could not be possibly be replicated by means of experiments. Nevertheless, the engineer has to treat with particular care the extrapolation of data obtained from simulation, as the model implemented could lead to gross errors if some parameters exceed the range of validity of such model.

1.2 Optimization

Optimization is the methodology of making the most effective use of a resource or of a situation; its implementation should guide a person in making a decision that results in valuable gains. Optimization applications can be found in almost all areas of engineering. A well-defined optimization problem is characterized by three essential elements:

- **Constraints**: set of equations and inequalities that define the behaviour of the system. In chemical engineering, the set of equations that describe the system comes from laws of conservation (mass, energy and momentum) and is commonly targeted as predictive model. Other constraints can come from process specifications of different nature, such as technical specifics, environmental constraints, space limitations and product quality. These constraints set a feasible region that defines limits of performance for the system.

- **Variables** that appear in the predictive model must be adjusted to satisfy the constraints. This can usually be accomplished with multiple instances of variable values, leading to a feasible region that is determined by a subspace of these variables. In many engineering problems, this subspace can be characterized by a set of decision variables that can be interpreted as degrees of freedom in the process.

- **Objective function**: performance measure, commonly a scalar quantity. This quantity is often referred to economic/financial indicators and needs to be minimized or maximized. Sometimes several objective functions are specified (e.g., minimizing cost while maximizing reliability); these are commonly combined into one function, or else one is selected for the optimization while the others are specified as constraints.

It goes without saying that adjusting variables will impact objectives and/or constraints; otherwise, such variables should not be included in the optimization study.

1.2.1 Optimization in Chemical Engineering

In chemical engineering, optimization is a critical decision-making tool. It has progressed from an academic approach to a technology having a substantial influence on engineering research and practice (*Perry's chemical engineers' handbook* 2008). Typical problems in chemical engineering arise in process design, process control, process identification, and real-time optimization. In the conceptual design, commonly, process optimization is applied to the problem of finding the best operating conditions to achieve the desired production rate. The capacity is indeed fixed from previous strategic considerations, including market research, supply chain and strategic evaluations. However, there might be a range in which the production capacity could be modified to meet profitability requirements. Figure 1.4 graphically reports a simple optimization problem of this nature: determining the most favorable rate of production in the operation of a manufacturing plant. From an analysis of the costs involved under different situations and consideration of other factors affecting the particular plant, it is possible to determine an optimum rate of production. In particular,

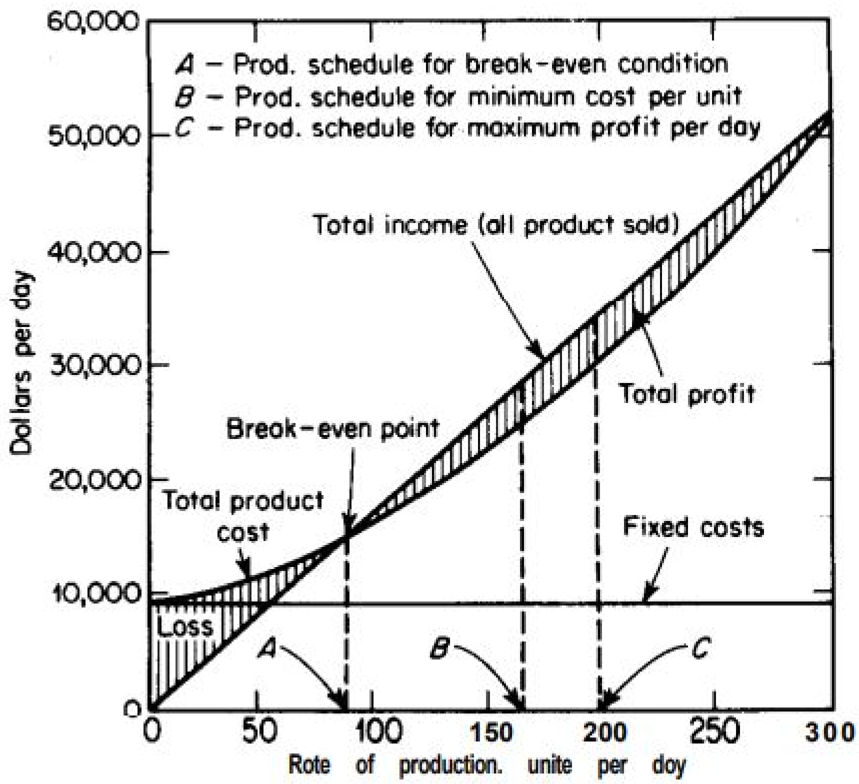

Figure 1.4: Break-even chart for operating production plant (Peters and Timmerhaus, 2001)

assuming the total production cost varies with the production rate following the curve reported in the diagram, Point C represent the rate of production at which the total profit is maximum and correspond to the optimum if the model built for the plant is accurate. Alternatively, if the production schedule is set at the value of point B, the minimum cost per unit is achieved. Point B solution might me optimal in the case where there is a certain degree of uncertainity in the capability of the market to absorb 200 units of product per day. In any case, the production schedule should never go below the break-even point, identified by point A in the Diagram. If this condition is not respected, the unitary cost of production outweighs the income that the product can generate and the operation of the plant will only cause losses.

It becomes clear that an analysis of this kind provides important support in the decision

making process. If the model describing the production is developed upon a meticulous study, the decision yielded can be trusted. On the contrary, even where the model is oversimplified, important information can be drawn, setting the basis for further analysis, and the domain of the decision might be narrowed down.
The optimization may be directed to single functions of the plant as well. One common example is energy consumption minimization also known as process integration or pinch technology. In a chemical process, distinct interactions between different units and streams can be observed. Process integration has the purpose of exploiting the interaction of different units in a process system in an optimal way, with special emphasis on efficient energy use. However, based on a more modern definition of process integration, it is not limited only to energy efficiency but also to efficient use of raw materials, emission reduction, controllability, operability, and so on (Haydary, 2019). In an ideal design, the engineer should be able to maximize the profit generated by the plant while minimizing its impact on a life cycle point of view and also keeping the risks associated with the operations as low as possible.

1.2.2 Optimization Strategies

The mathematical approach optimization, also referred to as optimization strategy, is essential for a robust and reliable optimization. Engineers and other applied scientists frequently deal with models of complex systems for which no rigorous mathematical solution can be calculated. To predict the behaviour of such systems, numerical approximations are frequently used. These approximation can be either based on measurements of real life systems or on the behaviour of simpler models (Buzzi-Ferraris and Manenti, 2013).
Some strategies are limited to find a local minimum point in the vicinity of the starting point for the search. An approach of this kind permits to find the global optimum only for "convex" problems, in which local minimum/maximum always correspond to the global one. For obvious reasons, these algorithms are much faster in finding a solution than the ones designed to find global optimum in nonconvex problems; consequently, their use is effective only for specific type of problems as the gain in speed corresponds to a loss in flexibility. It is worth noting that no algorithm exists that is always superior both in performance and accuracy, therefore, it is necessary to always recognize the problem type and address it with the most suitable resolution strategy.
The most common classes of optimization strategies are listed and briefly defined in the following:

- **Pattern Search**, also known as black-box search and direct search. This family of numerical optimization does not require a gradient, therefore it can be used on functions that are not continuous or differentiable. The idea behind this strategy is to evaluate the objective function in different points, each corresponding to a set of values of the independent variables, and iteratively move away for the worst point. The method takes large steps if the iterations are being successful in improving the objective function, otherwise, it collapses onto a set of points quite close to each other. The method works reasonably well, but it requires a lot of iterations, therefore is heavy from a computational point of view. Direct search methods are easy to apply to a wide variety of problem types and optimization models. Moreover, because their termination criteria are not based on gradient information and stationary points, they are more likely to favor the search for globally optimal rather than locally optimal solutions (Biegler, 2010).

- **Linear Programming**. One strategy for simplifying the approach to a programming problem is based on expressing the constraints and the objective in a linear mathematical form. With two variables, the constraint is a straight line on a two-dimensional plot, while a plane in a three-dimensional plot results for the case of three variables. Similarly, for more than three variables, the geometric representation of the constraint is a hyperplane.
  There are two families of techniques in wide use today, simplex methods and barrier or interior point methods. Both techniques generate an improving sequence of trial solutions until a solution is reached that satisfies the conditions for an optimal solution. Currently, LP solvers can handle millions of variables and constraints in an efficient way. For this reason, if the linearization of the problem is considered acceptable, it is suggested to apply this strategy rather than complicate the resolution by relying on Nonlinear Programming.

- **Nonlinear Programming** (NLP). The general form of a nonlinear programming problem is to minimize a scalar-valued function f of several variables x subject to constraints In mathematical terms,

$$\begin{aligned} & minimize && f(x) \\ & subject\ to && c_i(x) = 0 \quad \forall i \in E \\ & && c_i(x) \leq 0 \quad \forall i \in I \end{aligned} \tag{1.2.1}$$

  Where E and I are respectively the sets of Equality and Inequality to which the constraints $c_i(x)$ belong.
  For many general nonlinear programming problems, the objective function has many locally optimal solutions; finding the best of all such minima, the global solution, is often difficult. The main techniques that have been proposed for solving constrained optimization problems are reduced-gradient methods, sequential quadratic programming methods, methods based on augmented Lagrangians and exact penalty functions. These algorithms are suitable for the resolution of many problems in chemical engineering. For instance, the solution of a differential system with boundary conditions is usually brought back to the solution of a nonlinear system. The solution of nonlinear equations is, therefore, of significant interest not only as an independent problem but also in relation to the solution of DAE (differential algebraic equation) and ODE (ordinary differential equation) stiff problems with both initial and boundary conditions (Buzzi-Ferraris and Manenti, 2013).

For what concerns the mathematical resolution of the complex problems, the Capex/Opex Robust Optimizer relies on the library 'BzzMath' developed by Buzzi-Ferraris and Manenti,

2013. The library provides a wide variety of functions which apply different optimization strategies. In particular, the selected objective function (payback-time) is minimized through the 'BzzMinimizationRobust' method: a NLP algorithm that solves multi-variable constrained minimization problems. The program implements the penalty function method in order to apply unconstrained optimization techniques to constrained problems. In particular, the penalty functions modify the original objective function by adding special terms, which are null when the constraints are satisfied and become larger and larger as the constraints are violated. This function has been proven to ensure robustness against the formulation and the complexity of the problems.
It is important to remark that the different mathematical approaches for identifying optimum conditions described in this chapter indicate the conditions that best fulfill the requirements on a theoretical level. However, factors that are difficult to quantify or practical concerns may cause the final suggestion to differ from the theoretically accurate best condition. From here, the engineer must use his judgment to consider other important practical considerations, such as the fact that commercial equipment is typically available in discrete size intervals (Peters and Timmerhaus, 2001). The purpose of the discussion and examples presented in this chapter has been to give a basis for understanding the significance of optimum conditions. Costs due to taxes, time value of money, capital, efficiency or inefficiency of operation, and special maintenance are examples of factors that have not been emphasized in the preceding. Such factors may have a sufficiently important influence on an optimum condition that they need to be taken into account for final analysis. The engineer must have the practical understanding to recognize when such factors are important and when the added accuracy obtained by including them is not worth the difficulty they cause in the analysis. For this reason, a thorough review of process economics is provided in the next chapter.

Chapter 2

Process Economics

The term process economics refers to the estimation of capital and operating costs associated with the construction and realization of an industrial production process. In order to understand the particular methodologies for the estimation, it is worth to contextualise the assessment activities into the project lifetime. In particular, considering figure 2.1 as an illustrative description of the development of an industrial plant from the conceptual stage to the operating phase, the ‘art‘ of plant cost estimation would be included in the set of analyses of support to screening and feasibility studies.

It becomes clear that an industrial viability study goes far beyond the sheer appraisal of profit generated by the investment. On the contrary, a feasibility study should provide all data necessary for an investment decision. Therefore, the commercial, technical, financial, economic and environmental prerequisites for an investment project should be defined and critically examined on the basis of alternative solutions previously reviewed in the pre-feasibility study. The result of these efforts is a project with clearly defined background conditions and goals in terms of: possible marketing strategies, achievable market shares along with corresponding production capacities, plant location, existing raw materials, appropriate technology, mechanical equipment and, if required, an environmental impact assessment. Final estimates on investment and production costs, as well as later assessments of financial and economic profitability, are only valid if the scope of the project is well specified and all key components with their associated expenses are included (Behrens and Hawranek, 1991).

Generally, the project starts with a definition of a process flowsheet in which the entire process is broke down to single unit operations designed to perform the physical and chemical transformation necessary to convert the raw materials into products. On the basis of the Process Flow Diagram, the basic engineering can be performed (process simulators are frequently used to this end). The equipment are sized by means of first principle balances and, according to the methodologies that will shortly be explained, an estimation of the capital costs can be implemented.

Finally, an acceptable plant design must result in a plant that produces a product that can be sold at a price that generates profit (Peters and Timmerhaus, 2001): obviously, if a positive economic return is not reached the plant is unfeasible from this point of view and

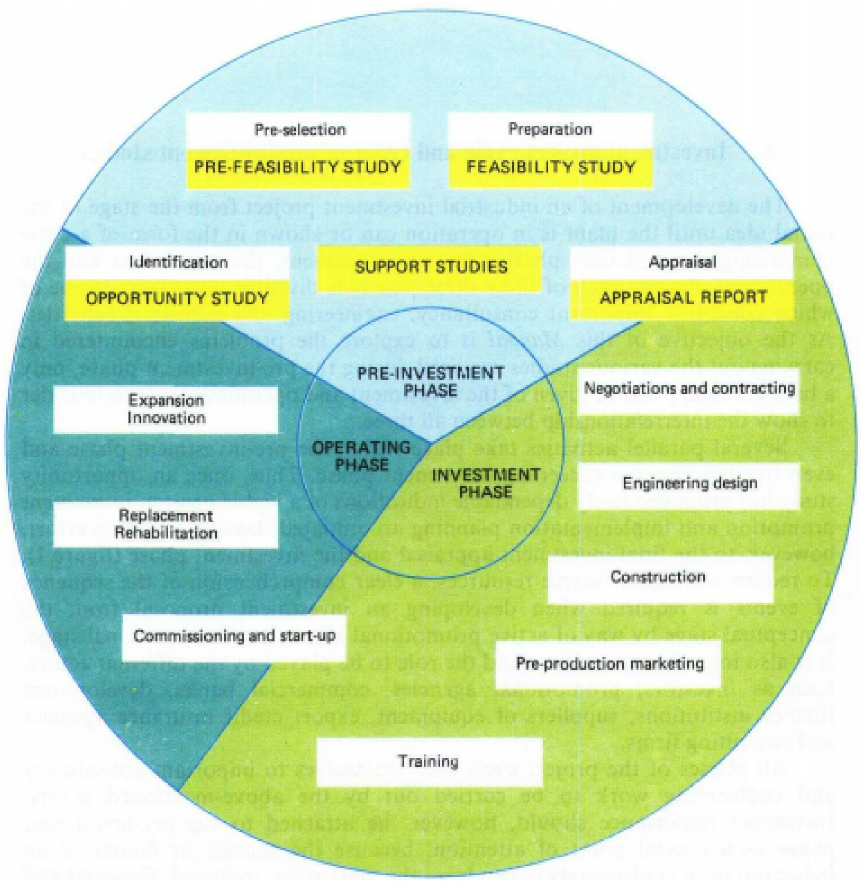

Figure 2.1: Pre-investment, investment and operating phases of the project cycle (Behrens and Hawranek, 1991)

the process configuration must be modified, where possible, or other project configuration must be analysed.

Over the years, several methodologies for the economic assessment of process plants have been developed: the aim of this chapter is to introduce the reader to all the theoretical aspects related to process economics and to the most common techniques used in the estimation of fixed capital investment, cost of manufacturing and revenues. Particular emphasis is dedicated to the methodologies proposed by Turton *et al.*, 2012 and Peters and Timmerhaus, 2001, as these two approaches to cost estimation are those implemented in the Capex/Opex Robust Optimizer.

Thereafter, the basic instruments to compare different investments will be provided. In particular, different measures of profitability along with the factors that could orientate the decision-making process are discussed.

2.1 Capital Investment

According to the definition given by Couper, 2003, the Total Capital Investment comprises expenditures for purchasing land, designing and purchasing equipment, structures and buildings, as well as bringing the facility into operation. In case the project consists in a revamping or expansion of the plant, the investment appraisal should include only the incremental expenses attributed directly to the project under consideration. Costs that have already been incurred (sunk costs) should be ignored as they are irrelevant to decisions concerning future projects. In order to have a reliable estimate, it is crucial to consider the proper boundary of the analysis. A simple but effective breakdown of the Fixed capital Investment (FCI) can be done considering the following budget headings:

- **ISBL** (Inside Battery Limits) plant expenses are the cost of procuring and installing all process equipment. They include purchasing and shipping costs of equipment, piping, catalysts, and any other material needed for final plant operation, or construction of the plant. ISBL costs also include any associated fees with construction such as permits, insurance, or equipment rental; even if these items are not needed once the plant is operational. In the early stages of a project, it is important to define the ISBL scope carefully, as other project costs are often estimated on its basis. If the ISBL scope is inadequately defined, the entire project economics can be grossly miscalculated (Towler and Sinnott, 2008).

- **Offsite Battery Limits** (OSBL) are defined as utilities, common facilities, and other equipment and components not included in the ISBL definition. OSBL refer to systems (equipment pieces and associated components) that support the production, such as cooling towers and water treatment facilities as well as essential infrastructures including shipping facilities, laboratory and offices. If precise information is not available, a rule of thumb is to use 40% of the ISBL costs as an estimate for offsite expenses. However, once detailed information such as the exact site and plant layout are known, OSBL costs can be calculated with a deterministic approach.

- **Engineering and Construction**: indirect expenses associated with the actual building of the plant such as supervision, engineering and legal expenses. Most of the time, these activities are handled by specialized companies that deliver the plant ready for production. For this reason, they are often referred to as *contractor charges*. These costs should be estimated individually as they do not scale that well with project size, but a rule of thumb is 10 − 30% of ISBL investment.

- **Working Capital**: is defined as the money required to start and run the already constructed plant until income can be obtained from the products. This money is normally obtained back at the end of plant life. Simple rules estimate WC as a proportion of ISBL.

- **Contingency**: allows for variation from the predicted cost estimate. Fluctuation can have many causes such as scope change, change in economic scenario, construction delays, validity of cost estimate and vendor quotes. Contingency should be at least 10% of ISBL and can be up to 50% if the process technology is uncertain.

The level of accuracy with which the capital expenses are estimated depends on the state of advancement of the project. The more the progress the more the information available are detailed the bigger the accuracy of the estimate.

2.1.1 Classification of Capital Costs Estimates

Within the framework of process industry, capital cost estimates are commonly classified in the following five categories, reported in ascending order of accuracy:

1. *Order-of-Magnitude Estimate*. It relies on cost information for a complete process taken from already existing plants: the available cost information is adjusted by means of appropriate scaling factors for capacity and inflation, to provide the estimated capital cost. Normally, only a Block Flow Diagram is required (BFD). The probable accuracy ranges from -30 to +50 percent.

2. *Study Estimate* (also known as Factored Estimate). It makes reference to a list of the major equipment present in the process, including pumps, compressors and turbines, columns and vessels, fired heaters and heat exchangers. Approximate sizing is performed for each piece of equipment and the approximate cost is determined. The total cost of equipment is then factored to get the estimated capital cost. It is based on the PFD and costs from generalized charts. It has a probable accuracy of -25 to +30 percent.

3. *Preliminary Estimate*: requires a more accurate equipment sizing than the one involved in the Study Estimate. An approximate layout of equipment is made with estimates of piping, instrumentation and electrical requirements. Utilities are also estimated. It is based on PFD, vessel sketches for main equipment, preliminary plot plant and elevation diagram. An accuracy of -20 to +25 percent can be reached.

4. *Definitive Estimate*: requires preliminary specifications for all the equipment, utilities, instrumentation, electrical and off-sites. It is based on final PFD, vessel sketches, plot plant and elevation diagrams, utility balances and a preliminary P&ID. The probable accuracy is increased to -10 to +15 percent.

5. *Detailed Estimate* (also known as Firm or Contractor's Estimate). It requires complete engineering of the process and all related off-sites and utilities, as well as vendor quotes for all expensive items. At the end of a detailed estimate, the plant is ready for construction. It is based on final PFD and P&ID, vessel sketches, utility balances, plot plan and elevation diagrams, piping isometrics. This estimate has a deterministic approach and ensures accuracy between -5 and +10 percent.

These classifications correspond to the five classes of estimate defined by the AACE, 2003. The Order-of-Magnitude Estimate and Study Estimate are generally used to compare many

process alternatives (Feasibility). More accurate estimates (Preliminary Estimate and Definitive Estimate) are used for the most profitable processes identified in the feasibility studies. Detailed Estimates are then performed for the most promising alternatives survived at the screening of the Preliminary Estimates. On the basis of the results obtained from the Detailed Estimate, the stakeholders should have all the elements to decide whether to continue the project and thus to build the plant or not.
The assessments produced by using the CORO fall within the category of Factorial estimate. In fact, all the equipment are sized exploiting tools and information provided by the process simulation and their cost is estimated on the basis of their characteristic dimension, whilst the remaining items of expense are inferred on the basis of factors available in literature. However, if a detailed process scheme is implemented in the simulator and the user provides detailed information on the the materials of construction of the equipment and on the nature of utilities, the accuracy of the estimate is considerably increased.
Since the unit operations constitute a significant share of the total expense and drive the complexity, thus the cost, of both the ISBL and offsite, many methodologies of appraisal, especially in early stages of the project, start from the computation of machinery purchase cost.

2.1.2 Equipment Cost

There are three sources of equipment cost data. These are: current vendor quotations, past vendor quotations, and literature estimates, in order of decreasing accuracy. Woods (1975, as cited in Silla, 2003) has stated that correlation of equipment costs in the literature can have large errors, by as much as 100%. A correlation with a large error is not completely useless, but it will limit the conclusions that one can draw. Vendor quotations are the most accurate, but the effort required to prepare detailed specifications and quotations are not usually warranted in the early stages of a project. Thus, it is common to rely on literature estimates and past quotations for quick estimates, in spite of their lower accuracy.
Although different methodologies implement different calculation strategies, a general procedure to assess equipment cost in *Study estimates* can be extrapolated. Generally, the following logical steps are executed:

1. Determination of the base cost in standard operative conditions, starting from a characteristic dimension.

2. Scaling of the cost taking into account the non-standard operative conditions (i.e. material of construction, pressure, temperature, or other non-standard factors).

3. Scale the cost with respect of a similar equipment with different capacity, if direct computation is not possible.

4. Adjusting of the cost considering the effect of inflation. Necessary because the quotation of the equipment cost, on which the estimate is based, is referred to the past.

Base cost in standard conditions

In order to follow this approach, firstly, it is necessary to define a characteristic dimension (or capacity) for each type of equipment. In this context, capacity is defined as the most important parameter affecting the machinery cost. For instance, exchange area is a typical characteristic dimension for heat exchangers, volume is generally selected for process vessels and diameter is used for trays of a distillation column. It is important to specify that characteristic dimension is not necessary a geometrical dimension: for compressors and pumps, for example, shaft power is the most common characteristic dimension, whilst volumetric gas flowrate is often used for dust collectors.
Secondly, the definition of standard conditions is required. Since equipment can operate in a very wide range of pressures, temperatures and can be built in different material, it is impossible to provide a correlation to estimate the cost in each specific case: the modus operandi adopted consists on providing a correlation for a standard case and move to other cases by multiplying the base cost by proper scaling factors. Usually, standard conditions are carbon steel and atmospheric pressure. For clarification, an example from Turton *et al.*, 2012 is reported as follows.
The purchased cost for a floating head, shell-and-tube heat exchanger having a heat transfer area of 100 m^2 has to be estimated. Turton's economic library gives the following correlation obtained from regression of data related to historical quotation of this type of exchanger. In this case, the correlation is valid for a capacity ranging between 10 and 1000 m^2.

$$\log_{10} C_P^0 = 4.8306 - 0.8509 \log_{10} A_e + 0.3187 \left[\log_{10} A_e\right]^2 \tag{2.1.1}$$

In this case equation 2.1.1 yields a cost of \$25,327.95 for the piece of machinery. More generally, the logarithmic shape of the expression is conserved whilst the coefficients are adapted to the type of the equipment. Therefore, the generic law to appraise the cost of equipment in standard conditions is:

$$\log_{10} C_P^0 = K_1 + K_2 \log_{10} A + K_3 \left[\log_{10} A\right]^2 \tag{2.1.2}$$

The values of the coefficients for some equipment units, together with the maximum and minimum values of capacity used in the correlation are given in Table 2.1 (Turton *et al.*, 2012).

Effect of Operating conditions on Purchased Cost

Once the cost in standard conditions has been obtained, the engineer has to take into account the conditions under which the equipment will be operated as these will affect the cost of the equipment.
In particular, the material of construction (MOC) used is determined by the chemicals that will come into contact with the unit walls. Ferrous alloys, particularly Carbon Steel (CS), are the most prevalent MOCs. Carbon steel, with a carbon content of less than 1.5% wt., provides hardness and durability, is easy to weld and, most importantly, is inexpensive.

Table 2.1: Equipment cost data to be used with equation 2.1.2

Equipment Type	Equipment Description	K_1	K_2	K_3	Capacity, Units	Min Size	Max Size
Compressors	centrifugal, axial, reciprocating	2.2897	1.3604	-0.1027	fluid power, kW	450	3000
Heat exchangers	floating head	4.8306	-0.8509	0.3187	area, m^2	10	1000
	u-tube	4.1884	-0.2503	0.1974	area, m^2	10	1000
	flat plate	4.6656	-0.1557	0.1547	area, m^2	10	1000
Process vessels	vertical	3.4974	0.4485	0.1074	volume, m^3	0.3	520
Pumps	centrifugal	3.3892	0.0536	0.1538	power, kW	1	300
Towers	tray and packed	3.4974	0.4485	0.1074	volume,m^3	0.3	520

Consequently, it is the material of choice in the chemical process industry when corrosion is not an issue.
Furthermore, the combination of operating temperature and pressure affects the choice of the MOC: when the process equipment is subject to severe operating conditions, more resistant hence expensive materials than carbon steel should be used. As the pressure at which a piece of equipment operates increases, the thickness of the walls of the equipment will also increase, therefore the cost rises. In some economic libraries (Ulrich, 1984) a multiplying factor for high temperatures is added. In fact, special technical arrangements and extra-material can be required to guarantee resistance at high temperatures.
For the purpose of cost assessment, the effect of the MOC and of the pressure on the equipment expected price are considered by adding proper multiplying factors to the standard conditions cost.

Effect of Capacity on Purchased Cost

Given the cost of an equipment with a certain characteristic dimension, how to estimate the cost of a similar one having different dimension?
The most simple way to establish a relationship based on the capacities of two distinct equipment of the same type is given by:

$$C_a = C_b \left(\frac{A_a}{A_b} \right)^n \tag{2.1.3}$$

where: A is the equipment cost attribute, C is the purchased cost, n is the cost exponent, subscripts a and b refer to equipment with the required and base characteristics, respectively.
This equation can be useful in the event where the capacity of the unit whose cost has to be

assessed exceeds the range of applicability of the correlation of reference.
The value of the cost exponent varies depending on the type of equipment. However, the value of n for different items of equipment is often around 0.6. Replacing this number in equation 2.1.3 yields the *six-tenths-rule*, which introduces the concept of economy of scale: the larger the equipment, the lower the cost of equipment per unit of capacity. Nevertheless, this rule has to be used with special care, as some equipment may scale with a cost exponent considerably different from 0.6. Table 2.2 shows a selection of units characterized by different cost exponents.

Table 2.2: Values of Cost Exponents for a selection of process equipment (Turton *et al.*, 2012)

Equipment Type	Range of Correlation	Unit of Capacity	Cost Exponent n
Reciprocating Compressor, motor drive	0.75 to 1490	kW	0.84
Heat Exchanger Shell&Tube	1.9 to 1860	m^2	0.59
Vertical Tank carbon steel	0.4 to 76	m^3	0.30
Centrifugal Blower	0.24 to 71	std m^3/s	0.60
Jacketed kettle glass lined	0.2 to 3.8	m^3	0.48

Effect of Time on Equipment Cost

The value of money will change because of inflation and deflation. Hence, cost data can be accurate only at the time when they are obtained and soon go out of date. Data from cost records of equipment and projects purchased in the past may be converted to present-day values by means of a cost index. The present cost of the item is found by multiplying the historical cost by the ratio of the present cost index divided by the index applicable at the previous date.

$$C_a = C_b \left(\frac{I_a}{I_b} \right) \tag{2.1.4}$$

Ideally, each cost item affected by inflation should be forecast separately. Labor costs, construction costs, raw materials and energy prices, and product prices all change at different rates. Composite indices are derived by adding weighted fractions of the component indices (*Perry's chemical engineers' handbook* 2008). Among the most popular cost indexes in process industry, there are: CEPCI (Chemical Engineering Plant Cost Index), Marshall and Swift (M&S), ENR (Engineering News Records), Nelson-Farrar. Their trends from 1996 to 2010 are reported in figure 2.2. It can be observed that their tendencies are very similar, but generally, CEPCI and M&S are preferred for process equipment and plant fixed investment estimate, due to their accuracy and their availability. Nelson-Farrar index is recommended for refinery applications. In both the economic libraries implemented in the CORO, CEPCI is the index of reference. The default value is 607.5 corresponding to 2019. The user can update this value in the dedicated input section whenever more recent information are accessible.

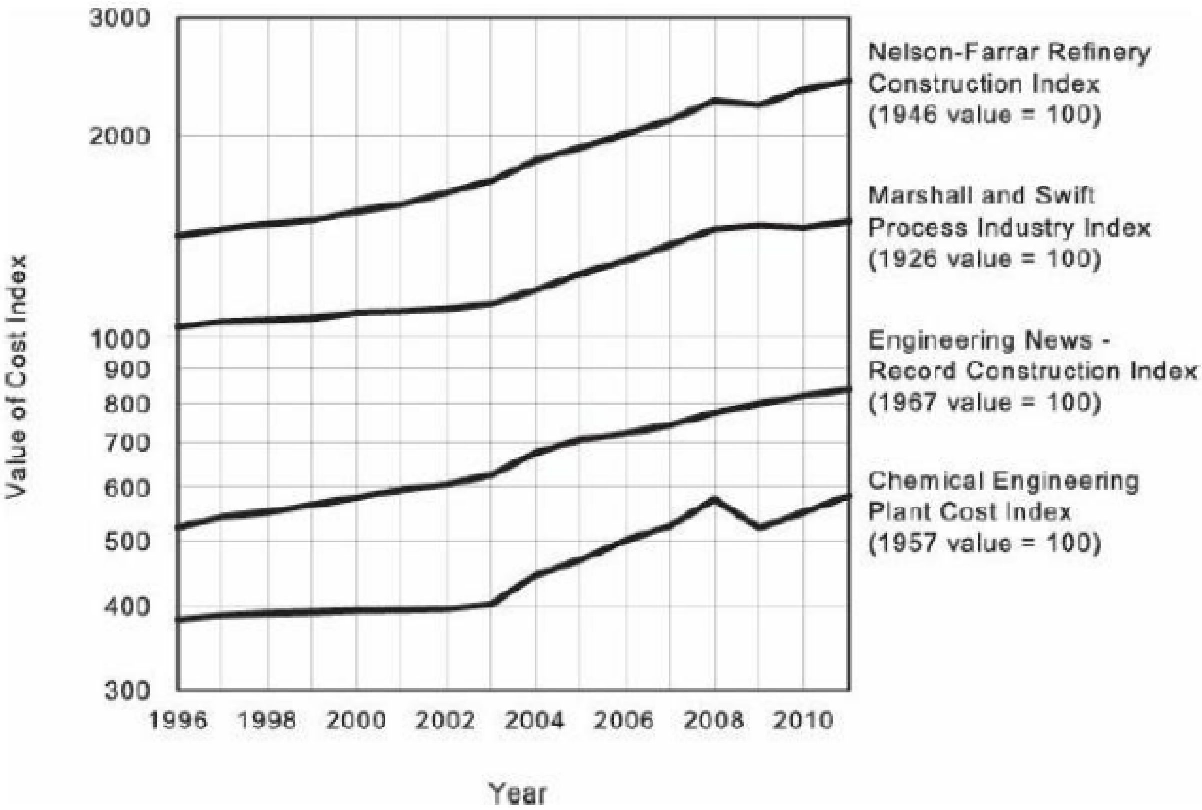

Figure 2.2: Trend of most common cost indexes (Turton *et al.*, 2012)

2.1.3 Percentage of delivered equipment methodology

The percentage of delivered equipment method for capital cost estimate is based on the assumption that each term of capital investment can be estimated as a proper percentage of the delivered equipment cost. This approach was proposed by Peters and Timmerhaus, 2001, and is one of the two implemented in the CORO. Generally, it can be assumed that cost of delivery is 10% of the purchased equipment cost: this is commonly true for f.o.b. (free on board delivery), but the percentage can vary as delivery cost is affected by size and weight of equipment, distance and type of transportation. The delivered equipment cost results from the addition of delivery cost and purchased equipment cost. Typical values of these percentage were proposed by Peters and Timmerhaus, 2001, and are reported in table 2.3 for different types of process plants (solid processing plant, solid-fluid processing plant and fluid processing plant). These percentages are average values proposed in literature on the basis of past experiences, estimated for capital investments in the range of 1-100 millions of dollars. As all the average-based approaches, this is convenient to address a wide range of problems but can generate inaccuracies for the single case. For this reason, if the user disposes of accurate information, the percentages can be tailored to the case in the dedicated user input section. The fixed (or the total) capital investment can be obtained by adding together the

Table 2.3: Ratio factors for estimating capital-investment items based on delivered equipment cost Peters and Timmerhaus, 2001

	Solid	Solid-fluid	Fluid
Direct costs			
Purchased delivered equipment	100	100	100
Purchased equipment installation	45	39	47
Instrumentation and controls	18	26	36
Piping (installed)	16	31	68
Electrical system (installed)	10	10	11
Buildings and services	25	29	18
Yard improvements	15	12	10
Service Facilities (installed)	40	55	70
Total direct plant cost	269	302	360
Indirect costs			
Engineering and supervision	33	32	33
Construction expenses	39	34	41
Legal expenses	4	4	4
Contractor fee	17	19	22
Contingency	35	37	44
Total indirect plant cost	128	126	144
Fixed-capital investment	397	428	504
Working capital (15% of TCI)	70	75	89
TCI	467	503	593

costs of each term:

$$FCI = \sum_{i=1}^{n} (Ef_i) \tag{2.1.5}$$

where E is the delivered equipment cost and f_i is the percentage associated to each contribution. This method is commonly used for preliminary economic analysis, and this is the reason why it was implemented in the Capex and Opex Robust Optimizer. Usually, the error associated to this method can be estimated to be in the range of ±20%-30%, but if data on similar process configuration are available error is reduced to almost ±10% (Peters and Timmerhaus, 2001).

2.1.4 Module Costing Technique

The equipment module costing technique is probably the most used technique in preliminary economic assessment of capital investment: it was originally proposed by Guthrie, 1974, and it was deeply discussed in literature (Ulrich, 1984, Navarrete, 1995, Turton *et al.*, 2012). The main difference between this method and the percentage of delivered equipment is that the direct and indirect costs are not determined by the total purchased equipment cost, but they are computed for each piece of equipment and referred to its purchased cost in standard condition. The resulting cost is defined as bare module cost (CBM) and it is a function of the purchased equipment cost in standard condition and material of construction, pressure and specific factors which take into account the direct and indirect cost relative to the type of equipment considered: all these terms are grouped in a single multiplying factor named bare module factor (FBM)

$$C_{BM} = C_P^0 F_{BM} \tag{2.1.6}$$

In order to estimate the fixed capital investment, other two elements must be considered, namely 'contingency and fee' and 'auxiliary facilities cost'.

Bare module cost

In standard conditions (i.e. atmospheric pressure and carbon steel as MOC) the bare module cost can be estimated according to the procedure proposed in table 2.4: for each contribution, a multiplying factor referred to the purchased cost (C_P^0) is assigned. The bare module cost is obtained by adding total direct and indirect costs. Ultimately, the following expression for the bare module factor is yielded:

$$F_{BM}^0 = (1 + \alpha_m)(1 + \alpha_L + \alpha_{FIT} + \alpha_L \alpha_O + \alpha_E) \tag{2.1.7}$$

Complications arise in non-standard condition, when the incremental cost due to more expensive material and higher operative pressure must be considered. Once again, multiplying factors (respectively F_M and F_P) are used to this end. Therefore, the purchased cost of the equipment can be expressed as:

$$C_P = C_P^0 F_M F_P \tag{2.1.8}$$

Then, with the assumption that installation complexity is not dependent on material, the installation cost in standard condition can be defined as:

$$Installation\, cost = C_P^0 (F_{BM}^0 - 1) \tag{2.1.9}$$

In non-standard conditions, instead, the installation cost has to be incremented by a factor:

$$Incremental\, installation\, cost = C_P^0 (F_P F_M - 1) f_{P\&I} \tag{2.1.10}$$

where $f_{P\&I}$ is the factor taking into account the incremental installation cost of piping and instrumentation due to non-standard conditions. At this point, the bare module cost of the equipment is obtained by adding the installation expenses to the purchased cost.

$$C_{BM} = C_P^0 F_P F_M + C_P^0 (F_{BM}^0 - 1) + C_P^0 (F_P F_M - 1) f_{P\&I} \tag{2.1.11}$$

Table 2.4: Composition of bare module cost (Turton *et al.*, 2012)

Factor	Basic Equation	Multiplying factor (to be used with C_P^0)
1. Direct		
Equipment	$C_P^0 = C_P^0$	1
Materials	$C_M = \alpha_M C_P^0$	α_M
Labour	$C_L = \alpha_L \left(C_P^0 + C_M\right)$	$(1+\alpha_M)\,\alpha_L$
Total Direct	$C_{DE} = C_P^0 + C_M + C_L$	$(1+\alpha_M)\,(1+\alpha_L)$
2.Indirect		
Freight services	$C_{FIT} = \alpha_{FIT} \left(C_P^0 + C_M\right)$	$(1+\alpha_M)\,\alpha_{FIT}$
Overhead	$C_O = \alpha_O C_L$	$(1+\alpha_M)\,\alpha_L\alpha_O$
Engineering	$C_E = \alpha_E \left(C_P^0 + C_M\right)$	$(1+\alpha_M)\,\alpha_E$
Total Indirect	$C_{IDE} = C_{FIT} + C_O + C_E$	$(1+\alpha_M)$ $(1+\alpha_{FIT}+\alpha_L\alpha_O+\alpha_E)$
Bare Module	$C_{BM}^0 = C_{DE} + C_{IDE}$	$(1+\alpha_m)$ $(1+\alpha_L+\alpha_{FIT}+\alpha_L\alpha_O+\alpha_E)$
3. Contingency and Fee		
Contingency	$C_{Cont} = \alpha_{Cont} C_{BM}^0$	$(1+\alpha_M)$ $(1+\alpha_L+\alpha_{FIT}+\alpha_L\alpha_O+\alpha_E)\,\alpha_{Cont}$
Fee	$C_{Fee} = \alpha_{Fee} C_{BM}^0$	$(1+\alpha_M)$ $(1+\alpha_L+\alpha_{FIT}+\alpha_L\alpha_O+\alpha_E)\,\alpha_{Fee}$
Total Module	$C_{TM} = C_{BM}^0 + C_{Cont}$ $+C_{Fee}$	$(1+\alpha_M)\,(1+\alpha_L+\alpha_{FIT}+\alpha_L\alpha_O+\alpha_E)$ $(1+\alpha_{Cont}+\alpha_{Fee})$

rearranging the terms of equation 2.1.11:

$$C_{BM} = C_P^0 \left[F_P F_M (1 + f_{P\&I}) + F_{BM}^0 - 1 - f_{P\&I}\right] \tag{2.1.12}$$

$$C_{BM} = C_P^0 \left[B_1 + B_2 F_P F_M\right] \tag{2.1.13}$$

where:

$$B_1 = F_{BM}^0 - 1 - f_{P\&I} \tag{2.1.14}$$

$$B_2 = 1 - f_{P\&I} \tag{2.1.15}$$

Equation 2.1.13 represents the typical way to compute bare module cost of an equipment in all the economic libraries based on Guthrie approach. The various factors α to compute the bare module factor in standard condition and the factor $f_{P\&I}$ are not to be separately evaluated for each piece of equipment: in the most common economic libraries, they are lumped in the factors B1 and B2 in order to simplify the procedure. The CORO estimation implements the module costing technique referring to the parameters proposed by Turton *et al.*, 2012.

Fixed Capital Investment

The total investment is estimated by adding up the costs associated to contingencies, fees and auxiliary facilities to the expenses derived by the equipment. By doing so, the amount of money to spend for site development, auxiliary buildings and, more broadly, off-sites is accounted. The fixed capital investment can be estimated for two different types of project:

- The construction of a completely new facility, started on undeveloped land. The capital to invest in this situation is referred to as *Grassroots cost* (C_{GR}). The C_{GR} can be computed by adding the cost of auxiliary facilities to the total module cost. This cost is usually unaffected by material of construction or operating pressure, consequently, it can be expressed as the bare module cost in standard conditions multiplied by a factor. This multiplying parameter generally lies in the range of 20-100% of the bare module cost. Turton *et al.*, 2012, proposes a multiplying factor of 0.5:

$$C_{GR} = C_{TM} + 0.5 \sum_{i=1}^{n} C^0_{BM,i} \tag{2.1.16}$$

- The renovation or expansion of an existing facility. The *Total Module Cost* (C_{TM}) is the investment required in this kind of venture. It can be computed by adding the cost associated to contingency and fees to the sum of bare module costs. In absence of specific information, contingency and fee can be computed, respectively, as 15% and 3% of the total bare module cost. Consequently, the expression of total module cost is:

$$C_{TM} = 1.18 \sum_{i=1}^{n} C_{BM,i} \tag{2.1.17}$$

  where n is the number of equipment in the plant.

When the user chooses to use Turton's economic library, the CORO estimates both total module and grassroots costs. In the latter case, the working capital has to be summed to have a correct estimation of the total capital investment. On the other hand, when the project consists in a revamping of an existing plant, it is reasonable to assume that the working capital has already been provided.

2.2 Operating Expenses

Management must consider both the overall capital needs and the production cost of the generated commodity when determining the financial viability of a process. Production cost is used as a synonym of operating cost and manufacturing cost (Silla, 2003). There are many different factors affecting the cost of manufacturing a chemical product and they are described in detail in table 2.5. All of the factors affecting the manufacturing costs can be classified in three main categories:

1. *Direct manufacturing costs.* These costs consist of the operating expenses varying with the production rate. For this reason, they are also known as Variable costs of production. If the product demand drops, the production rate is reduced below the design capacity, thus a reduction in the direct costs is expected.

2. *Fixed manufacturing costs.* These costs are not influenced by rate of production.

3. *General expenses.* These costs rarely vary with the production rate. They include management, sales financing and research functions.

Hence, the Cost of Manufacturing is given by the sum of the cost items previously described:

$$\begin{aligned} Cost\,of\,Manufacturing\ (COM) =& Direct\,Manufacturing\,Costs\ (DMC) + \\ & Fixed\,Manufacturing\,Costs\ (FMC) + \\ & General\,Expenses\ (GE) \end{aligned} \tag{2.2.1}$$

It is commonly accepted that the estimation of manufacturing cost is based on the knowledge of five elements:

1. Fixed capital investment (FCI)

2. Cost of operating labour (COL)

3. Cost of raw materials (CRM)

4. Cost of utilities (CUT)

5. Cost of waste treatment (CWT)

Once all these five terms are known, the other expenses can be either directly computed or estimated.
Whilst definition and estimation of fixed capital investment have been extensively covered in the previous paragraphs, the other main headings necessary to estimate total opex are discussed in detail in this section.

2.2.1 Cost of operating labour

This is the cost associated to the operators working in the plant, consequently their number must be estimated. The best way is to estimate the number of operators in a preliminary analysis is to scale up or down the number of operators of similar plant with different capacities. The relation between operators and capacity is not linear: usually a 0.2-0.25 power of the capacity ratio is used (Peters and Timmerhaus, 2001). This approach is not always possible, in particular for plants using new technologies. Another interesting approach, reported by Peters and Timmerhaus, 2001, is to divide the flowsheet in the main processing steps (e.g. pre-heating section, reaction section, separation section) with known capacity and compute the number of employee-hours per day per processing step. The number of operators can be obtained by summing all the operators for each processing step. Differences

Table 2.5: Factors affecting the *Cost of Manufacturing* (Turton *et al.*, 2012)

Factor	**Description**
1.Direct costs	**Factors that vary with rate of production**
A. Raw materials	Costs of chemical feedstocks required by the process
B. Waste treatment	Costs of waste treatment to protect the environment
C. Utilities	Cost of utility streams required by the process. Includes but not limited to: fuel gas, oil and/or coal; electric power; steam; cooling water; process water; boiler feed water; instrument air; inert gas (nitrogen); refrigeration.
D. Operating labor	Costs of personnel required for plant operations.
E. Direct supervisory and clerical labor	Cost of administrative/engineering and support personnel.
F. Maintenance and repairs	Costs of labor and materials associated with maintenance
G. Operating supplies	Costs of miscellaneous supplies that support daily operation not considered to be raw materials. Examples include chart paper, lubricants, chemicals, filters, respirators and protective clothing for operators.
H. Laboratory charges	Costs of routine and special laboratory tests required for product quality control and troubleshooting
I. Patents and royalties	Cost of using patented or licensed technologies.
Fixed costs	**Factors not affected by the level of production**
A . Depreciation	Costs associated with the physical plant. Legal operating expenses for tax purposes
B. Local taxes and insurance	Costs associated with property taxes and liability insurance. Based on plant location and severity of the process.
C. Plant overhead costs (factory expenses)	Catch-all costs associated with operations of auxiliary facilities supporting the manufacturing process. Costs involve payroll and accounting services, fire protection and safety services, medical services, cafeteria and any recreation facilities, payroll overhead and employee benefits
General expenses	**Costs associated with management level and administrative activities not directly related to the manufacturing process**
A. Administration costs	Costs for administration. Includes salaries, other administration, buildings and other related activities.
B. Distribution and selling costs	Costs of sales and marketing required to sell chemical products. Includes salaries and other miscellaneous costs.
C. Research and development	Costs of research activities related to the process and product. Includes salaries and funds for research-related equipment and supplies.

in type of processing plant (highly automated or batch processes) are considered. Even if this is an interesting method, it was not implemented in the Capex and Opex Robust Optimizer due to the programming difficulty in individuating the different processing steps. The method effectively implemented is the one suggested by Turton *et al.*, 2012. This procedure is based on a relation obtained by regression of archival plant data:

$$N_{OL} = \left(6.29 + 3.71P^2 + 0.23N_{np}\right)^{0.5} \tag{2.2.2}$$

where N_{OL} is the number of operators to run the process per unit of shift, P is the number of processing stages involving the handling of particulate solids (for example, transportation and distribution, particulate size control, particulate removal), N_{np} is the number of processing steps not dealing with solid particulate (including compression, heating/cooling, mixing and reaction). An important limitation of this approach is that capacity of the plant is not considered.

Once the number of operators per shift is determined, the cost of operating labour can be computed:

$$C_{OL} = N_{OL} \times Number\,of\,shifts \times Salary \tag{2.2.3}$$

Since a plant usually operates 24h per day and a shift is usually 8 hours, 3 shifts a day are necessary to satisfy the required operating labour. Salary is strongly dependent on the geographic area and on the company policy. A value of 52,900 $/year suggested by Turton *et al.*, 2012 is assumed by default in the CORO. As for all the other parameters for cost estimation, the value can be adjusted whenever more specific information are known.

2.2.2 Cost of raw materials

In the chemical industry, one of the major costs in a production operation is for the raw materials involved in the process. The amount of the raw materials which must be supplied per unit of time or per unit of product can be determined from process material balances. In many cases, certain materials act only as an agent of production and may be recoverable to some extent. Therefore, the cost should be based on the amount of raw materials actually consumed as determined from the overall material balances. Direct price quotations from prospective suppliers are preferable to published market prices. For preliminary cost analyses, market prices are often used for estimating raw-material costs. These values are published regularly in journals such as the Chemical Marketing Reporter (Peters and Timmerhaus, 2001) and are usually expressed in $/kg . In practice, looking solely at the current issue is insufficient for pricing of specific goods because not all compounds are mentioned in each issue. Furthermore, many chemicals may have substantial seasonal price variations, therefore the average price over a period of several months should be considered to have a reliable estimate.

In the particular case where the assessment is focused at a subsection of the plant, the raw material for that part of the plant may be a process stream from the global point of view. In order to be precise, the estimator should determine the cost of producing that material stream and assign it as its cost. Even if this expense is virtual as it does not correspond to an actual cash flow, this step is essential to assess the real added value of a block in a plant.

$$C_{RM} = \sum_{i=1}^{n} (F_i \times cost_i \times working\, hours/year) \tag{2.2.4}$$

where F_i is the flowrate of raw material expressed in kg/h and it is directly obtained by mass balances on the plant. The resulting cost has the dimensions of \$/year as all the other operating expenses.
Some consideration can be made on working hours term. Usually, a chemical plant works 24 hours/day, but due to maintenance interventions or contingencies, the plant does not operate continuously 365 days per year. Typical operating hours of a plant are taken as 90-96% of 8760 hours (i.e. a full year) and are an intrinsic part of the plant design. 8000 hours per year is commonly taken as a first guess value.

2.2.3 Cost of utilities and waste treatment

Utilities are all the materials or energy sources not directly transformed in the final product but fundamental to allow the proper operation of the plant. Fuels, cooling water, electricity, steam, catalyst, solvents, heating mediums or coolant and compressed air are the most common utilities used in a chemical plant. Their cost is subjected to high variability, is strongly influenced by the plant location and it can be influenced by the cost of fossil fuels. Similarly to what described for raw materials, the total cost of utilities can be obtained by multiplying the flowrate of each utility (in kg/h) estimated on the basis of the PFD, by its cost per unit of mass and the working hours of the plant. Accurate selection and supply strategy of the utilities in a plant is a key factor both from an operational point of view and for profitability. In the design phase, the engineers have to decide whether to purchase a utility from an external source or to produce it in the battery-limits of the plant. The advantage of the first case is that no capital costs are involved and the utility is delivered to the plant at fixed conditions. On the other hand, using a self-generated utility typically means to decrease opex whilst having an increase of capex due to the additional equipment necessary to the generation of such. The choice is, once again, to be made upon financial considerations. The CORO has a dedicated worksheet to properly estimate the cost derived from utilities consumption. It is implied that, in order for the tool to be able to evaluate the capital expenses related to unit operations producing utilities, the flowsheet provided to the software must include such equipment.
As regards to waste disposal: their cost can be distinguished between hazardous and non-hazardous waste or wastewater treatment, and it is strongly influenced by location of the plant and local policies. As environmental regulations continue to tighten, the problems and costs associated with the treatment of waste chemical streams will increase. In recent years, the trend has been to pursue waste minimization strategies to reduce or eliminate the volume of these streams. Such strategies involve utilizing alternative process technology and using additional recovery steps (Turton *et al.*, 2012).

2.2.4 Total Operating Expenses

As anticipated, once the main five terms are known, the other cost items can be subsequently computed. More specifically, table 2.6 summarizes the typical ranges of multiplying factors for each category and specifies the values used in the estimation. The equations for estimating the costs for each of the categories are as follows:

$$DMC = C_{RM} + C_{WT} + C_{UT} + 1.33C_{OL} + 0.069FCI + 0.03COM \tag{2.2.5}$$

$$FMC = 0.708C_{OL} + 0.068FCI + depreciation \tag{2.2.6}$$

$$GE = 0.177C_{OL} + 0.009FCI + 0.16COM \tag{2.2.7}$$

The total manufacturing cost is obtained by adding these three cost categories and by solving for the total COM:

$$COM = 0.280FCI + 2.73C_{OL} + 1.23\left(C_{UT} + C_{WT} + C_{RM}\right) \tag{2.2.8}$$

where the depreciation allowance impacts for 10% of FCI. Therefore, the cost of manufacture without depreciation, COM_d, is given by:

$$COM_d = 0.180FCI + 2.73C_{OL} + 1.23\left(C_{UT} + C_{WT} + C_{RM}\right) \tag{2.2.9}$$

2.3 Revenues

An investment venture is only financially viable if the project output has value for the consumers: when the product can be sold on the market (Behrens and Hawranek, 1991). The feasibility study has to analyse the present market situation and determine the capacity of the plant production as well as the product mix. Revenues can come not only from products but also from by-products that can be desired or undesired. In order to consider a product desirable, the margin between its price and the cost of its production should be large enough. However, since each market has its individual characteristics, the feasibility study should analyse very carefully each potential market-share and related profit. Table 2.7 schematically shows the classifications of plant output based on the aforementioned margin. The projection of sales revenues is essentially an extension of marketing research, on the basis of which a project is developed also in terms of specific sales volumes during different periods after the project goes into production. Estimating sales revenues, however, is an iterative process that should also take into account the optimal plant capacity, the appropriate technology, the technically feasible production programm and the alternative marketing strategies (Behrens and Hawranek, 1991).

The set of studies to determine the product optimal price and the projection of sales are not in the scope of this project. Nonetheless, a correct assessment of these aspects is crucial as the impact on profitability is tangible.

In case of plants producing electrical energy by means of turbines, the electricity produced has to be accounted as a source of profit. In the implementation, it was considered that

Table 2.6: Multiplication factors estimating manufacturing cost (Turton *et al.*, 2012)

Cost Item	Typical Range of Multiplying Factors	Value Used
1.Direct manufacturing costs		
A. Raw materials	C^*_{RM}	
B. Waste treatment	C^*_{WT}	
C. Utilities	C^*_{UT}	
D. Operating labour	C_{OL}	C_{OL}
E. Direct supervisory and clerical labour	$(0.1-0.25)\,C_{OL}$	$0.18C_{OL}$
F. Maintenance and repairs	$(0.02-0.1)\,FCI$	$0.06FCI$
G. Operating supplies	$(0.1-0.2)\,(Line\,1.F)$	$0.009FCI$
H. Laboratory charges	$(0.1-0.2)\,C_{OL}$	$0.15C_{OL}$
I. patents and royalties	$(0-0.06)\,COM$	$0.03COM$
Total direct manufacturing costs	$\boldsymbol{C_{RM}+C_{WT}+C_{UT}+1.33C_{OL}+0.03COM+0.069FCI}$	
2.Fixed manufacturing costs		
A . Depreciation	$0.1FCI^{+}$	$0.1FCI^{+}$
B. Local taxes and insurance	$(0.014-0.05)\,FCI$	$0.032FCI$
C. Plant overhead costs (factory expenses)	$(0.50-0.7)\,(Line\,1.D+Line\,1.E+Line\,1.F)$	$0.708C_{OL}$ $+0.036FCI$
Total fixed manufacturing costs	$\boldsymbol{0.708C_{OL}+0.068FCI+depreciation}$	
3. General manufacturing expenses		
A. Administration costs	$0.15\,(Line\,1.D+Line\,1.E+Line\,1.F)$	$0.177C_{OL}$ $+0.009FCI$
B. Distribution and selling costs	$(0.02-0.2)\,COM$	$0.11COM$
C. Research and development	$0.05COM$	$0.05COM$
Total general manufacturing costs	$\boldsymbol{0.177C_{OL}+0.009FCI+0.16COM}$	
TOTAL COSTS	$\boldsymbol{C_{RM}+C_{WT}+C_{UT}+2.215C_{OL}+0.190COM+0.146FCI+depreciation}$	
*Costs are evaluated from information given on the PFD +Depreciation costs are covered separately. 10% of FCI is a crude approximation		

all the electricity produced is sold at the same price at which electrical energy is bought. Although not rigorous, this approach allows to properly account operating costs in situations where turbines and compressors are combined. For example, if a compressor is driven by

Table 2.7: Contribution margin

VALUE ADDED		LOSS VALUE	
Product	By-product	By-product/Waste	Waste
$P >> C_P$	$P > C_P + C_T$	$P < C_P + C_T$	$P = 0$; $C_P + C_S > 0$
Desired	Desired/Undesired	Undesired	Undesired
$P = Price$		$C_P = Cost\,of\,Production$	
$C_T = Treatment\,cost$ (if any)		$C_S = Disposal\,cost$ (if any)	

a turbine, the operating expenses due to its electricity consumption are nullified by the virtual revenues derived by the electricity production of the expander. This will result in an overestimation of both revenues and opex; nevertheless, the derived financial parameter (result of interest of the analysis) will not be affected.

2.4 Profitability

Throughout this chapter, the methods to estimate capital investment, operating expenses and revenues have been presented. Although the knowledge of these categories can give an idea on the economic appeal of the project these same do not represent, singly, a financial performance of the investment. In order to generate an indicator of profitability, consequently, capex, opex and revenues must be considered together in a comprehensive evaluation.
The word profitability is used as the general term for the measure of the amount of profit that can be obtained from a given investment. Profitability, therefore, is the common denominator for all business activities.
Before capital is invested in a project or enterprise, it is necessary to know how much profit can be obtained and whether or not it might be more advantageous to invest the capital in another form of enterprise. Thus, the determination and analysis of profits obtainable from the investment of capital and the choice of the best investment among various alternatives are major goals of economic analysis. Capital investments are undertaken for a variety of reasons. Sometimes the goal is just to provide a service that cannot reasonably generate a monetary profit, such as providing recreation facilities for free use by employees. The profitability of this sort of venture cannot be directly measured by common criteria. The design engineer, however, usually deals with investments that are expected to yield a tangible profit (Peters and Timmerhaus, 2001).
In the following paragraph, the basic concepts of the cash flow analysis are synthesised, as this method represents the most rigorous way to assess the worth of an investment in the industrial field. In any case, the degree of accuracy of the evaluation of profitability can vary according to the project requirements: not all profitability indexes are necessarily based on a cash flow analysis. For instance, at a study estimate level, the determination of a detailed cash flow could be unreliable due to difficulties in providing accurate information.

2.4.1 Cash Flow Analysis

The net amount of cash and equivalents moving into and out of a business is referred to as cash flow. Inflows are represented by cash received, whereas outflows are represented by money spent. The cash flows are based on the best projections of investment, operational expenses, sales volume, and sales price that can be made for the project. A cash flow diagram gives a clear picture of the resources required for a project and the timing of the earnings (Towler and Sinnott, 2008). During any project, cash initially flows out of the company

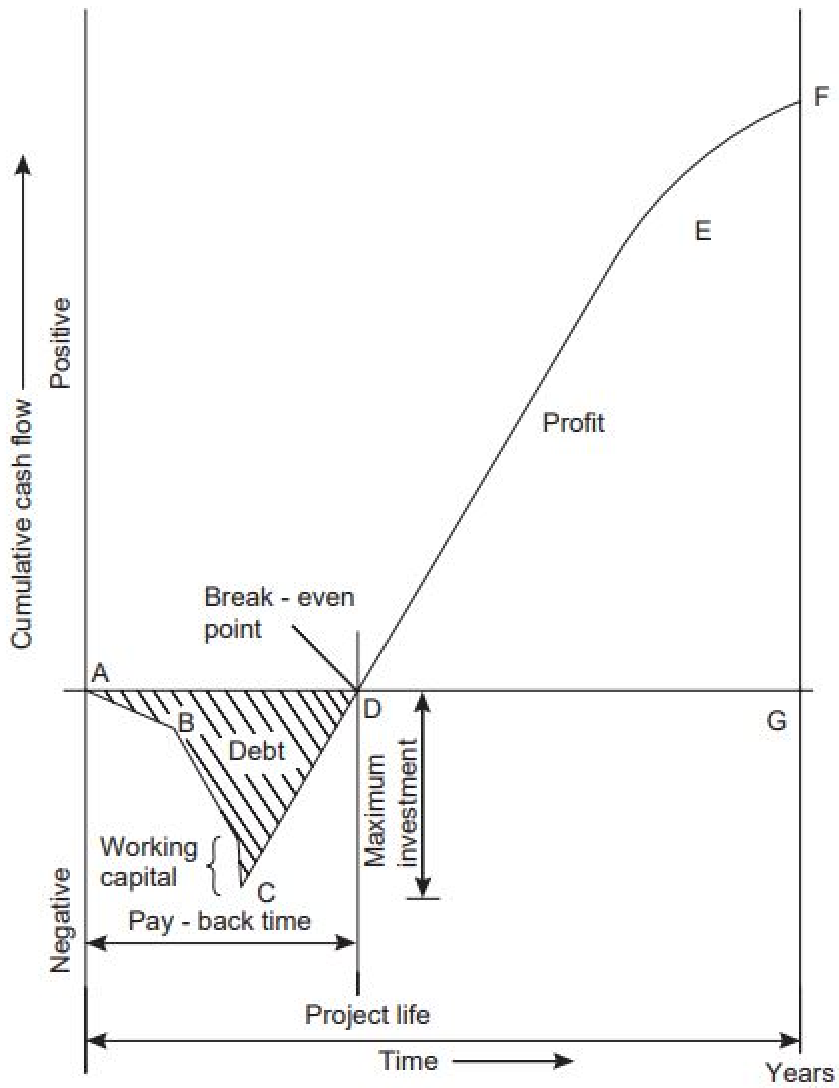

Figure 2.3: Cumulative cash flow diagram over the full life cycle of an industrial plant (Towler and Sinnott, 2008)

to pay for the costs of engineering, equipment procurement, and plant construction. From the time at which the plant is completely built and its operation can start, the revenues from sale of product begin to flow into the company. The *net cash flow* at any time is the difference between the earnings and expenditure. A cash flow diagram, such as the one shown in Figure 2.3, shows the forecast cumulative net cash flow over the life of a project. The diagram can be divided into the following characteristic regions:

- **A-B** The investment required to design the plant.
- **B-C** The large outflow of cash to develop the facility and provide startup funds, including working capital.
- **C-D** The curve changes direction at point C as the process begins the production and income is generated from sales. The net cash flow is now positive, but the cumulative amount is still negative until the investment is paid off, which occurs at point D. This point is known as *break-even point*.
- **D-E** In this region, the cumulative cash flow is positive. The venture is generating a return on the investment.
- **E-F** The rate of cash flow may tend to fall down at the end of project life due to higher operating expenses and declining sales volume and price due to plant obsolescence.

When the life time of the plant is terminated, the working capital and the cost of land are recovered by selling materials, supplies, equipment and land.
Net cash flow is a very simple and readily understood concept that serves as the foundation for the computation of more complicated metrics of profitability. 'Taxes and the effect of depreciation are not always taken into account in cash flow diagrams' (Towler and Sinnott, 2008). Moreover, this approach does not take into account the time value of money, which is a fundamental concept to establish the present worth of future earnings. This is a clearly strong approximation, but if the scope of the analysis is a comparison of different plant configurations, its impact may be negligible. Nevertheless, the profits generated are subject to taxation. Taxes have a significant influence on a project cash flows; thus, in order to conduct an economic appraisal of the project, the design engineer must have a fundamental grasp of taxation and tax allowances such as depreciation.
For these reasons and for the sake of completeness, the concepts of time value of money and depreciation are briefly introduced.

Time Value of Money

Money generated in a project can be reinvested, to generate a return, as soon as it becomes available. As a result, money gathered in the early years of the project is more valuable than money acquired later in the project's life. A modification of the well-known compound interest formula can be used to account for time value of money (TVM). The net cash flow for each year of the project is discounted at a selected compound interest rate to compute its value at the time of the appraisal.
The future worth of an amount of money P, invested at interest rate i, for n years is

$$Future\,worth\,in\,year\,n = P\,(i+1)^n \tag{2.4.1}$$

Therefore, the present value of a future capital is

$$present\, value\, of\, future\, sum = \frac{future\, worth\, in\, year\, n}{(i+1)^n} \tag{2.4.2}$$

The i used in discounting future values is known as the *discount rate* and is selected to reflect the earning capacity of money. In most companies the discount rate is set at the cost of capital (Towler and Sinnott, 2008). It is worth highlighting that discounting future cash flows should not be mistaken for allowing for price inflation. Inflation is a general increase in prices and expenses driven by a mismatch between supply and demand. Its impact is on the purchasing power of money and it is not related to the potentiality of producing profit. The consequence of discounting the future incomes in a cash flow analysis is that the final cumulative cash position will be lower with respect of the one estimated without considering the time value of money.

Depreciation of Capital Investment

Depreciation charges are the most common type of tax allowance used by governments to encourage investment. Depreciation is a non-cash charge that is recorded as an expense, reducing the taxable income. There is no cash outlay for depreciation, and no money is transferred to any fund or account. It is worth noting that most regulatory frameworks only allow for depreciation of fixed capital investments, not of total capital. In fact, working capital is not depleted and it may be entirely recovered at the conclusion of the project. In addition, if the project required the acquisition of land, the cost of the land cannot be depreciated and must be subtracted from the fixed capital cost since land is considered to keep its value. Different depreciation methods can be set by the law; the most common are the Straight-line and Double declining balance. A difference in the way depreciation is allowed, results in a slight discrepancy of the taxable income along the years.

2.4.2 Profitability Indicators

On the basis of what discussed so far, the choice of the particular profitability indicator depends on the context of the analysis as well as on the level of the detail required. This indicators are often the scalar quantity upon which process optimization is based. Some of the most popular profitability indexes are reported as follows:

- **Payback-time (PB)**
  The payback, also called pay-off period, is defined as the period required to recover the original investment through the accumulated net cash flows generated by the project. A simple method for estimating the payback time is to divide the total initial capital (fixed capital plus working capital) by the average annual cash flow:

$$PB = \frac{FCI}{Revenues - COM_d} \tag{2.4.3}$$

This is not the same payback time indicated by the cash flow diagram, as it assumes that all the investment is made in year 0 and revenues begin immediately. For most chemical plants projects, this is not realistic as investments are typically spread over 1 to 3 years and production may not reach the design capacity until the second year of operation. This simple approach also neglects taxes and depreciation. However, this indicator is particular convenient for effective comparison of plant configurations at low level appraisals. For this reasons, it was selected to be the index of reference for CORO estimations. The purpose of the optimization is to minimize this objective function by varying the degrees of freedom.
A short payback period corresponds on average to a high annual net cash flow, whereas a long payback period would imply that the ratio between the annual net cash flows and the initial investment is relatively poor. The reciprocal of the payback period can therefore be used as an appropriate measure of the profitability of an investment.

- **Net Present Value (NPV)**
The net present value of a project is defined as the value obtained by discounting, at a constant interest rate and separately for each year, all annual cash inflows throughout the life of a project.

$$NPV = \sum_{n=0}^{n=t} \frac{CF_n}{(1+i)^n} \tag{2.4.4}$$

where n represents the year, t is the time of activity of the plant and i is the interest rate applied to account for time value of money. This index can be also referred to as DNPV (Discounted Net Present Value).
This indicator can be very useful in advanced stages of an economic analysis as it is based on a comprehensive cash flow analysis; which, in turn, includes properly all the factors that could affect the economic success of the project. The disadvantage is that this type of index depends on projected cash flows that could be collected as far as 20-25 years (average plant life in chemical industry) from the time of the decision. Therefore accurate forecast of market for the raw materials, utilities and products of the plant are crucial for the reliability of the indicator.

- **Return On Investment (ROI)**
To calculate ROI, the benefit (or return) of an investment is divided by the cost of the investment. The result is expressed as a percentage or a ratio:

$$ROI = \frac{Net\,Income}{TCI} \times 100\% \tag{2.4.5}$$

ROI is a popular metric because of its versatility and simplicity. Essentially, ROI can be used as a rudimentary gauge of an investment profitability and it is applicable to a wide range of situations. However, in this formulation the time to recover the investment is not considered. This may produce inaccuracies: logically, between two investment having the same ROI, the one to prefer would be the one that guarantees the return in the shorter time. To avoid this problem, the following expression can be considered:

$$ROI = \frac{Cumulative\,Net\,Profit}{Plant\,Life \times Initial\,Investment} \times 100\% \tag{2.4.6}$$

In this way, the time factor is included: the sooner the investment is recovered, the higher the ROI.
To have an even more appropriate appraisal, one could use the NPV, which accounts for differences in the value of money over time, instead of the net profit.

In addition to profitability indicators, a thorough study should account for the impact of uncertainties in the forecasts on the viability of a project. As a matter of fact, the economic analysis of a project can only be based on the best estimates that can be made of the investment required and the cash flows. The actual cash flows achieved in any year will be affected by changes in raw materials costs and other operating costs and will be very dependent on the sales volume and price. A sensitivity analysis is a way of examining the incidence of this volatility. To begin the study, the investment and cash flows are computed using the most likely values for the individual components; this provides the base case for examination. The various parameters of the cost model are then modified one at a time, assuming a range of error for each element. This will point out how vulnerable the cash flows and economic criteria are to mistakes in the predicted figures. A sensitivity analysis gives some idea of the degree of risk involved in making judgments relying on certain forecasts (Towler and Sinnott, 2008).
Ultimately, alongside economic performances, many other factors have to be considered when evaluating projects, such as the following:

1. Safety;
2. Environmental problems (waste disposal);
3. Political considerations (government policies);
4. Location of customers and suppliers (supply chain);
5. Availability of labour and supporting services;
6. Corporate growth strategies;
7. Company experience in the particular technology.

These factors can have a major weight in the decision making process, possibly diverting the choice toward the less profitable solution.
With the objective of developing a tool that can be useful in a wide variety of cases, the choice has been to restrain the focus on economic performances and leave the more specific consideration to the user. It is clear, that whatever result obtained from the CORO has to be used as support to a wider analysis. Extrapolation may result in non-optimal decisions.

Chapter 3

Capex/Opex Robust Optimizer

Throughout this chapter, the actual implementation of the CORO is discussed. The separate layers of the application are individually presented, with a particular focus on the interface between them. The solutions implemented to overcome the complication that arose in the production and the practical arrangements made to ensure the proper functioning are closely depicted, providing, in some cases, the relative source code.
At this stage, it should be clear to the reader that the final purpose of the present thesis work is the development of a system application capable of performing cost estimation and of optimizing industrial processes, drawing the apposite information from the corresponding simulation flowsheet, previously designed in a process simulator. Nevertheless, the produced application has to respect some fundamental specifications. Particularly, the characteristics that the software is expected to have are:

- **Accessibility**: with the objective of building a user-friendly application, most of the information and instructions are displayed in an Excel workbook. In this way, the user can have a functional experience without the need to consult the user guide or to utilize impractical ways to interact with the application such as the command prompt.

- **Effectiveness**: the software has to produce accurate results in a reasonable amount of time for the required task.

- **Flexibility**: the algorithm must be adaptable to every flowsheet simulation developed in Aspen HYSYS. Users can change input options such as working hours of the plant, CEPCI index, and cost and nature of utilities to better tailor the cost estimation on the specific project. Moreover, the degrees of freedom are not limited to some classes; on the contrary, the user can choose any valid independent variable to carry out the optimization.

- **Comprehensiveness** in cost estimation: the assessment includes all the relevant expense items to be covered in an industrial project. As a consequence, the optimization is not limited to the minimization of a single class of costs but aims at optimizing a comprehensive economic index such as the payback time.

- **Robustness**: ability to provide a solution to the optimization problems, despite their particular formulation or their complexity.
- **Compatibility**: the product must provide a framework such that different process simulators can be attached to the tool without the necessity of rebuilding the whole application.

This section is intended to provide the necessary information to understand the logic and the functioning of the software. In this perspective, the discussion begins with an overview of the structure of the application.

3.1 Application Structure

The structure of the software is schematically represented in the flow diagram of figure 3.1. The prerequisite for the program to work is a functioning simulation compatible with Aspen HYSYS V10. The general procedure to build a serviceable simulation has been described in section 1.1.
The functionalities of the CORO are essentially two: cost estimation and process optimization. In the first case, the black lines of the diagram map out the procedures progressively executed to produce an assessment of the economics of the process. Specifically, by means of an Excel file, the user has to select the economic library of reference and specify the name of the simulation case that has to be analyzed. By activating a specialized routine, the data are extracted from the simulation and reported in the dedicated worksheets of the Excel workbook. Here, the user can browse through the available worksheets containing the different information and set the parameters essential for the economic estimation, this set of information is labeled as *'User Options'* in the flow diagram. Such input completes the details belonging to the *'Data for cost estimation'* block which comprises all the data necessary to estimate capex, opex, revenues and compute a payback time for the investment. Once such information is available, the Capex/Opex estimation can be initiated through a dedicated macro in the workbook. In particular, the macro retrieves and organizes in the *Buffer file (.XML)* all the information to be given as input to the CORO function, which is successively invoked. Such function executes the estimation of economic nature and produces an output to be read in the '*Economics Worksheet'*. A text file reporting the warnings eventually generated by the program is provided. For instance, if for some reason, the cost of the equipment results to be negative, the program will automatically set the cost variable to 0 and produce a warning line to notify the user that the input information is probably incorrect or senseless.
In the case the user chooses to exploit the optimization tool, the steps to produce the cost estimation are obviously still executed as the optimization has an objective function that is economics-related. Additionally, the steps linked to the red lines are launched in order to iterate over different values of the degrees of freedom, while respecting the constraints that are given by the model of the simulation. At each iteration a slightly new cost estimation is performed, until the optimization converges to the global optimum for the process.

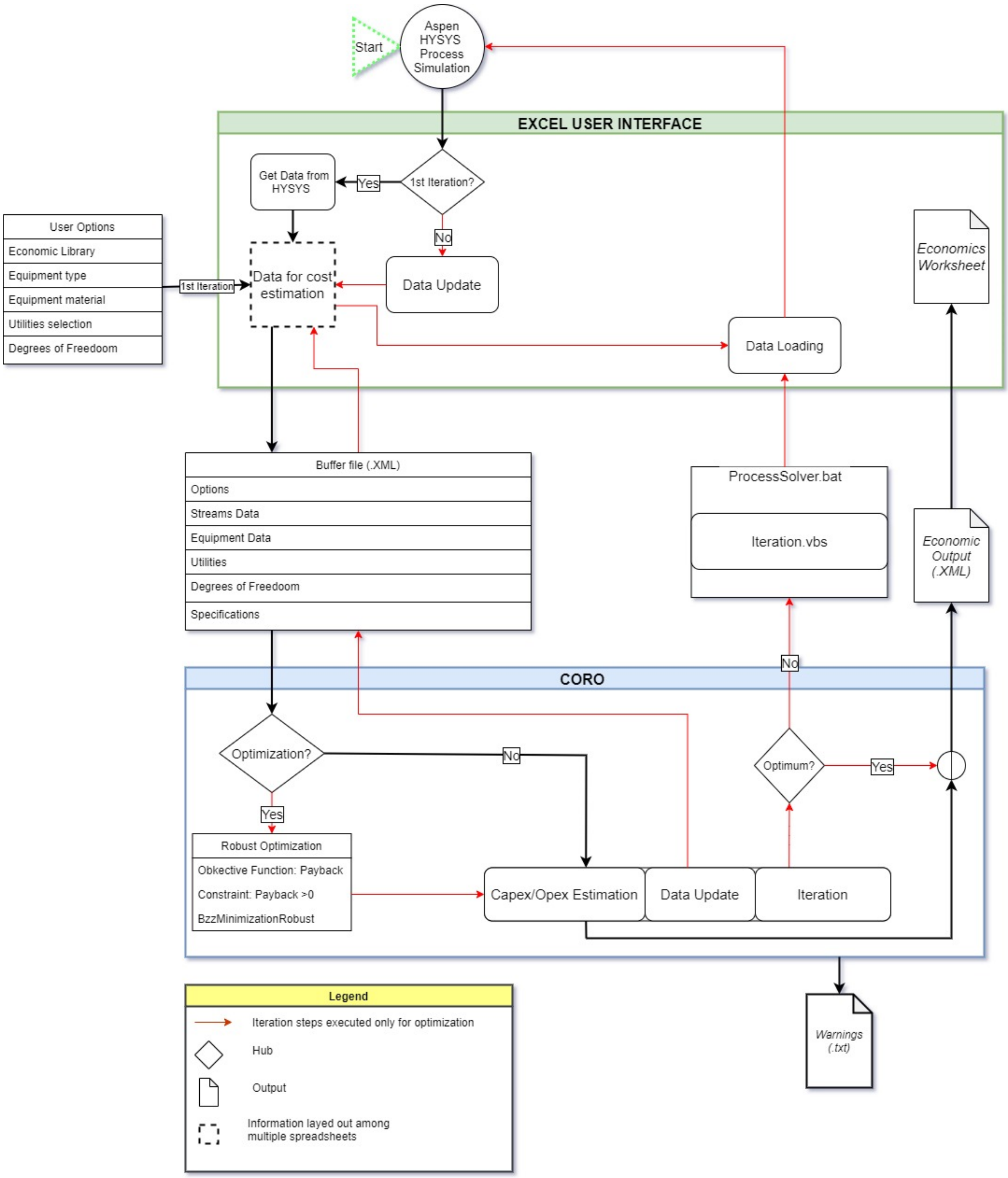

Figure 3.1: CORO algorithm

The hub that determines the main branching of the algorithm is marked as *'Optimization?'*. The program distinguishes whether the user desires to optimize the process or to simply obtain an economic estimate by analyzing the number of the Degrees Of Freedom (DOF):

- If DOF=0 the program just calls an auxiliary method that implements the factorial estimation, yielding a prediction of capital costs, operating expenses, revenues generated by the process and corresponding payback time.
- If DOF>0 the optimization routine is summoned.

The optimization proceeds thanks to a minimization function provided by a third-party library: BzzMath (Buzzi-Ferraris and Manenti, 2013). This function firstly computes the objective function at the initial conditions, then assigns new values to the DOFs, which are subsequently transferred to the process simulator (by passing through the Buffer file). The alteration in some design parameter determines a change for potentially all the data of the process, thus, after the resolution of the material and energy balances done by the simulation software, the data have to be updated and fed to the cost estimation function. The re-evaluation of the process economics allows the optimization function to understand how those alterations impacted the objective function. The cycle is repeated until the optimization converges to a point where the payback time is minimum. Once this condition is satisfied, the economic output can be consulted in the dedicated worksheet. Moreover, the set of values of the DOFs that guarantee an optimal economic performance are already loaded in the simulation and available in the CORO workbook.
Overall, as it has been emphasized in figure 3.1, the application is designed in a two-layer architecture. The first is represented by the Excel User interface, which allows the extraction of the data from the simulation, through dedicated macros developed in VBA language, and the interaction with the user. The second layer consists of the CORO function, enclosed in a Dynamic Linked Library (DLL), and is responsible for the data processing and for the logical operations that allow the optimization. The advantages brought by this kind of design are mainly two:

- The possibility to exploit the data processing layer with a different process simulator, since that part of the program has no direct interaction with the CPSS.
- The distinction between the functionalities avoids overburdening the CPU and the RAM as the data processing layer is only loaded when needed.

Further details on each of the layers are presented in the following paragraphs.

3.2 Excel User Interface

The interaction with the software is entirely managed from an Excel workbook, called 'CORO2.0.xlsb'. Through this file, the user can:

- Insert the information necessary to create a new case study.

- Specify the additional details to increase the accuracy of cost estimation and set the DOF for process optimization.
- Launch the macros performing the operations.
- Read the results obtained and gain useful knowledge on the economics of the process and, where desired, on its optimal operating conditions.

The choice of providing a user interface in Excel is dictated by the need to make the tool accessible to people who do not necessarily master process simulation software, nor have the required skills to properly interact with the software by means of the command prompt. In this perspective, Excel represents the most logical solution, as it is a familiar tool for everyone and offers spreadsheet functionalities that allow the display of information to be structured and clear.
Since this block of the software is the one that has a direct interface with the CPSS, it is also the one that has to be redesigned whereby, in future development, the tool will have to support a different process simulator. However, one can think of using the same workbook and the same logic structure, just modifying the syntax to retrieve data from the particular process simulator software. In this phase, the compatibility of the specific software with Excel would have to be taken into account. Anyhow, most of the software provides a library that can be imported and used through VBA Excel.

3.2.1 Data extraction

Figure 3.2 shows the upfront worksheet of the Excel User Interface.

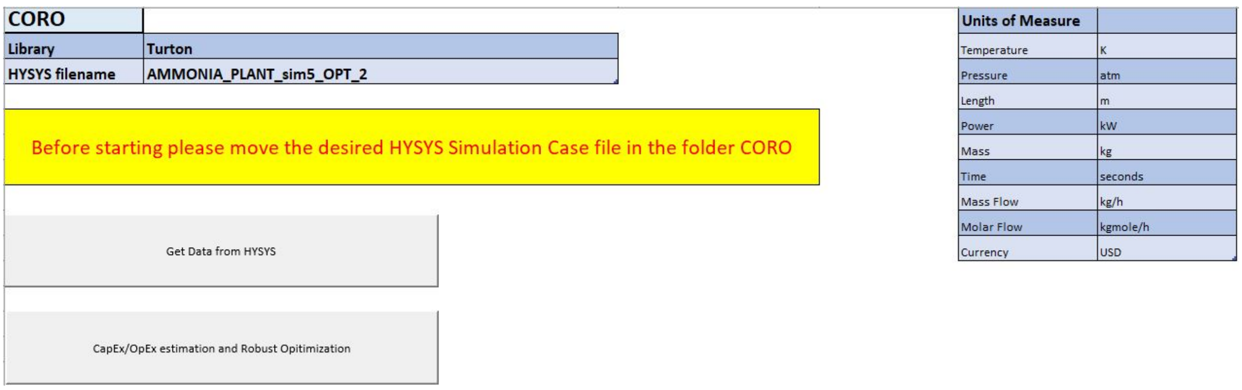

Figure 3.2: CORO starting Worksheet

Here, the user can specify the name of the simulation case to study, Units Of Measurement (UOM) and the economic library of reference for the cost estimation. The available options are the library developed by Turton *et al.*, 2012 and the one provided by Peters and Timmerhaus, 2001. The differences in the two approaches have been explicitly stated in chapter 2.
As regards the UOM, the applicable alternatives are displayed by means of drop-down lists

similar to that shown in Figure 3.3, so that the user knows which units are supported and cannot specify invalid options. The same strategy has been adopted whenever the user can modify a field whose valid values are limited to a finite list.

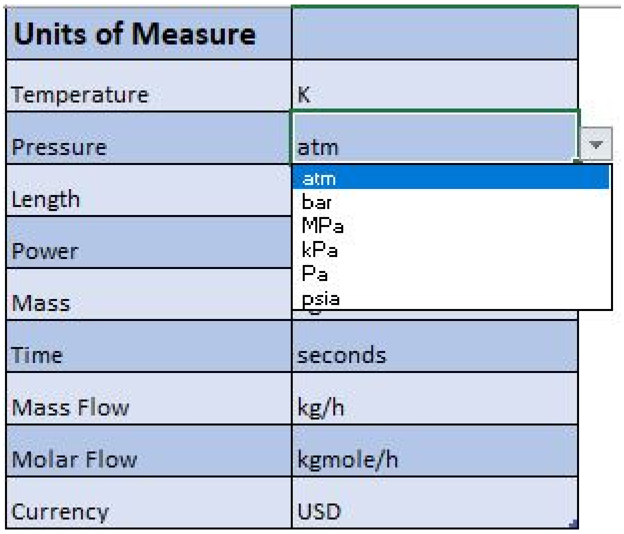

Figure 3.3: drop-down menu for preference selection

Once this set of input is given to the program, the routine attached to the button *'Get Data from HYSYS'* can be launched. This macro retrieves the simulation file (.hsc) from the folder and extracts the data of interest for assessing the related expenses. It is worth noting that, the specific data to draw out can change according to the selected methodology for the cost estimation. An explanatory example is given by the characteristic dimension of a pump: Turton bases the estimation of this equipment cost on the shaft power $[kW]$, whereas Peters and Timmerhaus consider the volumetric flowrate $[m^3/s]$ of liquid to process. For this reason, the selection of the library to use for cost estimation has to be done before the data are collected.

The two main information classes of interest are: material streams properties, to assess operating expenses and revenues from sales; equipment technical characteristics, to assess capital expenses. Consequently the *GetData* routine mostly consists in the respective loops. The source code that implements the first cycle is reported in Figure 3.4. Firstly, the object contained in *hyCase.Flowsheet.MaterialStreams* is assigned to the variable *hyStreams*. This object consists in an array of objects which are the singular material streams; each stream has a set of attributes. The attributes of interest for a process stream are name, mass flow, molar flow, temperature and pressure. It can be observed that all the process information are retrieved using the built-in *GetValue* method which allows specifying the desired UOM for the quantity by giving in input a parameter of type String. In this particular case, the strings *MassFlow_uom*, *MolarFlow_uom*, *T_uom* and *P_uom* have been previously initialized with the values established by the user in the 'User Options' worksheet.

Furthermore, additional fields are set out in order to allow external specifications for the

```
Set hyStreams = hyCase.Flowsheet.MaterialStreams
i = 0
For Each hyStream In hyStreams
    Cells(2 + i, 1).Value = hyStream.name
    Cells(2 + i, 2).Value = hyStream.MassFlow.GetValue(MassFlow_uom)
    Cells(2 + i, 3).Value = hyStream.MolarFlow.GetValue(MolarFlow_uom)
    Cells(2 + i, 4).Value = hyStream.Temperature.GetValue(T_uom)
    Cells(2 + i, 5).Value = hyStream.Pressure.GetValue(P_uom)
    Cells(2 + i, 6).Select
        Selection.Validation.Add Type:=xlValidateList, AlertStyle:=xlValidAlertStop, Operator:= _
        xlBetween, Formula1:="='Turton''s Codes'!$V$2:$V$7"
        Selection.Value = "1-Process stream"
    Cells(2 + i, 7).Select
        Selection.Value = 0
    Cells(2 + i, 8).Select
        Selection.Validation.Add Type:=xlValidateList, AlertStyle:=xlValidAlertStop, Operator:= _
        xlBetween, Formula1:="='Turton''s Codes'!$J$1:$J$2"
        Selection.Value = "No"
    Cells(2 + i, 9).Select
        Selection.Validation.Add Type:=xlValidateList, AlertStyle:=xlValidAlertStop, Operator:= _
        xlBetween, Formula1:="='Turton''s Codes'!$M$15:$M$17"
        Selection.Value = "F"
    Cells(2 + i, 10).Value = 0
    Cells(2 + i, 11).Value = 0
    i = i + 1
Next hyStream
Set hyStreams = Nothing
Range("A2").CurrentRegion.Select
    Selection.NumberFormat = "0.0000"
```

Figure 3.4: Loop to extract Material Streams properties

streams. Particularly, the user can indicate:

- **Type** of stream: the default value is set to *1-Process stream*, which identifies a stream generated and converted inside the battery limits of the plant or section of the plant studied. Other types of stream refer to input/output flows and can be of different nature; the options in the correspondent drop-down list include: *2-Raw stream*, *3-Product*, *4-Waste*, *5-Fuel* and *6-Utility*. This information is crucial for the estimation of the operating expenses.

- **Cost** $[USD/kg]$. This data is relevant only if the stream is entering or exiting the battery limits of the plant, therefore for streams whose type is between 2 and 6 in the aforementioned list. It is implied that the cost set for the material stream influences the revenues term if the streams represent a product, the opex term otherwise.

- **Degree of freedom**. It is set to *No* by default. In case an attribute of the correspondent stream can be changed to impact the economics of the process, this field should be changed to *Yes* by the user. It is hereby reminded that, if there is at least one DOF, the optimization is automatically performed by the CORO.

- **Optimization variable**. Wherein the field DOF is set to *Yes*, the particular attribute of the stream to be changed has to be set. The alternatives are: flowrate (F), temperature (T) or pressure (P).

- **Lower limit** for the optimization, significant only if 'Degree of Freedom?' is set to *Yes*. It is a required data for the optimization as the minimization function needs a range which the DOF can span.

- **Upper limit** for the optimization: represents the maximum value at which the specified design variable can be set.

Figures 3.5 and 3.6 show the table in which that information are registered in the dedicated worksheet, called 'Material Streams'. From there, the user is required to modify the default values where appropriate.

	A	B	C	D	E
1	Material Streams	Mass Flow [kg/h]	Molar Flow [kgmole/h]	Temperature [K]	Pressure [atm]
2	Feed	35876.7577	1550.0000	353.1500	3.9477
3	bypass	7175.3515	310.0000	353.1500	3.9477
4	to flash	28701.4061	1240.0000	353.1500	3.9477
5	purified	28271.3064	1216.1269	298.2908	0.9869
6	liquid	430.0997	23.8731	298.2908	0.9869
7	cooled to flash	28701.4061	1240.0000	313.1500	3.9477
8	laminated to flash	28701.4061	1240.0000	298.2908	0.9869
9	waste	430.0997	23.8731	334.7308	0.9376
10	feed2	7175.3515	310.0000	348.1500	3.8983
11	Additive	7650.1081	150.0000	343.1500	2.9363
12	mixed	14825.4596	460.0000	344.7751	2.9363
13	cooled	14825.4596	460.0000	293.1500	2.8870
14	vapour	13483.0177	411.9988	293.1500	2.8870
15	liq	1342.4419	48.0012	293.1500	2.8870
16	heated vapour	13483.0177	411.9988	313.1500	2.8870
17	sour natural gas	25628.0225	1010.3125	303.1500	54.2808
18	Partially purified	14244.4340	725.8724	210.0859	49.3462
19	bottom	11383.5885	284.4401	283.0728	49.4449
20	Solvent In	204166.0004	2000.0000	333.1500	60.1000
21	Gas In	6588.4876	304.5114	333.1500	60.1000
22	Gas Out	2798.3097	170.1069	333.4235	60.1036
23	Bottom liquid product	207956.1783	2134.4045	334.8983	60.1000

Figure 3.5: Material Streams part 1

The second major loop present in the macro is the one programmed to retrieve technical characteristics of all the equipment. This cycle is more complicated than the former one as each unit operation is represented by a different kind of object which has completely different attributes and methods. For this reason, a conditional statement, which allows to distinguish the instruction to be executed from case to case, is enclosed in the 'for'

F	G	H	I	J	K
Type	Cost [USD/kg](Insert only for input/output streams)	Degree of Freedom?	Optimization Variable	Lower limit	Upper limit
2-Raw stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
3-Product	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
4-Waste	0.0000	No	F	0.0000	0.0000
2-Raw stream	0.0000	No	F	0.0000	0.0000
6-Utility	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
1-Process stream	0.0000	No	F	0.0000	0.0000
6-Utility	0.0000	No	F	0.0000	0.0000
6-Utility	0.0000	No	F	0.0000	0.0000
3-Product	0.0000	No	F	0.0000	0.0000

Figure 3.6: Material Streams part 2

loop. Figure 3.7 shows a simplified code snippet for clarification. In this case, *unitClass* is the vector containing the classes of the equipment. At each iteration, the 'Select Case' statement compares the string *unitClass(k)*, also called 'test expression', with the strings identifying the different possibilities (expression list), once a match is found, the particular instructions for that event are carried out and the program exits the 'Select Case', to re-enter for the next value of k. The 'Case Else' clause is used to indicate the instructions to be executed if no match is found between the test expression and the expression list. In the CORO, whenever a unit belongs to a class that is not supported, its name is reported in a worksheet called 'Neglected Units'. Often, the classes of the equipment not considered for cost estimation are objects which do not have correspondent real equipment. In fact, HYSYS classifies manipulator objects as 'Operation', therefore, when performing a loop on all the 'Operations' of the flowsheet, such elements are not differentiated from the real unit operations. Regarding all the other equipment, the data extracted are laid out in multiple spreadsheets. In particular, in order to make the data easy to find, each class of equipment has a dedicated worksheet, where the user can read the obtained data and specify details on the units following the instructions provided in the opposite block. The complete list of the supported equipment and the correspondence between the HYSYS objects and unit operations included in the economic libraries are reported in Appendix A.
Figure 3.8 shows part of the worksheet dedicated to compressors. It can be observed that each table corresponds to a single compressor, having a set of features. More specifically, the information taken from the simulation are *Shaft Power* and *Pressure*, whilst the other attributes have been placed and set to default values through the macro in order to let the user add details.

```
For k = 0 To countUnits - 1
    Select Case unitClass(k)
            Case "Heat Exchanger"
                ...
            Case "Heater"
                ...
            Case "Cooler"
                ...
            Case "Air cooler"
                ...
            Case "LNG"
                ...
            Case "Plate Exchanger"
                ...
            Case "Compressor"
                ...
            Case "Pump"
                ...
            Case "Valve"
                ...
            Case "Distillation"
                ...
            Case "Separator"
               ...
            Case "Absorber"
                ...
            Case "Cont. Stirred Tank Reactor"
                ...
            Case "Plug Flow Reactor"
                ...
            Case "Conversion Reactor"
                ...
            Case "Equilibrium Reactor"
                ...
            ...
            Case Else
               ...
    End Select
Next k
```

Figure 3.7: Simplified code: Select Case in for loop

As mentioned before, each case implements a different set of instructions; since it would be impossible to present all the individual procedures, the most comprehensive case is

	A	B
1	**In this worksheet the following HYSYS units are reported: Compressor**	
2		
3		
4	**K-107**	(Compressor)
5	Type	1-Centrifugal
6	Shaft Power	141.96
7	Pressure	1.94
8	Material	1-CS
9	Optimize?	No
10	Optimization Variable	P
11	Lower limit	
12	Upper limit	
13		
14	**K-108**	(Compressor)
15	Type	1-Centrifugal
16	Shaft Power	2837.06
17	Pressure	5.32
18	Material	1-CS
19	Optimize?	No
20	Optimization Variable	P
21	Lower limit	
22	Upper limit	

Figure 3.8: Compressors Worksheet

shown: Distillation Column. Figure 3.9 reports the actual VBA code executed whenever the equipment belongs to the class of 'Distillation'. Firstly, there is a control to check if it is the first piece of equipment to be added to the worksheet 'Towers'. If that is the case, the worksheet is created and the formatting is done, otherwise, the worksheet already exists and it is just activated. Then, in order to access particular information such as 'Tray spacing' and Column 'Diameter', a special type of variable is needed, a backdoor variable. Through this variable, it is possible to access attributes that are not available otherwise. Once all

```
Case "Distillation"
    If Col_count = 0 Then
        ActiveWorkbook.Sheets.Add After:=ActiveWorkbook.Worksheets("Equipment")
        ActiveSheet.name = "Towers"
        ActiveWindow.DisplayGridlines = False
        Range("A1").Value = "In this worksheet the following HYSYS units are reported:
        _Distillation Column, Blank Column, Separator, Absorber, Tank"
        Call format.Title
    Else
        Worksheets("Towers").Activate
    End If

    Set hyColumn = hyCase.Flowsheet.Operations.Item(k)
    Set colFS = hyColumn.ColumnFlowsheet
    Set colBD = colFS

    Col_Trayspacing = colBD.BackDoorVariable
    _("TraySection.507.0/TrayStageData.550:Length.204").Variable.GetValue("m") * L_cf
    Col_D = colBD.BackDoorVariable
    _("TraySection.507.0/TrayStageData.550:Length.210").Variable.GetValue("m") * L_cf
    Col_N = colFS.ColumnStages.count - 2
    Col_RR = colFS.RefluxRatio
    Col_H = 1.05 * (Col_N * Col_Trayspacing) * L_cf
    Col_V = 3.14 * Col_D ^ 2 / 4 * Col_H
    Col_AT = 3.14 * Col_D ^ 2 / 4
    Col_P = hyColumn.BtmLiquidProduct.Pressure.GetValue("atm") * P_cf
    Qcond = hyColumn.ColumnFlowsheet.EnergyStreams.Item(0).HeatFlow.GetValue("kW") * Power_cf
    Qreb = hyColumn.ColumnFlowsheet.EnergyStreams.Item(1).HeatFlow.GetValue("kW") * Power_cf
    Call towers.Towers_Sheet(unitMatrix(2, k), unitMatrix(1, k), Col_count,
    _Library, Col_V, Col_P, Col_D, Col_AT, Col_N, Col_RR, Col_H, Qcond, Qreb)
    Col_count = Col_count + 1
```

Figure 3.9: Distillation Column data *GetData* macro

the data have been extracted, an auxiliary function that manages the correct display of information is called. In the present case, the function 'Towers_Sheet', belonging to the module 'towers'. This method requires a set of parameters which basically correspond to all the data that have to be printed in the worksheet. Lastly, the variable counting the number of columns in the worksheet is updated. Additional instructions relative to the addition of a heater and a cooler corresponding to reboiler and condenser of the column are implemented but not shown in this figure. More particular information on the treatment of these units

are provided in the next paragraph.
The same approach seen for the class ‘Distillation’ can be generalized for all the units, with the due adjustment to be made due to differences in the data to be extracted and structure of the objects.
It is worth highlighting that it is not mandatory for the simulation case to be opened at the invocation of *GetData* sub-routine. However, the performances of the program are considerably affected, as the time of loading the CPSS is usually large. A drawing of data of a simple simulation takes around 2 seconds if Aspen HYSYS is already running in the system, whereas more than 15 seconds are needed if the simulation software has to be launched at runtime.

3.2.2 Plant details Input

Upon extraction of the data related to the simulation, the user has the possibility to add specific information about the process plant which are relevant for cost estimation. Without this input, the macro used sets all the additional information to default values, therefore the resulting estimation would not be accurate. Particularly, the user can update the following details:

- Material Streams data, as it can be seen from Figures 3.5 and 3.6.
- Materials of construction and specific type for each equipment. The information on the possible values for these fields are accessible through a drop-down list associated to the cell where the detail has to be specified.
- Degrees of freedom for the optimization. It is important to remark that, whenever a DOF is introduced, also the limits within the variable can change have to be set. To add flexibility, the DOF can be set not only to parameters of streams but also to specifications of the unit operations. This feature is particularly useful for optimization of distillation columns. The number of DOF the user can select is not limited; however, as one might imagine, the time to perform the optimization increases exponentially with the number of independent variables.
- Utilities used in heaters and coolers.

The last point represents a particular issue and deserves to be covered in more detail. As a matter of fact, Aspen HYSYS allows the user to insert units called ‘heaters’ and ‘coolers’, which are heat exchangers in which the utility fluid employed to heat-up or cool down the process stream is not specified: the process simulator only evaluates the duty to be given or removed to the material stream. The same approach is used when including reboilers and condensers in distillation columns. It is clear that such methodology does not allow to represent an heat exchanger with a rigorous model; consequently a proper sizing of the unit cannot be done, impairing the possibility to carry out an estimation of both capital and operating costs.
The problem of not having an heat transfer area for the exchanger is solved in the phase

of pulling of the data. Specifically, when heaters or coolers are encountered, the program extract all the information useful to implement Equation 3.2.1

$$Area = \frac{Q}{U \cdot LMTD \cdot Ft} \tag{3.2.1}$$

Where Q is the duty taken from the simulation. U is the global heat transfer coefficient estimated by looking at the temperatures and the states of the process stream at the inlet and at the outlet and assigning a suitable utility depending on these information. The $LMTD$ is evaluated knowing the temperature of the assigned utility. Finally, the correction factor Ft is simply assumed to be 0.9 as its computation would require a rigorous design.
After having executed this auxiliary instructions, the heat exchanger is reported in the dedicated sheet displaying the evaluated Heat transfer area and the pressure at which operates; so that the estimation of its cost can be performed normally. It is worth emphasizing that this same commands are recalled for reboilers and condenser of columns.
On the other hand, the solution to the problem of evaluating the opex is reported in Figures 3.10 and 3.11. This worksheet constitutes an important support to the correct

HEATING	T [k]	Latent Heat Of Vaporization [kJ/kg]	Cost [$/kg]
LP STEAM (6 bar)	433.00	2508.03	0.027700
MP STEAM (11 bar)	457.00	1998.55	0.028310
HP STEAM (42 bar)	527.00	1697.79	0.029970

COOLING	Tin [K]	Tout [K]	ΔT [K]	cp [kJ/kg/K]	Cost [$/kg]
Cooling water	293.00	303.00	10.00	4.1860	0.0000148

Working Hours per year	8760
TOTAL UTILITIES COST [USD/year]	233,448.89

COLD UTILITIES

Unit	Duty [kW]	Utility	Flowrate [kg/s]	Utility cost [USD/kg]	Annual cost [USD/year]
E-101	1089.49	1-Cooling water	26.02705818	0.0000148	12,147.68
E-102	942.85	1-Cooling water	22.52390097	0.0000148	10,512.64
Condenser_T-100	2095.73	1-Cooling water	50.06518277	0.0000148	23,367.06
E-105	706.62	1-Cooling water	16.88054183	0.0000148	7,878.70
Totale					**53,906.09**

Figure 3.10: Utilities worksheet part 1

Instructions:
- This worksheet is done to estimate cost of the utilities related to heaters and coolers units.
-The total OpEx are NOT the sum of cold, hot utilities and electricity. Depending on the selected library, different approaches are used to estimate total operating cost
-Electricity consumption is evaluated automatically in the external CORO
-The user can either custom the data relative to the standard utilities or add a different utility by selecting refrigerant/heating fluid in the Utility column and providing the required data
-Duties are always reported in [kW] in this worksheet in order to stay consistent with the other data (conversion is automatic even if the selected uom for Power is not kW). It is suggested to the user to do not change reference in this worksheet.

HOT UTILITIES

Unit	Duty [kW]	Utility	Latent Heat [kJ/kg]	Flowrate [kg/s]	Utility Cost [USD/kg]	Annual cost [USD/year]
E-103	132.58	3-LP steam	2508.03	0.052863675	0.0277	46,178.92
Reboiler_T-100	382.90	3-LP steam	2508.03	0.152669348	0.0277	133,363.88
Totale						**179,542.80**

Figure 3.11: Utilities worksheet part 2

estimation of operating expenses and adds flexibility to the tool. The solution adopted is quite simple: compute how much a certain duty costs in terms of utility by assigning an appropriate service stream to each exchanger. Therefore, in the 'Utilities' spreadsheet, a row is added to the table 'HOT UTILITIES or 'COLD UTILITIES' every time that there is, respectively, a heater or a cooler. The row reports the name of the unit and its duty, assigns a utility and calculates the required flowrate of satisfy the duty. Equation 3.2.2 reports the case of an exchanger using cooling water as service fluid.

$$Flowrate\left[\frac{kg}{s}\right] = \frac{Q\,[kW]}{\Delta T\,[K] \cdot cp\left[\frac{kJ}{kg \cdot K}\right]} \tag{3.2.2}$$

Knowing the cost of the stream, the calculation of the annual cost for that equipment becomes trivial, see Equation 3.2.3.

$$\begin{aligned} Annual\,cost\left[\frac{USD}{year}\right] &= Flowrate\left[\frac{kg}{s}\right] \cdot Utility\,cost\left[\frac{USD}{kg}\right] \\ &\cdot 3600\left[\frac{s}{h}\right] \cdot Working\,hours\,per\,year\left[\frac{h}{year}\right] \end{aligned} \tag{3.2.3}$$

The Total Utilities Cost per year is simply the sum all of the costs in the tables.
Moreover, the user can either custom the data relative to the standard utilities or add a different utility by selecting refrigerant/heating fluid in the 'Utility' column of the tables and providing the required data. The default values are cooling water when a cold utility is needed and Low Pressure steam for the heaters.
Wherein the simulation has been developed employing only process-process heat exchangers and all the utilities are included in the flowsheet, their cost can be set in the 'Material Streams' table, so there is no need to use the 'Utilities' worksheet, which will be empty. This solution ensures flexibility as the user can have a reliable cost estimation even if the simulation was not designed with total accuracy.
On the basis of what presented so far, it is clear that the routines implemented in the Excel workbook are not exclusively dedicated to data retrieving and visualization, but implement some auxiliary functions to provide robustness and accuracy to the CORO. By means of such functions, the data that are given to the data-processing layer are always meaningful and complete.

3.2.3 Interface between software layers

The interface between the user interface and the data processing layer is managed by means of an XML (eXtensible Markup Language) file. This file is pivotal for the logic of the tool as it allows to have the information well ordinated in a data three and easily accessible from both layers.
After the user has specified all the desired details, the data-processing functions can be called by activating the second button on the first worksheet of the Excel workbook. When the macro connected to the button is launched, all the data to be processed in the CORO function are taken from the spreadsheets and properly disposed in tables to be exported. At

this point, a useful functionality provided by Excel allows to map each cell of such tables with a correspondent XML file. The correspondence generated by the mapping enables a simple import and export of information, which is a key feature for the iteration.
Figure 3.12 shows the structure of the XML file used in CORO. Each tag represents a node

```xml
<?xml version="1.0"?>
<rootElement xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
    <Options library="Peters_Timmerhaus">···
    </Options>
    <Streams>···
    </Streams>
    <UnitsList>···
    </UnitsList>
    <Utilities opex="233448.887057885" />
    <Specifications>···
    </Specifications>
</rootElement>
```

Figure 3.12: XML file storing plant data

that can have attributes and child nodes. This arrangement permits to store information and to easily retrieve them. Specifically, all the nodes are child of the ‘rootElement’, and each node has child nodes or attributes depending on the data to forward. A brief description of the nodes structure is reported as follows:

- **Options**: comprise all the parameters related to economic libraries and units of measurement. The attribute of this node specifies the methodology selected for cost estimation.
- **Streams**: has a set of child nodes corresponding to the single material streams; each of them includes all the attributes specified in the workbook.
- **UnitsList**: this node wraps all the nodes for the equipment. In order to have a well-structured table, all the equipment have the same number of attributes. If a certain attribute does not belong to a class of unit, its value is automatically set to 0.
- **Utilities**: has only one attribute corresponding to the opex of utilities computed as shown above. This costs have to be added to the other operating expenses such as cost of electricity and cost of labour.
- **Specifications**: this nodes incorporates all the nodes reporting a specification for a unit operation.

The same approach has been used to forward the economic results obtained in the data processing layer to the Excel workbook, so that the user can visualize them in tables of dedicated worksheets.

It is suggested to not directly change data in this type of files, as incorrect syntax could invalidate the document object model resulting in premature termination of the program.

3.3 Data Processing Layer (C++)

The level of data-processing of CORO has been developed in C++ language. The choice of such programming language is driven by the advantages connected with it: portability, flexible memory management, fast system application and, most of all, Object-oriented programming (OOP). Moreover, being C++ popular, many useful libraries are available to be exploited. In this particular case, the 'BzzMath' library developed by Buzzi-Ferraris and Manenti, 2013, has been used to implement the robust optimization, 'pugixml' library allowed to facilitate the access to XML files and 'magicenum' library has been employed to ease the operations with enumeration classes.
The features of OOP have been useful to treat the equipment as objects with their attributes and methods. The method of interest for this particular application is the equipment cost estimation. Depending on the unit, the method takes different properties as arguments and evaluates the cost on the basis of different data. Consequently, according to the category of the equipment a specific function has to be recalled. However, the differentiation between categories complicates the standardization of the equipment to a single type of object. On the other hand, it would be inconvenient to construct each object singularly. The Builder design pattern solves this problem; its structure is depicted in 3.13. Builder is a

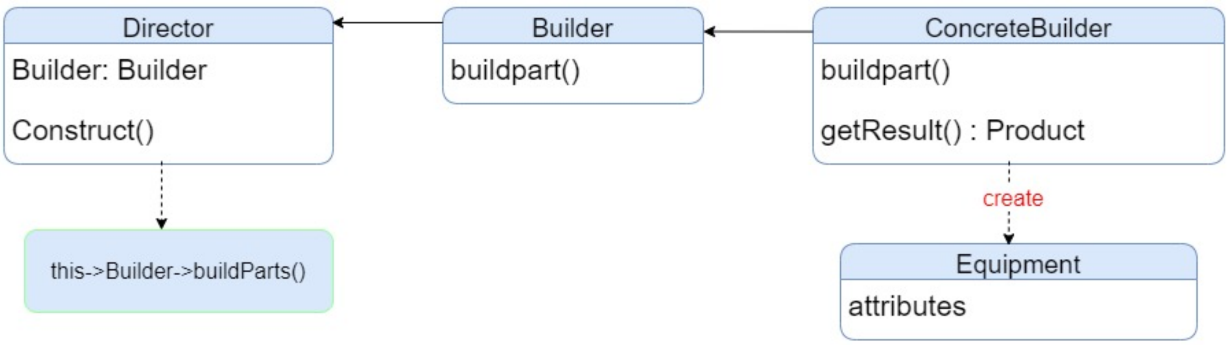

Figure 3.13: UML of Builder design pattern

creational design pattern, which allows constructing complex objects step by step. Unlike other creational patterns, Builder does not require products to have a common interface, enabling to produce different products using the same construction process. This is the case for chemical processing equipment, which differ from each other for having different attributes, not only in nature but also in number. For instance, it is sufficient to specify pressure, MOC and a characteristic dimension to estimate the cost of a compressor whereas additional parameters are required when forecasting the cost of a distillation column, such as information on its internals.
The Builder class includes methods to build different part of an item. Therefore, the

attributes of an object of type 'Equipment' are set one by one by such methods. The value to be assigned to the attribute is retrieved from the xml file by recalling a dedicated class called 'Input'. In particular, by knowing the name of the equipment and the name of the property to be initialized, the value can be easily found in the XML file.
Furthermore, the application of the design pattern allows encapsulation of all the equipment in a unique object. In this particular case, vectors data type have been employed for the necessity to add elements in a dynamic way. Thereby, iteration is simple and information is stored in an a structured way.
Following the management of the input data and the creation of the objects, the functional part of the program is implemented, namely, economic estimation and robust optimization.

3.3.1 Payback estimation function

The objective function chosen for the optimization of the processes is the payback time. As discussed above, this economic index combines capex and opex to give a measure of the profitability of the investment.
The most important distinction to be made is the methodology to use for the assessment. This information is read from the 'Options' node of the 'input.xml' file, and assigned to the string variable *library*. A check on the value of *library* directs the execution on the instructions implementing the desired approach.
According to what presented in chapter 2, the main point of factorial estimate procedures is to evaluate the cost associated to the equipment, therefore the program performs a loop between all the units, evaluates their cost and progressively updates the total equipment cost. Figure 3.14 reports the instruction executed for the evaluation of the cost of an heat exchanger with the Turton library. After having checked that the equipment i belongs to the class of heat exchangers, the apposite cost function, with the correspondent parameters, is recalled. In this function, the factors provided from the economic library are employed, together with the equations presented in the process economics chapter, to estimate a cost. The result returned by the function is assigned to the variable *Equipment_cost* which is a vector of two values: purchased cost and bare module cost. This distinction is needed in the Turton approach to estimation because the grassroots costs are evaluated on the basis of the total bare module cost. Then, a control block is inserted to check if the result obtained make sense. In the case were the cost is infinite or not a number, it is set to 0 to not compromise the entire estimation, and a warning is sent to the user. Generally, the probable cause for this kind of problem is that an input data did not make sense from a physical point of view. Finally, the cost of the exchanger is written in the economics XML file and the total costs are updated. This sequence of operation is identical for all the equipment of the plant, the only thing changing is the cost function, according to the class of the equipment.
Once the total equipment cost is known, the capital cost estimation comes down to a series of calculations considering the factors specified by the economic library.
The operating expenses, instead, are evaluated through a loop between the material streams. As explained previously, raw materials, utilities, fuels and waste flows impact the opex.

```
// Loop for the equipment cost estimation

for (size_t i = 0; i < plant_data.Units.size(); i++)
{
    if (plant_data.Units[i]->u_class == "heatExchanger")
    {
        turton::heatExchanger he;

        std::vector<double> Equipment_cost = he.cost_T(plant_data.Units[i]->type,
            plant_data.Units[i]->A * pow(Length_conv,2), (plant_data.Units[i]->P) * P_conv,
            plant_data.Units[i]->material);


        double Purchased_cost = Cost_index * Equipment_cost[0];
        double Bare_module_cost = Cost_index * Equipment_cost[1];


        if (isnan(float(Purchased_cost)) == 1 || isinf(float(Purchased_cost)) == 1)
        {
            Purchased_cost = 0;
            out.warning("Error in computing the cost of equipment: " + plant_data.Units[i]->name +
                ", check the input data");
        }

        if (isnan(float(Bare_module_cost)) == 1 || isinf(float(Bare_module_cost)) == 1){ ... }



        out.economic_output(plant_data.Units[i]->name, Purchased_cost, options::output::unit);
        Total_bare_module_cost = Total_bare_module_cost + Bare_module_cost;
        Total_purchased_cost = Total_purchased_cost + Purchased_cost;

        plant_data.Units[i]->cost = Purchased_cost;
        out.to_simulation("UnitsList", plant_data.Units[i]->name, "cost", plant_data.Units[i]->cost);

        Nnp = Nnp + 1;
    }
```

Figure 3.14: Estimation of equipment cost implementation

Thus, each time a stream belongs to one of these categories, its annual cost is evaluated and added to the opex. Through the same loop, also the revenues can be computed by considering the price of product outflows. Considering capex, opex and revenues, a payback time can be computed for the process.
This function is invoked once if only a cost estimation is required, at each iteration if the process optimization feature is exploited.

3.3.2 Robust Optimization

One of the main goals of the software is to be able to optimize a process starting from its simulation. The structure created allows to have the data needed for cost estimation from the simulation along with the input of the user specifying the DOFs on the basis of which the optimization has to be carried out. In order to ensure a robust optimization, a numerical library developed specifically for complex problems in chemical engineering, BzzMath from Buzzi-Ferraris and Manenti, 2013, has been employed. More specifically, the function 'BzzMinimizationRobust' was found to be suitable for this application. This function extends high-performance methods for solving unconstrained optimization problems to constrained minimization by applying penalty function methods. Figure 3.15 reports the instruction to call this function. Firstly, the scalar objective function y, corresponding to

```
if (optimization_name.size() == 0)
        pb = functions::payback(x0,0);
else
{
    y0 = functions::payback(x0, 0);

    if (y0 < 0)
    {
        bzzUnfeasible = 1;
        BzzError("The starting point must be feasible");
    }
    BzzMinimizationRobust m(x0, y0, functions::Optimization, xL, xU);
    m.SetTolRelF(1.e-3);
    m.SetTolRelX(1.e-4);
    m();
    m.BzzPrint("Results");
    BzzVector xSolution;              //Generating Vector where to store the solution
    m.GetSolution(&xSolution);        //saving the solution
    xSolution.BzzPrint("xSolution");

    BzzPause();
}
```

Figure 3.15: BzzMinimizationRobust exploitation

the payback time, is evaluated at the initial conditions. If the payback is negative, meaning that the yearly operating expenses outweigh the revenues from sales, the process will be certainly unfeasible. Also it would be impossible to optimize as the minimum value for the objective function will be always negative. At this point, the BzzMinimizationRobust is initialized with the object *m*. The method requires the initial values of the independent variables (*x0*), the initial value of the objective function *y0*, the function to run to adjourn it (*Optimization*), and the limits, lower and upper, for the DOFs. The data type requested to run this method is 'BzzVector', therefore, the vectors *x0*, *xL* and *xU* have been previously initialized with the values specified from the user as DOFs. The function *Optimization* simply recalls the payback estimation function presented above and checks, at every iteration if the payback time is still positive. The instruction *m();* triggers the minimization, which modifies the independent variables in order to find the conditions where the objective function is minimum; the number of iterations executed depends strongly on the number of independent variables and on the complexity of the problem.
It is clear that, in order to be able to find a minimum, the payback has to be estimated in

different points. Consequently, the simulation has to be run iteratively. This raises the issue to be able of updating the data and feed them to the process simulation software.

Iteration

As stated in the introduction to this chapter, the data processing layer is designed to be independent from the process simulation software. Therefore, the update of operating conditions is done by calling macro contained in the Excel user interface which, in turn, interfaces with Aspen HYSYS. In particular, after that the minimization function modifies the independent variables, the procedure is managed by implementing the following operations:

1. Assign the new values of the independent variables to the objects representing the information of the plant and, contextually, updating such information in the file XML containing them.

2. Call the macro of the Excel file by means of a batch file, as shown in Figure 3.16. Such macro updates the new values in the simulation, activates the solver and overwrites the XML file with the data corresponding to the new operating conditions. This step is deepened in the next paragraph.

3. The process information corresponding to the up-to-date conditions are introduced into objects exploiting again the builder design pattern.

4. The cost estimation and payback computation is executed on the basis of the new information.

This steps allow a proper simulation-based optimization and represent the way an external minimization function can be linked to a process simulation software.
It is worth emphasizing that the instructions from 1 to 3 are always enclosed in control blocks and are executed only when there is at least one degree of freedom. Therefore, they are never executed if the CORO is used just for economic estimation, avoiding to slow down this functionality.
At this point, the usefulness of having an XML file to function as vessel between the two

```
if (optimization_name.size()>0)
{
    std::filesystem::path current_path = std::filesystem::current_path();
    std::string path_string = current_path.parent_path().string();
    std::string bat = path_string.append("\\ProcessSolver.bat");
    system(bat.c_str());
}
```

Figure 3.16: Batch launch

layers can be appreciated. Furthermore, by using this system the data-processing layer has been made completely independent from the process simulation software.
To complete the discussion, the set of routines implemented in the Excel Workbook to interface with Aspen HYSYS are described

Data updating

The set of operations of interface XML/Excel and Excel/HYSYS are executed by exploiting the tables mapped with the XML file. These tables are included in a worksheet called 'XML' that is hidden from the user, as inappropriate interferences could cause the routine to stop working.
The macro called from the batch file is responsible for launching two sub-routines in series. The first is the data loading: changing the values of the independent variables in the simulation with the values provided by the optimizer. In implementing this macro, it is important to stop the solver of the process simulator before setting new values. Figure 3.17 shows how the data are loaded in HYSYS. In the particular case, the specification of

```
For Each tbl_cell In Spec_tbl.ListColumns("DOF").DataBodyRange.Rows
    If tbl_cell.Value = "Yes" Then
        opt_unit = tbl_cell.Offset(0, -4)
        u_type = tbl_cell.Offset(0, -3)
        opt_value = tbl_cell.Offset(0, -1)
        spec_name = tbl_cell.Offset(0, -2)
        If u_type = "Distillation" Or u_type = "Absorber" Then
            Set hyColumn = hyFlowsheet.Operations.Item(opt_unit)
            Set Spec = hyColumn.ColumnFlowsheet.ActiveSpecifications.Item(spec_name)
            DOF = Spec.Goal.CanModify
            If DOF = True Then
                Spec.Goal.SetValue (opt_value)
                hyCase.Solver.CanSolve = True
                hyCase.Solver.CanSolve = False
            Else
                MsgBox (spec_name & " is not a Degree of Freedom for item " & opt_unit)
                tbl_cell.Value = "No"
            End If
        End If
    End If

Next tbl_cell
```

Figure 3.17: Uploading of values in HYSYS

a column is the DOF for the optimization. Therefore, a row of the table reporting the Specifications has the value of the field 'DOF' set to *Yes*. In correspondence of that row, the required information, such as unit name, unit type, optimization value and name of the specifications are reported. Before trying to set a new value in the simulation, the program checks if that variable is modifiable, if so the new value is set and the solver is activated. In case the new value is in conflict with process conditions, the solver is not able to solve the balances; therefore, proceeds to notify the error and the optimization procedure is stopped. For this reason, it is important that the user inserts numbers having a physical meaning. This procedure is similarly implemented for DOFs corresponding to a material stream or to a design variable for an equipment.

To get the adjourned values from the process simulation, a routine similar to the one used to extract the data in the first place is employed, with the difference that the results are stored directly in the tables connected with the XML file. From there, also the values in the worksheets visible to the user are updated. Finally, the export of the values in the tables overwrites the XML file, making the new information available to the data-processing layer.

Chapter 4

Validation and Case studies

In order to give a demonstration of the functionalities of the software, in this last chapter of the thesis, the results obtained from the application of the CORO to demonstrative case studies are examined. The experiments are designed to test the functionalities of the program and to appraise its potential.
In particular, two simulations have been linked to the Capex/Opex Robust Optimizer: a tailored flowsheet, specifically designed to contain several types of equipment; an industrial case study with a complex flowsheet. For each of them, the simulation case will be described, the assumptions made stated and, finally, the outcome of the applications will represent the basis to draw general conclusions.

4.1 Case Study 1

4.1.1 Simulation

This flowsheet has been developed to test the proper functioning of the CORO, therefore, it does not represent a real industrial process. In order to obtain reasonable results, costs associated with input and output streams have been made up. As a general indication, the cost of raw materials has been assumed to be around one order of magnitude smaller than the price of the products, so that the revenues could guarantee an acceptable payback time. Moreover, the cost of waste streams has been adjusted in order to create a situation where a trade-off between maximizing the production and minimizing the operating expenses has to be found. The experiment is also useful to validate the consistency between the estimations executed on the basis of the different libraries. Figure 4.1 shows a snapshot of the flowsheet simulated in Aspen HYSYS. The simulation comprises all kinds of equipment, such as distillation columns, absorbers, flash separators, air coolers, heat exchangers, splitters, pumps, compressors and turbines. This allows to control that the CORO can manage all the cases without malfunction.

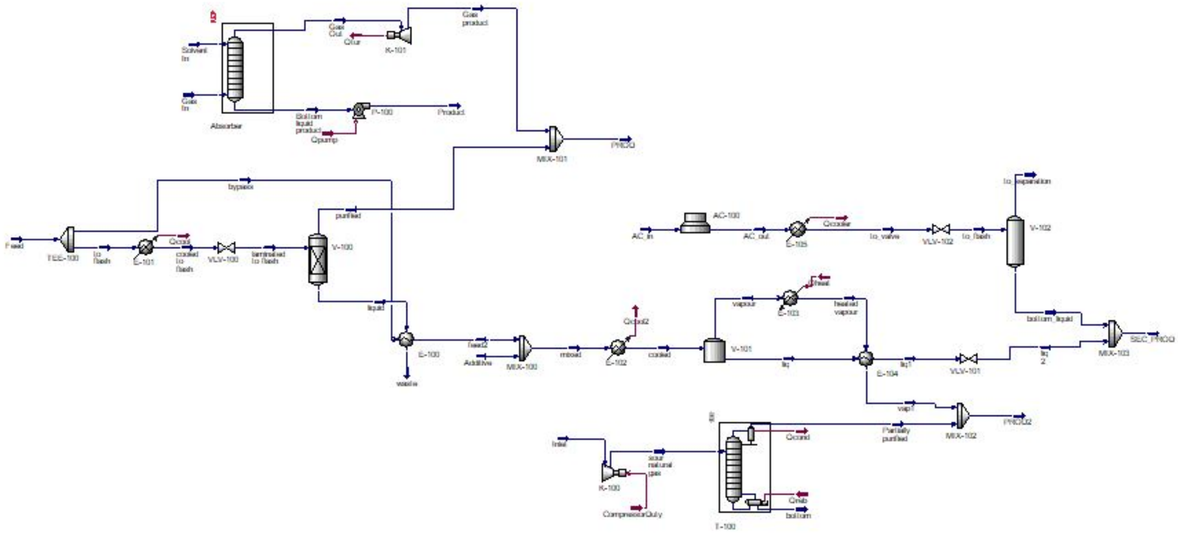

Figure 4.1: Simulation Flowsheet Case Study 1

4.1.2 Cost Estimation

In comparing equipment cost obtained from the two different economic libraries, one has to keep in mind that the two voices have a different scope:

- Equipment cost in Turton estimation refers to the module cost, which includes installation, delivery and all the direct cost associated with the machinery.
- Equipment cost in Peters & Timmerhaus estimation does not include installation, delivery, instrumentation and piping, which are computed separately. This cost refers to the simple purchase price for the piece of machinery.

For this reason, looking simply at the estimation of equipment cost it seems that the second approach heavily underestimates the expenses. In truth, the cost item that is meaningful to compare is the Total Capital Investment (TCI), which necessarily has the same significance, regardless of which methodology has been used to appraise it.
Table 4.1 reports the estimations of the cost for all the unit operations of the process, and Table 4.2 contains the final results of the assessment. Three parallel cost assessments have been carried out on the same simulation: two by using the CORO, with the different economic libraries, whilst the third has been executed by exploiting the Aspen Process Economics Analyzer (APEA), which is the built-in tool of Aspen HYSYS for cost estimation. APEA bases its assessment on a different methodology, which considers the weight of the equipment to estimate installation cost. While this approach may be more rigorous, it requires a larger amount of data, possibly slowing down the procedure.
Even though the three approaches to cost estimation are completely different, the *Total Operating Cost* and the *Total Installed Cost* are very similar. The biggest difference is found by comparing the *Total Capital Cost*: the APEA estimate the TCI to be around

Table 4.1: Equipment cost comparison Test simulation

Equipment Name	**Installed Cost [USD]**		
	APEA	**TURTON**	**PETERS-TIMMERHAUS**
K-101	238,100	439,657	88,727
AC-100	95,300	190,611	46,727
E-105	61,800	83,531	7,767
Absorber	337,200	332,070	113,254
V-101	69,300	11,401	23,812
V-100	136,100	25,765	5,854
K-100	884,400	274,748	121,280
E-100	76,200	23,726	2,524
E-103	61,900	110,302	15,563
P-100	93,100	93,724	19,088
E-102	81,200	109,181	15,234
E-101	72,100	157,962	29,020
V-102	96,000	17,888	2,592
T-100	819,200	507,292	199,375
E-104	72,600	88,738	9,283

Table 4.2: Summary of cost estimation results for Case Study 1

COST ITEM	**APEA**	**CORO_TURTON**	**CORO_PETERS&TIMMERHAUS**
Total Capital Cost $[USD]$	8,764,720	5,099,617	4,868,715
Total Operating Cost $[USD/Year]$	3,984,250	4,680,622	4,122,115
Equipment Cost $[USD]$	1,488,800	-*	840,013
Total Installed Cost $[USD]$	3,194,500	3,343,157	3,024,047
Revenues $[USD/Year]$	5,808,721	5,808,721	5,808,721
Payback time $[Years]$	4.80	4.52	2.88
*Turton library estimates directly the installed cost for the equipment, therefore no information is available on purchased equipment cost			

75% bigger than the one estimated by the CORO using the module cost technique, whereas the difference between the Turton and Peters & Timmerhaus assessments is less than 5%. This overestimation certainly derives from the application of higher factors to compute the indirect expenses related to the construction of the plant, as the forecast of the Total Installed Cost of APEA ($3,194,500) is between the one found by implementing Turton

($3,343,157) and the correspondent evaluated with Peters & Timmerhaus ($3,024,047). It is impossible to affirm which evaluation is correct, as indirect cost may appreciably vary depending on location, regulation and political reasons. However, the CORO is designed to be flexible, and allows the user to change multiplication factors from case to case.
Regarding the smaller differences found by comparing the other cost items, it is important to remark that the Factored estimates, by definition, have an error margin that can be up to 30%; for this reason, the differences found in the comparison are completely acceptable for this kind of analysis. Revenues, on the other hand, do not depend on the economic library but only on the price of the product, the flowrate and the working hours of the plant; which are variables characteristic of the plant.
On these bases, it can be affirmed there is no gross error in the estimation. Thus, the procedures for factorial estimation have been correctly automated. Moreover, the time to produce the results using the CORO is considerably smaller than the time required by APEA. As anticipated, APEA bases its assessments on a wider set of data, however, the fact that the results are similar proves the efficiency of CORO. Besides, it can be affirmed that the CORO has been able to provide comparable results based on a restricted set of information with respect to the one required by APEA, indicating particular effectiveness.

4.1.3 Process Optimization

The goal is to prove that CORO is able to find the global minimum for an optimization problem and to demonstrate the correct functioning of the simulation-based optimization. It is reminded that the objective function for the CORO optimizations is always the payback time of the investment to be made to build and operate the plant. The independent variables for the optimization, instead, can be chosen by the user among all the variables that the user can actually input in the simulation studied. In this case, the degree of freedom selected is the split ratio of the splitter 'TEE-100'. The output streams connected to this unit are 'bypass' and 'to flash'. The first contributes to increase the flowrate of the product 'SEC_PROD' whilst the second goes to a separator, where the bottom represents a waste for the process, constituting an operating expense, and the top output contributes to the product 'PROD' which is the product stream that produces more revenues from sales. Therefore, decreasing the split ratio means to increase the production of stream 'PROD', but at the same time, the waste generated is larger and the separator size increases. The aim is to find the optimum condition in terms of profitability. In this case, the initial conditions correspond to the one of the assessment done by following Turton economic library: the initial value for the payback time is 4.52 years, corresponding to a split ratio of 0.5. The limits specified for the independent variable are 0.2 as lower limit and 0.8 as upper limit.
Figures 4.2 and 4.3 report, respectively, the trends of the independent variable and of the objective function with the number of iteration steps, obtained by applying the CORO. It can be noted that the convergence is reached in a short number of iterations, in this particular case after 10 steps the objective function had already achieved a value very close to the minimum. The amplitude of the steps progressively reduces until it becomes smaller

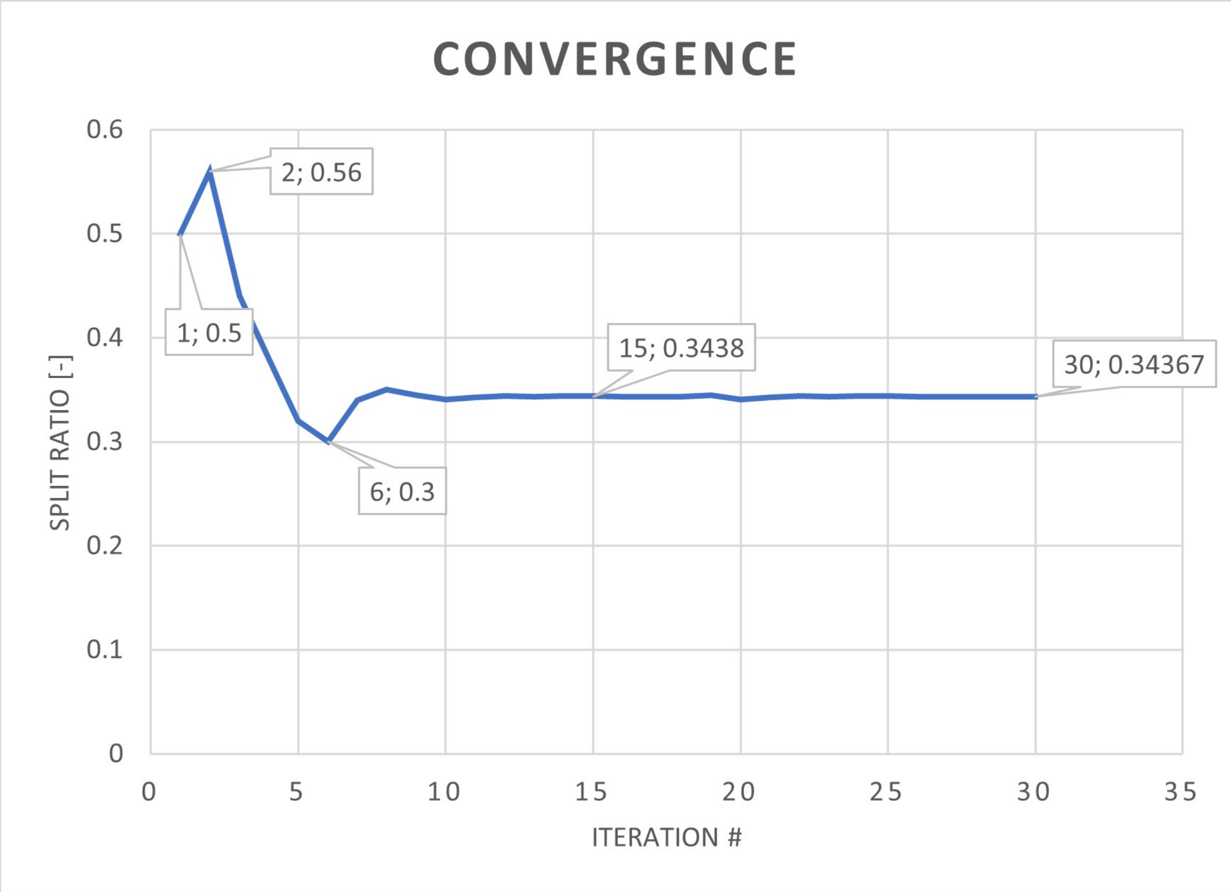

Figure 4.2: Convergence of Optimization

than the tolerance of the function. It was observed that the optimizer tends to oscillate around the optimum condition before automatically stopping the optimization and yielding the result, sometimes introducing a sudden variation of the DOF to check that the minimum to which is converging is not only local but a global one.

The trend of the payback time guides, to some extent, the variation of the DOF set by the solver. In general, at the first iteration a random change is assigned to the independent variable; the objective function is calculated in this new point and a first clue on its trend can be generated. In this case study, the split ratio of 'TEE-100' changed from 0.5 to 0.56, for this last value the CORO produced an estimation of the payback of 5.398 years, indicating that the economic performance has become worse with respect to the initial conditions. Thus, the variation changed direction, and iteratively converged at the optimum point, which is achieved for a split ratio equal to 0.34367. Specifically, with this condition, the production rate of 'PROD' is incremented from 851.46 to 1064.55 $kgmol/h$, with a contextual reduction of 'SEC_PROD' from 241.83 to 174.72 $kgmol/h$ and growth of the waste flowrate from 218.65 to 287.01 $kgmol/h$. The corresponding estimations of the CORO are: $TCI = \$5,118,742$, $Revenues = 6232943\$/year$, '$Opex = 4,830,762\$/year$ yielding a payback time of 3.195 years.

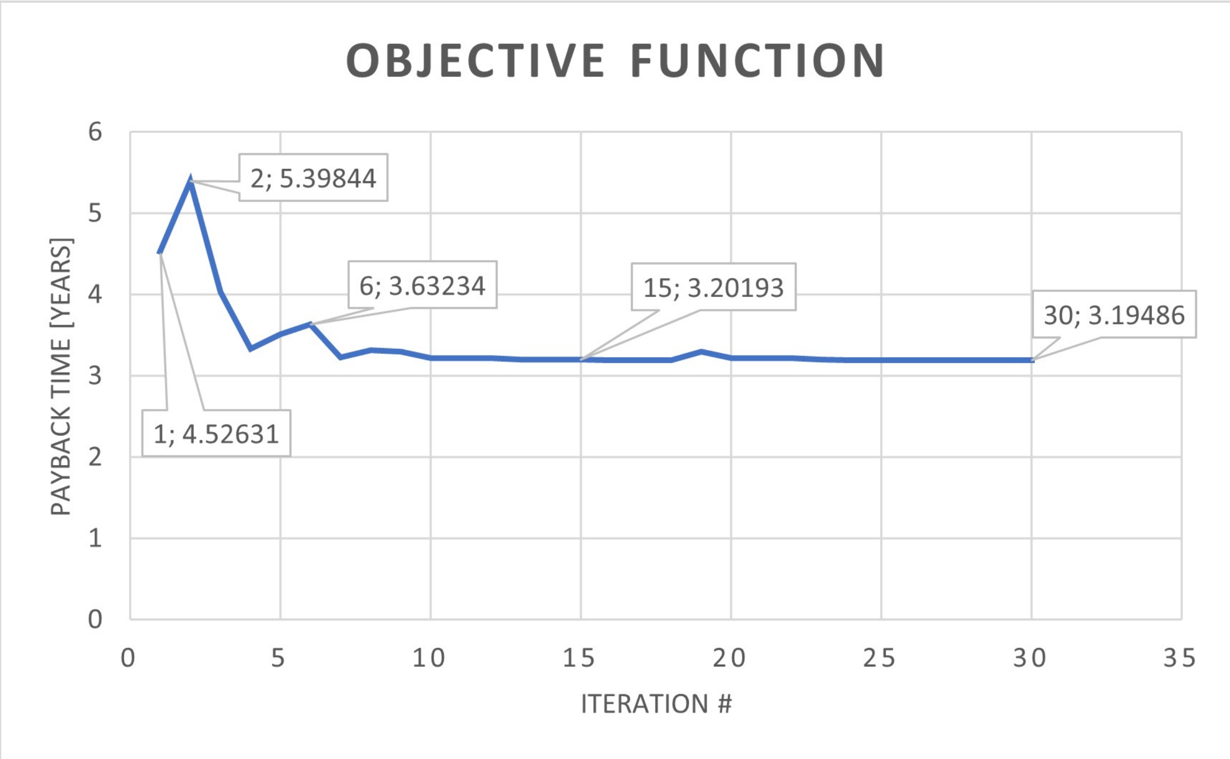

Figure 4.3: Payback time optimization

Ultimately, the optimization resulted in a reduction of payback time of almost 30%, thanks to a change in the production strategy which involved the maximization of the revenues that could withstand an increase of both capex and opex.
It appears evident that issues due to the market request of the products have been neglected, therefore, the optimization was carried out under the assumption that the commodities produced would be all sold, despite of the rate of production of the plant. Moreover, it is important to remark that the optimum conditions depend significantly on the cost assigned to the input/output streams, as these can dramatically affect the revenues and the operating expenses of the process. For this reason, the user should take care in using accurate values and in not neglecting streams that have a cost or that can be sold.
The performance of the Optimizer was satisfactory: the minimum was attained in a relatively short amount of iterations and time. Indicatively, the time deployed to perform one iteration is one second, which is more than acceptable considering that the routines get through two interfaces, two times per step (From HYSYS to Excel, from Excel to DLL, from DLL to Excel and from Excel to HYSYS again). Moreover, the tolerance for the solver could be set to be lower, to reduce the redundant iteration steps. Clearly, the time of the iteration depends on the complexity of the flowsheet of the simulation. In this regard, the rate-determining step is represented by the sub-routines of the Excel workbook: VBA has some known performance issues when using certain functionalities.
The robustness of the optimization is guaranteed by the *BzzMinimizationRobust* function,

which has already been extensively tested by Buzzi-Ferraris and Manenti, 2013. Therefore, even if the optimization carried out in this section is simple, it serves as a demonstration that the minimization function is correctly linked to the simulation; the properties of the function applied are consequently inherited.
On a final note, a limitation that emerged from this case study is that the CORO does not support the changing of the price of a commodity: for instance, the price of a product could be dependent by its purity, which in turn can vary when changing the operating conditions. In this version of the software, the price of a stream has to be set initially and it is constant throughout the optimization.

4.2 Case Study 2

4.2.1 Simulation

In this case study, the cost estimation feature of CORO is applied to an Ammonia separation plant simulation provided by a known EPC contractor. The simulation flowsheet of the process includes a significant number of unit operations and material streams, therefore it represents the ideal case to test the capability of the software of adapting to real industrial situations without losing effectiveness. The plant consists in an intricate series of flash separators, compressors and turbines to obtain pure ammonia from a mixture with carbon dioxide and heavier components, performing low temperatures separations. The main equipment involved are: compressors, turbines, vessels for separation, pumps and heat exchangers. The flowsheet includes all the cooling water utilities, therefore it represents a well-designed simulation, as long as the streams are identified as utilities and the relative cost is added from the user. Otherwise, by default the CORO treats them as process flows, neglecting the associated operating expenses.

4.2.2 Cost Estimation

Also in this case, the evaluation of costs has been carried out following the three different available approaches, as shown in Table 4.3. The first observation to be made is relative to the failure of APEA in estimating the cost of some equipment. In particular, all the expanders have been neglected because their characteristic dimensions exceed the range of the correlations provided by the economic libraries. With regard to this, it has to be emphasized that the equipment exploited to perform the operations are particularly large in terms of capacity. To overcome this problem, in the CORO, a six-tenths rule was automatically used to extend the estimation outside of that range. In general, this practice reduces the accuracy of the estimate, however, the results obtained seem to be coherent between them, proving the reliability of the estimations. Moreover, this solution allows having an estimation of the costs which is considerably more accurate than the one carried out by APEA.
It is worth noting that, apart from the turbines, the differences in equipment costs are relatively small and within the degree of accuracy of factorial estimates, even though the methodologies applied are different. This proves, once again, the reliability of CORO cost

Table 4.3: Equipment cost comparison Ammonia plant

Equipment Name	**Installed Cost [USD]**		
	APEA	**TURTON**	**PETERS-TIMMERHAUS**
K-100	0	3,089,304	1,178,814
K-101	0	5,051,110	1,927,399
K-102	0	2,754,952	1,051,233
K-103	0	1,529,592	344,606
K-104	0	1,792,148	483,822
K-105	0	1,392,246	291,455
K-106	0	1,861,768	537,030
P-102	39,900	15,197	4,637
P-104	37,700	15,532	5,109
E-100	347,500	743,772	146,819
E-101	1,044,900	941,777	185,905
E-102	2,063,100	552,917	114,542
E-103	2,074,200	356,696	75,476
E-104	1,823,300	425,070	89,154
E-105	2,371,200	323,573	68,524
V-100	204,700	227,059	159,774
V-101	216,200	239,785	247,534
V-102	480,900	3,755,784	187,408
V-103	217,400	170,175	122,336
V-104	235,700	73,946	40,778
K-107	929,300	313,815	140,724
K-108	4,611,000	2,202,463	959,714
K-109	4,206,400	4,105,969	5,480,989
K-110	0	4,744,310	1,810,331
K-111	0	1,493,775	329,855
K-112	0	1,216,277	234,550
K-113	0	820,203	139,946
K-114	0	446,068	82,895
K-115	0	467,428	82,466
E-106	181,100	160,583	29,710
E-107	283,800	353,776	79,884
V-105	190,700	201,423	55,461
V-106	102,600	25,191	4,161
V-107	98,700	34,812	9,817
E-108	323,000	207,981	44,035
E-109	207,900	127,164	20,850
V-108	198,900	127,758	29,302
V-109	109,800	30,158	3,356

estimation.
The gap in the equipment cost estimated by Peters & Timmerhaus and the other two methodologies is explained by what presented for Case study 1. This is proved by the fact that the resulting total capital cost does not carry this discrepancy. On the contrary, by estimating the single indirect cost items as a percentage of delivered cost, this approach turns out to be more conservative than the others, yielding higher predicted costs. Table 4.4 summarizes the results obtained from the economic estimations.

Table 4.4: Summary of cost estimation results for Ammonia Plant

COST ITEM	APEA	CORO_TURTON	CORO_PETERS&TIMMERHAUS
Total Capital Cost $[USD]$	37,123,400	90,947,990	124,178,729
Total Operating Cost $[USD/Year]$	8,994,820	21,525,931	24,218,866
Equipment Cost $[USD]$	16,087,400	-*	21,424,901
Total Installed Cost $[USD]$	23,305,100	57,861,033.96	59,989,724.48
*Turton library estimates directly the installed cost for the equipment, therefore no information is available on purchased equipment cost			

The equipment impacting the most on the cost of a plant are, generally, distillation towers, compressors and turbines. However, some of them have been neglected by APEA because of failure of the tool in estimating such large units. As a result, capex are completely miscalculated and no decision can be taken on this basis. On the other hand, using the estimation of CORO, all the equipment are considered and a more accurate estimate is produced. It is not rare to have information not completely precise at the conceptual design stage; the lack of flexibility found in APEA can represent an important obstacle in the production of studies of support to decision making. In this sense, the CORO exhibits robustness to the size of machinery of the plant to be studied.
The other considerable difference in the estimation generated by APEA is the Total Operating Cost. Two main factors contribute to this discrepancy. Firstly, the opex depend in some extent on the capital costs, as the labour, and more in general, expenses to cover for the operations depend on the magnitude of the plant. Neglecting a significant part of the capex results in underestimating the size of the plant, and by consequence the opex. Secondly, as explained in chapter 3, the CORO does not directly subtract the energy produced by the turbines from the energy required to run the compressors, rather it considers the energy produced as a product that can be sold. For these reasons, also in this case, the estimation of CORO is more likely to be correct than the estimation of Aspen.

Conclusions and future developments

The present project has produced a functional software capable of performing cost estimation and robust process optimization starting from any flowsheet designed in Aspen HYSYS. Its structure enables clear visualization of data and results, allowing, at the same time, the user to set the desired parameters for cost estimation and process optimization. This characteristic makes the CORO stand out from all the comparable tools, which do not always ensure a user-friendly experience.

Throughout the thesis, overviews on process simulation and process economics have highlighted the importance of implementing accurate algorithms for optimization problems and the necessity of ensuring accuracy in the cost estimation for correct objective function evaluation.

Two different cost estimation methodologies have been successfully implemented in the software: Turton and Peters & Timmerhaus. In particular, the exploitation of CORO for cost estimation of an industrial case study has provided additional accuracy and flexibility with respect to the built-in tool of Aspen HYSYS.

Additionally, the robustness in the optimization has been achieved thanks to the *BzzMinimizationRobust* algorithm included in the 'BzzMath' numerical library. The case studies have demonstrated the ability of the tool to reach fast convergence on the global minimum despite the complexity of the problem. Moreover, the procedure implemented to allow an external optimization routine to be linked with a process simulation software can be considered as a general template to enable simulation-based optimization.

A natural limitation is represented from the dependency on simulation design accuracy: not always the object implemented in a process simulation corresponds to a real unit. In the worst cases, this might result in meaningless estimations as, for obvious reasons, the software is not designed to be able to discern. In any case, the closer to reality is the simulation, the better is the quality of the results produced.

In conclusion, the structure provided allows the re-utilization of the functional part of the tool for future extension to other chemical process simulation software. This represents an important achievement of this project, as the efforts taken to complete it can be followed up to extend its scope.

Future Developments

The produced software can represent the starting point for a number of attractive applications, especially since the interest, and investments, in process digitalization are constantly growing driven by increasing market competitivity and environmental concern. It is quite clear, indeed, that extensive implementation of digital solutions is a key factor in improving sustainability and avoiding waste of resources in the chemical industry.

In this work, the development has been limited to one process simulation software, however, the CAPE-OPEN Interface standard provides a common framework for all the commercial software of this kind. In this perspective, the development of a program respecting the CAPE-OPEN standard would be attractive as the increased portability would enhance its field of application. Moreover, it could result useful to implement a third economic library to single out eventual gross errors of the libraries already implemented.

The optimization has been aimed to steady-state conditions, but conceptually it can be extended considering the process dynamics. Dynamic optimization is at the basis of digital twin applications and, if implemented, can ensure important margins in terms of plant performance and profit. However, this kind of optimization would have to rely on more accurate models for cost estimation. Consequently, the cost estimation functionality would have to be redeveloped.

The data processing layer of CORO has been developed to be a function of a Dynamic Linked Library, meaning that the library can easily be expanded, considering also that the C++ programming language ensures the lightness and speed of the compiled program. This interesting feature of the application core could be exploited to centralize several digital support applications, such as data reconciliation and digital twin implementation (e.g. Real-Time Dynamic Optimization), producing a comprehensive package that could be very appealing for companies operating in the process industry.

Appendix A

CORO support information

Table A.1: Equipment correspondence

HYSYS UNITS	TURTON		PETERS-TIMMERHAUS	
	class	type	class	type
Mixer	-	-	-	-
Heater	heater	+	heatExchanger	+
Cooler	heatExchanger	+	heatExchanger	+
Heat Exchanger	heatExchanger	+	heatExchanger	+
Pump	pump	+	pump	+
Control Valve	-	-	-	-
Relief Valve	-	-	-	-
Separator	processVessel	+	processVessel	+
3 Phase Separator	processVessel	+	processVessel	+
Tank	tank	+	tank	+
Compressor	compressor	+	compressor	+
Expander	turbine	+	turbine	+
Distillation Column	tower	+	tower	+
Blank Column	tower	+	tower	+
Component Splitter	tower	+	tower	+
Pipe Segment	-	-	-	-
Gas Pipe	-	-	-	-
Fired Heater	furnace	+	furnace	+
Air Cooler	heatExchanger	Air_cooler	heatExchanger	Air_cooled
LNG Exchanger	heatExchanger	+	heatExchanger	+
Plate Exchanger	heatExchanger	Flat_plate	heatExchanger	Flat_plate

Absorber	tower	+	tower	+
Refluxed Absorber	tower	+	tower	+
Reboiled Absorber	tower	+	tower	+
Three Phase Distillation	tower	+	tower	+
Shortcut Column	tower	+	tower	+
Refining Short-Cut Column	tower	+	tower	+
Liquid-Liquid Extractor	-	-	-	-
Continuosly Stirred Tank Reactor	reactor	+	reactor	+
Plug Flow reactor	reactor	+	reactor	+
Conversion Reactor	reactor	+	reactor	+
Equilibrium Reactor	reactor	+	reactor	+
Gibbs Reactor	reactor	+	reactor	+
Yield Shift Reactor	reactor	+	reactor	+
3 Stripper Crude	tower	+	tower	+
4 Stripper Crude	tower	+	tower	+
Vacuum Resid Tower	tower	+	tower	+
Product Blender Isomerization	-	-	-	-
Naphtha Hydrotreater	-	-	-	-
Catalytic Reformer	-	-	-	-
Hydrocracker	-	-	-	-
Hydroproccessing Bed	-	-	-	-
Fluidized Catalytic Cracking	-	-	-	-

FCCU Main Frac	-	-	-	-
CatGas Hydrotreater SHU	-	-	-	-
CatGas Hydrotreater HDS	-	-	-	-
Delayed Coker	-	-	-	-
Visbreaker	-	-	-	-
Petroleum Shift Reactor	-	-	-	-
Simple Solid Separator	centrifuge	+	separator	+
Cyclone	dustCollector	Cyclone	-	-
Hydrocyclone	-	-	-	
Liquid-liquid Hydrocyclone	-	-	-	-
Baghouse Filter	dustCollector	Baghouse	dustCollector	+
Rotary Vacuum Filter	filter	Disc_drum	filter	+
Precipitator	dustCollector	Electrostatic	dustCollector	+
Crystallizer	crystallizer	+	-	-
Legend: +: Multiple type options -: Equipment not supported				

Bibliography

References

AACE (2003). "AACE International Recommended Practice No. 17R-97". *AACE International* 17, pp. 1–7 (see p. 20).

Behrens, W. and P. M. Hawranek (1991). *Manual for the preparation of industrial feasibility studies*. United Nations Industrial Development Organization (see pp. 17, 18, 34).

Biegler, L. (1985). "Improved infeasible path optimization for sequential modular simulators—I: The interface". *Computers & Chemical Engineering* 9.3, pp. 245–256. DOI: https://doi.org/10.1016/0098-1354(85)80003-X. URL: https://www.sciencedirect.com/science/article/pii/009813548580003X (see p. 2).

— (2010). *Nonlinear Programming: Concepts, Algorithms, and Applications to Chemical Processes*. MOS-SIAM Series on Optimization. Society for Industrial and Applied Mathematics (SIAM, 3600 Market Street, Floor 6, Philadelphia, PA 19104). URL: https://books.google.it/books?id=VdB1wJQu0sgC (see pp. 2, 6, 14).

Buzzi-Ferraris, G. and F. Manenti (2013). *Nonlinear Systems and Optimization for the Chemical Engineer: Solving Numerical Problems*. Wiley. URL: https://books.google.it/books?id=flh0AgAAQBAJ (see pp. 3, 13, 14, 46, 59, 62, 73).

Cai, Z., J. Wang, Y. Chen, L. Xia, and S. Xiang (2017). "The development of chemical process simulation software according to CAPE-OPEN". *Chemical Engineering Transactions* 61, pp. 1819–1824. DOI: 10.3303/CET1761301 (see p. 5).

Couper, J. (2003). *Process engineering economics*. New York: Marcel Dekker (see p. 19).

Guthrie, K. (1974). *Process Plant Estimating, Evaluation and Control*. Solana Beach, CA, Craftsman Book Company of America. URL: https://books.google.it/books?id=vcgctAEACAAJ (see p. 27).

Haydary, J. (2019). *Introduction to Computer-Aided Process Design and Simulation*, pp. 1–14. DOI: 10.1002/9781119311478.ch1 (see pp. 6, 7, 10, 13).

Martin, P., J.-Y. Dantan, A. Siadat, X. Houin, and Q. Daniel (Nov. 2017). "Cost estimation and conceptual process planning"," in: (see p. 1).

Navarrete, P. (1995). *Planning, Estimating and Control of Chemical Construction Projects*. Taylor & Francis. URL: https://books.google.it/books?id=A6CwQgAACAAJ (see p. 27).

Perry's chemical engineers' handbook (2008). eng. 8th ed. / prepared by a staff of specialists under the editorial direction of editor-in-chief, Don W. Green, late editor, Robert H. Perry. New York: McGraw-Hill (see pp. 11, 24).

Peters, M. S. and K. D. Timmerhaus (2001). *Plant design and economics for chemical engineers.* McGraw-Hill (see pp. 3, 12, 15, 17, 18, 25, 26, 30, 32, 36, 47).

Silla, H. (2003). *Chemical Process Engineering: Design And Economics.* Chemical Industries. Taylor & Francis. URL: https://books.google.it/books?id=lWmIX0r-XggC (see pp. 21, 29).

Thomé, B. (1993). *Systems Engineering: Principles and Practice of Computer-Based Systems Engineering.* Wiley Series in Software-Based Systems. Wiley. URL: https://books.google.it/books?id=O4FRAAAAMAAJ (see p. 6).

Towler, G. and R. K. Sinnott (2008). *Chemical engineering design: Principles, practice and economics of plant and process design.* Elsevier/Butterworth-Heinemann (see pp. 19, 37–39, 41).

Turton, R., R. C. Bailie, D. Bhattacharyya, J. A. Shaeiwitz, and W. B. Whiting (2012). *Analysis, synthesis, and design of chemical processes.* 4th. Upper Saddle River, NJ: Pearson Education International (see pp. 3, 18, 22, 24, 25, 27–29, 31–33, 35, 47).

Ulrich, G. (1984). *A Guide to Chemical Engineering Process Design and Economics.* Wiley. URL: https://books.google.it/books?id=pdVTAAAAMAAJ (see pp. 23, 27).

Colophon

This document was created using $\LaTeX\,2_\varepsilon$ and edited within the TEXWorks editor, with the help of arara (by Paulo Cereda) typesetting directives. The text body is set in 11 pt Latin Modern Roman, a typeface derived from the Computer Modern fonts designed by Donald E. Knuth. Most of the graphics were generated by PUT PRORGRAM, and diagrams were typeset in PUT PROGRAM. The bibliography was typeset using BIBLATEX.

Copyright Notice