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E DELL'INFORMAZIONE

CORO (Capex/Opex Robust Optimizer) A Simulation-based Process Optimization Package

TESI DI LAUREA MAGISTRALE IN
CHEMICAL ENGINEERING - INGEGNERIA CHIMICA

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Academic year:
2023-2024

Abstract: The feasibility study of chemical plants occurs when not all process information is available. The choice of process configuration significantly impacts plant costs, and changing the layout in later stages can be very expensive. Therefore, it is crucial to have reliable economic estimates from the beginning, when decisions have a greater impact on profitability. The Capex Opex Robust Optimizer (CORO) has been developed to address this need.

CORO uses process simulations in Aspen HYSYS to gather the necessary data to estimate operating and capital expenses. This tool enables rapid, automated, and reliable estimates, minimizing the risk of human error. The data is transferred to a graphical interface in Microsoft Excel via VBA functions, allowing users to make adjustments based on additional information.

Economic estimates are performed using C++ functions that utilize Turton's economic package. Information is transferred from Excel to DLLs using XML schemas. CORO can optimize processes economically by employing the "BzzMath" library developed by Buzzi-Ferraris and Manenti, implemented in C++. The goal is to minimize the project's payback time. This iterative procedure is managed through VBScript functions.

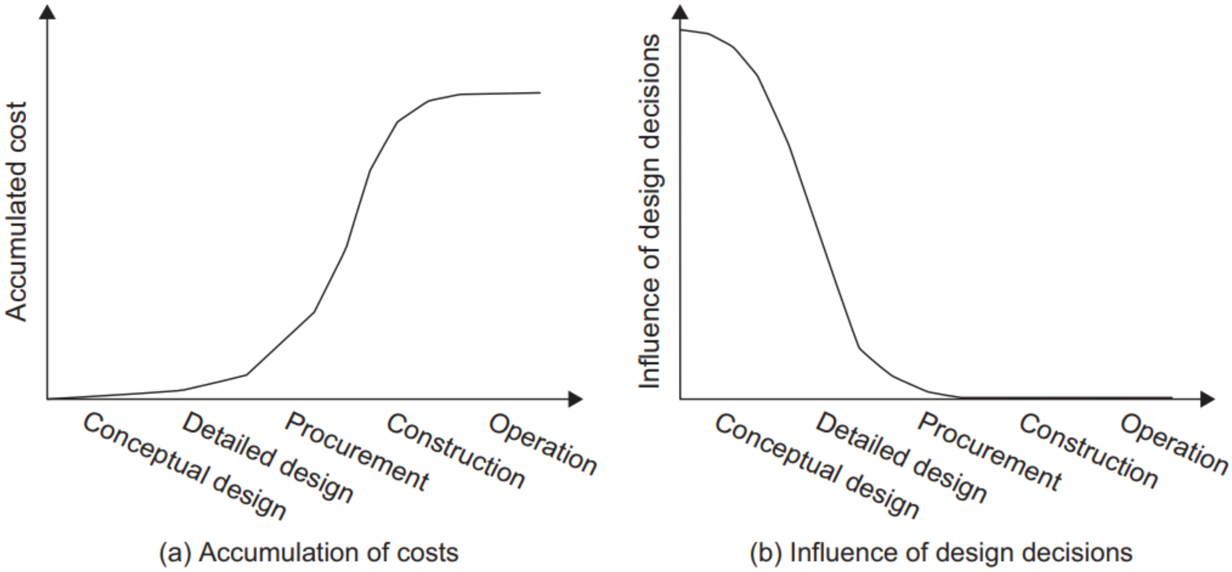
CORO provides a comprehensive and accurate economic analysis, revealing the payback time, net present value, and internal rate of return of the project, as well as the cash flow. The application has proven to be highly flexible and reliable, even with complex process simulations, thanks to its implemented error-handling procedure.

The case study analyzed, related to the economic estimation and optimization of a methanol synthesis plant, demonstrated CORO's accuracy and efficiency. Thus, CORO proves to be a valuable tool for the economic evaluation and optimization of industrial plants.

Key-words: Cost estimation, Process Optimization, CORO, Process Simulation

1. Introduction

At the start of project development, precise information regarding physical and chemical data and details about the equipment involved in the process is often unavailable. Consequently, economic analyses conducted at this stage tend to be imprecise and inadequate. As the project progresses, costs accumulate, and the overall cost estimate becomes increasingly accurate, as illustrated in Figure 1. Simultaneously, the influence of design decisions on project costs diminishes. An understanding of capital and operational expenditures during the early stages of the project lifecycle is fundamental. This allows companies to make reasoned decisions that are cost-effective and impactful, thus minimizing the need for costly modifications to the plant layout in the later stages of the project. It is essential to have a reliable and efficient tool capable of evaluating project profitability. In particular, the ability to explore optimal process configurations and determine the values of key variables that maximize project profitability is of paramount importance.



(a) Accumulation of costs

(b) Influence of design decisions

Figure 1: Influence of design decisions on project cost *Towler*(2022)[20].

The availability of process simulators addresses the challenge of obtaining accurate physical and chemical data. These tools allow for the virtual representation of the process, enabling the acquisition of extensive data that would otherwise require substantial time and financial resources. Consequently, process simulation software becomes an invaluable asset in comparing alternatives during the preliminary stages of project development.

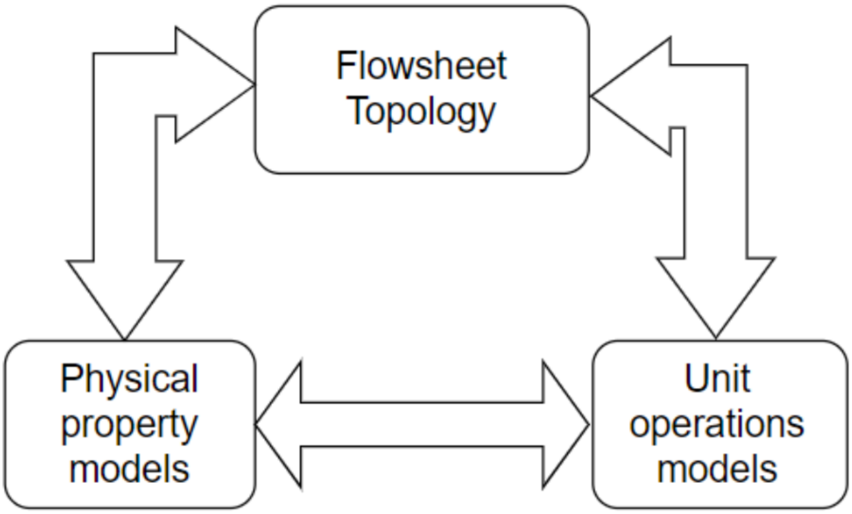


Figure 2: Process simulator's structure *Haydary*(2019)[10].

All process simulators are built upon a fundamental structure, as depicted in Figure 2:

- Physical Property Models: Thermodynamic packages are included to comprehensively describe the physical properties of the components, facilitating the determination of phase equilibrium. Furthermore, when the process involves chemical reactions, the simulator can predict the chemical equilibrium among species, providing estimates of production rates.
- Unit Operations Models: The operation of each unit is simulated by solving mathematical equations of mass and energy balances, as well as physical and chemical equilibrium equations, based on the specific equipment involved.
- Flowsheet Topology: All streams and unit operations within the simulation are interconnected according to their intended use and location, resulting in a coherent and consistent overall process flowsheet.

Chemical process simulation software plays a crucial role in both designing new processes and improving existing plants. It allows for the prediction of product outputs and facilitates process intensification and optimization, applicable during both the design and operational phases. These capabilities are essential for meeting stringent environmental regulations, enhancing market competitiveness, and addressing shrinking profit margins.

Process simulation offers three primary classes of improvements:

- Cost Improvements: Traditional experiments often require substantial financial investments due to the expenses associated with equipment, materials, and facilities. These costs can quickly escalate, particularly for complex or large-scale experiments involving specialized instruments. In contrast, simulations provide a cost-effective alternative by replicating physical and chemical phenomena without the need for physical resources. This approach significantly reduces overall expenditure. Additionally, simulations offer remarkable flexibility, allowing multiple scenarios to be tested without incurring additional costs.
- Time Improvements: Simulations can be conducted at any desired speed, offering a significant advantage over real-world experiments, which may take months to complete. While real-time experiments require waiting for their natural conclusion, simulations can be accelerated to complete in a fraction of the time, or slowed down in cases where detailed analysis of the retrieved data is necessary, such as in biological processes. This flexibility is particularly useful when large amounts of data must be analyzed within a limited timeframe.
- Knowledge Improvements: Simulating plant behavior independent of actual operations enables the acquisition of new competencies. While certain extreme or specialized conditions may be challenging to replicate in physical experiments, simulations provide a means to explore these scenarios. However, it is important to approach data extrapolation from such simulations with caution, as exceeding the model's valid range can lead to significant errors.

When it comes to economic optimization, the economic assessment of a plant is typically based on calculating both capital and operational expenses. These estimates are usually derived from historical data of similar plants and parametric correlations based on the key variables of each unit. Conducting a feasibility study is a tedious and complex task, prone to human error and demanding significant time and financial resources. In chemical engineering, multiple solutions to a given problem may exist, thus the challenge lies in identifying the global optimum among numerous local optima. This is achieved through numerical algorithms that maximize project profitability by optimizing certain process variables.

To address these challenges, the Capex/Opex Robust Optimizer (CORO) package has been developed. The primary objective of this tool is to facilitate cost estimation and process optimization with varying amounts of information. Designed for use in the preliminary stages of a project, this software ensures both precision and significant savings in terms of time and money. This goal is achieved starting from processes simulated on Aspen HYSYS, provided by AspenTech.

2. State of the Art

The optimization of a chemical process can be assessed following different methods according to the type of optimization, which can be single-objective or multi-objective, to the function to be maximized or minimized, and to the numerical algorithm used. In the scientific literature, various examples of optimization can be found.
In the study by *Zhou et al.*(2022)[24], a novel hierarchical catalytic cracking process for crude oil is investigated to enhance control over the cracking depth. The process optimization is achieved using four different temperatures as degrees of freedom. A multi-objective function is developed to maximize the output value while minimizing greenhouse gas emissions, wastewater generation, and non-renewable energy consumption. The study aims to strike a balance between economic optimization and environmental sustainability. The branch and bound (BAB) method is employed as the optimization algorithm.
In the study by *Park et al.*(2021) [14], an adiabatic four-stage CO2 methanation process is examined for the production of synthetic natural gas. This process is optimized by manually varying the pressure and temperature of the reactors, as well as the recycle ratio to the first reactor. Instead of employing optimization algorithms, the degrees of freedom are adjusted manually. The total levelized cost method, which accounts for capital and operational expenditures, is used to identify the optimal process configuration. The configuration that minimizes the cost of synthetic natural gas is considered the best, making this optimization purely a techno-economic assessment.
In the study by *Zhang et al.*(2020) [23], a techno-economic optimization of CO2 hydrogenation for the synthesis of green methanol, integrated with a solid-oxide electrolysis process, is examined. The process optimization involves adjusting the steam and sweep-gas feed flow rates, operating pressure, and steam utilization of the electrolyzer. These variables are tuned using an in-house optimization platform developed by the Group of Industrial Process and Energy Systems Engineering at École Polytechnique Fédérale de Lausanne [8]. The algorithm performs a multi-objective techno-economic optimization, considering both system efficiency, assessed through a life cycle assessment model, and methanol production cost, evaluated based on the project's payback time. The study concludes that the optimal solution is a trade-off between system efficiency and methanol production cost.
In the study by *Chiou et al.*(2023) [6], six alternative process configurations for methanol production via CO2 hydrogenation are evaluated. Each configuration is optimized using the simulated annealing method, which minimizes the required selling price for methanol under different target internal rates of return and various hydrogen price scenarios. This approach results in more energy-efficient configurations with reduced hydrogen demand and increased methanol production rates. The environmental impact of each optimized configuration is subsequently assessed, although it is not included as part of the objective function.
In the study by *Lombardelli et al.*(2022) [12], a methanol production plant utilizing biogenic CO2 and H2 through electrolysis is examined. Three scenarios are investigated by varying the purge fraction of unconverted gases. The economic assessment, conducted using the total levelized cost method, evaluates the methanol production cost. A sensitivity analysis is then performed on the scenario with the lowest methanol cost, varying the gas hourly space velocity and the pressure in the methanol synthesis reactor to further optimize the process.
In the study by *Maroukis et al.*(2022) [13], the performance of a membrane process is compared with that of a cryogenic distillation process using an optimization-based techno-economic analysis. The cryogenic distillation process is optimized by varying the number of theoretical stages. Two configurations of the membrane process are evaluated: one without recycling and one with a fraction of the retentate recycled. In both configurations, the inlet pressure to the membrane serves as an optimization variable. For the configuration with recycle, the recycle ratio is also considered as a degree of freedom. The overall optimization problem is formulated as a Non-Linear Programming (NLP) problem and solved in gPROCESS™ using the NLPSQP solver, aiming to minimize the annualized production cost of argon.
In the study by *Hamedi et al.* (2023) [9], H2 extraction from natural gas distribution grids through pressure swing adsorption process is analyzed. The objective function to be minimized is the levelized H2 separation cost varying seven different variables characterizing the adsorption process. The particle swarm optimization is selected as the optimization algorithm.
In the study by *Pietrek et al.* (2021) [16], immobilized multi-enzyme cascades in a flow system are analyzed. The optimization focuses on maximizing an objective function that balances techno-economic indicators: space-time yield and biocatalytic productivity (techno indicators), and product cost (an economic indicator). The aim is to achieve a trade-off between high yield and economic viability. Both reactor and flow parameters are used as degrees of freedom in optimizing the system, which is carried out using a genetic algorithm.
In the study by *Lee et al.*(2022) [11], novel processes for synthesizing hydroxypropyl acrylate from diluted aqueous acrylic acid and propylene glycol are proposed. The investigation focuses on three different configurations: the conventional reaction/distillation process, an intensified process utilizing a side reactor, and a configuration with multiple side reactors coupled with feed splitting. Optimization of these configurations is performed using the simulated annealing method with the reactor temperature as the degree of freedom. The optimization algo-

rithm is implemented in Python. Each optimized configuration undergoes an environmental impact assessment, calculating the indirect CO2 emission rate. Among the configurations, the multiple side reactors with feed splitting emerges as the best option, excelling in both techno-economic and environmental performance. For this configuration, the minimum required selling price of hydroxypropyl acrylate is also determined.

In the study by *Vlysidis et al.* (2011) [22], alternative strategies for the co-production of biofuels (specifically biodiesel) and chemicals (such as succinic acid) in biorefineries are analyzed. The system's key variables include the cycle time of batch fermentation and the water flow rate entering the bioreactor. Both single-objective and multi-objective optimizations are conducted to maximize profit and/or minimize the overall environmental impact of the process. The primary objective function aims to maximize the net present value (NPV) of the project. Additionally, a single-objective optimization is performed to maximize NPV while accounting for the environmental impact by incorporating a penalty cost per ton of CO2 produced to the product cost. For the multi-objective optimization, a series of optimization runs are conducted for various levels of CO2 emissions per year, allowing the calculation of the optimal NPV at different emission levels. The optimization is carried out using the simulated annealing, a stochastic optimization algorithm implemented in Matlab.

In the study by *Soltani et al.* (2023) [19], a biomass gasification energy system incorporating a supercritical CO2 cycle for hydrogen fuel and electricity production is analyzed. The study employs a multi-objective optimization based on a genetic algorithm, with exergy efficiency and the levelized cost of energy serving as the objective functions. To speed up the optimization process, an artificial neural network is used as an intermediary to reduce computation time. Five different process variables serve as the system's degrees of freedom.

Therefore, various strategies for process optimization are explored in the scientific literature. Some adopt a rudimentary approach, examining processes under different conditions without employing algorithms for optimization. Others incorporate environmental factors into the objective function, while some rely on basic techniques for economic estimation, in contrast to more sophisticated methods.

In the industrial sector, it is common to focus only on minimizing operating expenses or maximizing profit, overlooking capital expenses. However, profitability indexes are significantly influenced by both fixed investment costs and operating expenses.

CORO addresses this by adopting a holistic approach to techno-economic assessment and process optimization. By minimizing the project's payback time, CORO considers all potential expenses, including taxes, the time value of money, depreciation, capital, and operational efficiency or inefficiency. Furthermore, the "BzzMath" library developed by Buzzi-Ferraris and Manenti [4], is robust and reliable in minimizing the objective function.

3. Methods: CORO

The aim of this thesis is to provide a tool that automates the economic estimation and performs the process optimization of a project starting from a process layout designed in Aspen HYSYS. The Capex Opex Robust Optimizer (CORO) addresses the need for a fast and reliable estimation during the initial stages of a project to determine the feasibility of a plant. This package facilitates and enhances the conceptual design of a plant with minimal investment of time and money. Moreover, CORO has been designed to ensure flexibility and robustness for the user, who is allowed to customize the cost estimation based on available or missing information.

3.1. General Framework

Economic estimation and optimization can be assessed using a simulation developed with the Aspen HYSYS package, which provides a type library between Excel and the software.
CORO has been structured as follows (Figure 3):

- An Excel pre-defined workbook that acts as a Graphical User Interface (GUI). This workbook includes all the macros that link the commercial process simulation software Aspen HYSYS with the workbook itself;
- Extensible Markup Language (XML) files where data are stored and transferred between the different package components.
- A Dynamic Link Library (DLL) developed in C++. This DLL contains the core analytics for cost estimation and optimization.
- A Dynamic Link Library developed in VBScript, which updates variable values from the C++ environment to the Aspen HYSYS environment and vice versa during process optimization. It is also used for error handling in case of failed convergence of Aspen HYSYS during the iterations.

The main components of the software are decoupled to ensure high flexibility and independence of the application core from the process simulator. These sections are strictly interconnected and different operating systems produce a high level of complexity.
To better understand how the CORO works a block diagram of the successive steps followed by the iterative algorithm is reported (Figure 4).

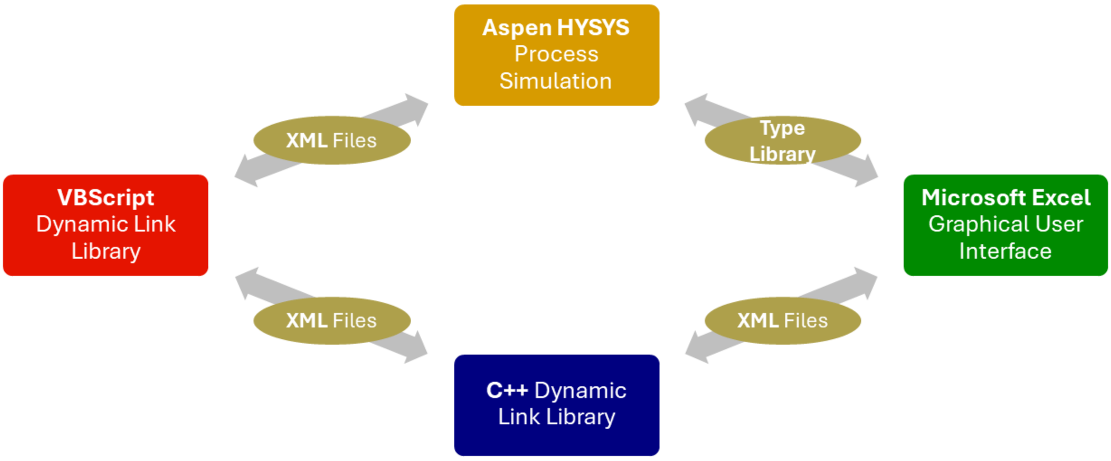


Figure 3: CORO structure

The Graphical User Interface (GUI) has been built in Microsoft Excel because of its extensive applicability, user-friendly interface and interconnection with Aspen HYSYS. To start CORO it is necessary to activate the "Get Data" function providing the name of the simulation, the economic package, and the units of measure that the user wants to apply. Therefore CORO retrieves from Aspen HYSYS all the physical and chemical data that describe the process and that are used to size the units. These data are stored in different worksheets according to their class.
The user can then customize the economic parameters for cost estimation and add information about the unit's materials and type, as well as the type and cost or value of both material and energy streams. Additionally, the "Custom Unit" and "Neglected Unit" functions allow the user to personalize one or more operating units by adding cost or cost curve parameters, or to exclude one or more units from the economic estimation.

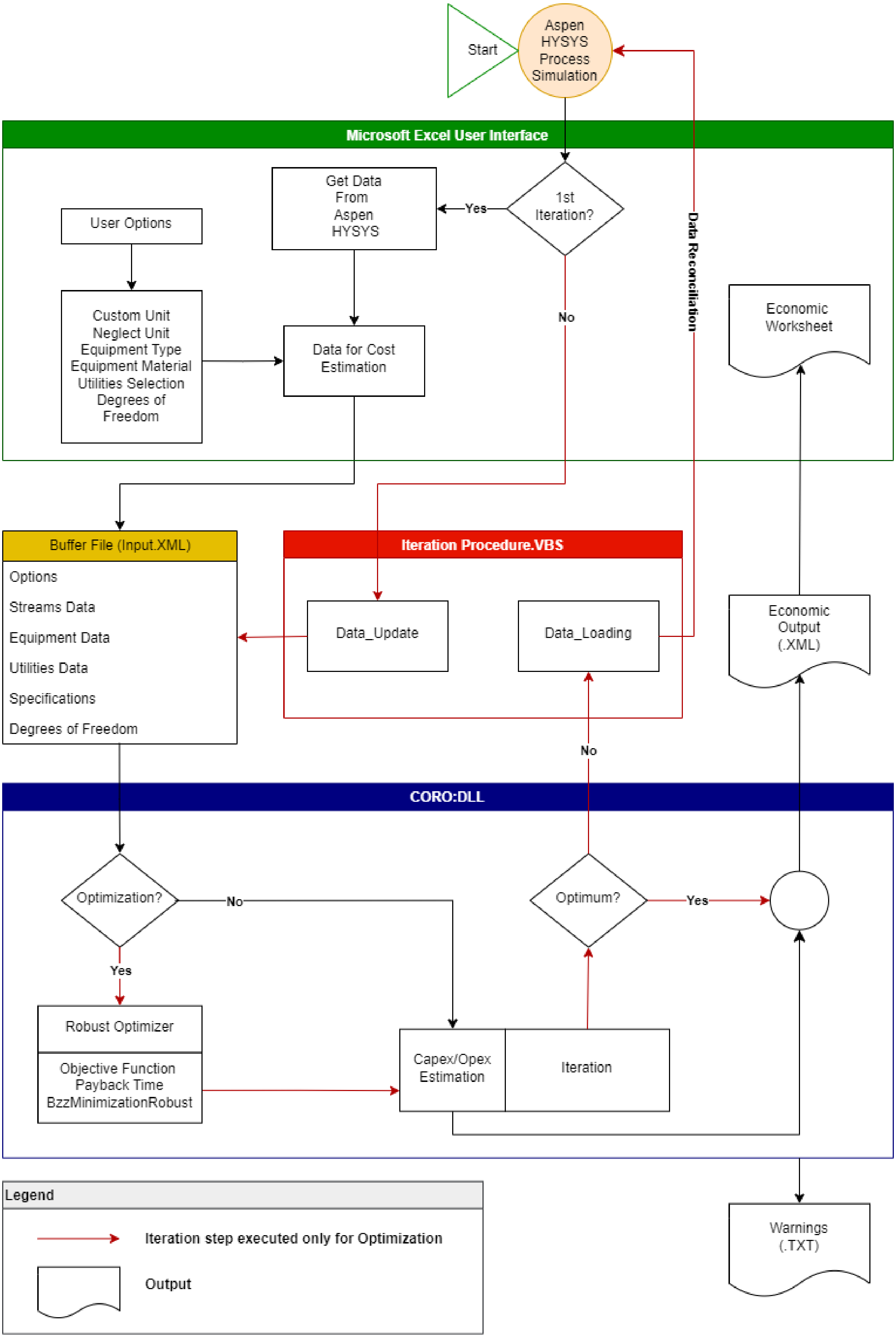


Figure 4: CORO iterative algorithm

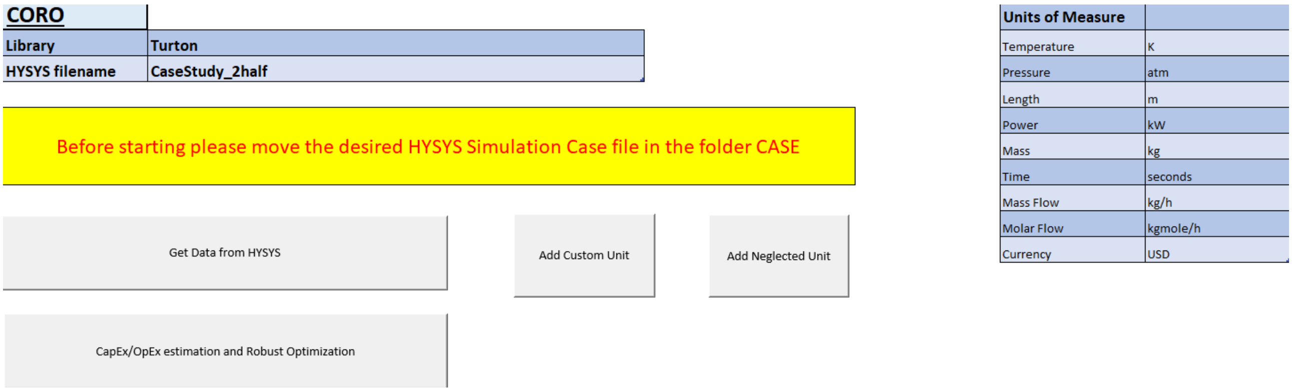
The user can also select the degrees of freedom (DOF) among the simulation variables and set their boundaries to perform process optimization.
Specifically, the possible optimization variables include molar flow, temperature, and pressure for material streams, and duty for utility streams. Each unit operation also has its optimization variable (for example, the split ratio for splitters).

- if DOF $= 0$, performs only the economical estimation of the process, following the black line of Figure 4.
- if DOF > 0, CORO calls the iterative optimization procedure, described by the red line in Figure 4 until the global optimum is attained.

The relevant data are exported from the Microsoft Excel application in XML file format to "CORO.dll", where, depending on the value of the degrees of freedom (DOF), either an economic evaluation is performed, calculating the costs divided into CAPEX and OPEX and the revenues of the process, or the iterative procedure for process optimization begins.
Specifically, the software evaluates the payback time of the project, which is the key parameter used for optimization. The payback time serves as the objective function that the algorithm aims to minimize through the iterative procedure. For the mathematical resolution of the optimization, the Capex/Opex Robust Optimizer relies on the 'BzzMath' library developed by Buzzi-Ferraris and Manenti [4].
The iterative procedure uses two main functions, executed by a different Dynamic Link Library written in VBScript: "Data Loading" and "Data Update". The "Data Loading" function retrieves the modified variables from the "BzzMinimizationRobust" library and loads them into the process simulator to solve the balances and collect the dependent variables' values. The "Data Update" function takes the reconciled data from the simulation and updates "CORO.dll" for a new economic estimation.
Data transfer between environments within the software occurs via XML files. The iterations continue until the minimum payback time value is reached, and the results of the economic evaluation are reported in the economic worksheet of Microsoft Excel. In case of discrepancies within "CORO.dll", a .txt warning file is generated to describe the error. Furthermore, error handling is managed: if the Aspen simulation fails to converge and produces unreasonable system variable values, the faulty simulation is terminated, and the last saved simulation with successful convergence is restored to allow the iterative procedure to continue.
Each part of the package will be examined more in detail in the following sections.

3.2. Get Data

To start the "Get Data" process and download all necessary data from the HYSYS simulation, specific information must first be provided. Specifically, the simulation name, the economic library, and the units of measurement must be selected.
The simulation name should correspond to the name of the simulation located in the "CASE" folder of the software. To initiate data collection, the case study of interest must be placed in this folder, allowing the software to trace the file path and transfer all required data to Microsoft Excel.
For the economic library and units of measurement, they can be selected using a drop-down list. This method ensures that the data entry process is error-free by providing predefined options for the user to choose from.



CORO

Library	**Turton**
HYSYS filename	**CaseStudy_2half**

Before starting please move the desired HYSYS Simulation Case file in the folder CASE

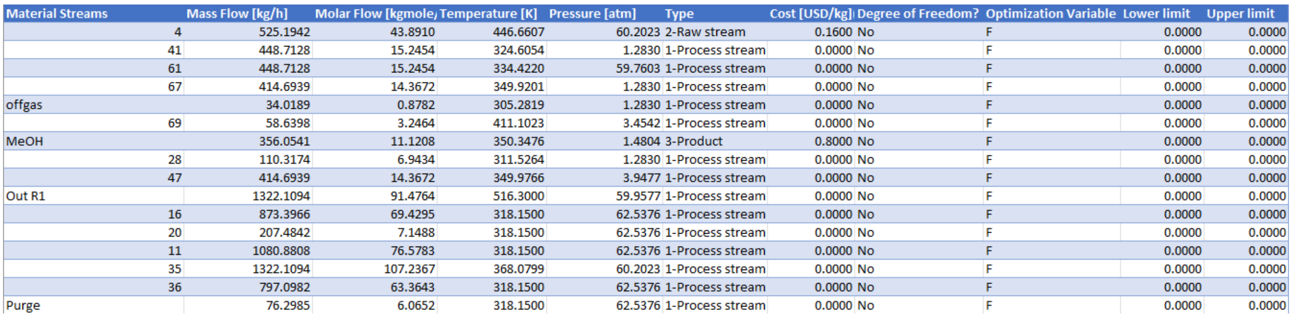
Units of Measure	
Temperature	K
Pressure	atm
Length	m
Power	kW
Mass	kg
Time	seconds
Mass Flow	kg/h
Molar Flow	kgmole/h
Currency	USD

Figure 5: CORO Entry Environment

Pressing the "Get Data from HYSYS" button triggers a macro written in VBA in the Excel workbook. This function retrieves all the information from the Aspen HYSYS simulation and organizes it into different worksheets.
The first worksheet created is the "Material Streams" worksheet, which collects all the material streams from

the simulation. Specifically, the worksheet stores the name, mass and molar flow, temperature, and pressure, as shown in Figure 6.

The meaning of the other columns (Type, Cost, Degree of Freedom, Optimization Variable, Lower Limit, and Upper Limit) will be further investigated in the Data Customization section 3.3. This applies to material streams as well as utilities, specifications, and various equipment worksheets that will be addressed next.

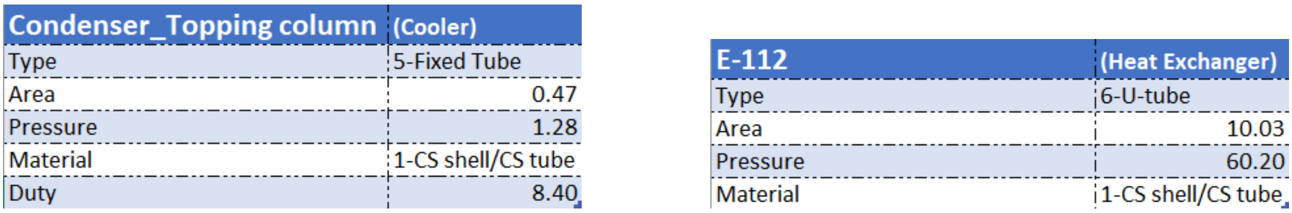


Material Streams	Mass Flow [kg/h]	Molar Flow [kgmole/	Temperature [K]	Pressure [atm]	Type	Cost [USD/kg]	Degree of Freedom?	Optimization Variable	Lower limit	Upper limit
4	525.1942	43.8910	446.6607	60.2023	2-Raw stream	0.1600	No	F	0.0000	0.0000
41	448.7128	15.2454	324.6054	1.2830	1-Process stream	0.0000	No	F	0.0000	0.0000
61	448.7128	15.2454	334.4220	59.7603	1-Process stream	0.0000	No	F	0.0000	0.0000
67	414.6939	14.3672	349.9201	1.2830	1-Process stream	0.0000	No	F	0.0000	0.0000
offgas	34.0189	0.8782	305.2819	1.2830	1-Process stream	0.0000	No	F	0.0000	0.0000
69	58.6398	3.2464	411.1023	3.4542	1-Process stream	0.0000	No	F	0.0000	0.0000
MeOH	356.0541	11.1208	350.3476	1.4804	3-Product	0.8000	No	F	0.0000	0.0000
28	110.3174	6.9434	311.5264	1.2830	1-Process stream	0.0000	No	F	0.0000	0.0000
47	414.6939	14.3672	349.9766	3.9477	1-Process stream	0.0000	No	F	0.0000	0.0000
Out R1	1322.1094	91.4764	516.3000	59.9577	1-Process stream	0.0000	No	F	0.0000	0.0000
16	873.3966	69.4295	318.1500	62.5376	1-Process stream	0.0000	No	F	0.0000	0.0000
20	207.4842	7.1488	318.1500	62.5376	1-Process stream	0.0000	No	F	0.0000	0.0000
11	1080.8808	76.5783	318.1500	62.5376	1-Process stream	0.0000	No	F	0.0000	0.0000
35	1322.1094	107.2367	368.0799	60.2023	1-Process stream	0.0000	No	F	0.0000	0.0000
36	797.0982	63.3643	318.1500	62.5376	1-Process stream	0.0000	No	F	0.0000	0.0000
Purge	76.2985	6.0652	318.1500	62.5376	1-Process stream	0.0000	No	F	0.0000	0.0000

Figure 6: "Material Streams" worksheet

The next worksheet to be created is the "Equipment" worksheet, where the class and name of each piece of equipment are stored. Subsequently, a worksheet is created in Excel for each class of equipment. Depending on the type of unit, the fundamental information required for economic estimation is reported. Although the specific details vary by unit, they generally include: equipment class, characteristic size, operating pressure, and material. The types of classes can be summarized as follows:

- **Heat exchangers**: This class comprises process to process "Heat Exchanger", "Heater", "Cooler", "Air Cooler", "LNG", "Plate Exchanger".



Condenser_Topping column	(Cooler)
Type	5-Fixed Tube
Area	0.47
Pressure	1.28
Material	1-CS shell/CS tube
Duty	8.40

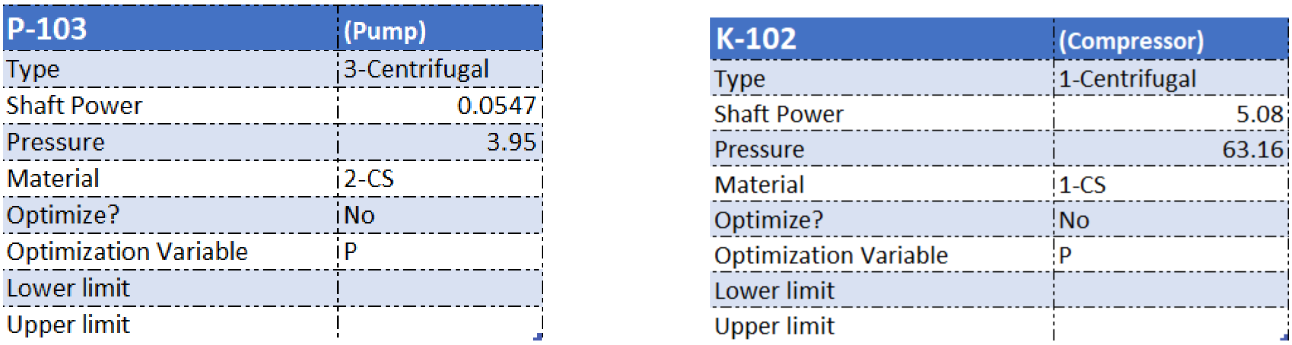
(a)

E-112	(Heat Exchanger)
Type	6-U-tube
Area	10.03
Pressure	60.20
Material	1-CS shell/CS tube

(b)

Figure 7: Examples of heat exchangers.

- **Furnaces**: This class comprises only "Fired Heater"
- **Compressors**: This class comprises only "Compressor".
- **Pumps**: This class comprises only "Pump".



P-103	(Pump)
Type	3-Centrifugal
Shaft Power	0.0547
Pressure	3.95
Material	2-CS
Optimize?	No
Optimization Variable	P
Lower limit	
Upper limit	

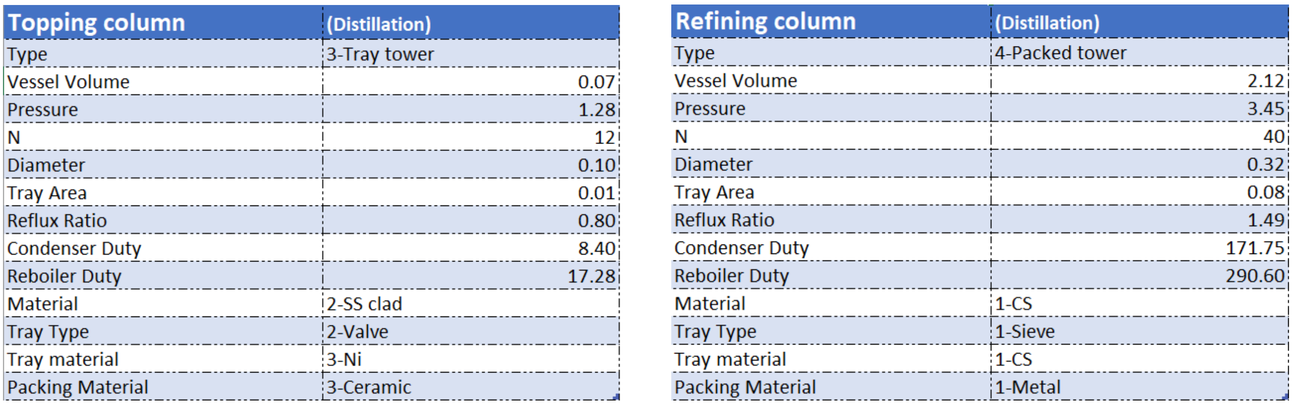
(a)

K-102	(Compressor)
Type	1-Centrifugal
Shaft Power	5.08
Pressure	63.16
Material	1-CS
Optimize?	No
Optimization Variable	P
Lower limit	
Upper limit	

(b)

Figure 8: Examples of pump and compressor.

- **Turbines**: This class comprises only "Expander".
- **Valve**: This class comprises "Control Valve", "Relief Valve" and "Valve".
- **Towers**: This class comprises "Distillation", "Vacuum Resid Tower", "Liquid-Liquid Extractor", "Separator", "3 Phase Separator", "Tank", "Absorber", "Refluxed Absorber", "Reboiled Absorber".



Topping column	(Distillation)
Type	3-Tray tower
Vessel Volume	0.07
Pressure	1.28
N	12
Diameter	0.10
Tray Area	0.01
Reflux Ratio	0.80
Condenser Duty	8.40
Reboiler Duty	17.28
Material	2-SS clad
Tray Type	2-Valve
Tray material	3-Ni
Packing Material	3-Ceramic

(a)

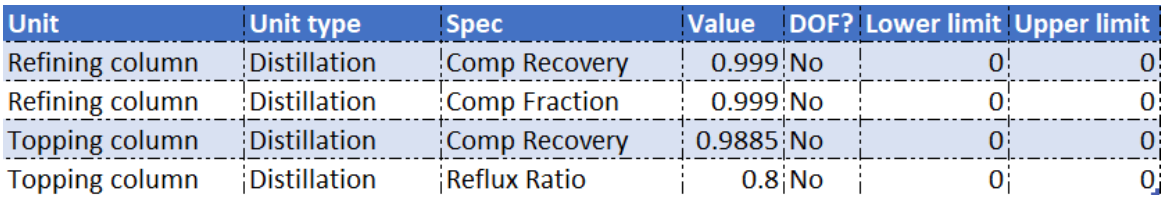
Refining column	(Distillation)
Type	4-Packed tower
Vessel Volume	2.12
Pressure	3.45
N	40
Diameter	0.32
Tray Area	0.08
Reflux Ratio	1.49
Condenser Duty	171.75
Reboiler Duty	290.60
Material	1-CS
Tray Type	1-Sieve
Tray material	1-CS
Packing Material	1-Metal

(b)

Figure 9: Examples of distillation columns.

- **Reactors**: This class comprises "Continous Stirred Tank Reactor", "Plug Flow Reactor", "Conversion Reactor", "Equilibrium Reactor", "Gibbs Reactor" and "Yield Shift Reactor".
- **Splitters**: This class comprises only "Tee".

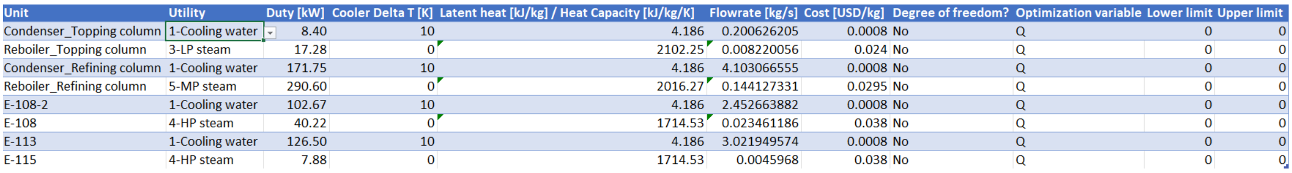
For more complex units, such as distillation columns, a dedicated worksheet called "Specifications" is provided. This worksheet contains detailed design specifications, including the information used for sizing the column.



Unit	Unit type	Spec	Value	DOF?	Lower limit	Upper limit
Refining column	Distillation	Comp Recovery	0.999	No	0	0
Refining column	Distillation	Comp Fraction	0.999	No	0	0
Topping column	Distillation	Comp Recovery	0.9885	No	0	0
Topping column	Distillation	Reflux Ratio	0.8	No	0	0

Figure 10: "Specifications" worksheet

Finally, the last worksheet to be created is the "Utilities" worksheet. This worksheet contains all the units equipped with an energy stream that is treated as a utility and must be provided to the process. This scenario applies particularly to heaters, coolers, and the reboiler and condenser of distillation columns. The table includes all the necessary information to calculate the cost of the utilities. The flow rate is calculated differently depending on the value of the duty, the type of heat exchanger, and the type of service fluid.



Unit	Utility	Duty [kW]	Cooler Delta T [K]	Latent heat [kJ/kg] / Heat Capacity [kJ/kg/K]	Flowrate [kg/s]	Cost [USD/kg]	Degree of freedom?	Optimization variable	Lower limit	Upper limit
Condenser_Topping column	1-Cooling water	8.40	10	4.186	0.200626205	0.0008	No	Q	0	0
Reboiler_Topping column	3-LP steam	17.28	0	2102.25	0.008220056	0.024	No	Q	0	0
Condenser_Refining column	1-Cooling water	171.75	10	4.186	4.103066555	0.0008	No	Q	0	0
Reboiler_Refining column	5-MP steam	290.60	0	2016.27	0.144127331	0.0295	No	Q	0	0
E-108-2	1-Cooling water	102.67	10	4.186	2.452663882	0.0008	No	Q	0	0
E-108	4-HP steam	40.22	0	1714.53	0.023461186	0.038	No	Q	0	0
E-113	1-Cooling water	126.50	10	4.186	3.021949574	0.0008	No	Q	0	0
E-115	4-HP steam	7.88	0	1714.53	0.0045968	0.038	No	Q	0	0

Figure 11: "Utilities" worksheet

3.3. Data Customization

Once all the relevant information from the Aspen HYSYS simulation is stored in the Excel worksheet, the user can customize the data. The first parameters that can be modified are those in the "Turton's Library" worksheet. This worksheet contains all the parameters related to the economic package needed for estimating the cost of various equipment and utilities. It also includes input parameters for payback time and cash flow evaluation, such as the discount rate, taxation rate, project lifetime, and residual value of the process. Further details on how the economic estimation and cash flow calculation are performed will be provided in section 3.4.

Considering the "Material Streams" worksheet, the second part of the figure presented above (Figure 6) can now be analyzed in detail.

The initial step involves selecting the type of stream from the drop-down list, which includes the following options:

1. **Process stream**
2. **Raw stream**
3. **Product**
4. **Waste**
5. **Fuel**
6. **Utility**

Depending on this selection, the stream will be categorized as either a potential profit source (product) or a cost factor (raw stream, waste, fuel, utility), or neither (Process stream).

Next, the price associated with the chosen stream must be input. The remaining columns are designated for optimization purposes. Each stream may be treated as a degree of freedom for optimization. If stream optimization is required, the subsequent column must specify the optimization variable, which may include molar flow, temperature, or pressure.

Finally, the lower and upper limits within which the optimization should be performed must be entered. It is crucial to ensure that the chosen variable is allowed to vary within Aspen HYSYS for the optimization to be successfully executed; otherwise, CORO will generate an error message. This is also valid for the optimization variables of the units and utilities.

The user can customize the process units by selecting the type of equipment and the material of construction from a drop-down list. For instance, there are 13 different types of heat exchangers and 17 different materials to choose from. Additionally, the size of compressors, splitters, pumps, and valves can be optimized by selecting "Yes" in the "Optimize?" cell (Figure 8). For more complex units, such as distillation columns, the user can choose the type and material of each part of the column, including the external vessel, trays, or packaging (Figure 9).

In the "Specification" worksheet is possible to optimize the performances of the towers. In this case the optimization variables are the specifications selected by the user to make the column converge in Aspen HYSYS such as reflux ratio or component recovery (Figure 10).

Regarding the utilities in the "Utilities" worksheet (Figure 11), the user can select the type of heating or cooling fluid depending on whether it is a heater or a cooler. Specifically, for coolers, the user can choose from:

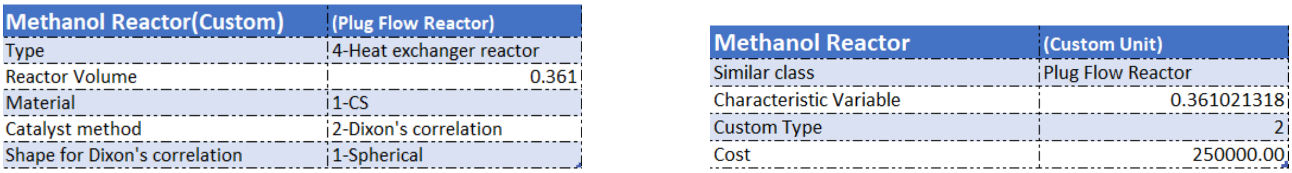
1. **Cooling Water**
2. **Refrigerant**
3. **Neglected Utility**

Cooling Water is a standard cooling fluid whose properties are already included in the worksheet for flow rate calculations, with the fluid's temperature change set at 10 K, although this can be modified. Refrigerant refers to a generic cooling fluid selected by the user, and its properties must be entered manually. Neglected Utility indicates that the cost of that utility should be disregarded. For heaters, user can choose from:

1. **Low Pressure Steam**
2. **High Pressure Steam**
3. **Medium Pressure Steam**
4. **Heating Fluid**
5. **Neglected Utility**

Steam at three different pressures, like Cooling Water, is a standard heating fluid with properties for flow rate calculations already entered into the system. Heating Fluid and Neglected Utility perform the same functions for heaters as Refrigerant and Neglected Utility do for coolers.

Moreover, there are two functions, "Add Custom Unit" and "Add Neglected Unit" (Figure 5). The "Add Neglected Unit" function allows users to exclude one or more units from the economic estimation. When this button is clicked, a macro activates the "Equipment" Excel sheet and prompts the user to enter the name of the unit to be neglected. The unit's classification then changes to "Neglected," and its cost is not evaluated.



Methanol Reactor(Custom)	(Plug Flow Reactor)
Type	4-Heat exchanger reactor
Reactor Volume	0.361
Material	1-CS
Catalyst method	2-Dixon's correlation
Shape for Dixon's correlation	1-Spherical

(a) Methanol Reactor in "Reactor" worksheet

Methanol Reactor	(Custom Unit)
Similar class	Plug Flow Reactor
Characteristic Variable	0.361021318
Custom Type	2
Cost	250000.00

(b) Methanol Reactor in "Custom Unit" worksheet

Figure 12: Reactor customization

The "Add Custom Unit" function allows the user to customize the cost of one or more units in two different ways. When using "Add Custom Unit," the "Equipment" worksheet is activated, and a box asks for the name of the unit. Then another box appears, asking for the customization type. The user can enter either the cost of the unit or the new parameters for the cost curve. These units then appear as "Custom" in their worksheet and are contained in a new worksheet called "Custom Unit."

3.4. Economic Estimation

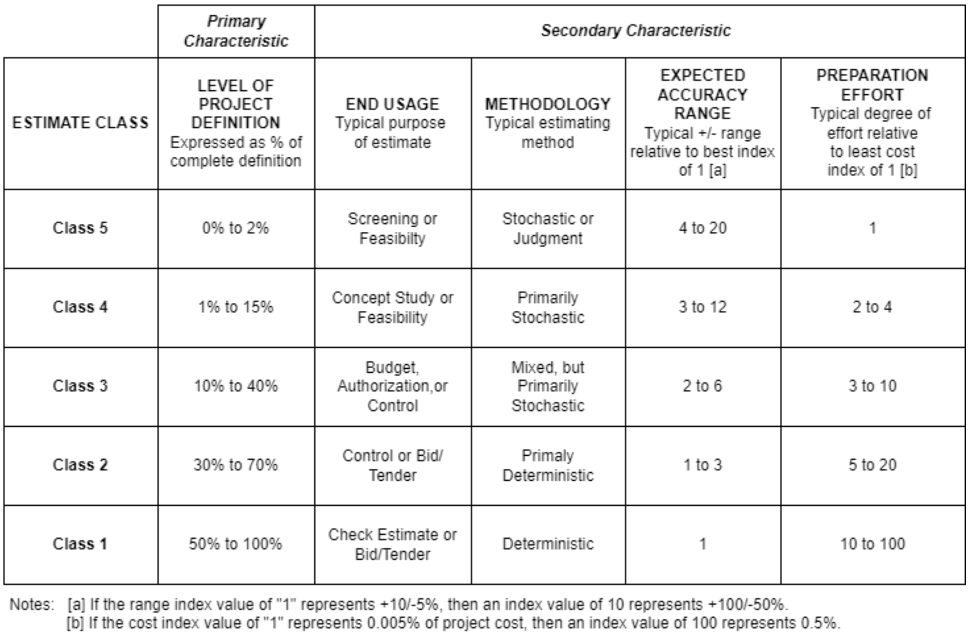
Economic estimation is performed when the degrees of freedom are zero by selecting the "CapEx/OpEx Estimation and Robust Optimization" command. An Excel macro is activated, and in the initial phase, it generates a worksheet named "XML" where all the necessary data for conducting the economic estimation of the process are compiled. Specifically, this xml file is organized into several sections:

- Options: this node includes the name of the simulation, the name of the economic package and its parameters, the preferred unit of measures and the values of the economic parameters for the cash flow evaluation.
- Material Streams: this node includes the thermodynamic data of each stream, the type of stream and its cost or value.
- Units: this node includes the parameters that completely describe each unit operation of the process.
- Specifications: this node includes particular unit operation specifications.
- Utilities: this node includes the data regarding the energy streams of the process and its respective cost.

Subsequently, the data are mapped into a pre-loaded XML map in Excel to export them as an XML file named "Input.xml". The Excel macro calls a function defined within a Dynamic-Link Library (DLL) named "CORO.dll", developed in C++. This enables the transfer of the necessary information from the Excel GUI to the C++ section of the package, where the economic estimation is actually performed.

The cost estimation of a project can be carried out with different levels of precision. According to Turton [21] there are five levels, listed from most to least accurate:

1. Detailed estimates.
2. Definitive estimates.
3. Preliminary estimates.
4. Study estimates.
5. Order of magnitude estimates.



	Primary Characteristic	*Secondary Characteristic*			
ESTIMATE CLASS	LEVEL OF PROJECT DEFINITION Expressed as % of complete definition	END USAGE Typical purpose of estimate	METHODOLOGY Typical estimating method	EXPECTED ACCURACY RANGE Typical +/- range relative to best index of 1 [a]	PREPARATION EFFORT Typical degree of effort relative to least cost index of 1 [b]
Class 5	0% to 2%	Screening or Feasibilty	Stochastic or Judgment	4 to 20	1
Class 4	1% to 15%	Concept Study or Feasibility	Primarily Stochastic	3 to 12	2 to 4
Class 3	10% to 40%	Budget, Authorization,or Control	Mixed, but Primarily Stochastic	2 to 6	3 to 10
Class 2	30% to 70%	Control or Bid/ Tender	Primaly Deterministic	1 to 3	5 to 20
Class 1	50% to 100%	Check Estimate or Bid/Tender	Deterministic	1	10 to 100

Notes: [a] If the range index value of "1" represents +10/-5%, then an index value of 10 represents +100/-50%.
[b] If the cost index value of "1" represents 0.005% of project cost, then an index value of 100 represents 0.5%.

Figure 13: Classification of cost estimates [21].

The accuracy of the estimation produced by CORO can be compared to preliminary estimates based on the process flow diagram (PFD) of the project. This diagram provides an approximate layout of equipment and includes estimates for piping, instrumentation, and electrical requirements, as well as utilities [21].

Turton's book claims that class 1 is typically +6% to -4% accurate, therefore the accuracy level in the cost estimation of CORO, with a project definition ranging from 10% to 40% compared to the complete definition, varies from +36% to -24% when the project definition is closer to the lower end. Conversely, when the project definition approaches the higher end, the range narrows to between +12% and -8%. Moreover, the economical effort of the 5th class estimate covers generally between 0.015% and 0.3% of the total installation cost of the plant. Consequently, for the third class the cost range varies between 0.045% and 3% [21]. Therefore, CORO is capable of providing a reasonably accurate economic estimate of plant costs, while also offering savings in terms of both time and money.

3.4.1. Turton's correlations

The cost estimation in CORO relies on Turton's correlation techniques[21]. It is based on the calculation of capital expenditures (Capex) and operational expenditures (Opex). Capex is determined using empirical parametric correlations based on the real purchase cost of existing units, linking the characteristic variable of each unit to its cost through cost curves. Opex is estimated through additional correlations related to Capex and as a function of the main costs specified by the user, such as raw materials, waste treatment, and utilities.

Capital expenditures are commonly estimated using the Module Costing Technique. This technique links the purchase cost of equipment under base conditions to the characteristic variable of each unit. Base conditions imply that the equipment is made of carbon steel and operates near atmospheric pressure. Deviations from these conditions are managed by applying specific multiplying factors based on the type of equipment, operating conditions, and construction material.

The procedure implemented in CORO for estimating the cost of each unit involves the following steps:

1. Estimating the purchase cost under base conditions: Utilizing correlations that link the cost to the unit's characteristic variable. If the value of this variable exceeds the upper limit of the correlation range, the six-tenths rule is applied.
2. Evaluating correction factors: Taking into account the actual operating conditions of the unit.
3. Determining the Bare Module Cost: Including the direct costs of the unit (not under base conditions) and related indirect costs.
4. Updating costs: Using equations to adjust the unit's cost to the present time, given that the correlation parameters are derived from historical data.

The overall project cost is estimated, which includes:

1. Contingency and Fee Costs: Protection against unexpected situations, estimated to be between 3% and 15% of the Bare Module Cost, with CORO overestimating at 18%.
2. Auxiliary Facilities Costs: These are variable and unpredictable, estimated to be between 20% and 100% of the Bare Module Cost, with an assumed value of 50%.

The total capital expenditure (CAPEX) of the plant, known as the Grassroots cost, is calculated by summing these costs. The final step involves assessing the Working Capital,which is the funds, in addition to the fixed capital, that a company must contribute to a project. It must be adequate to get the plant in operation and to meet subsequent obligations when they come due [15]. This is estimated to be between 15% and 20% of the Fixed Capital Investment, with CORO assuming 15%. All these parameters can be adjusted by the user via the graphical user interface (GUI).

It is crucial to evaluate the operation of the process, investigating and quantifying aspects such as available markets, production costs, potential selling prices, and other operational elements of the plant.

The estimation of operating expenditures, also known as the Cost of Manufacturing (COM), requires the assessment of fixed capital investment and the process flow diagram (PFD) provided by Aspen HYSYS. The COM includes costs related to the production rate (variable costs) and costs unaffected by the production rate (fixed costs and general expenses).

The correlations provided by Turton allow the estimation of these costs by considering the following elements:

1. Fixed Capital Investment (C_{GR})
2. Cost of Operating Labor (C_{OL})
3. Cost of Utilities (C_{UT})
4. Cost of Waste Treatment (C_{WT})
5. Cost of Raw Materials (C_{RM})

CORO uses the Module Costing Technique to evaluate fixed capital investment. The cost of operating labor includes wages, employee benefits, and payroll taxes. Utilities, which include steam, electricity, and water, have variable costs depending on the plant's location, historical period, and method of supply.

The cost of waste treatment and raw materials is estimated similarly. Waste treatment refers to activities required to minimize environmental impact, often regulated by law. The cost of raw materials depends on the commercial price of the material. CORO calculates these costs using the information about the type of streams chosen by the user in the Microsoft Excel workbook.

3.4.2. Payback time and cash flow calculation

Once both CAPEX and OPEX have been estimated, the annual revenues are calculated based on the material streams selected by the user as products. Annual revenues are determined as product sales in kg/year times the product sales price in \$/kg. At this point, it is possible to estimate the project's payback time using the Discounted Cash Flow Method.

A cash flow diagram, like Figure 14, illustrates the forecasted cumulative net cash flow over the project's life, based on estimates of investment, operating costs, sales volume, and prices. This diagram helps visualize the required resources and the timing of earnings[20]. There are three main indicators which can be obtained from the Discounted Cash Flow Method:

- Payback time (PBT), i.e. the time required for an investment to recover its initial outlay in terms of profits or savings, also known as the break-even point of the project, as illustrated by point E in Figure 14.
- Net Present Value (NPV), i.e. the difference between the present value of cash inflows and the present value of cash outflows over a period of time as illustrated by point G in Figure 14. The NPV is calculated as follows, where $\mathrm{INV_0}$ is the initial investment, CF is the cash flow, DR is the discount rate, N is the number of periods of the timespan of interest of the investment/project, $\mathrm{RV_i}$ is the residual value at i-th period:

$$NPV = \sum_{i=1}^{N} \frac{CF_i}{(1+DR)^i} - INV_0 + \frac{RV_i}{(1+DR)^i} \quad [\$] \tag{1}$$

- Internal Rate of Return (IRR), i.e. the interest rate at which the NPV is equal to zero at the end of the project life. This financial indicator is more useful than NPV for comparing projects of different sizes. IRR is analogous to an interest rate, and so allows projects to be compared with other investments [20].

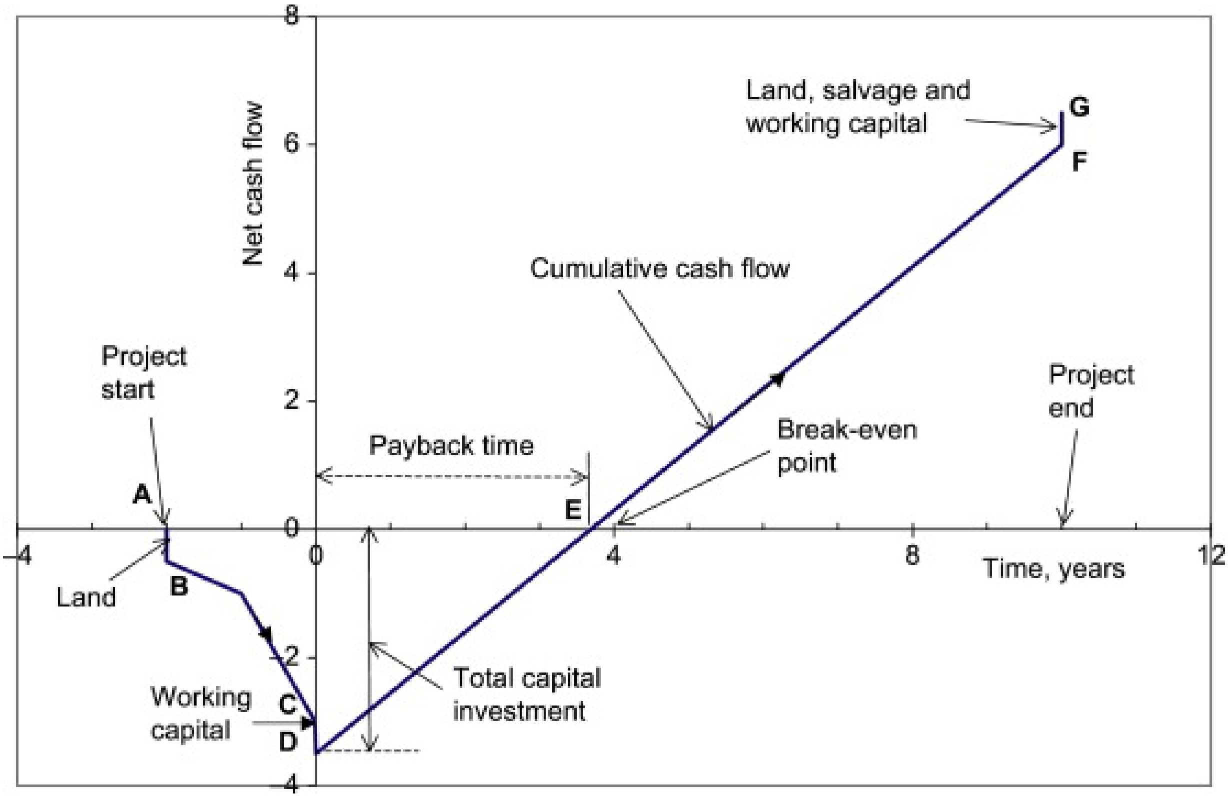


Figure 14: Project cash flow diagram *Dimian*(2014)[7]

The cash flow is not simply calculated as annual reveneus minus Opex. It takes into account both taxes and depreciation. Depreciation is an accounting practice used to spread the cost of a tangible or physical asset over its useful life [2], which increases after-tax cash flow and makes investments more attractive. For capital expenditures, a linear depreciation is used over the entire life of the plant. Therefore, annual depreciation is calculated as:

$$\text{Depreciation} = \frac{\text{Total Capital Investment}}{\text{Lifetime of the Plant}} \left[\frac{\$}{\text{year}}\right]$$

The Income is calculated as:

$$\text{Income} = \text{Annual Reveneus} - \text{Opex} \left[\frac{\$}{\text{year}}\right]$$

The taxable income is determined as:

$$\text{Taxable Income} = \text{Income} - \text{Depreciation} \left[\frac{\$}{\text{year}}\right]$$

Taxation is then calculated as:

$$\text{Taxation} = \text{Tax Rate} \times \text{Taxable Income} \left[\frac{\$}{\text{year}}\right]$$

only if the taxable income is positive, otherwise Taxation is equal to zero. The cash flow is then:

$$\text{Cash Flow} = \text{Income} - \text{Taxation} \left[\frac{\$}{\text{year}}\right]$$

The user can customize the values of the input parameters needed for the calculation of the economic indicators and the cash flow, such as the discount rate, the taxation rate, the lifetime of the project, and the residual value of the process. Once all these values are calculated, they are stored in an XML file named after the economic package, which is already loaded in the Excel file. Finally, the last step of the macro maps the final results in a new sheet called "Economics-Turton".

3.5. Optimization

The objective of CORO's optimization is to minimize the project's payback time. This iterative procedure utilizes the "BzzMinimizationRobust" function, contained in the BzzMath Library written in C++ [4]. The program employs the penalty function method to apply unconstrained optimization techniques to constrained problems. Specifically, the penalty functions modify the original objective function by adding special terms that are null when the constraints are satisfied and increase progressively as the constraints are violated. This approach has been proven to improve the process robustness.

This iterative process is initiated when the number of degrees of freedom is equal to or greater than one, and the user clicks the same button for the economic estimation.

Initially, a copy of the original Aspen HYSYS simulation is created and saved under the name "SimulationName_optimized.hsc." This approach allows the optimization to be conducted on the new simulation, preserving the integrity of the original simulation. As a result, the user can more easily compare the outcomes of the optimized and original simulations. If the user is not satisfied with the optimization, the original simulation can be reverted and the iterative procedure restarted, making adjustments to the degrees of freedom as required.

The same steps of the evaluation of unit costs are followed. Then, CORO.dll calls the "BzzMinimizationRobust" function, which takes as input the payback time value, the original variable values, and the lower and upper bounds of the degrees of freedom entered by the user in the Excel worksheet.

The iterative procedure is carried out by two functions written in VBScript due to its compatibility with Aspen HYSYS. These functions are:

- **Data Loading**
- **Data Update**

The iterative algorithm followed by CORO to perform this task is described by the red line in Figure 4. The following analysis starts from the box "Optimum?". After the new values of the degrees of freedom are uploaded to the "input.xml" file to be accessible to the iterative procedure, the first function to execute is "Data Loading". Its role is to load the new values of the degrees of freedom into Aspen HYSYS. This step is crucial because the degrees of freedom are optimized from a strictly numerical standpoint and may not conform to the material and energy balances in the Aspen simulation.

Additionally, only the modified degrees of freedom are loaded into Aspen, and the Aspen solver is turned off and on with each transfer of a new variable value to boost solver convergence. By the end of the Data Loading process, data reconciliation is completed, and the new simulation adheres to all material and energy balances. The new values of the degrees of freedom meet the specifications set by the user.

At this stage, the second function, "Data Update," is executed. Its purpose is to transfer the reconciled values from the Aspen simulation into the "Input.xml" file, thereby making these values accessible to "CORO.dll" and enabling a new economic estimation of the plant, including the evaluation of the payback time. This iterative procedure continues until the optimal values of the degrees of freedom are identified, which minimizes the payback time.

Another feature that ensures the robustness of CORO's iterative procedure is the implementation of error handling. Specifically, there are two additional functions written in VBScript that enable the iterative process to proceed even in the event of convergence failures in the Aspen HYSYS simulation. The two functions are:

- **Data Recovery**
- **Simulation Saving**

Particularly in complex simulations, it is possible that, once the new values from the optimization are loaded into Aspen, the solver may fail to converge. This issue is especially likely when very broad boundaries are set for the degrees of freedom. Such failures result in the Aspen simulation being unable to find a physically meaningful solution, leading to the simulation streams changing color from blue to light blue and variables assuming a value of -32767.

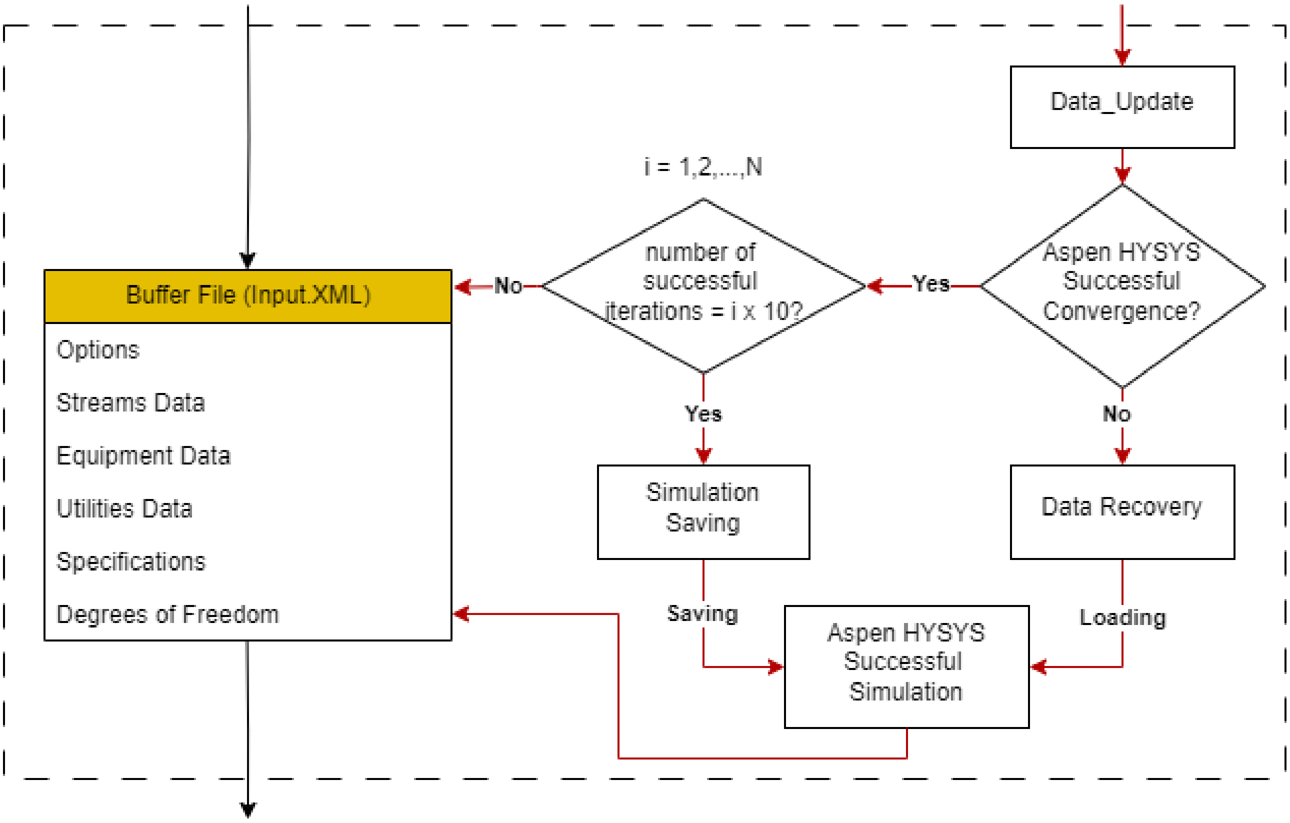


Figure 15: Error Handling Environment.

After the "Data Update," if a variable in the simulation streams has a value of -32767, the "CORO.dll" calls the "Data Recovery" function. This function ends the erroneous simulation without saving it and recovers the most recently saved simulation. Consequently, the iterative procedure continues with the search for optimal degrees of freedom values through the "BzzMinimizationRobust" function.

Additionally, "CORO.dll" includes counters that track the number of times the Aspen HYSYS solver successfully converges versus the number of failures. These counters are crucial for the "Simulation Saving" function, which is designed to save the currently optimized simulation. This function is called by "CORO.dll" only after every 10 successful iterations. This approach prevents excessive slowing of the iterative process and, in the event of a solver failure, ensures that progress is not lost by avoiding a return to the degrees of freedom values of the original simulation. Thus, the optimization process consistently relies on simulations that have successfully converged.

At the conclusion of the iterative procedure, once the payback time has been minimized, the system records the number of successful iterations, failed iterations, and the percentage of successful iterations. These parameters help the user assess the effectiveness of the optimization. The percentage of successful iterations allows the user to determine whether the optimization process is reliable and robust.

These data are stored in an XML file, named after the economic package, which is already integrated into the Excel file and mapped in the "Economics-Turton" worksheet. This worksheet also displays the elapsed time required for the simulation optimization. These indicators provide a measure of the quality of the optimization process.

4. Case Study

To evaluate the functionalities of CORO and demonstrate its reliability and robustness, a specific case study was developed involving a "Biogas to Methanol" plant. The simulation comprises the majority of the unit operations implemented in CORO. Moreover, to achieve a comprehensive economic assessment, it was necessary to incorporate some custom units. After the initial economic evaluation, an optimization process was carried out by adjusting five key variables. This optimization resulted in a tangible improvement in the plant's economic performance. Through this case study, all the main features of CORO were rigorously tested, allowing for an accurate assessment of the software's capabilities.

4.1. Introduction

The case study focuses on the revamping of an existing plant that produces syngas from biogas (see the figures in Appendix A). The existing process is divided into two main sections: the partial upgrading of biogas and the steam reforming. The output of this first part is syngas, which has a production cost of \$0.16/kg, evaluated in the study of *Salano et al.*(2024)[17]. The initial part of the process does not undergo economic evaluation or optimization because the only relevant data, the cost of the syngas, has already been assessed and will be used as input for the second part of the process.

The second section of the plant, where syngas is converted into methanol, is the focus of the detailed analysis. In this phase, both economic evaluation and optimization are carried out to enhance the efficiency and profitability of the methanol production process.

The sections of the plant are described in detail:

1. **Biogas to syngas:**
    - **Partial upgrading of biogas:** The biogas stream, characterized by a molar composition of 56.56% methane, 40.95% CO2, 0.01% H2S, and 2.48% water vapor (corresponding to 80% relative humidity under system conditions), is cooled and sent to a flash separator to remove the water. The stream is then pressurized, cooled again, and fed into a component splitter to simulate the removal of H2S. At this stage, the stream is split using a tee. One part is directed to the biogas upgrading section and will be used as feed for the catalytic tube reactors for syngas production. The other part, together with a recycle stream from the methanol production section, containing mainly methane, hydrogen, and CO2, and an air stream, is sent to a fired heater. The fired heater and the catalytic tube reactor serve as the shell side and tube side, respectively, of the same reactor. The tee's split ratio is adjusted to ensure the process is autothermal. This is achieved using the adjust function in Aspen HYSYS.

      The part of syngas directed to the upgrading section is pressurized with intercooling bar and then sent to an absorption column. In this column, CO2 is absorbed in a water scrubbing unit, where the biogas passes through water inside a packed tower in a counter-current configuration. The upgraded syngas exits from the top of the column, while the CO2-enriched water exits from the bottom and is sent to a flash separator to remove the CO2. This allows for partial water recirculation after repressurization.
    - **Steam reforming:** Both the fired heater and the catalytic tube reactor are simulated using Gibbs reactors. The flue gases from the furnace are utilized for heat recovery purposes. Specifically, they are used to preheat both the steam from the reactor's recirculation loop and the upgraded biogas. Additionally, the reformed gases exiting the reactor are employed to heat and vaporize the recycled water. After cooling, the reaction product is sent to a flash separator to divide the desired syngas from the condensate. The condensate is then directed to another flash separator for CO2 removal. To this primarily water-based stream, a recycle stream from the methanol production section, also mainly consisting of water, is added along with a makeup water stream. This combined stream is recirculated to the reactor, after being heated by the reactor's outlet gases as previously mentioned. The makeup flow rate of water is adjusted to achieve a 4:1 stoichiometric ratio of steam to methane at the inlet of the steam reforming reactor. Finally, the syngas is compressed.
2. **Syngas to methanol:** The two methanol reactors are simulated as plug flow reactors and are assumed to be isothermal. To the syngas stream, composed mainly of hydrogen, CO, and CO2, a recycle stream of unreacted reagents from the methanol reactors is added. The feed is preheated before entering the first reactor. The products from the first reactor are cooled and sent to a flash separator to separate the produced methanol, enhancing conversion in the second reactor. The unreacted reagents from the top of the flash separator are recompressed and reheated before being fed into the second reactor. The products are once again cooled and sent to another flash separator to separate the obtained methanol. The stream exiting the top of the second flash contains mainly hydrogen, methane, and CO2, which

is partially recycled to the first methanol reactor and partially recycled to the shell side of the steam reforming reactor to be used as fuel.

The streams from the bottom of the two flash separators, besides containing methanol, also include other impurities such as water, CO2, methane, and hydrogen. Therefore, a distillation section is necessary to purify the methanol to make it marketable. Specifically, a first distillation column is used to remove gaseous light compounds, such as CO2, methane, and hydrogen. These gases are recycled back to the steam reforming furnace. As a result, a stream rich in methanol and water exits from the bottom. The second distillation column is used to remove the water. Thus, from the top of the second distillation column, the desired methanol stream exits with a 99.9% w/w purity, while water is recycled back to the tube side of the steam reforming reactor from the bottom.

4.2. Economic Evaluation

At this stage, the focus shifts to the economic feasibility of the syngas-to-methanol plant as an extension of the existing facility. The first step involves inserting the required parameters into the "Turton's Library" Excel worksheet. The initial parameters required include those from the Turton library and the costs of standard utilities. The default values from Turton[21] were employed, with some exceptions:

- The CEPCI index[1] and utility costs have been updated to reflect the 2024 values.

	CEPCI	Electricity	Cooling water	LP steam	MP steam	HP steam
Value	800.7	0.12	0.8	0.024	0.0295	0.038
UoM	[-]	[\$/kWh]	[\$/ton]	[\$/kg]	[\$/kg]	[\$/kg]

Table 1: CEPCI index and utility costs values.

- In the equation for the cost of manufacturing, the contributions from the grassroots cost and the cost of operating labor were set to zero. This adjustment is justified by the fact that the plant under analysis (syngas-to-methanol, Figure 21) is an expansion of an existing facility (biogas-to-syngas, Figures 19,20). These two contributions are incorporated into the first part of the plant and are accounted for in the syngas price, which serves as the input for the process under consideration.

Next, the input values for the cash flow assessment must be entered. The discount rate is set to a value close to the current inflation rate [3]. The taxation rate includes both the corporate income tax (IRES) and the regional production tax (IRAP) [5]. The plant's operational lifetime is assumed to be 15 years. As a first approximation, the residual value of the plant at the end of its life is considered to be zero.

	Discount Rate	Taxation Rate	Timespan	Residual Value
Value	6	28	15	0
UoM	[%]	[%]	[years]	[\$]

Table 2: Cash flow parameters.

At this stage, all the necessary information is available within CORO, and the "Get Data" function can be executed. This function transfers all the required data from the Aspen simulation to the Excel workbook, allowing for the customization of the data. For this simulation, three actions are required to appropriately modify the data:

- A cost is assigned to the incoming raw material, syngas, corresponding to stream "4" and the type of stream is changed to "Raw Stream" from the drop-down list. The value used is \$0.16 per kg, as estimated in the study by *Salano et al.*(2024)[17]. A price is also assigned to the produced methanol stream, referred to as "MeOH," set at \$0.8 per kg and the type of stream is changed to "Product" from the drop-down list. This price is significantly higher than that of methanol on the conventional market, which is justified by the fact that it is green methanol, produced from biogas. Biogas is generated through the anaerobic digestion of biomass, which is playing a paramount role in the energy transition by enabling the production of energy and chemicals with a significant reduction in CO2 emissions. Companies benefit from government incentives for producing green energy or chemicals, helping to bridge the price gap between methanol produced from fossil fuels and green methanol.

- The cost of the methanol reactors is determined using the "Add Custom Unit" function because Turton's library does not provide correlations for estimating the cost of this specific type of equipment. This is due to the significant variability among reactor types, as they can differ widely in design, function, and operational parameters. To account for this diversity and ensure a consistent approach in the analysis, a cost of 250,000$, derived from an internal source, is assigned to each methanol reactor.
- In the "Utilities" worksheet, the default settings are "Cooling Water" for coolers and "Low-Pressure Steam" for heaters. However, according to the guidelines in *Silla*(2003)[18], which recommend selecting heating or cooling media based on the temperature of the process stream, there are inconsistencies in the use of "Low-Pressure Steam" for heaters "E-108" and "E-115". Due to the high temperature of the process streams in these heat exchangers, "High-Pressure Steam" is required to reach the desired temperature. For all other utilities, the default heating and cooling media are appropriate.
- The material of all units containing hydrogen was changed from carbon steel to stainless steel to prevent embrittlement caused by hydrogen exposure.

Once the data are all set the economic estimation can be performed with the following results.

Equipment Name	**Cost [$]**	**Characteristic Variable**	**Value**
VLV-101	0.00	[-]	[-]
Topping column	32351.75	Volume $[m^3]$	0.07
Condenser_Topping column	31542.55	Area $[m^2]$	0.80
Reboiler_Topping column	23792.12	Area $[m^2]$	0.89
Refining column	113364.45	Volume $[m^3]$	2.12
Condenser_Refining column	26947.10	Area $[m^2]$	1.09
Reboiler_Refining column	118928.86	Area $[m^2]$	37.83
P-103	3495.99	Power $[kW]$	0.0546
Methanol Reactor	250000.00	Volume $[m^3]$	0.361
V-102	93385.55	Volume $[m^3]$	0.41
TEE-101	0.00	[-]	[-]
E-108-2	65853.59	Area $[m^2]$	2.11
E-112	224674.62	Area $[m^2]$	9.95
E-108	108475.83	Area $[m^2]$	4.90
E-113	99389.88	Area $[m^2]$	4.24
V-105	90059.42	Volume $[m_3]$	0.41
Methanol Reactor-2	250000	Volume $[m^3]$	0.343
E-114	68198.75	Area $[m^2]$	1.35
E-115	99232.40	Area $[m^2]$	4.18
K-102	107541.49	Power $[kW]$	4.30

Table 3: Bare Module Cost of each unit operation.

Table 3 presents the bare module cost for each piece of equipment. The costs associated with mixers, tees, and valves are omitted by CORO due to their minimal impact on the overall plant cost. Figure 16 illustrates the percentage contribution of each unit type to the total cost. The most significant contributors are the two methanol reactors. As previously mentioned, the cost of the reactors was manually input using the "Add Custom Unit" function. The high cost is due to the complexity of the tubular reactors.

The refining column accounts for 14% of the total cost, which includes not only the vessel itself but also the associated condenser and reboiler. This column, with 40 stages and substantial duties (171.4 kW for the condenser and 290.1 kW for the reboiler), requires large heat exchangers. This is justified by the fact that the separation of water and methanol occurs in this column, with methanol being extracted from the top as a product, necessitating high purity.

On the contrary, the impact of the topping column is significantly lower. This column has only 12 stages, and its duties are at least ten times smaller at both the condenser (9.112 kW) and the reboiler (25.87 kW). The primary function of this column is to separate gaseous impurities from the main water and methanol stream, which requires fewer stages and lower duties compared to the refining column.
Significant contributions to the overall cost are from the two process-to-process heat exchangers (E-112, E-114) and the four heat exchangers that utilize external utilities (E-108, E-113, E-115, E-108-2).

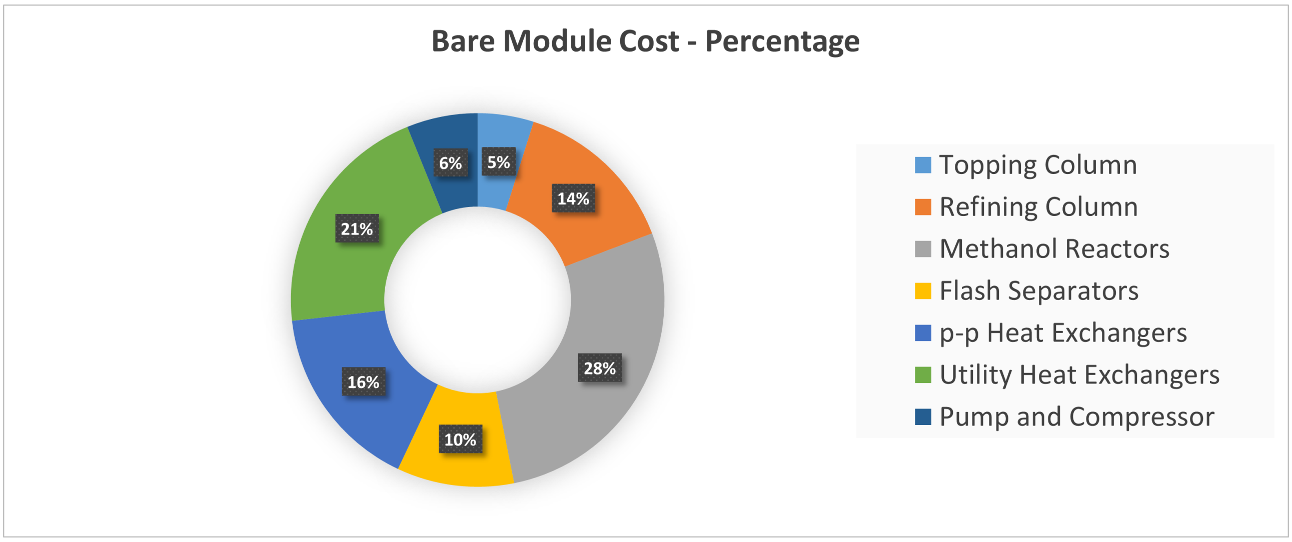


Figure 16: Bare Module Cost - Percentage

Table 4 provides a detailed breakdown of the costs and revenues for the entire plant. The Total Capital Investment is calculated as the sum of the grassroots cost and working capital. Operational expenditures include only the costs of utilities and raw materials, as there are no waste treatment processes involved, and the contribution of operating labor is omitted, as previously discussed. Revenues are generated from the sale of the methanol stream produced by the plant. The income is then determined as the difference between revenues and operational expenditures.

	Total Capital Investment	Opex	Reveneus	Income
Value	3,214,047.70	1,308,596.22	2,276,668.92	968,072.70
UoM	[$]	[$/year]	[$/year]	[$/year]

Table 4: Cost estimation of methanol plant.

Table 5 presents key indicators of the plant's economic feasibility, including economic measures such as payback time and net present value, as well as the financial indicator of internal rate of return.

	Payback Time	Net Present Value	Internal Rate of Return
Value	5.05	4,138,201.51	22.42
UoM	[years]	[$]	[%]

Table 5: Economic and financial indicators.

Figure 17 illustrates the cumulative cash flow of the project. The x-axis represents the project's lifetime, while the y-axis shows the cumulative cash flow, calculated as the sum of the discounted net present value (NPV) for each year. At year 0, the cumulative cash flow is equal to the negative total capital investment. As time progresses, this value increases until it reaches zero, marking the break-even point, which corresponds to the project's payback time. By the end of the 15th year, the cumulative cash flow curve aligns with the net present value.
Although the income remains constant over the years, the cumulative cash flow forms a curve rather than a straight line. This curvature arises from cash flow discounting. Referring to the first term of Equation 1, the

discounted cash flow for each year is defined as $CF_i \times DI_i$, where DI is the discount item, given by $\frac{1}{(1+\text{DR})^i}$. As the years progress, the discount factor diminishes, resulting in the slope of the curve in Figure 17 becoming progressively less steep over time.

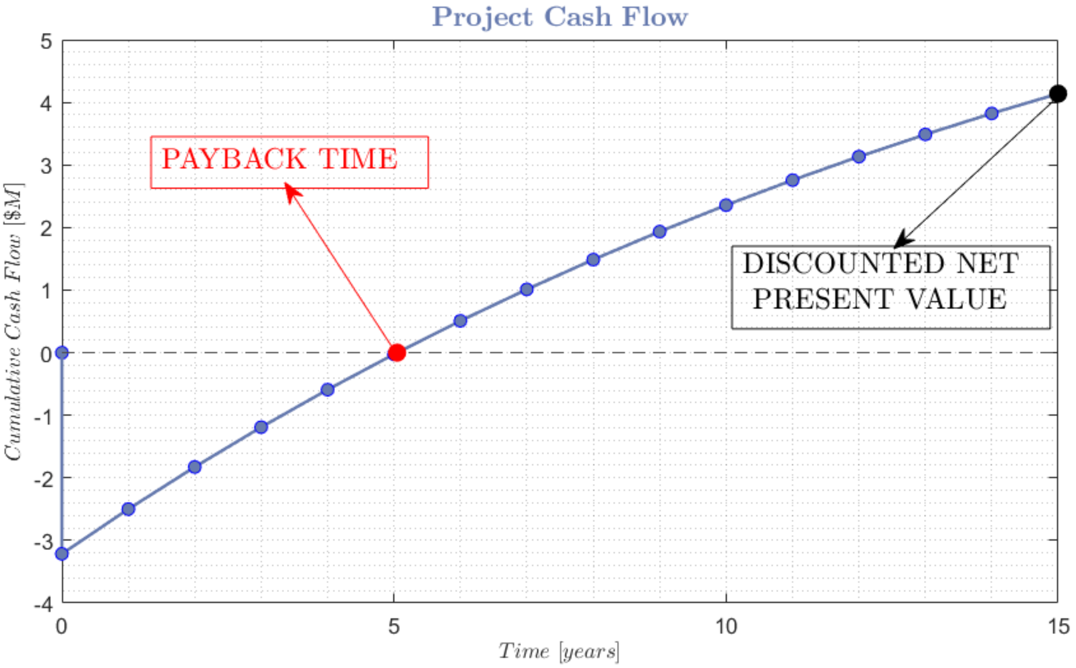


Figure 17: Project Cash Flow

4.3. Optimization

Once the initial economic assessment is completed, the next step is to optimize the process using the "BzzMinimizationRobust" numerical algorithm. The primary goal is to minimize the project's payback time by adjusting the system's variables. However, only those variables that are manually specified by the user can be treated as degrees of freedom. If other variables are set as degrees of freedom, it leads to an over specification issue, which stops the optimization process and triggers an error message to the user.

To optimize the methanol production process, five key variables are considered:

- The temperature of the "Methanol Reactor".
- The temperature of the stream "55".
- The temperature of the "Methanol Reactor-2".
- The temperature of the stream "11".
- The split ratio of "TEE-101".

The variation of each of these variables has a significant impact on the characteristics of the process streams and units. Specifically, the temperature of the two methanol reactors affects the reactivity of the mixture, influencing the flow rate and molar composition of the streams exiting the reactors. Moreover, the temperature of these exiting streams impacts the sizing and the duty of the subsequent process-to-process heat exchangers (E-112, E-114). The temperatures of streams "55" and "11" mainly affect the sizing and the duty of the heat exchangers "E-113" and "E-108-2". Since these heat exchangers are served by external utilities, changes in heat duty directly impact the amount of cooling fluid required, thus influencing operating expenses. Additionally, both of these streams are directed to flash separators. The temperature of the incoming streams, and consequently the temperature of the flash separators since they are isothermal, affects the quality of the separation between unreacted gaseous reactants and the produced methanol and water. Lastly, the split ratio of "TEE-101" alters the recycling flow of unreacted gases, which in turn affects the flow rate and composition of the stream entering the first reactor.

Given the system's complexity, manually optimizing the process would be a long and tedious task. However, by relying on CORO, it is possible to rapidly and reliably find the system's economic optimum.

The optimization procedure initially involves setting all five variables as degrees of freedom, with their respective lower and upper boundaries defined in Table 6. This approach allows CORO to reduce the payback time effectively when the simulation is still distant from the minimum by varying all the variables together. As the simulation approaches the optimum, each variable is subsequently optimized individually, with a narrower range, to enhance precision.

When multiple degrees of freedom are employed together in proximity to the economic optimum, the procedure tends to become less precise, potentially leading to higher payback time values compared to earlier stages. Therefore, it is recommended to use multiple DOFs simultaneously during the initial phase, where the system is far from the optimum, to quickly converge towards the optimal values for each variable and generally reduce the payback time. For a more precise refinement and to achieve greater profitability, optimizing each variable individually is preferred, as this approach is more robust and accurate.

Furthermore, when the numerical algorithm suggests new values for multiple variables at the same time and these are input into the Aspen HYSYS simulation via the "Data_Loading" function, the process simulator may struggle to achieve convergence and produce reconciled data. This can lead to the generation of physically unreliable data, which triggers the error-handling procedure. As a result, the optimization process slows down and becomes less effective.

	T "OutR1"	**T "55"**	**T "OutR2"**	**T "11"**	**SR "TEE-101"**
Original	240.00	45.00	240.00	45.00	0.905
Optimized	243.9	70.11	243.9	74.45	0.9422
Optimization Range	235 - 243.9	42 - 82	235 - 243.9	42 - 82	0.89 - 0.95
UoM	[°C]	[°C]	[°C]	[°C]	[-]

Table 6: Degrees of freedom values.

Table 6 shows a slight increase in temperature in both the first and second methanol reactors, which enhances the reactivity of the mixture. Although the reactions involved are overall exothermic and thus thermodynamically disfavored by an increase in temperature, the reaction kinetics are improved, leading to greater methanol production. The temperature is not increased further because doing so would require switching the heating medium for the heat exchangers E-108 and E-115 from high-pressure steam to a more expensive thermal oil. According to [18], high-pressure steam would no longer be sufficient to heat the mixture above 244°C. In this case, it is preferable to accept a lower conversion rate in the reactors, resulting in reduced methanol production, but with significant savings on utility costs.

The inlet temperature of the two flash separators increases in both cases, leading to less effective separation of methanol from the unreacted gases. As a result, both the molar flow rate and the molar fraction of methanol exiting the bottom of the two flash separators decrease. This means that a larger amount of methanol is fed to the second reactor and recirculated, respectively, in the first and second flash separators. From a technical perspective, this is a drawback for the plant because having more methanol entering the second reactor reduces the reactivity and conversion of the mixture, as well as increases the recirculation load. However, from a techno-economic standpoint, this results in lower duties for heat exchangers E-113 and E-108-2. This translates to smaller, less expensive heat exchangers and a reduced flow rate of cooling water, which lowers operating expenses.

The split ratio of "TEE-101" is defined as the ratio of the molar flows of stream "36" to stream "16". The split ratio increases, allowing unreacted hydrogen and CO2 to be added to the main flow of reactants "4", which then enters the first reactor. The remaining flow becomes a purge stream, which is recirculated to the steam reforming reactor on the furnace side and used as fuel. The split ratio is not increased further because the recirculated stream contains a high amount of methane, which acts as an inert gas in the methanol reactors. Without the purge, the methane fraction entering the reactors would increase, eventually rendering the reaction ineffective.

CORO allows for more accurate economic analysis; otherwise, there is a risk of focusing merely on technical optimization and productivity without adequately accounting for the associated costs.

The variations in temperature, flowrate, and composition of optimized streams "69" and "28" compared to the initial simulation, which are recirculated to the initial "Biogas to syngas" section of the plant, are negligible and do not affect the characteristics of the syngas stream "4" entering the section of interest of the plant.

The performance of the optimization procedure can be evaluated by examining the number of successful iterations, the percentage of successful iterations, and the time required for each optimization run. When all degrees of freedom are varied simultaneously, CORO requires between fifty and seventy iterations, with each optimization taking between four and seven minutes. When only a single degree of freedom is optimized, CORO completes the process in fifteen to forty-five iterations, with a time span ranging from 30 seconds to two minutes. The percentage of successful iterations remains at 100% across all optimization scenarios.

	Total Capital Investment	**Opex**	**Reveneus**	**Income**
Value	3,005,285.53	1,278,933.92	2,320,999.80	1,042,065.88
UoM	[\$]	[\$/year]	[\$/year]	[\$/year]
% difference [1]	-6.50 %	-2.27 %	+1.95 %	+7.64%

Table 7: Cost estimation of methanol plant after optimization.

Table 7 shows the new plant cost values. Both Capex and Opex have decreased compared to the initial simulation. On the contrary, revenues have increased, resulting in an overall increase in the plant's income. [1]

	Payback Time	**Net Present Value**	**Internal Rate of Return**
Value	4.35	4,826,537.03	25.99
UoM	[years]	[\$]	[%]
% difference [1]	-13.82%	+16.63%	+15.92%

Table 8: Economic and financial indicators after optimization.

Table 8 shows the new values of the economic and financial indicators. The payback time of the plant has decreased, while both the net present value and the internal rate of return have increased. These changes indicate a more profitable project.

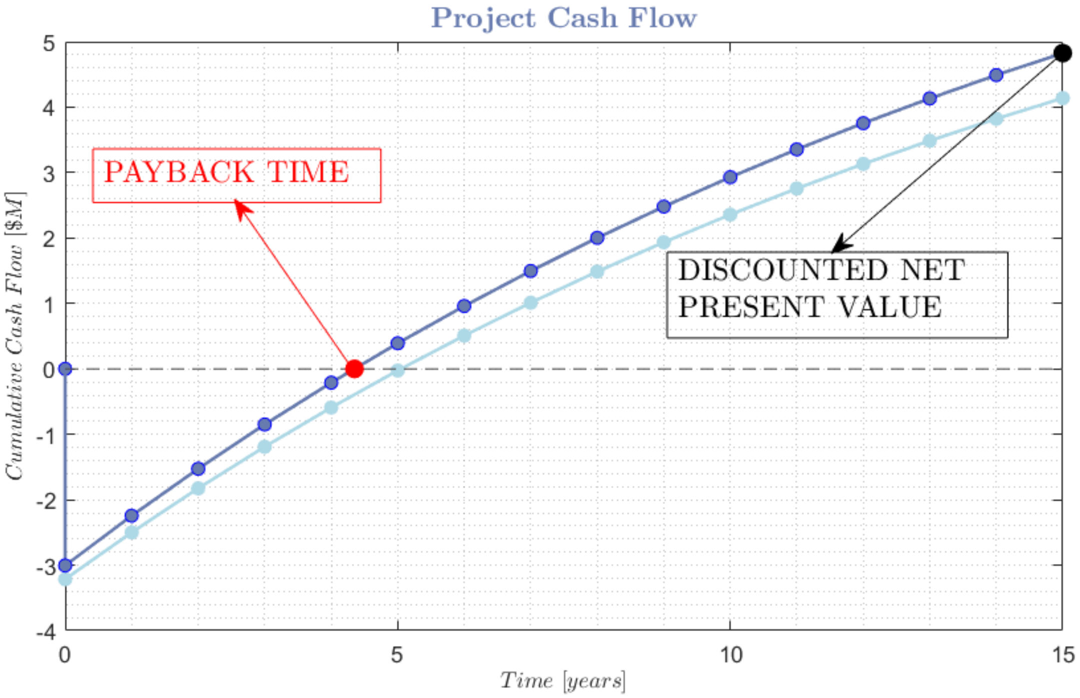


Figure 18: Project Cash Flow after Optimization.

Figure 18 presents a comparison between the original cumulative cash flow, shown in light blue, and the optimized cumulative cash flow, shown in blue."

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[1] "% difference" refers to the difference in the costs between the original and the optimized plant, evaluated as : $\left(\frac{\text{optized plant value}}{\text{original plant value}} - 1\right) \times 100$.

5. Conclusions and Future Developments

This thesis aimed to develop a robust application capable of performing economic estimations and process optimizations based on any simulation generated in Aspen HYSYS. The application, named CORO, was designed with a highly flexible and user-friendly architecture. CORO allows users to visualize the entire process through worksheets that organize material streams and units effectively.

The thesis begins by highlighting the importance of process simulators and optimization tools in project development. As the complexity of engineering challenges grows, there is an increasing demand for powerful, automated tools capable of providing rapid and continuous solutions. CORO fulfills these demands by offering a responsive and versatile tool.

A key feature of CORO is its integration with process simulation software, which facilitates the rapid execution of multiple optimization scenarios for the same process.

CORO also offers a customization function for economic estimations, which is particularly valuable when users have access to supplementary information or need to evaluate non-standard units. This feature enhances CORO's flexibility in handling unconventional unit operations and simulations.

The robustness of CORO in optimization tasks is secured by the BzzMinimizationRobust numerical algorithm, which consistently identifies optimal operating conditions, even in large and complex simulations.

CORO's exceptional reliability is further demonstrated by its advanced error-handling procedure, which ensures successful optimization even when dealing with complex Aspen HYSYS simulations that fail to converge.

The integration of economic indicators, such as payback time, net present value, internal rate of return, and a comprehensive cash flow analysis, provides users with a thorough perspective on the project's profitability, enabling effective comparisons with alternative investments.

A case study on methanol production from syngas, presented in this thesis, further illustrates CORO's effectiveness in achieving optimal solutions.

CORO serves as a strong foundation for future developments in project assessment and design. The creation of digital and automated solutions is crucial in minimizing time and resource wastage in the process industry. However, CORO can be further enhanced to broaden its applicability, improve the accuracy of its results, and increase its overall appeal.

Several potential enhancements could further improve the application:

- Expansion of CORO's compatibility with multiple process simulators. The underlying structure of CORO is designed to accommodate such extensions without requiring a complete revamp, potentially allowing the application to meet the CAPE-OPEN standard for interoperability among commercial process simulation software. This would broaden CORO's applicability and attract more interest from investors.
- Development of an advanced cash flow model. A potential improvement involves refining the depreciation strategy, which is currently assumed to span the entire project lifespan. By implementing a non-linear depreciation method over a shorter period, the model can accelerate capital recovery, resulting in a reduced payback time and enhanced financial performance.
- Implementation of a sensitivity analysis on user-customizable input parameters would be beneficial. This feature would identify which parameters have the most significant impact on the economic estimation and, consequently, on the plant's overall profitability. By understanding which variables are most influential, users can better focus on optimizing key aspects of the process.
- The incorporation of a Monte Carlo analysis would add another layer of robustness to the economic assessment. This function would simulate numerous "what-if" scenarios by varying the input parameters, generating a distribution curve that indicates the probability of achieving positive plant profitability. In this way, assessing the economic risks and uncertainties associated with different operational conditions would be possible.
- The integration of a Life Cycle Assessment (LCA) section would enhance the application. By assigning environmental impact values to each material and energy stream entering and exiting the process, as well as to each unit operation, the LCA would enable the assessment of emissions across multiple impact categories. This addition would help users make more informed decisions regarding the sustainability of the plant design and operations.

References

[1] Cost Indices – Towering Skills.

[2] Depreciation: Definition and Types, With Calculation Examples.

[3] Global inflation rate from 2000 to 2029 | Statista.

[4] Guido Buzzi-Ferraris and Flavio Manenti. *Nonlinear systems and optimization for the chemical engineer: solving numerical problems.* Wiley-VCH-Verl, Weinheim, 2014.

[5] Nomad Capitalist. Taxes in Italy: The Ultimate Guide 2024, May 2023.

[6] Hsuan-Han Chiou, Chi-Jui Lee, Bo-Sheng Wen, Jian-Xun Lin, Cheng-Liang Chen, and Bor-Yih Yu. Evaluation of alternative processes of methanol production from CO2: Design, optimization, control, techno-economic, and environmental analysis. *Fuel*, 343:127856, July 2023.

[7] Alexandre C. Dimian, Costin S. Bildea, and Anton A. Kiss. Chapter 19 - Economic Evaluation of Projects. In Alexandre C. Dimian, Costin S. Bildea, and Anton A. Kiss, editors, *Computer Aided Chemical Engineering*, volume 35 of *Integrated Design and Simulation of Chemical Processes*, pages 717–755. Elsevier, January 2014.

[8] Léda Gerber. *Integration of Life Cycle Assessment in the conceptual design of renewable energy conversion systems.* PhD thesis, Lausanne, EPFL, 2012.

[9] Homa Hamedi, Torsten Brinkmann, and Thorsten Wolff. Techno-economic assessment of H2 extraction from natural gas distribution grids: A novel simulation-based optimization framework for pressure swing adsorption processes. *Chemical Engineering Journal Advances*, 16:100541, November 2023.

[10] Juma Haydary. *Chemical process design and simulation: Aspen Plus and Aspen HYSYS applications.* Wiley, Hoboken, N.J, 2019.

[11] Ming-Ting Lee and Bor-Yih Yu. Evaluation on the intensified hydroxypropyl acrylate (HPA) production processes: Rigorous design, optimization, techno-economic and environmental analysis, and control. *Process Safety and Environmental Protection*, 167:671–685, November 2022.

[12] G Lombardelli, S Consonni, A Conversano, M Mureddu, A Pettinau, and M Gatti. Process Design and Techno-Economic Assessment of biogenic CO $_2$ Hydrogenation-to-Methanol with innovative catalyst. *Journal of Physics: Conference Series*, 2385(1):012038, December 2022.

[13] Georgios Maroukis and Michael C. Georgiadis. Modeling, simulation, and techno-economic optimization of argon separation processes. *Chemical Engineering Research and Design*, 184:165–179, August 2022.

[14] Sungho Park, Kwangsoon Choi, Changhyeong Lee, Suhyun Kim, Youngdon Yoo, and Daejun Chang. Techno-economic analysis of adiabatic four-stage CO2 methanation process for optimization and evaluation of power-to-gas technology. *International Journal of Hydrogen Energy*, 46(41):21303–21317, June 2021.

[15] Robert H. Perry and Don W. Green, editors. *Perry's chemical engineers' handbook.* McGraw-Hill, New York, NY, 8. ed edition, 2008.

[16] Philip Pietrek, Manfred Kraut, and Roland Dittmeyer. Towards a Novel Computer-Aided Optimization of Microreactors: Techno-Economic Evaluation of an Immobilized Enzyme System. *Symmetry*, 13(3):524, March 2021.

[17] Loretta Salano, Marcello M. Bozzini, and Flavio Manenti. Techno-Economic Analysis for Biogas Reforming using PSWA: Case Study on Methanol Synthesis. In Flavio Manenti and Gintaras V. Reklaitis, editors, *Computer Aided Chemical Engineering*, volume 53 of *34 European Symposium on Computer Aided Process Engineering / 15 International Symposium on Process Systems Engineering*, pages 1045–1050. Elsevier, January 2024.

[18] Harry Silla. *Chemical process engineering: design and economics.* Number 96 in Chemical industries. M. Dekker, New York, 2003.

[19] Mohammad Mohsen Soltani, Pouria Ahmadi, and Mehdi Ashjaee. Techno-economic optimization of a biomass gasification energy system with Supercritical CO2 cycle for hydrogen fuel and electricity production. *Fuel*, 333:126264, February 2023.

[20] Gavin P. Towler and R. K. Sinnott. *Chemical engineering design: principles, practice and economics of plant and process design*. Butterworth-Heinemann, Oxford [England] ; Cambridge, MA, third edition edition, 2022.

[21] Richard Turton, editor. *Analysis, synthesis, and design of chemical processes*. Prentice Hall international series in the physical and chemical engineering sciences. Prentice Hall, Boston, 5th edition edition, 2018.

[22] Anestis Vlysidis, Michael Binns, Colin Webb, and Constantinos Theodoropoulos. A techno-economic analysis of biodiesel biorefineries: Assessment of integrated designs for the co-production of fuels and chemicals. *Energy*, 36(8):4671–4683, August 2011.

[23] Hanfei Zhang and Umberto Desideri. Techno-economic optimization of power-to-methanol with co-electrolysis of CO2 and H2O in solid-oxide electrolyzers. *Energy*, 199:117498, May 2020.

[24] Xin Zhou, Shangfeng Li, Yuan Wang, Jiewenjing Zhang, Zhibo Zhang, Changgui Wu, Xiaobo Chen, Xiang Feng, Yibin Liu, Hui Zhao, Hao Yan, and Chaohe Yang. Crude oil hierarchical catalytic cracking for maximizing chemicals production: Pilot-scale test, process optimization strategy, techno-economic-society-environment assessment. *Energy Conversion and Management*, 253:115149, February 2022.

A. Appendix

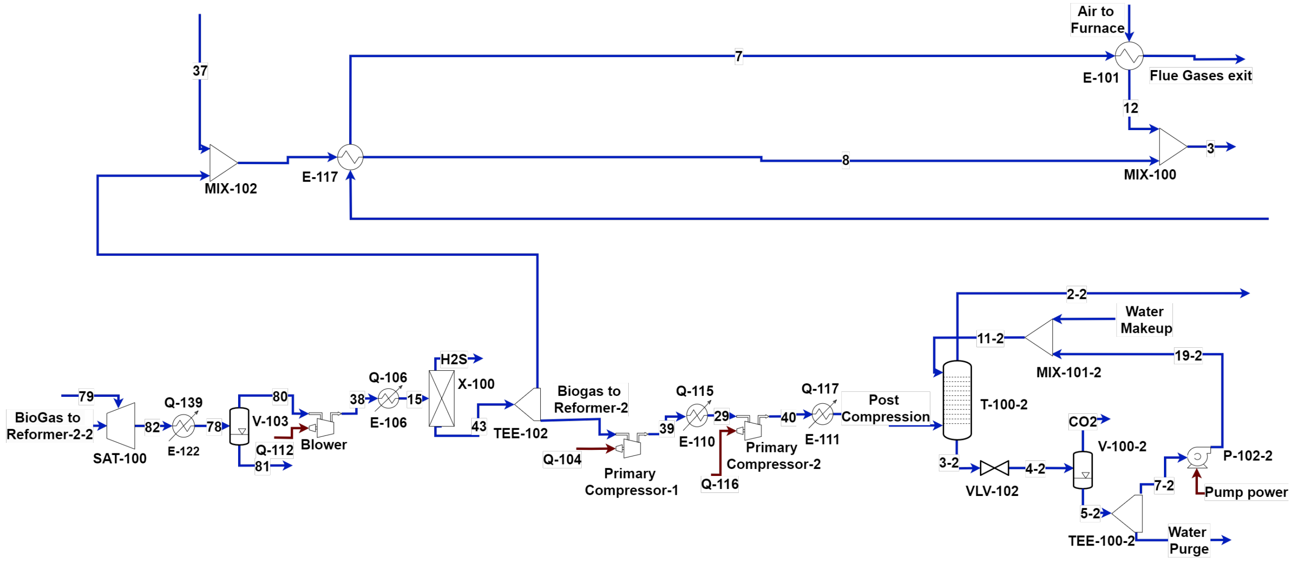

Figure 19: Upgrading section

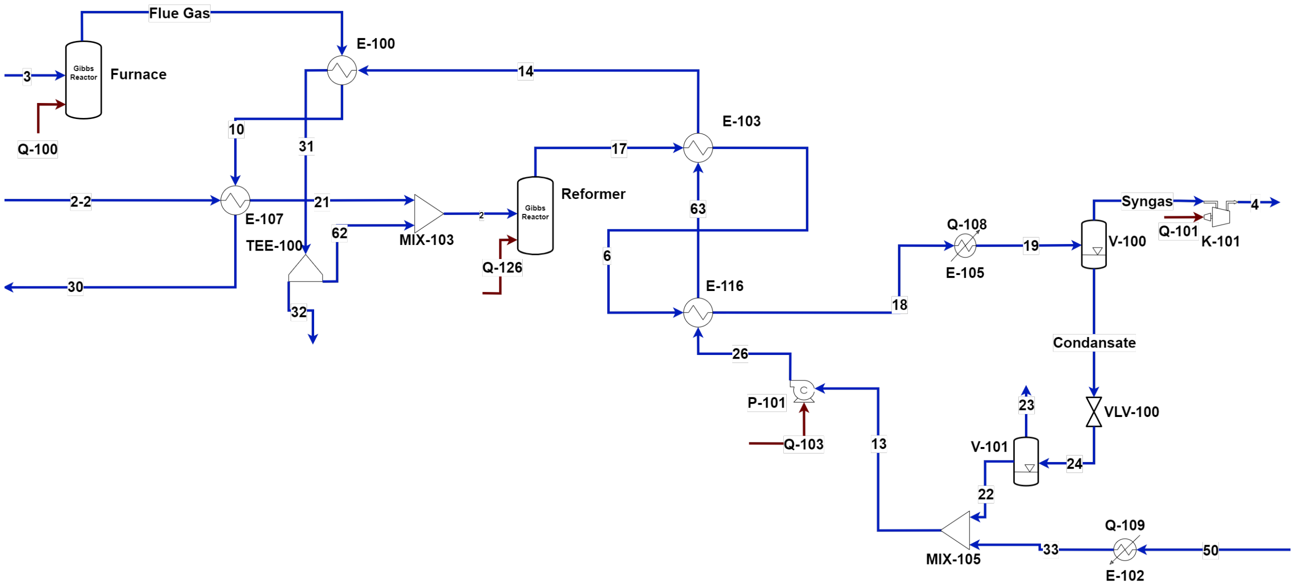

Figure 20: Reformer section

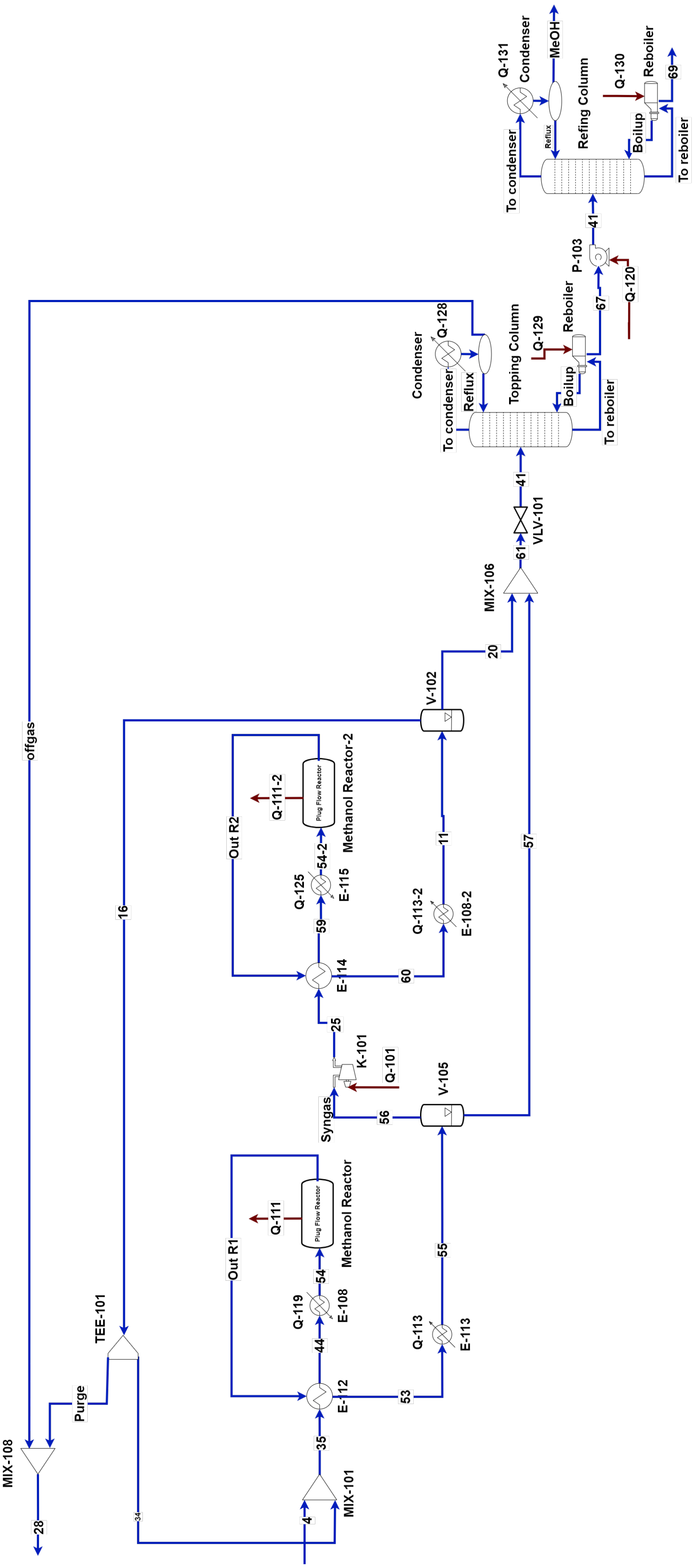

Figure 21: Methanol section

Abstract in lingua italiana

Lo studio di fattibilità degli impianti chimici avviene quando non tutte le informazioni del processo sono ancora disponibili. La scelta della configurazione dei processi ha un impatto significativo sui costi dell'impianto, e modificare il layout successivamente può risultare molto costoso. Pertanto, è fondamentale avere stime economiche affidabili fin dall'inizio, quando le decisioni hanno un impatto maggiore sul profitto. Per affrontare questa esigenza, è stato sviluppato il Capex Opex Robust Optimizer (CORO).

CORO utilizza simulazioni di processo in Aspen HYSYS per raccogliere i dati necessari alla stima economica delle spese operative e capitali. Questo strumento consente di ottenere stime rapide, automatizzate e affidabili, riducendo al minimo il rischio di errore umano. I dati vengono trasferiti su un'interfaccia grafica in Microsoft Excel tramite funzioni scritte in VBA, permettendo all'utente di apportare modifiche basate su informazioni aggiuntive.

Le stime economiche sono effettuate tramite funzioni scritte in C++ che utilizzano il pacchetto economico del Turton. Le informazioni sono trasferite da Excel alle DLL tramite schemi XML. CORO è in grado di ottimizzare i processi dal punto di vista economico, utilizzando la libreria "BzzMath" sviluppata da Buzzi-Ferraris e Manenti, ed implementata in C++. L'obiettivo è minimizzare il payback time del progetto. La procedura iterativa di ottimizzazione è gestita tramite funzioni scritte in VBScript.

CORO fornisce un'analisi economica completa e accurata, rivelando il payback time, il valore attuale netto e il tasso di rendimento interno del progetto, oltre al cash flow. L'applicazione si è dimostrata molto flessibile e affidabile, anche con simulazioni di processi complessi, grazie alla procedura di gestione degli errori implementata.

Il caso studio analizzato, relativo alla stima economica e ottimizzazione di un impianto di sintesi di metanolo, ha dimostrato l'accuratezza e l'efficienza del CORO. Per cui, CORO si dimostra uno strumento valido per la valutazione economica e ottimizzazione di impianti industriali.

Parole chiave: Stima dei costi, Ottimizzazione di processo, CORO, Simulazione di processo